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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.

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SUPPORTING FILE 4

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

55
name = lig-etoh-Water-frame_1

C	5.040017	-1.737589	1.503713	38.54
H	5.215639	-0.671932	1.244402	20.62
C	4.897911	-4.046266	0.868532	59.03
H	5.007524	-4.639949	-0.027886	25.34
C	4.807502	-4.473940	2.233329	23.16
O	4.509728	-5.799401	2.671955	179.17
C	4.364890	-6.867654	1.685772	116.62
H	5.243155	-7.049633	1.019033	25.40
H	3.410536	-6.775468	1.168482	27.24
H	4.336029	-7.719995	2.368237	25.95
C	4.800276	-3.484077	3.196151	26.53
O	4.541520	-3.659612	4.566115	120.76
H	4.959911	-4.508221	4.958738	21.12
C	5.023177	-2.143886	2.827827	56.60
H	4.950795	-1.362273	3.612783	30.60
C	4.943783	-2.680265	0.522525	36.09
C	5.000074	-2.247387	-0.923230	84.08
H	5.362919	-3.141475	-1.424149	26.52
O	5.960869	-1.236341	-1.281195	148.42
H	5.781693	-0.362563	-0.859092	26.36
C	3.618433	-1.887613	-1.503185	89.30
H	3.017778	-2.808031	-1.363722	28.67
C	3.714006	-1.558816	-3.011057	105.96
O	3.889692	-2.762252	-3.809880	279.11
H	4.666484	-2.582472	-4.379103	25.74
H	4.562402	-0.855369	-3.205918	27.47
H	2.694932	-1.185446	-3.260579	27.53
C	-0.499224	-1.668856	0.173330	67.54
H	-1.267689	-2.510825	0.180425	27.62
C	-0.205610	0.786671	0.252440	72.32
H	-0.645310	1.748503	0.280074	26.31
C	1.134169	0.606806	-0.100739	7.39
O	1.944958	1.717000	-0.434063	216.16
C	1.450514	3.014402	-0.106451	119.22
H	2.270666	3.648037	-0.169066	28.47
H	0.644936	3.378393	-0.878977	26.99
H	1.035117	3.027813	0.932650	28.50
C	1.696561	-0.674707	-0.342359	10.55

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 O       3.022021    -0.777736    -0.775750     118.96
 C       0.834563    -1.841795    -0.244633      56.68
 H       1.277164    -2.794783    -0.512589      29.55
 C      -1.030475    -0.370445     0.409621       6.21
 C      -2.511165    -0.261059     0.813486      91.30
 H      -2.689034    -1.234448     1.400660      28.34
 O      -2.817955     0.859114     1.635271     257.20
 H      -2.355520     0.739737     2.551687      28.23
 C      -3.445966    -0.258879    -0.358593      92.78
 H      -3.129792     0.557508    -1.102752      29.33
 O      -3.394650    -1.554577    -1.048357     181.38
 H      -3.520566    -1.343696    -2.061361      26.48
 C      -4.912873    -0.005625     0.078023     109.50
 O      -5.417086     1.344408     0.078979     203.10
 H      -4.861882     1.910614     0.689467      29.13
 H      -5.025128    -0.412979     1.146092      27.80
 H      -5.480181    -0.637736    -0.587779      29.80
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name = lig-etoh-Waterframe_2
 C       5.058965    -1.689689     1.514629      55.46
 H       5.251440    -0.651559     1.213197      26.02
 C       4.924655    -4.080701     0.855984      57.72
 H       5.025167    -4.914622     0.185368      22.88
 C       4.756263    -4.498404     2.190007      59.82
 O       4.532935    -5.748093     2.663585     163.77
 C       4.382623    -6.862711     1.713807     126.24
 H       5.105301    -6.818617     0.867363      25.93
 H       3.379044    -6.800378     1.251074      28.36
 H       4.335207    -7.763514     2.344692      26.57
 C       4.800404    -3.464897     3.257798      26.89
 O       4.556537    -3.653850     4.573568      29.87
 H       4.948070    -4.516601     4.963069      19.62
 C       4.997385    -2.114874     2.866428      57.63
 H       4.997454    -1.356642     3.664064      25.49
 C       4.976418    -2.704801     0.504433      32.75
 C       5.007908    -2.296145    -0.941039      65.62
 H       5.363533    -3.158294    -1.517943      21.58
 O       6.003253    -1.236898    -1.266747      71.02
 H       5.918841    -0.511620    -0.611748      30.03
 C       3.614494    -1.916640    -1.515040      80.38
 H       2.948454    -2.810352    -1.498244      26.69
 C       3.662240    -1.534624    -3.010479     101.72
 O       3.885793    -2.767971    -3.789715     277.62
 H       4.678228    -2.862527    -4.334198      24.26
 H       4.472038    -0.799042    -3.243162      27.10
 H       2.696101    -1.076169    -3.318506      27.88
 C      -0.499226    -1.639435     0.159550      58.54
 H      -1.073076    -2.552787     0.436460      28.76
 C      -0.231478     0.755578     0.244716      85.48
 H      -0.526378     1.731446     0.447215      29.39
 C       1.142393     0.624675    -0.132329     -48.46
 O       1.948624     1.677617    -0.436930     219.18
 C       1.441409     3.025041    -0.102821     112.82
 H       2.303027     3.623206    -0.183896      28.03
 H       0.679569     3.311358    -0.909414      27.73
 H       0.926417     3.171931     0.874036      28.50
 C       1.688135    -0.737746    -0.360197      -7.03
 O       3.032343    -0.751338    -0.768894     122.96
 C       0.864766    -1.794228    -0.215855     117.07
 H       1.290556    -2.768891    -0.360882      31.77
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 C      -1.022768    -0.372658     0.392023      39.00
 C      -2.440376    -0.325210     0.836277      83.19
 H      -2.695862    -1.264028     1.394403      30.38
 O      -2.812637     0.907478     1.665809     248.58
 H      -2.439041     0.844595     2.605425      29.04
 C      -3.479758    -0.236132    -0.391387      85.86
 H      -3.168528     0.552768    -1.135724      30.34
 O      -3.401867    -1.555599    -1.065184     170.33
 H      -3.721019    -1.453764    -2.045622      27.43
 C      -4.928064    -0.036068     0.119181     108.76
 O      -5.433697     1.327881     0.078508     204.85
 H      -4.907340     1.806773     0.785114      29.34
 H      -5.016535    -0.567916     1.109869      28.39
 H      -5.588783    -0.567584    -0.577309      29.43
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name = lig-etoh-Waterframe_3
 C       5.077760    -1.712215     1.525122      63.36
 H       5.088528    -0.644979     1.370173      28.80
 C       4.936382    -4.132874     0.856674      49.12
 H       4.912701    -4.914641     0.095607      20.32
 C       4.709882    -4.423870     2.221559      15.12
 O       4.567421    -5.742674     2.659054     227.18
 C       4.345718    -6.817484     1.739653     123.18
 H       5.159756    -6.800863     0.983903      29.80
 H       3.332665    -6.743761     1.279096      30.50
 H       4.459218    -7.789954     2.239750      28.86
 C       4.802487    -3.421472     3.227748      -1.38
 O       4.567260    -3.671303     4.622409     105.68
 H       5.097005    -4.541911     4.746076      20.89
 C       4.963242    -2.065685     2.901431      53.69
 H       5.151635    -1.409850     3.736872      21.42
 C       5.045309    -2.706499     0.514527      11.42
 C       5.034266    -2.333179    -0.997022      77.24
 H       5.286498    -3.116142    -1.738693      23.55
 O       6.039893    -1.249932    -1.238393      58.80
 H       5.917274    -0.622813    -0.495624      31.48
 C       3.578464    -1.923655    -1.532311      70.46
 H       2.898832    -2.781513    -1.371958      25.90
 C       3.640855    -1.513432    -3.044693     102.93
 O       3.851829    -2.792975    -3.755839     287.77
 H       4.689280    -2.801401    -4.195803      27.56
 H       4.392858    -0.723434    -3.178883      27.15
 H       2.693033    -1.055832    -3.360612      27.92
 C      -0.459900    -1.652383     0.165005      80.70
 H      -0.987781    -2.557995     0.402896      28.37
 C      -0.183188     0.760827     0.226701      71.07
 H      -0.677907     1.642107     0.572571      23.30
 C       1.122893     0.570746    -0.198527      24.29
 O       1.974238     1.658984    -0.406700     206.17
 C       1.438569     3.044550    -0.143142     112.81
 H       2.303382     3.766522    -0.171040      26.21
 H       0.739727     3.350081    -0.904984      28.96
 H       1.070515     3.061606     0.892205      28.36
 C       1.714895    -0.669859    -0.417331      15.13
 O       3.060923    -0.738707    -0.766896     109.57
 C       0.865361    -1.828205    -0.181599      45.25
 H       1.165384    -2.862144    -0.188994      27.73
 C      -1.027850    -0.399389     0.403160      28.48
 C      -2.469772    -0.312148     0.855184      82.34
 H      -2.774364    -1.149308     1.451810      28.75
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 O      -2.794336     0.927026     1.677628     278.81
 H      -2.322865     0.676072     2.505315      29.49
 C      -3.494223    -0.257273    -0.411685      88.02
 H      -3.248947     0.613003    -1.005762      30.63
 O      -3.412897    -1.547780    -1.073413     194.86
 H      -3.608787    -1.481459    -2.084366      26.51
 C      -4.969397    -0.093327     0.130826     102.56
 O      -5.436938     1.294790     0.109498     222.42
 H      -4.937916     1.850642     0.777883      28.62
 H      -5.135866    -0.497442     1.118821      28.40
 H      -5.715432    -0.561844    -0.549531      28.44
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name = lig-etoh-Waterframe_10
 C       5.000389    -1.587218     1.656417      59.93
 H       4.989279    -0.518132     1.509011      21.07
 C       4.849239    -3.929396     0.926725      58.77
 H       4.842520    -4.672776     0.133380      23.15
 C       4.822522    -4.324047     2.332803       9.50
 O       4.642592    -5.681025     2.761567     236.41
 C       4.111131    -6.711893     1.850775     112.12
 H       4.900352    -7.112343     1.219874      26.09
 H       3.250878    -6.380038     1.228925      28.22
 H       3.755895    -7.513396     2.538307      26.03
 C       4.952979    -3.377495     3.370251      14.60
 O       4.853277    -3.601332     4.710253     195.81
 H       5.134285    -4.526754     4.856662      23.27
 C       5.118203    -1.986036     2.989076      46.68
 H       4.997589    -1.355899     3.846273      24.86
 C       5.057608    -2.542993     0.661031      33.47
 C       5.028840    -2.165747    -0.912340      93.29
 H       5.496435    -3.047261    -1.437558      24.70
 O       5.970804    -1.095803    -1.198758     232.19
 H       5.825214    -0.387631    -0.577804      27.67
 C       3.642456    -1.968052    -1.462316      91.47
 H       3.042572    -2.839801    -1.216888      26.49
 C       3.605472    -1.683021    -3.010672      99.31
 O       3.715896    -2.956178    -3.777320     247.17
 H       4.537486    -3.061122    -4.439558      24.01
 H       4.306258    -0.937728    -3.384456      27.45
 H       2.651502    -1.176648    -3.274052      27.68
 C      -0.409513    -1.716359     0.026153      65.53
 H      -1.027480    -2.560162     0.122109      26.13
 C      -0.191054     0.704535     0.057970      64.08
 H      -0.665776     1.698082     0.056162      24.93
 C       1.170276     0.539722    -0.243501       7.42
 O       2.044453     1.635195    -0.422118     181.15
 C       1.572253     3.033451    -0.250480     113.25
 H       2.409115     3.729707    -0.740869      24.62
 H       0.638033     3.253147    -0.698064      27.52
 H       1.638434     3.198414     0.844657      26.97
 C       1.776294    -0.739112    -0.437943      16.88
 O       3.094095    -0.744563    -0.837512     139.56
 C       0.934256    -1.867154    -0.266451      72.42
 H       1.244239    -2.862842    -0.536541      26.59
 C      -0.972475    -0.495488     0.253125      34.97
 C      -2.472575    -0.400496     0.744816      79.91
 H      -2.614219    -1.326630     1.370416      27.73
 O      -2.673781     0.909357     1.515552     257.01
 H      -2.236990     0.726749     2.459245      27.25
 C      -3.531708    -0.386391    -0.427685      88.89
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 H      -3.326635     0.420379    -1.165960      28.72
 O      -3.462348    -1.697124    -1.081980     203.80
 H      -3.694441    -1.663771    -2.034997      28.43
 C      -4.998463    -0.320062     0.177448     102.91
 O      -5.597568     0.978688     0.544547     206.60
 H      -4.826335     1.577927     0.809029      30.37
 H      -5.043384    -1.081417     0.965596      29.35
 H      -5.639114    -0.645334    -0.700883      28.12
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name = lig-etoh-Waterframe_11
 C       5.042970    -1.511910     1.664360      49.92
 H       4.922406    -0.520675     1.293412      23.15
 C       4.901770    -3.884442     1.021685      51.58
 H       4.959842    -4.624549     0.206259      23.52
 C       4.813744    -4.356879     2.339367      33.35
 O       4.639605    -5.637198     2.722417     241.16
 C       4.103938    -6.708889     1.873094     119.24
 H       4.804756    -7.176526     1.185694      27.32
 H       3.160674    -6.405134     1.414978      29.44
 H       3.911867    -7.446884     2.671011      26.78
 C       4.994046    -3.355709     3.397075      26.87
 O       4.913319    -3.613760     4.770156     108.03
 H       4.963391    -4.564059     5.011361      19.53
 C       5.128585    -2.006610     3.022859      59.94
 H       5.258909    -1.204599     3.719133      24.45
 C       5.027205    -2.511810     0.625005      29.91
 C       5.064861    -2.180970    -0.854281      94.67
 H       5.468250    -3.023967    -1.443499      24.91
 O       5.919739    -1.070110    -1.161147     234.68
 H       5.609864    -0.287058    -0.706997      28.91
 C       3.650540    -1.935003    -1.480471      87.89
 H       3.041241    -2.826017    -1.383663      26.19
 C       3.626414    -1.693943    -3.025355      95.12
 O       3.710846    -2.977909    -3.778737     242.24
 H       4.689150    -2.994586    -4.230097      22.59
 H       4.386765    -0.946102    -3.328892      26.02
 H       2.541902    -1.361726    -3.186654      26.77
 C      -0.469064    -1.737780    -0.033179      50.05
 H      -1.029143    -2.601160     0.147151      25.20
 C      -0.157764     0.665145     0.052574      67.36
 H      -0.637021     1.650030     0.358540      23.68
 C       1.172747     0.547296    -0.292981      17.45
 O       2.080677     1.632341    -0.459483     183.30
 C       1.589787     3.017615    -0.228312     114.56
 H       2.384191     3.690576    -0.760714      25.26
 H       0.630785     3.217802    -0.716421      27.47
 H       1.535817     3.268539     0.853699      27.22
 C       1.732619    -0.747949    -0.449027      22.52
 O       3.080501    -0.775641    -0.844273     166.04
 C       0.952300    -1.868513    -0.287571      67.48
 H       1.428257    -2.830619    -0.453166      25.54
 C      -1.019926    -0.453538     0.255928      42.13
 C      -2.421634    -0.364954     0.684606      81.05
 H      -2.781774    -1.263630     1.315145      26.21
 O      -2.656578     0.867493     1.491176     261.84
 H      -2.238521     0.624459     2.429152      25.88
 C      -3.541746    -0.412133    -0.465427      85.71
 H      -3.264455     0.349599    -1.280767      28.01
 O      -3.453436    -1.716482    -1.071523     203.60
 H      -3.395762    -1.533975    -2.018154      28.61
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 C      -5.041701    -0.354678     0.148618     103.27
 O      -5.572857     0.922362     0.620483     225.28
 H      -4.733830     1.453882     0.797786      29.84
 H      -5.053252    -1.082819     1.022268      28.04
 H      -5.807287    -0.740406    -0.577126      28.57
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name = lig-etoh-Waterframe_12
 C       5.093573    -1.544982     1.654908      56.33
 H       5.123998    -0.466832     1.577933      23.85
 C       4.975190    -3.843346     1.060811      66.59
 H       4.949600    -4.655235     0.301734      21.29
 C       4.825288    -4.298306     2.361210      20.25
 O       4.647928    -5.632159     2.714113     278.20
 C       4.094530    -6.702959     1.940738     108.90
 H       4.768338    -6.920770     1.080260      27.57
 H       3.145328    -6.405147     1.483326      31.29
 H       3.916413    -7.559168     2.608737      26.59
 C       5.011596    -3.338127     3.412511     -12.17
 O       4.967925    -3.616685     4.811874     134.76
 H       5.156839    -4.598518     4.941260      21.18
 C       5.124025    -1.952469     3.016666      48.03
 H       5.412682    -1.297834     3.856565      21.54
 C       4.972431    -2.508951     0.645611      38.52
 C       5.080095    -2.187999    -0.825130      92.99
 H       5.509999    -3.043643    -1.325177      25.93
 O       5.896312    -1.018077    -1.126835     236.62
 H       5.385034    -0.228972    -0.960789      27.07
 C       3.662658    -1.937122    -1.517272      82.63
 H       3.082440    -2.839499    -1.288909      25.05
 C       3.618638    -1.727298    -3.029381     101.53
 O       3.732831    -2.960063    -3.747415     266.97
 H       4.704291    -3.048771    -4.154660      24.51
 H       4.417326    -1.022608    -3.369489      25.41
 H       2.593973    -1.299394    -3.306212      26.13
 C      -0.470860    -1.774468    -0.043411      42.61
 H      -1.058300    -2.679282     0.063632      22.01
 C      -0.187273     0.662897     0.095929      80.12
 H      -0.426487     1.693261     0.509270      20.52
 C       1.207974     0.591827    -0.334122       9.11
 O       2.095405     1.636870    -0.493908     229.45
 C       1.616260     2.980118    -0.213092     119.29
 H       2.377539     3.604487    -0.670364      26.02
 H       0.591000     3.058101    -0.695952      26.90
 H       1.445706     3.232069     0.836108      27.99
 C       1.736489    -0.737692    -0.508926      18.59
 O       3.062707    -0.788422    -0.834732     175.58
 C       0.895060    -1.894746    -0.328015      56.64
 H       1.374602    -2.883474    -0.276406      23.05
 C      -0.998660    -0.468855     0.193855      44.43
 C      -2.481357    -0.302713     0.643991      83.29
 H      -2.615362    -1.203959     1.323254      25.38
 O      -2.649188     0.808574     1.457415     276.16
 H      -2.241615     0.720373     2.397119      27.21
 C      -3.579407    -0.424430    -0.460893      92.03
 H      -3.525039     0.452036    -1.187023      27.63
 O      -3.439102    -1.742914    -1.095312     223.62
 H      -3.048131    -1.667068    -1.963177      28.91
 C      -5.053653    -0.392843     0.126992     109.93
 O      -5.523659     0.871462     0.670216     230.94
 H      -4.775171     1.418606     1.063816      30.02
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 H      -5.008443    -1.107489     1.009708      28.06
 H      -5.736233    -0.826966    -0.597335      29.61
55
name = lig-etoh-Waterframe_13
 C       5.133106    -1.552691     1.723336      59.07
 H       5.431814    -0.518208     1.461563      21.99
 C       4.999781    -3.868111     1.027108      61.63
 H       4.938232    -4.638424     0.228346      14.78
 C       4.847236    -4.251147     2.419919      25.35
 O       4.678494    -5.621763     2.784171     274.31
 C       4.079505    -6.657602     1.945166     116.90
 H       4.764666    -6.891361     1.067422      28.67
 H       3.054774    -6.410941     1.607679      30.44
 H       4.090508    -7.581287     2.534677      26.78
 C       4.997189    -3.290835     3.456133       0.75
 O       5.027143    -3.619008     4.793147     136.22
 H       5.509534    -4.523183     4.899984      19.68
 C       5.147717    -1.961274     3.044803      56.03
 H       5.299423    -1.211381     3.877269      22.52
 C       4.961917    -2.492293     0.685124      38.07
 C       5.048035    -2.141644    -0.862365      95.02
 H       5.605212    -2.963770    -1.290342      25.46
 O       5.892884    -0.968968    -1.097177     248.27
 H       5.339504    -0.195095    -1.044607      26.18
 C       3.664487    -1.992617    -1.488758      78.28
 H       3.049700    -2.882069    -1.234528      23.26
 C       3.619844    -1.715240    -3.041172     106.34
 O       3.769177    -2.960749    -3.711894     284.72
 H       4.581335    -3.048760    -4.293604      26.46
 H       4.404463    -0.994014    -3.361150      25.48
 H       2.720471    -1.177025    -3.321410      26.38
 C      -0.467340    -1.774890    -0.039207      41.40
 H      -1.165851    -2.664320     0.013321      20.20
 C      -0.110076     0.707812     0.130714      88.42
 H      -0.681794     1.612677     0.443622      19.09
 C       1.170477     0.552758    -0.339030      12.65
 O       2.111279     1.633471    -0.511346     190.73
 C       1.611559     2.943700    -0.213314     124.88
 H       2.273417     3.653217    -0.536028      27.85
 H       0.651256     3.189855    -0.799050      25.39
 H       1.587111     3.006078     0.875851      26.48
 C       1.695709    -0.740926    -0.586280      17.08
 O       3.086287    -0.791797    -0.832240     150.32
 C       0.881839    -1.894275    -0.370578      56.59
 H       1.261536    -2.931746    -0.327430      21.57
 C      -1.009499    -0.496828     0.110104      56.87
 C      -2.498402    -0.363697     0.625454      83.68
 H      -2.659056    -1.258899     1.195068      25.90
 O      -2.681205     0.843979     1.449863     279.49
 H      -2.166099     0.567221     2.276503      27.22
 C      -3.641401    -0.415913    -0.460539      99.31
 H      -3.598684     0.384734    -1.193994      26.75
 O      -3.428374    -1.753940    -1.122949     244.09
 H      -2.879597    -1.689238    -1.890634      28.56
 C      -5.006709    -0.459045     0.175606     113.75
 O      -5.490888     0.829009     0.684738     238.76
 H      -4.723603     1.123259     1.277931      29.20
 H      -5.091697    -1.293569     0.894812      28.55
 H      -5.685824    -0.622243    -0.640275      28.66
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name = lig-etoh-Waterframe_14
 C       5.177245    -1.532742     1.746768      43.77
 H       5.474249    -0.539351     1.351077      22.01
 C       4.944316    -3.892972     1.043493      53.10
 H       4.955445    -4.638159     0.241605      20.56
 C       4.870181    -4.291321     2.395172      19.93
 O       4.716034    -5.583282     2.888134     237.45
 C       4.106710    -6.592926     1.932115     116.56
 H       4.655493    -6.768566     0.968122      26.05
 H       3.032067    -6.364737     1.746801      28.43
 H       4.171589    -7.446028     2.603750      24.96
 C       4.983814    -3.285795     3.463919      35.33
 O       5.094247    -3.625686     4.783494     151.99
 H       5.571806    -4.521787     5.020509      21.71
 C       5.182324    -1.936496     3.131724      58.43
 H       5.227732    -1.086151     3.860456      23.98
 C       5.013498    -2.501625     0.678952      17.19
 C       5.055111    -2.088671    -0.835537      84.30
 H       5.524180    -2.917984    -1.435233      23.14
 O       5.884125    -0.927530    -1.084508     234.29
 H       5.461185    -0.088583    -0.862591      26.24
 C       3.635192    -1.994066    -1.473316      76.67
 H       3.070985    -2.937808    -1.311690      24.99
 C       3.658069    -1.671043    -3.013329     106.14
 O       3.784459    -2.992648    -3.703533     277.04
 H       4.532823    -2.854443    -4.273475      27.01
 H       4.518573    -1.029456    -3.198505      26.03
 H       2.690869    -1.322781    -3.244155      26.94
 C      -0.489631    -1.739142    -0.064743      58.73
 H      -1.120297    -2.694470     0.071813      20.98
 C      -0.168994     0.652414     0.132349      77.93
 H      -0.541897     1.678013     0.253459      20.20
 C       1.186700     0.552926    -0.342078       7.16
 O       2.103113     1.583282    -0.542218     208.57
 C       1.611050     2.939751    -0.195238     115.12
 H       2.401934     3.594678    -0.465967      26.50
 H       0.604646     3.195660    -0.626793      26.98
 H       1.382962     2.999255     0.899953      27.84
 C       1.692028    -0.789475    -0.643804      18.22
 O       3.086236    -0.800982    -0.836218     154.71
 C       0.905137    -1.898979    -0.416363      61.55
 H       1.383426    -2.872092    -0.615929      23.36
 C      -1.025041    -0.435752     0.097151      56.54
 C      -2.480597    -0.424382     0.577786      79.85
 H      -2.751203    -1.221450     1.218607      24.82
 O      -2.708508     0.853000     1.460009     267.25
 H      -2.253528     0.748300     2.339309      29.02
 C      -3.611713    -0.453909    -0.476245     100.49
 H      -3.546667     0.328144    -1.191510      26.22
 O      -3.437670    -1.745797    -1.130708     282.61
 H      -2.993519    -1.489944    -1.923103      29.62
 C      -5.035271    -0.517932     0.189976     106.21
 O      -5.433507     0.770156     0.713309     252.98
 H      -4.787734     1.014196     1.449405      30.35
 H      -5.170838    -1.356324     0.860797      29.20
 H      -5.724976    -0.706409    -0.654204      28.03
55
name = lig-etoh-Waterframe_15
 C       5.220465    -1.564627     1.720397      42.12
 H       5.315883    -0.485825     1.619802      23.23
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 C       4.864549    -3.886476     1.053512      61.40
 H       4.874754    -4.663882     0.306845      21.95
 C       4.890667    -4.289179     2.414947      16.64
 O       4.741091    -5.562920     2.929754     260.62
 C       4.155254    -6.519755     1.996397     106.52
 H       4.670067    -6.504536     1.038920      24.81
 H       3.105891    -6.221602     1.800755      28.57
 H       4.191532    -7.529274     2.428838      25.08
 C       5.025393    -3.307964     3.430799      -9.80
 O       5.152883    -3.631396     4.814776      93.72
 H       5.350719    -4.657804     4.880106      21.28
 C       5.192920    -1.872891     3.123256      22.24
 H       5.332317    -1.249934     4.020790      21.02
 C       5.098786    -2.514468     0.709206      39.65
 C       5.073384    -2.076528    -0.782478      77.25
 H       5.556656    -2.895005    -1.409156      26.03
 O       5.878743    -0.883095    -1.085203     195.90
 H       5.530865    -0.141819    -0.560414      27.03
 C       3.653800    -1.925597    -1.465484      92.46
 H       3.122977    -2.869371    -1.272799      28.31
 C       3.686969    -1.704723    -2.939194     104.86
 O       3.801207    -2.978783    -3.694915     278.45
 H       4.572020    -3.042884    -4.253849      27.15
 H       4.453871    -0.995390    -3.253723      28.15
 H       2.760272    -1.182051    -3.275385      28.25
 C      -0.448538    -1.718058    -0.124285      51.34
 H      -1.096817    -2.619577     0.095023      23.82
 C      -0.173129     0.663851     0.046198      71.59
 H      -0.476001     1.666421     0.275924      21.70
 C       1.177745     0.485326    -0.348506      17.76
 O       2.055251     1.554023    -0.560064     200.76
 C       1.600494     2.920857    -0.141439     111.42
 H       2.490182     3.578866    -0.445150      24.72
 H       0.770116     3.150595    -0.797656      27.93
 H       1.421611     3.014645     0.970674      27.66
 C       1.718486    -0.745324    -0.637571      29.19
 O       3.046841    -0.825878    -0.849142     173.76
 C       0.867627    -1.910755    -0.479740      58.56
 H       1.232163    -2.916437    -0.721388      25.01
 C      -1.057514    -0.471335     0.152383      54.78
 C      -2.481096    -0.370338     0.623272      93.56
 H      -2.522507    -1.281757     1.288821      26.10
 O      -2.738127     0.822820     1.447074     306.58
 H      -2.300190     0.665820     2.308241      29.53
 C      -3.594067    -0.516893    -0.458717     101.96
 H      -3.558691     0.360144    -1.111656      27.59
 O      -3.434740    -1.736386    -1.166528     274.25
 H      -3.348324    -1.648071    -2.110498      29.50
 C      -5.063062    -0.544315     0.151604     100.45
 O      -5.398862     0.708196     0.757459     237.24
 H      -4.695123     0.924939     1.448776      30.12
 H      -5.046090    -1.310420     0.940180      29.45
 H      -5.809834    -0.845030    -0.643592      28.46
55
name = lig-etoh-Waterframe_16
 C       5.256882    -1.546086     1.777908      61.25
 H       5.274299    -0.513602     1.414059      28.49
 C       4.827383    -3.870246     1.073661      62.75
 H       4.646005    -4.569950     0.270430      23.11
 C       4.892237    -4.239451     2.458481       7.37
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 O       4.767471    -5.566682     2.952355     224.46
 C       4.197289    -6.459587     2.042813     126.19
 H       4.792578    -6.410931     1.150238      26.67
 H       3.147499    -6.223777     1.796086      29.09
 H       4.290635    -7.504446     2.375338      26.74
 C       5.118351    -3.247830     3.468163      21.26
 O       5.195362    -3.631951     4.792261      61.92
 H       5.192007    -4.665213     4.925219      23.27
 C       5.191290    -1.965983     3.085803      74.53
 H       5.402154    -1.221061     3.834769      18.22
 C       5.143520    -2.526382     0.716377      -4.18
 C       5.110498    -2.070240    -0.765821      76.35
 H       5.622283    -2.901123    -1.300767      24.51
 O       5.874371    -0.858080    -1.066118     187.67
 H       5.582442    -0.140568    -0.478652      27.88
 C       3.713589    -1.926527    -1.400794      90.61
 H       3.129737    -2.814683    -1.179202      28.43
 C       3.732920    -1.727759    -2.968142      99.88
 O       3.807831    -2.948540    -3.667917     281.55
 H       4.629006    -2.977051    -4.196412      26.04
 H       4.572961    -1.064531    -3.238659      26.83
 H       2.721876    -1.202795    -3.217727      26.58
 C      -0.486426    -1.731854    -0.145734      52.84
 H      -1.064864    -2.645666    -0.069309      24.80
 C      -0.189312     0.660901    -0.044331      75.95
 H      -0.511184     1.588483     0.311007      24.89
 C       1.136991     0.497225    -0.359869       6.40
 O       2.013913     1.557335    -0.544659     222.19
 C       1.614225     2.873741    -0.131840     118.01
 H       2.542724     3.593194    -0.352603      25.00
 H       0.799779     3.284819    -0.688182      29.74
 H       1.393351     2.927206     0.958077      28.49
 C       1.680850    -0.820370    -0.600797      32.13
 O       3.042752    -0.788987    -0.847471     160.81
 C       0.863166    -1.886977    -0.576660      79.02
 H       1.106905    -2.928261    -0.696815      28.20
 C      -0.999303    -0.462167     0.180034      48.03
 C      -2.481665    -0.375744     0.709160      85.43
 H      -2.647206    -1.304677     1.404477      26.13
 O      -2.761958     0.784056     1.442147     323.81
 H      -2.311378     0.616677     2.276296      29.46
 C      -3.635820    -0.527525    -0.447670      91.25
 H      -3.507443     0.382397    -1.124313      27.68
 O      -3.410604    -1.769081    -1.237130     214.93
 H      -3.656715    -1.554080    -2.129295      29.80
 C      -5.019908    -0.585251     0.155901     105.98
 O      -5.406147     0.669828     0.797658     223.44
 H      -4.529097     0.849654     1.265506      28.92
 H      -5.041970    -1.445018     0.902143      28.56
 H      -5.831284    -0.757521    -0.607947      28.21
55
name = lig-etoh-Waterframe_17
 C       5.272268    -1.561852     1.714521      61.72
 H       5.430903    -0.484180     1.526760      26.99
 C       4.834419    -3.836846     1.119293      72.86
 H       4.446687    -4.529435     0.377426      23.41
 C       4.887869    -4.220917     2.476326      17.34
 O       4.800397    -5.515111     3.000626     223.93
 C       4.241867    -6.467629     2.009225     119.89
 H       4.801308    -6.508733     1.068445      28.33
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 H       3.179522    -6.265181     1.818748      30.05
 H       4.324773    -7.382639     2.618629      26.68
 C       5.186654    -3.323392     3.502487       1.88
 O       5.228492    -3.603021     4.787789      52.83
 H       5.318890    -4.627980     4.973839      24.07
 C       5.242622    -1.925763     3.105586      22.84
 H       5.311115    -1.128831     3.823840      16.97
 C       5.130481    -2.490438     0.743616      40.30
 C       5.158767    -2.065694    -0.747343      92.98
 H       5.595482    -2.824819    -1.379501      26.18
 O       5.893911    -0.858381    -1.031077     213.90
 H       5.504953    -0.028556    -0.660869      26.99
 C       3.746361    -1.962662    -1.366109      79.75
 H       3.190158    -2.864277    -1.133632      26.53
 C       3.777828    -1.699484    -2.953772      95.49
 O       3.826798    -2.957702    -3.657696     285.00
 H       4.543406    -2.915490    -4.362799      25.92
 H       4.639504    -1.047697    -3.194961      25.76
 H       2.770054    -1.221492    -3.200574      25.92
 C      -0.536730    -1.761792    -0.164113      58.16
 H      -1.175936    -2.588196    -0.156518      24.25
 C      -0.239785     0.670308    -0.061598      67.14
 H      -0.531325     1.635063     0.180927      23.94
 C       1.128310     0.514665    -0.403054      14.30
 O       2.001866     1.552801    -0.531614     209.90
 C       1.622940     2.874303    -0.107836     117.32
 H       2.604281     3.471499    -0.236151      24.74
 H       0.724750     3.271815    -0.562588      27.67
 H       1.372299     2.810683     0.942713      28.07
 C       1.695994    -0.803846    -0.586578      11.55
 O       3.067486    -0.728293    -0.825472     128.04
 C       0.784993    -1.949579    -0.639495      64.66
 H       1.295819    -2.881577    -0.835346      27.12
 C      -1.018153    -0.499386     0.191255      46.22
 C      -2.477780    -0.498539     0.694537      76.88
 H      -2.730324    -1.317863     1.423106      26.88
 O      -2.769930     0.783039     1.480886     284.00
 H      -2.378697     0.778691     2.345608      30.47
 C      -3.602159    -0.540611    -0.446005      88.70
 H      -3.538539     0.362187    -1.149380      27.51
 O      -3.396317    -1.774895    -1.292637     215.01
 H      -3.538083    -1.442179    -2.174679      28.24
 C      -5.022721    -0.624387     0.183724     109.02
 O      -5.403517     0.626017     0.843890     204.61
 H      -4.619198     1.115972     1.217518      30.60
 H      -5.135672    -1.557370     0.814116      29.01
 H      -5.700713    -0.755851    -0.676247      28.92
55
name = lig-etoh-Waterframe_19
 C       5.343703    -1.475003     1.777163      73.97
 H       5.555744    -0.483870     1.403578      22.76
 C       4.820027    -3.814418     1.127811      46.45
 H       4.751775    -4.592219     0.334825      22.48
 C       4.983095    -4.172646     2.499089       9.52
 O       4.796830    -5.525592     2.939601     283.17
 C       4.327373    -6.549007     2.090489     114.72
 H       5.073442    -6.626028     1.236607      24.55
 H       3.333205    -6.312261     1.656955      28.23
 H       4.292353    -7.499315     2.651781      23.63
 C       5.243973    -3.204880     3.532889       3.88
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 O       5.309514    -3.556661     4.896371      78.19
 H       5.532553    -4.537120     4.982864      24.53
 C       5.382165    -1.862242     3.143675      51.63
 H       5.562026    -1.118478     3.944978      21.10
 C       5.071952    -2.436409     0.774522      14.10
 C       5.143863    -2.057762    -0.761281      91.26
 H       5.602900    -2.925687    -1.260377      24.22
 O       5.989637    -0.854628    -0.947513     207.74
 H       5.435036    -0.013208    -0.914277      24.56
 C       3.746948    -1.883202    -1.389101      90.80
 H       3.153120    -2.795440    -1.196515      24.35
 C       3.831727    -1.680163    -2.908049     102.99
 O       3.851707    -2.972331    -3.628836     268.73
 H       4.738053    -2.883532    -4.162105      25.02
 H       4.778819    -1.158138    -3.099996      25.42
 H       2.941411    -1.196727    -3.189386      27.56
 C      -0.546096    -1.832547    -0.239918      54.35
 H      -1.026468    -2.820890    -0.206435      21.06
 C      -0.292639     0.543998    -0.008060      65.59
 H      -0.701141     1.508569     0.112695      21.63
 C       1.063560     0.496552    -0.422002       3.86
 O       2.018703     1.562208    -0.540140     200.29
 C       1.625633     2.879866     0.009758     118.03
 H       2.434682     3.485521    -0.148772      26.53
 H       0.663870     3.288201    -0.507412      25.29
 H       1.299001     2.893552     1.072191      26.44
 C       1.658723    -0.817423    -0.687357      11.33
 O       3.080602    -0.771261    -0.768808     164.77
 C       0.819620    -1.905836    -0.658526      62.27
 H       1.102048    -2.894676    -1.052568      22.84
 C      -1.067415    -0.585848     0.115989      45.44
 C      -2.500488    -0.526035     0.692761      86.49
 H      -2.647195    -1.329710     1.380625      26.09
 O      -2.739834     0.690959     1.478411     284.59
 H      -2.302663     0.514271     2.379939      27.13
 C      -3.572345    -0.599937    -0.437087     102.73
 H      -3.397095     0.312228    -0.960252      27.49
 O      -3.397785    -1.725529    -1.293586     284.50
 H      -3.027500    -1.395897    -2.141639      28.31
 C      -5.018226    -0.642676     0.153613     106.56
 O      -5.443697     0.544971     0.911133     234.76
 H      -4.619201     0.790951     1.429176      31.09
 H      -5.070249    -1.503028     0.814512      28.95
 H      -5.742927    -0.822584    -0.628250      28.02
55
name = lig-etoh-Waterframe_20
 C       5.364859    -1.459298     1.780566      57.13
 H       5.510537    -0.435771     1.532277      23.21
 C       4.862688    -3.771022     1.132825      52.71
 H       4.842230    -4.542066     0.339552      23.15
 C       5.000577    -4.180985     2.493318      10.17
 O       4.810993    -5.508064     2.955299     276.42
 C       4.377426    -6.582397     2.073020     120.32
 H       5.137772    -6.866584     1.317278      25.58
 H       3.396658    -6.428014     1.583591      28.09
 H       4.289884    -7.378615     2.806409      25.36
 C       5.244918    -3.216505     3.593015       0.30
 O       5.355598    -3.521205     4.888917     135.35
 H       5.299749    -4.485317     5.039203      26.74
 C       5.457904    -1.814771     3.177040      34.99
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 H       5.858645    -1.030944     3.874525      21.01
 C       5.056646    -2.409763     0.814316      40.66
 C       5.115426    -2.027363    -0.695213      89.93
 H       5.601968    -2.843584    -1.312534      24.46
 O       6.024831    -0.885632    -0.927126     192.76
 H       5.593621     0.011341    -0.683861      23.87
 C       3.735613    -1.885458    -1.386333      82.54
 H       3.221141    -2.856372    -1.236386      24.66
 C       3.855725    -1.683615    -2.950444     102.52
 O       3.868623    -2.941360    -3.595543     265.23
 H       4.786368    -3.143021    -4.073188      25.03
 H       4.733833    -1.080663    -3.255407      25.77
 H       3.006530    -1.073328    -3.334827      26.90
 C      -0.478572    -1.857596    -0.286957      33.78
 H      -1.086616    -2.833391    -0.199157      20.91
 C      -0.256327     0.527027    -0.015742      83.73
 H      -0.745895     1.412099     0.401082      19.61
 C       1.105118     0.467779    -0.405374      16.78
 O       1.963086     1.575647    -0.507255     213.24
 C       1.593458     2.868098     0.032524     118.72
 H       2.454439     3.486972    -0.072449      24.98
 H       0.673493     3.303272    -0.482398      25.52
 H       1.434181     2.654068     1.146372      26.12
 C       1.671873    -0.763667    -0.731458      23.83
 O       3.029912    -0.804748    -0.747854     182.12
 C       0.829149    -1.932555    -0.688627      46.13
 H       1.359952    -2.865114    -0.888336      21.62
 C      -1.096326    -0.669384     0.083132      74.55
 C      -2.488606    -0.537631     0.707550      83.35
 H      -2.706108    -1.427956     1.378036      25.22
 O      -2.705896     0.615328     1.467340     297.30
 H      -2.243900     0.571394     2.384091      27.22
 C      -3.622286    -0.525017    -0.424580      98.36
 H      -3.551065     0.325730    -1.097348      26.84
 O      -3.386506    -1.734393    -1.246908     257.98
 H      -3.217838    -1.390414    -2.168139      26.56
 C      -5.027749    -0.673573     0.151545     103.06
 O      -5.440616     0.510892     0.917164     233.42
 H      -4.820938     0.681254     1.668593      32.07
 H      -5.027562    -1.619018     0.729810      29.01
 H      -5.771351    -0.772996    -0.676330      27.73
55
name = lig-etoh-Waterframe_21
 C       5.363025    -1.456270     1.864883      57.34
 H       5.539750    -0.437798     1.602163      23.18
 C       4.945588    -3.737988     1.198148      57.39
 H       4.742039    -4.464379     0.404946      20.99
 C       4.978436    -4.182209     2.526103      26.25
 O       4.836032    -5.457347     2.972441     216.52
 C       4.438000    -6.625908     2.073389     121.44
 H       5.204749    -6.966254     1.398991      27.86
 H       3.500867    -6.347305     1.561512      28.53
 H       4.212873    -7.417803     2.779742      26.06
 C       5.255870    -3.154292     3.499411       9.69
 O       5.393784    -3.512057     4.908512     168.12
 H       5.301270    -4.456220     5.074054      23.72
 C       5.532828    -1.846482     3.176098      78.70
 H       5.879055    -1.145922     3.969150      24.75
 C       5.053767    -2.390688     0.786503      10.16
 C       5.106377    -1.972472    -0.637091      85.37
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 H       5.596744    -2.867969    -1.134598      23.74
 O       6.045248    -0.918428    -0.915542     175.28
 H       5.648189    -0.088597    -0.454205      25.27
 C       3.742266    -1.889118    -1.407438      78.11
 H       3.262353    -2.870704    -1.269771      25.29
 C       3.881606    -1.624476    -2.962163      93.46
 O       3.890566    -2.963435    -3.584203     252.33
 H       4.705400    -3.053730    -4.275622      23.70
 H       4.775517    -1.023598    -3.218404      24.92
 H       2.938960    -1.060310    -3.349613      25.21
 C      -0.474096    -1.939447    -0.325315      58.93
 H      -1.159624    -2.873384    -0.230242      18.71
 C      -0.258326     0.487234     0.003791      67.46
 H      -0.521942     1.462895     0.521695      19.60
 C       1.086602     0.493082    -0.388039      20.16
 O       1.924075     1.578572    -0.492566     230.95
 C       1.551015     2.824824     0.094529     119.65
 H       2.424457     3.544827    -0.114427      24.41
 H       0.707086     3.287901    -0.391700      27.22
 H       1.383126     2.782770     1.223052      26.64
 C       1.637950    -0.770797    -0.739868      20.96
 O       3.025007    -0.819794    -0.747743     158.32
 C       0.927200    -1.947897    -0.738530      63.26
 H       1.367188    -2.942941    -0.718120      23.92
 C      -1.054438    -0.657544     0.070102      53.64
 C      -2.505556    -0.607328     0.648876      70.01
 H      -2.651393    -1.645564     1.151128      23.65
 O      -2.669940     0.617555     1.491699     299.65
 H      -2.063371     0.359530     2.299037      25.34
 C      -3.631803    -0.500637    -0.424578      93.17
 H      -3.637084     0.485644    -1.000001      26.16
 O      -3.381084    -1.729838    -1.202854     220.78
 H      -3.490556    -1.667826    -2.219380      26.38
 C      -5.044324    -0.679406     0.168645      99.52
 O      -5.468259     0.470329     0.920825     234.10
 H      -4.814816     0.467670     1.665535      31.60
 H      -5.156909    -1.638087     0.765642      28.76
 H      -5.769678    -0.684929    -0.705815      27.88
55
name = lig-etoh-Waterframe_22
 C       5.353000    -1.426892     1.855252      66.69
 H       5.578639    -0.399055     1.641966      21.79
 C       4.985539    -3.737077     1.199888      63.35
 H       4.721914    -4.483903     0.465859      20.76
 C       4.963742    -4.124206     2.543516      17.47
 O       4.855957    -5.473512     2.984242     245.11
 C       4.488036    -6.598329     2.117479     120.77
 H       5.346669    -6.805410     1.489505      28.12
 H       3.668450    -6.302217     1.430676      29.85
 H       4.182347    -7.429308     2.768294      26.35
 C       5.290265    -3.207000     3.546777      12.73
 O       5.417356    -3.486034     4.874656     186.61
 H       5.533421    -4.436005     4.941766      20.27
 C       5.581187    -1.876446     3.186311      44.84
 H       5.775732    -1.238734     4.054957      24.76
 C       5.077589    -2.332288     0.890705      27.38
 C       5.125330    -1.999395    -0.664805      91.79
 H       5.564529    -2.908392    -1.088229      25.30
 O       6.048264    -0.925520    -0.896892     210.78
 H       5.754739     0.004072    -0.549855      22.68
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 C       3.775246    -1.854827    -1.424836      89.73
 H       3.239291    -2.806699    -1.332232      25.62
 C       3.895165    -1.597125    -2.938053      94.84
 O       3.928430    -2.970798    -3.598463     266.81
 H       4.514977    -2.768260    -4.435261      24.73
 H       4.823937    -1.054510    -3.142808      24.98
 H       2.927200    -1.082984    -3.253519      24.88
 C      -0.459882    -1.928910    -0.357946      41.07
 H      -0.956326    -2.923600    -0.348557      21.20
 C      -0.250840     0.505311     0.067231      67.95
 H      -0.737264     1.479252     0.433155      19.09
 C       1.042356     0.466046    -0.407586      15.89
 O       1.915759     1.572747    -0.476014     199.36
 C       1.501630     2.839230     0.161775     112.60
 H       2.430894     3.523762    -0.090746      23.53
 H       0.604820     3.159452    -0.271191      26.43
 H       1.307962     2.813228     1.241773      26.40
 C       1.663150    -0.802719    -0.728065       8.94
 O       3.049939    -0.801481    -0.766794     159.31
 C       0.878766    -2.006489    -0.725944      55.00
 H       1.462762    -2.928555    -0.850661      23.56
 C      -1.017318    -0.718433     0.042383      53.81
 C      -2.487688    -0.622403     0.559073      82.28
 H      -2.717895    -1.496140     1.226111      25.43
 O      -2.621341     0.567938     1.516541     277.39
 H      -2.132679     0.438714     2.440293      27.12
 C      -3.628934    -0.552652    -0.430938      99.60
 H      -3.473488     0.448156    -0.987605      25.80
 O      -3.395714    -1.732426    -1.194995     236.85
 H      -3.561797    -1.461206    -2.191540      24.94
 C      -5.085949    -0.667895     0.154537     102.63
 O      -5.505344     0.437726     0.954670     248.75
 H      -4.786420     0.614648     1.615073      31.71
 H      -5.180744    -1.631440     0.735456      28.85
 H      -5.756411    -0.799417    -0.734307      28.34
55
name = lig-etoh-Waterframe_23
 C       5.387667    -1.355572     1.909508      48.27
 H       5.515023    -0.310134     1.624072      20.83
 C       4.962463    -3.712083     1.198930      68.46
 H       4.870382    -4.417968     0.382829      22.26
 C       4.975027    -4.171620     2.541186      19.87
 O       4.861552    -5.475413     3.014889     229.52
 C       4.553090    -6.507637     2.126474     135.09
 H       5.480968    -6.862718     1.596297      27.91
 H       3.736512    -6.334725     1.398964      28.84
 H       4.243401    -7.371288     2.767118      26.97
 C       5.347479    -3.207056     3.582377      13.74
 O       5.446983    -3.506443     4.879017     110.09
 H       5.504377    -4.472208     5.114382      17.77
 C       5.566121    -1.878621     3.210366      67.31
 H       5.801185    -1.144674     3.959751      24.08
 C       5.086719    -2.357168     0.867914      12.85
 C       5.153692    -2.045368    -0.650969      81.23
 H       5.634268    -2.831202    -1.188736      25.29
 O       6.074057    -0.917986    -0.904750     173.91
 H       5.505832    -0.057282    -0.740081      22.75
 C       3.805692    -1.842570    -1.404586      90.60
 H       3.260893    -2.786849    -1.281083      25.87
 C       3.904460    -1.630433    -2.916632     107.93
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 O       3.960560    -2.900460    -3.615201     291.97
 H       4.520893    -2.975800    -4.476683      25.70
 H       4.740434    -1.005095    -3.232220      25.26
 H       3.094507    -1.004937    -3.266082      26.18
 C      -0.456984    -1.948472    -0.385905      34.33
 H      -1.093281    -2.797882    -0.378918      20.15
 C      -0.278530     0.470668     0.096953      74.89
 H      -0.886914     1.385437     0.339367      18.86
 C       1.067542     0.427824    -0.422186       8.72
 O       1.913423     1.564867    -0.437795     179.84
 C       1.446621     2.839348     0.201789     106.83
 H       2.249965     3.651389     0.016728      25.19
 H       0.540268     3.216144    -0.265609      25.39
 H       1.413025     2.603932     1.227677      26.41
 C       1.674722    -0.845141    -0.693889      25.11
 O       3.072575    -0.747583    -0.796475     175.91
 C       0.904691    -2.000705    -0.708652      60.09
 H       1.250816    -2.988184    -1.079067      22.30
 C      -1.049698    -0.722538     0.040124      48.60
 C      -2.436346    -0.607655     0.632338      94.06
 H      -2.607033    -1.507751     1.196665      24.60
 O      -2.595067     0.518469     1.495190     308.22
 H      -2.181801     0.207545     2.386081      27.45
 C      -3.626357    -0.579121    -0.423794     101.05
 H      -3.545535     0.240686    -1.158124      25.45
 O      -3.436792    -1.752110    -1.252653     239.85
 H      -3.346216    -1.466809    -2.270807      23.83
 C      -5.089447    -0.674382     0.134349     103.90
 O      -5.555986     0.428606     0.998368     264.17
 H      -4.713681     0.785084     1.374276      31.69
 H      -5.082146    -1.620496     0.677234      29.58
 H      -5.809297    -0.698320    -0.675593      28.46
55
name = lig-etoh-Waterframe_24
 C       5.396543    -1.407498     1.893700      48.03
 H       5.477009    -0.319309     1.734423      22.98
 C       4.920079    -3.719292     1.215613      48.28
 H       4.943207    -4.422064     0.378999      24.73
 C       5.040455    -4.172714     2.568347      21.21
 O       4.856174    -5.431216     3.053151     241.86
 C       4.621327    -6.499375     2.102693     112.19
 H       5.549705    -6.803298     1.511503      26.12
 H       3.823416    -6.177466     1.412632      27.94
 H       4.239166    -7.316851     2.756015      27.03
 C       5.373934    -3.217756     3.512998     -23.82
 O       5.492998    -3.547296     4.964585      87.87
 H       5.230004    -4.557861     5.076545      23.63
 C       5.528974    -1.803801     3.230706      46.34
 H       5.856960    -1.165106     4.031503      16.79
 C       5.124870    -2.332794     0.845563      -2.82
 C       5.206630    -2.037349    -0.645361      75.70
 H       5.610252    -2.938557    -1.128579      25.39
 O       6.077817    -0.907137    -0.921553     167.69
 H       5.512317    -0.039943    -0.818969      22.63
 C       3.818138    -1.872269    -1.361533      80.47
 H       3.246281    -2.782542    -1.140248      27.08
 C       3.946867    -1.612503    -2.954732     103.81
 O       3.960582    -2.864843    -3.635298     289.58
 H       4.760666    -2.851345    -4.221433      27.07
 H       4.858248    -1.025497    -3.134075      25.58
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 H       3.035307    -1.138970    -3.211106      28.36
 C      -0.508753    -1.941628    -0.377913      35.76
 H      -1.113706    -2.782070    -0.479140      19.43
 C      -0.259180     0.406095     0.031694      71.48
 H      -0.599582     1.377983     0.366415      18.53
 C       1.064103     0.431518    -0.356169      26.15
 O       1.914018     1.566885    -0.411872     231.02
 C       1.405392     2.788928     0.228646     118.30
 H       2.171048     3.525274     0.053873      25.08
 H       0.380578     3.179588    -0.129753      24.49
 H       1.274764     2.645736     1.299637      26.38
 C       1.720244    -0.817726    -0.651786      23.69
 O       3.090712    -0.703705    -0.836971     172.09
 C       0.916435    -2.019911    -0.725914      59.19
 H       1.261409    -2.971163    -1.160631      22.65
 C      -1.058608    -0.712089     0.055077      42.58
 C      -2.460282    -0.661062     0.684819      84.09
 H      -2.571728    -1.589012     1.196384      24.95
 O      -2.589715     0.494029     1.486026     322.92
 H      -2.161603     0.409120     2.401243      27.89
 C      -3.615417    -0.584529    -0.461013      92.31
 H      -3.553839     0.352128    -0.987778      25.34
 O      -3.484792    -1.805778    -1.311717     244.98
 H      -3.238525    -1.598044    -2.328000      24.00
 C      -5.074838    -0.680620     0.142275     103.11
 O      -5.572663     0.419963     1.030628     275.86
 H      -4.761846     0.938069     1.221720      32.56
 H      -5.213082    -1.612425     0.672598      29.26
 H      -5.741363    -0.692175    -0.703650      28.39
55
name = lig-etoh-Waterframe_25
 C       5.386343    -1.445211     1.870979      69.93
 H       5.543252    -0.383031     1.571671      22.76
 C       4.924739    -3.711957     1.220504      67.76
 H       4.759074    -4.523030     0.488041      22.48
 C       5.103429    -4.115839     2.545498      -1.50
 O       4.854242    -5.413370     3.072013     242.81
 C       4.657920    -6.491495     2.080671     120.79
 H       5.607690    -6.640933     1.521526      26.56
 H       3.896871    -6.172777     1.359771      26.07
 H       4.315987    -7.404758     2.588679      26.81
 C       5.404242    -3.156986     3.635040      -3.89
 O       5.521085    -3.546639     4.948943      60.93
 H       5.439278    -4.637843     5.070384      22.78
 C       5.493241    -1.829034     3.246510      49.75
 H       5.725110    -1.129103     4.054707      20.21
 C       5.162610    -2.368697     0.874384      29.35
 C       5.221482    -1.991598    -0.650180      91.04
 H       5.723324    -2.904055    -1.102157      24.06
 O       6.083496    -0.904055    -0.957085     205.09
 H       5.682738    -0.023452    -0.612158      23.42
 C       3.833222    -1.876906    -1.355535      86.35
 H       3.246623    -2.789589    -1.164568      25.48
 C       3.957734    -1.597521    -2.902000      96.60
 O       3.978238    -2.863660    -3.665807     287.89
 H       4.746656    -2.924965    -4.280027      26.45
 H       4.846777    -0.956359    -3.116853      24.39
 H       3.065814    -1.014642    -3.219847      26.43
 C      -0.479509    -1.940194    -0.385989      31.55
 H      -1.029863    -2.845497    -0.503586      20.94
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 C      -0.234662     0.449689    -0.018034      82.47
 H      -0.613876     1.311968     0.434009      19.35
 C       1.138728     0.398580    -0.296026      20.79
 O       1.887144     1.569513    -0.377374     235.24
 C       1.368273     2.737341     0.274053     123.75
 H       2.078788     3.452315     0.058310      26.69
 H       0.380557     3.022603    -0.292853      24.84
 H       1.233394     2.666479     1.398646      26.63
 C       1.738421    -0.813180    -0.625513      18.35
 O       3.112940    -0.695713    -0.876729     174.03
 C       0.867476    -1.981151    -0.743215      49.75
 H       1.382504    -2.864457    -1.065167      22.30
 C      -1.075494    -0.768278     0.077011      62.35
 C      -2.499794    -0.742235     0.643240      79.69
 H      -2.738914    -1.596515     1.330048      24.52
 O      -2.619470     0.518265     1.498605     302.91
 H      -2.126157     0.422320     2.348861      27.94
 C      -3.610764    -0.626260    -0.447496      91.97
 H      -3.400509     0.314585    -0.943779      25.90
 O      -3.524241    -1.830212    -1.325257     215.40
 H      -3.441773    -1.488371    -2.320386      23.49
 C      -5.081984    -0.676496     0.148217      99.44
 O      -5.547886     0.401235     1.034281     278.03
 H      -4.821395     1.021756     1.237299      32.27
 H      -5.247179    -1.626536     0.701126      28.35
 H      -5.700234    -0.709111    -0.767688      27.78
55
name = lig-etoh-Waterframe_26
 C       5.389106    -1.454506     1.895114      54.74
 H       5.646711    -0.425033     1.564948      22.29
 C       4.965366    -3.745212     1.243520      53.38
 H       4.533854    -4.435939     0.486573      20.50
 C       5.133154    -4.078472     2.615648      15.21
 O       4.853695    -5.406216     3.048924     240.69
 C       4.697964    -6.441767     2.050559     117.98
 H       5.647931    -6.600958     1.566837      26.63
 H       3.886890    -6.294330     1.323967      27.98
 H       4.499824    -7.371358     2.573201      26.62
 C       5.402661    -3.157379     3.676445      33.61
 O       5.551258    -3.530930     4.936346     125.43
 H       5.699419    -4.547605     5.073229      23.94
 C       5.474813    -1.821585     3.265897      52.73
 H       5.521147    -0.948808     3.944002      23.15
 C       5.179816    -2.400471     0.840293       4.62
 C       5.216206    -1.989502    -0.635828      92.96
 H       5.734554    -2.793100    -1.240234      23.13
 O       6.110245    -0.880165    -0.986272     191.68
 H       5.725389    -0.097698    -0.518824      25.17
 C       3.852480    -1.856711    -1.389981      90.08
 H       3.322865    -2.818429    -1.247169      25.06
 C       3.962122    -1.613964    -2.866213      96.78
 O       3.995045    -2.862038    -3.673764     300.49
 H       4.536694    -2.848201    -4.466229      27.99
 H       4.866857    -1.002664    -3.087154      23.52
 H       3.084464    -0.959644    -3.216865      24.64
 C      -0.446890    -1.977640    -0.394964      51.40
 H      -1.013563    -2.944097    -0.397254      20.08
 C      -0.290247     0.428087     0.017367      55.38
 H      -0.784885     1.289764     0.335015      20.06
 C       1.147537     0.398838    -0.254043      10.74
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 O       1.903030     1.548337    -0.327367     226.80
 C       1.325989     2.730027     0.286449     120.29
 H       2.006735     3.544745     0.145156      26.64
 H       0.365129     3.048427    -0.215501      25.75
 H       1.178196     2.516595     1.401954      26.29
 C       1.750881    -0.846767    -0.629837      28.48
 O       3.111388    -0.728344    -0.892065     178.25
 C       0.925053    -1.907924    -0.762472      72.43
 H       1.265251    -2.885571    -1.004926      24.23
 C      -1.041775    -0.762030     0.083558      42.33
 C      -2.513862    -0.740998     0.644848      79.56
 H      -2.712819    -1.684237     1.310042      23.73
 O      -2.667934     0.527271     1.473698     301.73
 H      -2.210786     0.257556     2.270130      28.92
 C      -3.628700    -0.685913    -0.394999     102.66
 H      -3.432495     0.153604    -1.105632      25.96
 O      -3.556259    -1.804856    -1.306233     194.03
 H      -3.660382    -1.526272    -2.292243      24.28
 C      -5.080337    -0.659839     0.139099     102.07
 O      -5.516303     0.385735     1.018562     271.72
 H      -4.678261     0.848565     1.240038      30.99
 H      -5.144876    -1.666310     0.677046      28.45
 H      -5.823113    -0.637459    -0.712981      27.28
55
name = lig-etoh-Waterframe_27
 C       5.413010    -1.474156     1.881947      51.14
 H       5.586573    -0.409199     1.762492      24.29
 C       5.005865    -3.738795     1.280372      58.18
 H       4.609807    -4.507099     0.588329      23.31
 C       5.103041    -4.132858     2.636746      23.70
 O       4.851049    -5.388585     3.028883     224.59
 C       4.767106    -6.418834     2.027475     109.96
 H       5.652082    -6.491069     1.405295      27.70
 H       3.883887    -6.267124     1.360540      28.43
 H       4.601709    -7.254765     2.693039      26.80
 C       5.392621    -3.152786     3.602968     -15.53
 O       5.601513    -3.511126     5.000065     194.65
 H       5.477957    -4.494735     5.092075      27.16
 C       5.450473    -1.754402     3.254431      41.88
 H       5.520605    -0.996134     4.078029      18.86
 C       5.199786    -2.392797     0.843298       9.92
 C       5.243655    -2.013083    -0.686903      83.44
 H       5.623921    -2.925883    -1.181845      25.22
 O       6.130757    -0.853447    -0.977064     190.82
 H       5.692336    -0.025577    -0.724744      25.34
 C       3.858754    -1.877363    -1.396688      93.21
 H       3.314855    -2.819037    -1.223310      26.84
 C       4.000736    -1.621233    -2.945548     101.05
 O       3.979669    -2.863262    -3.650732     301.80
 H       4.522113    -2.665756    -4.406801      28.22
 H       4.937774    -1.071506    -3.081175      26.06
 H       3.038439    -1.073070    -3.186404      25.75
 C      -0.419153    -1.951055    -0.359193      44.07
 H      -0.934222    -2.980004    -0.359071      21.85
 C      -0.286947     0.393769     0.085111      82.83
 H      -0.793621     1.331070     0.182635      20.92
 C       1.043060     0.401024    -0.233481      18.81
 O       1.943783     1.539390    -0.274987     182.67
 C       1.286047     2.741513     0.303268     118.32
 H       2.081702     3.556596     0.281357      24.74
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 H       0.365251     3.007110    -0.132192      27.03
 H       1.046445     2.530284     1.381292      26.46
 C       1.768095    -0.773586    -0.634121      12.45
 O       3.099122    -0.765844    -0.875639     151.33
 C       0.947701    -1.990221    -0.778897      47.31
 H       1.423683    -2.898199    -1.139097      23.93
 C      -1.045347    -0.802997     0.070631      58.87
 C      -2.483112    -0.694291     0.661584      83.93
 H      -2.552149    -1.632673     1.296617      25.14
 O      -2.715180     0.481529     1.436724     303.06
 H      -2.400542     0.495447     2.337846      31.44
 C      -3.661899    -0.672249    -0.433961      97.44
 H      -3.530379     0.359600    -0.936274      25.82
 O      -3.585494    -1.812292    -1.271842     235.42
 H      -3.598984    -1.498075    -2.229951      25.22
 C      -5.097356    -0.693074     0.139364     103.79
 O      -5.458073     0.400739     1.010102     265.82
 H      -4.623216     0.651215     1.458800      31.24
 H      -5.278963    -1.682154     0.646995      29.11
 H      -5.783306    -0.691870    -0.761025      28.63
55
name = lig-etoh-Waterframe_28
 C       5.439749    -1.397351     1.872246      49.45
 H       5.422659    -0.399861     1.496308      22.71
 C       5.026075    -3.716213     1.273265      81.88
 H       4.945630    -4.501111     0.518392      23.53
 C       5.066516    -4.110882     2.589866       7.73
 O       4.856479    -5.408184     3.045316     223.47
 C       4.813029    -6.425810     2.022481     109.61
 H       5.709543    -6.397726     1.355131      26.83
 H       3.860610    -6.289936     1.443599      28.11
 H       4.768180    -7.434752     2.488444      26.03
 C       5.392884    -3.121108     3.657406       6.98
 O       5.632108    -3.472835     4.996924     196.39
 H       5.343882    -4.349008     5.230003      25.51
 C       5.428039    -1.804864     3.252904      53.99
 H       5.666778    -1.067189     4.051994      19.44
 C       5.227112    -2.382788     0.857842       4.30
 C       5.270429    -2.022629    -0.708370      77.54
 H       5.819925    -2.824565    -1.182541      24.84
 O       6.135321    -0.867131    -0.964653     188.54
 H       5.562692    -0.111999    -0.828019      27.53
 C       3.856502    -1.907771    -1.411654      83.22
 H       3.329918    -2.855346    -1.242767      26.69
 C       3.999996    -1.615994    -2.962881     104.96
 O       3.962075    -2.879578    -3.646833     298.36
 H       4.643039    -3.076981    -4.360648      25.90
 H       4.857517    -1.025003    -3.259832      26.35
 H       3.217676    -0.939614    -3.331363      26.61
 C      -0.361734    -1.999327    -0.333371      54.98
 H      -1.027074    -2.927979    -0.368241      20.93
 C      -0.299551     0.396487     0.129918      79.47
 H      -0.820416     1.366815     0.323134      19.02
 C       1.094529     0.411684    -0.261969       8.22
 O       1.914936     1.548456    -0.204810     207.83
 C       1.278991     2.735114     0.349117     113.65
 H       2.090096     3.595755     0.280775      25.23
 H       0.545992     3.026319    -0.324230      27.99
 H       0.990483     2.606065     1.377406      27.27
 C       1.673222    -0.829791    -0.653940      20.32
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 O       3.114133    -0.754156    -0.834513     146.22
 C       0.977561    -1.998419    -0.761464      67.45
 H       1.434127    -2.891728    -1.218446      24.12
 C      -1.067847    -0.788470     0.082875      56.32
 C      -2.467440    -0.722252     0.648552      88.27
 H      -2.681667    -1.552123     1.285297      25.38
 O      -2.764707     0.477727     1.419588     288.12
 H      -2.294123     0.418124     2.271816      30.07
 C      -3.677965    -0.614679    -0.415582      95.68
 H      -3.582955     0.353250    -0.993003      25.59
 O      -3.585899    -1.807587    -1.274556     239.64
 H      -3.373077    -1.596513    -2.203142      27.62
 C      -5.129027    -0.739699     0.154439     106.13
 O      -5.401646     0.426124     1.004109     257.77
 H      -4.643924     0.453357     1.614901      31.36
 H      -5.333040    -1.677058     0.661160      29.52
 H      -5.774172    -0.626915    -0.723406      29.03
55
name = lig-etoh-Waterframe_29
 C       5.412357    -1.366716     1.847093      56.17
 H       5.441709    -0.321270     1.611216      22.21
 C       5.056938    -3.705011     1.203895      46.66
 H       5.138918    -4.415824     0.400480      22.69
 C       5.055580    -4.060934     2.648411       1.28
 O       4.880505    -5.439540     3.071896     207.88
 C       4.834408    -6.454166     2.005509     104.10
 H       5.727485    -6.262446     1.331091      26.20
 H       3.917582    -6.392974     1.385226      28.44
 H       4.953218    -7.469377     2.461929      25.29
 C       5.350571    -3.174752     3.669607      12.35
 O       5.642462    -3.419755     4.970362     192.77
 H       5.495052    -4.336661     5.167322      26.64
 C       5.459789    -1.793933     3.233382      16.56
 H       5.706834    -1.027794     3.968308      20.51
 C       5.257693    -2.331147     0.848138       7.92
 C       5.303835    -2.030024    -0.671644      83.75
 H       5.798168    -2.843359    -1.216013      25.82
 O       6.112749    -0.889669    -0.958969     196.92
 H       5.670534    -0.045502    -0.728486      24.92
 C       3.873115    -1.880487    -1.441531      74.41
 H       3.350579    -2.836964    -1.335472      26.95
 C       4.001089    -1.598691    -2.975600     102.61
 O       3.926506    -2.941610    -3.662187     268.42
 H       4.779646    -3.047600    -4.254809      24.99
 H       4.968663    -1.145617    -3.164895      25.98
 H       3.154905    -1.038874    -3.310726      27.91
 C      -0.410790    -2.026274    -0.299794      47.47
 H      -0.947073    -2.982166    -0.417764      20.54
 C      -0.265615     0.423062     0.119215      64.58
 H      -0.759195     1.311711     0.645016      17.24
 C       1.098552     0.409141    -0.265803      13.31
 O       1.887204     1.536980    -0.128188     227.45
 C       1.293782     2.756982     0.359683     115.07
 H       2.183966     3.495508     0.399163      24.47
 H       0.487590     3.128367    -0.322467      27.12
 H       0.835851     2.667180     1.317506      27.73
 C       1.728437    -0.827393    -0.680636      18.46
 O       3.107752    -0.760572    -0.793409     156.76
 C       0.931529    -2.024361    -0.734615      55.62
 H       1.363157    -2.978631    -1.123767      24.64
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 C      -1.005252    -0.794611     0.101419      60.72
 C      -2.557287    -0.758649     0.609191      79.58
 H      -2.746022    -1.652716     1.162535      26.97
 O      -2.765972     0.496647     1.442602     286.46
 H      -2.138824     0.356890     2.178216      28.79
 C      -3.674360    -0.647900    -0.406792     106.65
 H      -3.584931     0.220405    -1.029156      27.03
 O      -3.551755    -1.786380    -1.300542     248.17
 H      -3.268302    -1.509002    -2.170526      28.48
 C      -5.130567    -0.705224     0.178440     111.35
 O      -5.378098     0.431982     1.006335     260.15
 H      -4.642954     0.436845     1.641614      31.07
 H      -5.236165    -1.675913     0.658743      29.34
 H      -5.867243    -0.656932    -0.606017      29.20
55
name = lig-etoh-Waterframe_30
 C       5.364344    -1.371945     1.889850      60.47
 H       5.600997    -0.329301     1.800799      23.51
 C       5.117406    -3.665315     1.236397      69.69
 H       5.033239    -4.450824     0.502172      24.58
 C       5.038635    -4.144903     2.601383      -3.32
 O       4.908780    -5.442926     3.073383     209.27
 C       4.882616    -6.451256     1.985591     115.60
 H       5.727340    -6.312840     1.268221      25.94
 H       3.933445    -6.464814     1.457965      27.89
 H       4.982267    -7.364241     2.600251      25.17
 C       5.319267    -3.097263     3.602116       0.15
 O       5.635691    -3.407790     4.970284     172.54
 H       5.706986    -4.344987     5.148161      20.64
 C       5.506729    -1.765548     3.188379      55.96
 H       5.649855    -1.054698     3.971791      26.14
 C       5.254631    -2.333868     0.808103      30.97
 C       5.280124    -2.005265    -0.661315      93.87
 H       5.678917    -2.944240    -1.125869      25.36
 O       6.121358    -0.889223    -0.971720     222.47
 H       5.719983    -0.074798    -0.545974      25.64
 C       3.892574    -1.843441    -1.427703      83.68
 H       3.313799    -2.771026    -1.306307      27.26
 C       4.005503    -1.651288    -2.970170      99.50
 O       3.903332    -2.977366    -3.656558     263.53
 H       4.580687    -2.897157    -4.471765      24.14
 H       4.958765    -1.128213    -3.209314      25.35
 H       3.166180    -1.033322    -3.296286      26.82
 C      -0.467331    -2.015562    -0.294365      47.43
 H      -1.026696    -2.912212    -0.281205      23.63
 C      -0.240029     0.384763     0.115717      65.51
 H      -0.616631     1.317546     0.644664      19.34
 C       1.080505     0.388253    -0.249566      19.62
 O       1.899173     1.513806    -0.064829     206.69
 C       1.298314     2.798391     0.364458     113.86
 H       2.150182     3.440313     0.547264      25.54
 H       0.507185     3.259432    -0.383693      26.16
 H       0.838376     2.645347     1.349465      26.92
 C       1.758468    -0.816427    -0.680339      12.35
 O       3.127257    -0.793840    -0.777984     159.27
 C       0.901971    -2.024307    -0.707466      48.16
 H       1.356210    -3.012131    -0.937419      24.34
 C      -1.037894    -0.808817     0.135148      44.20
 C      -2.572228    -0.735879     0.607957      76.16
 H      -2.706047    -1.682655     1.207392      25.96
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 O      -2.721442     0.466367     1.470521     291.52
 H      -2.202280     0.484070     2.321079      28.37
 C      -3.693131    -0.686285    -0.480931     107.04
 H      -3.540345     0.272975    -0.923390      28.69
 O      -3.503645    -1.790302    -1.338841     253.72
 H      -3.360935    -1.441741    -2.211671      27.75
 C      -5.097277    -0.670950     0.190709     115.40
 O      -5.387944     0.439065     1.035062     258.44
 H      -4.595935     0.643515     1.562456      30.09
 H      -5.198124    -1.623097     0.797503      28.33
 H      -5.847193    -0.728014    -0.603644      29.44
55
name = lig-etoh-Waterframe_31
 C       5.353657    -1.361269     1.849545      60.23
 H       5.568131    -0.355748     1.508288      22.79
 C       5.141878    -3.709854     1.276785      66.24
 H       4.889360    -4.410173     0.475330      26.34
 C       5.069925    -4.106780     2.582214      19.38
 O       4.944471    -5.428204     3.021991     212.89
 C       4.922788    -6.459703     2.014083     117.18
 H       5.742721    -6.417192     1.304663      25.96
 H       3.949775    -6.428087     1.538589      27.50
 H       5.006649    -7.433046     2.505341      25.44
 C       5.327825    -3.115507     3.574239      12.08
 O       5.607560    -3.392650     4.930307     154.45
 H       5.606859    -4.359907     5.117704      20.62
 C       5.513640    -1.769777     3.228137      59.06
 H       5.713227    -1.040749     3.990958      27.16
 C       5.218274    -2.314346     0.864955      -9.02
 C       5.227625    -1.990640    -0.695216      81.01
 H       5.784483    -2.822302    -1.217329      22.71
 O       6.156756    -0.882005    -0.985148     191.02
 H       5.703931    -0.045753    -0.620079      26.05
 C       3.879430    -1.871477    -1.386389      86.44
 H       3.392508    -2.851242    -1.192134      26.23
 C       4.001504    -1.705939    -2.961299      97.24
 O       3.888291    -2.969643    -3.637548     291.06
 H       4.390823    -3.138218    -4.537528      25.17
 H       4.916925    -1.172467    -3.338072      24.84
 H       3.175272    -1.006344    -3.284811      25.75
 C      -0.483349    -1.987850    -0.299606      48.74
 H      -1.039895    -2.865358    -0.194327      24.98
 C      -0.280623     0.322518     0.150101      61.60
 H      -0.705715     1.305003     0.408163      21.96
 C       1.134138     0.366362    -0.234518      -2.82
 O       1.925097     1.507525    -0.025893     191.22
 C       1.313276     2.803763     0.399074     112.20
 H       2.095838     3.454082     0.517025      28.48
 H       0.708295     3.232754    -0.503656      27.16
 H       0.750103     2.692343     1.375150      26.99
 C       1.685358    -0.872536    -0.649853      13.85
 O       3.156284    -0.795707    -0.775801     146.95
 C       0.911198    -1.986378    -0.667337      74.88
 H       1.375888    -2.950946    -0.850908      25.52
 C      -1.129636    -0.784859     0.145061      35.71
 C      -2.480787    -0.709705     0.671445      81.22
 H      -2.783345    -1.627025     1.322091      25.54
 O      -2.687076     0.441999     1.485373     282.13
 H      -2.267545     0.220097     2.392726      28.59
 C      -3.671207    -0.635715    -0.492382      86.90
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 H      -3.574191     0.298808    -1.101552      28.35
 O      -3.463189    -1.806167    -1.390520     198.19
 H      -3.556686    -1.652998    -2.325947      26.52
 C      -5.066432    -0.694342     0.204435     106.21
 O      -5.412337     0.472019     1.061458     241.51
 H      -4.528474     0.790232     1.310954      30.27
 H      -5.162417    -1.639925     0.843376      28.28
 H      -5.856128    -0.707930    -0.593995      28.78
55
name = lig-etoh-Waterframe_32
 C       5.388027    -1.340665     1.843291      48.58
 H       5.369442    -0.302213     1.485061      27.18
 C       5.102127    -3.711583     1.205017      71.80
 H       4.933602    -4.491101     0.422084      25.96
 C       5.134235    -4.071846     2.602223      21.94
 O       4.999592    -5.406371     2.992349     203.32
 C       4.934185    -6.490665     2.028744     114.19
 H       5.750593    -6.362008     1.335621      25.97
 H       4.018740    -6.424246     1.395880      27.32
 H       4.968005    -7.417887     2.587306      25.85
 C       5.382170    -3.127394     3.616860      22.38
 O       5.562448    -3.399019     4.887069     145.24
 H       5.390189    -4.356588     5.172264      22.93
 C       5.479970    -1.746261     3.213935      38.57
 H       5.809280    -1.072527     4.017176      19.14
 C       5.169146    -2.366237     0.869213       7.79
 C       5.267352    -1.985667    -0.685833      75.07
 H       5.737783    -2.852640    -1.211838      24.75
 O       6.165032    -0.865360    -0.984113     155.06
 H       5.761263     0.073949    -0.924930      23.81
 C       3.861150    -1.936223    -1.379028      79.30
 H       3.369717    -2.907913    -1.184004      27.69
 C       3.985989    -1.710402    -2.964982      96.99
 O       3.835190    -3.000606    -3.616727     262.37
 H       4.691137    -3.008256    -4.219160      23.21
 H       4.995190    -1.269531    -3.128803      26.67
 H       3.074810    -1.114781    -3.237965      26.47
 C      -0.489107    -1.970775    -0.283111      56.31
 H      -0.929287    -2.956990    -0.304614      24.35
 C      -0.263350     0.367789     0.154481      76.05
 H      -0.805284     1.251221     0.354835      21.77
 C       1.080619     0.363962    -0.168793      12.12
 O       1.952360     1.494717    -0.000140     201.86
 C       1.345330     2.772374     0.399504     118.54
 H       2.171340     3.401457     0.578835      26.46
 H       0.691289     3.113430    -0.409562      28.34
 H       0.634427     2.751907     1.290241      27.23
 C       1.743755    -0.836773    -0.597618      10.47
 O       3.112517    -0.792497    -0.779358     135.42
 C       0.861761    -2.029780    -0.622685      56.29
 H       1.325705    -2.956106    -0.891004      26.91
 C      -1.077884    -0.800338     0.103666      52.01
 C      -2.518871    -0.706527     0.681713      76.87
 H      -2.699675    -1.694964     1.216237      26.05
 O      -2.656135     0.446812     1.526102     282.77
 H      -2.296961     0.290332     2.497410      28.35
 C      -3.601410    -0.610062    -0.473893      86.00
 H      -3.535076     0.321261    -1.143099      26.29
 O      -3.442907    -1.816953    -1.377672     205.80
 H      -3.641702    -1.526897    -2.284307      26.42
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 C      -5.060985    -0.700308     0.216719      95.91
 O      -5.413442     0.487781     1.052515     255.12
 H      -4.593990     0.962759     1.243959      31.35
 H      -5.062907    -1.667330     0.775205      29.21
 H      -5.864909    -0.799149    -0.576252      28.36
55
name = lig-etoh-Waterframe_33
 C       5.389808    -1.380335     1.856357      52.50
 H       5.364194    -0.280720     1.708269      25.79
 C       5.039606    -3.714846     1.189270      70.45
 H       5.053956    -4.534696     0.429445      23.05
 C       5.190991    -4.095739     2.531255       7.44
 O       5.055753    -5.395150     3.013412     202.68
 C       4.945407    -6.481254     2.005757     113.27
 H       5.876955    -6.552435     1.405438      26.13
 H       3.993387    -6.456486     1.389155      27.52
 H       4.895859    -7.344848     2.658011      25.64
 C       5.424719    -3.069604     3.550006      -2.14
 O       5.519246    -3.419690     4.941389      74.30
 H       5.436694    -4.447331     5.190147      21.24
 C       5.467351    -1.729174     3.181698      57.70
 H       5.674579    -0.961399     3.970046      19.00
 C       5.171012    -2.341953     0.791532       2.72
 C       5.290257    -1.995793    -0.649787      72.95
 H       5.791747    -2.852150    -1.090549      24.89
 O       6.164001    -0.856942    -0.989489     164.04
 H       5.542747    -0.032506    -0.949426      24.90
 C       3.849927    -1.947676    -1.384951      84.68
 H       3.285141    -2.865588    -1.186145      27.24
 C       3.926150    -1.728343    -2.878914     108.18
 O       3.817267    -3.018246    -3.610899     274.38
 H       4.659076    -3.282431    -4.156157      24.74
 H       4.858566    -1.220302    -3.150078      26.79
 H       3.209734    -0.996523    -3.303337      26.67
 C      -0.462037    -2.036242    -0.276038      39.89
 H      -1.169077    -2.929172    -0.364458      19.39
 C      -0.296624     0.434297     0.137181      48.68
 H      -0.700818     1.319695     0.515565      16.79
 C       1.108266     0.391729    -0.105096      23.91
 O       1.954455     1.462012     0.025991     229.93
 C       1.355181     2.729863     0.372149     117.34
 H       2.203984     3.438622     0.656192      24.57
 H       0.809749     3.163773    -0.398103      29.24
 H       0.829372     2.565651     1.337966      26.87
 C       1.712733    -0.861124    -0.518967      28.97
 O       3.077906    -0.803156    -0.793196     161.08
 C       0.933238    -2.017570    -0.607017      65.94
 H       1.231705    -2.987772    -0.950995      25.08
 C      -1.037169    -0.765269     0.102969      53.71
 C      -2.525434    -0.722976     0.628727      79.02
 H      -2.713748    -1.626149     1.171349      26.28
 O      -2.652009     0.467551     1.566227     279.16
 H      -2.118332     0.338288     2.477564      25.75
 C      -3.598872    -0.638960    -0.436844     102.98
 H      -3.367393     0.349400    -0.941810      25.73
 O      -3.440056    -1.787927    -1.293047     269.17
 H      -3.446013    -1.466609    -2.232428      26.75
 C      -5.019347    -0.669116     0.210568     105.37
 O      -5.418280     0.471645     1.007798     286.78
 H      -4.608020     0.924700     1.276706      31.91
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 H      -5.030820    -1.518727     0.872278      29.87
 H      -5.789519    -0.815660    -0.574468      28.24
55
name = lig-etoh-Waterframe_34
 C       5.347452    -1.396878     1.797347      54.51
 H       5.543457    -0.338500     1.512236      21.61
 C       5.024357    -3.700078     1.169667      53.48
 H       4.973435    -4.446460     0.363116      21.24
 C       5.230069    -4.084307     2.506446       4.73
 O       5.113228    -5.394853     3.012401     239.59
 C       4.964195    -6.476913     2.032925     109.52
 H       5.883974    -6.669289     1.400843      25.26
 H       4.066091    -6.257935     1.385272      28.02
 H       4.770124    -7.383876     2.614929      25.00
 C       5.435189    -3.119030     3.542703      -2.03
 O       5.476230    -3.394765     4.947372     184.33
 H       5.638820    -4.439356     5.123236      18.31
 C       5.480262    -1.742359     3.200533      38.97
 H       5.423688    -0.889503     3.926462      23.41
 C       5.207025    -2.298623     0.813919      32.91
 C       5.274259    -2.015292    -0.692427      90.34
 H       5.811155    -2.825089    -1.166674      25.45
 O       6.115278    -0.861607    -0.989831     212.13
 H       5.613253     0.024059    -0.759341      23.52
 C       3.819076    -1.918447    -1.337020      92.21
 H       3.370290    -2.893817    -1.114828      27.00
 C       3.910900    -1.740129    -2.874960     103.33
 O       3.795389    -3.037718    -3.584725     265.71
 H       4.503916    -3.068088    -4.322918      24.91
 H       4.850570    -1.306402    -3.164716      26.22
 H       3.035847    -1.142525    -3.157281      26.37
 C      -0.432419    -1.991102    -0.260440      36.87
 H      -1.117936    -2.919404    -0.382092      19.75
 C      -0.281744     0.468271     0.133276      63.06
 H      -0.718353     1.333589     0.572993      14.19
 C       1.119997     0.368312    -0.072573      23.93
 O       1.985009     1.437648     0.031518     228.43
 C       1.386062     2.705222     0.392136     105.49
 H       2.321529     3.416015     0.579960      23.15
 H       0.760666     3.119342    -0.384238      27.94
 H       0.767682     2.611640     1.281952      27.68
 C       1.680192    -0.879697    -0.446686      21.07
 O       3.084659    -0.808555    -0.801658     179.28
 C       0.939036    -2.061426    -0.600227      46.73
 H       1.523539    -2.894594    -1.020731      22.17
 C      -1.051928    -0.770020     0.119161      88.07
 C      -2.441808    -0.716691     0.658042      87.26
 H      -2.644041    -1.565016     1.254191      27.03
 O      -2.667858     0.469353     1.557911     294.85
 H      -2.067576     0.197894     2.352880      26.55
 C      -3.604620    -0.609323    -0.387632     108.68
 H      -3.512770     0.285497    -1.003379      25.85
 O      -3.446936    -1.759298    -1.217253     276.55
 H      -3.236867    -1.590946    -2.176551      27.00
 C      -4.987344    -0.660487     0.215409     111.86
 O      -5.424505     0.481105     0.945844     290.57
 H      -4.620324     0.750696     1.418187      32.04
 H      -5.053052    -1.547541     0.846728      30.01
 H      -5.676945    -0.815199    -0.607205      28.87
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name = lig-etoh-Waterframe_36
 C       5.398040    -1.363771     1.786722      54.43
 H       5.507262    -0.288079     1.712799      28.84
 C       5.119911    -3.739465     1.208562      64.42
 H       4.831617    -4.476854     0.490815      24.59
 C       5.239194    -4.101304     2.553552      31.17
 O       5.251271    -5.406800     2.998503     235.56
 C       4.944259    -6.442713     2.037337     115.82
 H       5.868978    -6.776828     1.556021      25.78
 H       4.141037    -6.245889     1.362501      29.57
 H       4.644550    -7.299619     2.676277      25.92
 C       5.386380    -3.106402     3.484660       3.84
 O       5.429152    -3.304575     4.910562     120.93
 H       5.260165    -4.276126     5.087531      23.76
 C       5.413288    -1.758252     3.141723      42.67
 H       5.642165    -1.065620     3.939621      16.12
 C       5.247888    -2.318067     0.773151     -11.59
 C       5.193845    -1.976062    -0.701449      78.22
 H       5.705445    -2.794179    -1.297992      23.01
 O       6.026627    -0.827139    -1.022720     176.74
 H       5.511442    -0.027828    -0.622204      26.26
 C       3.803216    -1.924685    -1.336698      90.34
 H       3.239523    -2.828940    -1.056334      26.65
 C       3.795457    -1.752186    -2.858681     106.81
 O       3.776814    -3.044352    -3.547759     293.62
 H       4.462656    -3.280523    -4.187762      26.84
 H       4.670762    -1.163667    -3.225910      26.85
 H       2.960243    -1.138954    -3.217819      26.92
 C      -0.428388    -1.968282    -0.246699      38.24
 H      -1.079337    -2.818719    -0.162700      21.37
 C      -0.208567     0.411371     0.202149      92.49
 H      -0.684625     1.431484     0.293483      19.26
 C       1.189990     0.322175    -0.071471      15.23
 O       2.038471     1.403887     0.051651     218.75
 C       1.464115     2.710794     0.405659     110.03
 H       2.272329     3.443692     0.447300      26.52
 H       0.753480     3.124138    -0.430834      27.08
 H       1.028791     2.600499     1.386885      28.70
 C       1.776435    -0.917884    -0.457050      35.33
 O       3.107467    -0.770903    -0.725726     167.71
 C       0.955474    -2.028168    -0.570883      70.79
 H       1.130976    -3.088407    -0.816279      25.22
 C      -1.011947    -0.751471     0.173013      56.08
 C      -2.441058    -0.664080     0.729105      80.18
 H      -2.661474    -1.670648     1.304616      23.48
 O      -2.684284     0.495065     1.550200     290.70
 H      -2.213109     0.265120     2.409724      28.86
 C      -3.549115    -0.603213    -0.327664      99.49
 H      -3.355335     0.339037    -0.857107      27.07
 O      -3.449082    -1.804281    -1.175920     232.93
 H      -3.261212    -1.593025    -2.163392      26.41
 C      -5.005394    -0.700495     0.207565     102.69
 O      -5.440617     0.540486     0.860306     234.32
 H      -4.851772     0.663286     1.608575      32.95
 H      -5.128866    -1.587605     0.930321      29.22
 H      -5.712344    -0.809712    -0.638568      29.13
55
name = lig-etoh-Waterframe_37
 C       5.444844    -1.378599     1.779189      65.80
 H       5.441623    -0.332097     1.511892      30.21
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 C       5.170175    -3.721820     1.193110      78.68
 H       5.133075    -4.528163     0.464271      25.16
 C       5.238947    -4.123774     2.526893      10.12
 O       5.296136    -5.415199     3.016065     211.89
 C       4.939287    -6.480082     2.037004     119.19
 H       5.763715    -6.799949     1.406373      27.55
 H       4.117714    -6.174177     1.381953      27.84
 H       4.586632    -7.273198     2.722062      26.12
 C       5.329485    -3.050225     3.537381       6.17
 O       5.403051    -3.270706     4.885364     134.25
 H       5.404094    -4.204887     5.190411      23.09
 C       5.413583    -1.727781     3.120133      63.66
 H       5.644604    -0.951382     3.808683      19.93
 C       5.244189    -2.345326     0.793243       8.25
 C       5.214718    -2.001500    -0.710556      74.66
 H       5.798003    -2.853029    -1.152382      24.20
 O       5.978121    -0.784104    -1.040806     175.85
 H       5.497385     0.107459    -0.863453      24.38
 C       3.747902    -1.905655    -1.349547      90.00
 H       3.236699    -2.861539    -1.131446      27.38
 C       3.747087    -1.715198    -2.879817     101.43
 O       3.758744    -3.061920    -3.537830     275.46
 H       4.628234    -3.136044    -3.891819      26.98
 H       4.692607    -1.170374    -3.151368      26.61
 H       2.755069    -1.265189    -3.130383      27.33
 C      -0.453678    -1.956989    -0.186919      44.89
 H      -0.984436    -2.852366    -0.256669      24.24
 C      -0.135413     0.418862     0.209544      77.71
 H      -0.566153     1.423635     0.519726      20.38
 C       1.205954     0.331446    -0.067114      20.86
 O       2.069214     1.416396     0.053812     223.51
 C       1.516805     2.706739     0.385400     120.94
 H       2.334361     3.300576     0.394713      27.21
 H       0.652839     3.041287    -0.261139      27.57
 H       1.036292     2.674670     1.401702      27.56
 C       1.780390    -0.883597    -0.483991      12.98
 O       3.181609    -0.780092    -0.693098     167.49
 C       0.915455    -2.070799    -0.554474      52.42
 H       1.506770    -2.939153    -0.826032      25.43
 C      -1.026462    -0.751860     0.224839      64.22
 C      -2.471534    -0.711851     0.723551      83.19
 H      -2.628186    -1.543415     1.474000      26.76
 O      -2.691458     0.545060     1.598991     289.63
 H      -2.139756     0.353568     2.391159      29.36
 C      -3.569365    -0.686155    -0.343013      97.40
 H      -3.418860     0.259569    -0.965887      26.77
 O      -3.426224    -1.826151    -1.186972     225.81
 H      -3.482624    -1.575371    -2.208532      24.16
 C      -5.005115    -0.637062     0.215142     111.42
 O      -5.478983     0.544237     0.828389     255.28
 H      -4.789347     0.785274     1.462567      32.43
 H      -5.079419    -1.495908     0.929535      29.98
 H      -5.673594    -0.920305    -0.645755      29.41
55
name = lig-etoh-Waterframe_100
 C       5.504110    -1.572753     1.846548      50.72
 H       5.624196    -0.545333     1.594695      23.91
 C       5.402626    -3.889374     1.207419      48.82
 H       5.350872    -4.688561     0.420669      21.64
 C       5.504350    -4.231976     2.602582      14.60
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 O       5.662994    -5.562208     2.929245     263.12
 C       4.597267    -6.490110     2.543225     117.83
 H       4.265394    -6.433383     1.481610      27.04
 H       3.732951    -6.513403     3.243254      25.49
 H       5.115390    -7.462054     2.670969      26.43
 C       5.543322    -3.271005     3.650767       9.98
 O       5.543618    -3.564047     4.965676     166.27
 H       5.132818    -4.540711     5.109563      21.66
 C       5.553051    -1.904458     3.251479      11.74
 H       5.523732    -1.163181     4.119229      21.31
 C       5.430044    -2.543572     0.823163       9.52
 C       5.333155    -2.212172    -0.714900      82.19
 H       5.743053    -3.158049    -1.259019      23.75
 O       6.192510    -1.130239    -1.179194     223.28
 H       5.726797    -0.204525    -0.968878      24.08
 C       3.884310    -2.149379    -1.299855      75.87
 H       3.345172    -3.022278    -0.862461      27.21
 C       3.779897    -2.224195    -2.932856      99.55
 O       4.024745    -3.564852    -3.506542     244.20
 H       4.938138    -3.561667    -3.868896      28.26
 H       4.511791    -1.526751    -3.360787      25.76
 H       2.793335    -1.958636    -3.276102      29.09
 C      -0.307913    -1.814186    -0.181023      47.02
 H      -0.994357    -2.756789    -0.117052      23.53
 C      -0.029905     0.618878    -0.097031      65.30
 H      -0.483409     1.621692    -0.026397      22.54
 C       1.358315     0.481991    -0.460707       7.39
 O       2.328991     1.495144    -0.558800     206.23
 C       1.804281     2.848584    -0.147811     107.60
 H       2.667101     3.602152    -0.182454      24.69
 H       0.854151     3.084935    -0.670364      26.78
 H       1.296274     2.749676     0.796933      28.07
 C       1.875732    -0.879089    -0.684488      16.75
 O       3.271048    -0.858358    -0.856762     150.91
 C       1.035568    -1.993530    -0.539871      69.20
 H       1.423582    -2.973027    -0.783741      25.96
 C      -0.800915    -0.508495     0.113246      46.16
 C      -2.220912    -0.540834     0.593491      81.69
 H      -2.400292    -1.497547     1.185245      25.50
 O      -2.487238     0.580451     1.504814     292.05
 H      -2.178626     0.370020     2.406663      28.47
 C      -3.344735    -0.534652    -0.531104      80.45
 H      -2.988462     0.423586    -1.192698      26.17
 O      -3.130993    -1.810752    -1.260192     214.85
 H      -2.848014    -1.550110    -2.180019      27.26
 C      -4.837377    -0.417592    -0.023910     108.53
 O      -5.214443     0.785068     0.680394     246.51
 H      -4.478196     0.968860     1.278730      31.57
 H      -5.110030    -1.305217     0.615046      28.17
 H      -5.506519    -0.546270    -0.943477      27.49
55
name = lig-etoh-Waterframe_101
 C       5.449706    -1.544442     1.885980      34.72
 H       5.628346    -0.545156     1.517603      20.70
 C       5.343885    -3.911588     1.243803      33.19
 H       5.358064    -4.725873     0.529294      19.61
 C       5.527611    -4.249353     2.636968      21.49
 O       5.685546    -5.606612     3.009956     215.83
 C       4.605439    -6.494144     2.590230     127.71
 H       4.388975    -6.208635     1.563751      25.87
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 H       3.773414    -6.359786     3.256206      25.36
 H       5.058115    -7.519031     2.620333      26.91
 C       5.560808    -3.277481     3.626583      18.38
 O       5.503470    -3.584044     4.970061     182.97
 H       5.016879    -4.544787     5.193579      19.71
 C       5.569225    -1.915697     3.249546      44.98
 H       5.507954    -1.201994     4.106259      23.45
 C       5.441109    -2.564805     0.816977      12.77
 C       5.317060    -2.213220    -0.659583     103.30
 H       5.780958    -3.041608    -1.159523      26.04
 O       6.172296    -1.134104    -1.157982     216.24
 H       5.746393    -0.230901    -0.839808      23.90
 C       3.930170    -2.159834    -1.370255      70.39
 H       3.371092    -3.054316    -1.039559      27.24
 C       3.807633    -2.184739    -2.903255      94.52
 O       4.008284    -3.581256    -3.483777     243.10
 H       4.808711    -3.398216    -3.972115      28.29
 H       4.582068    -1.496663    -3.369188      24.23
 H       2.755584    -1.927749    -3.159785      27.36
 C      -0.276680    -1.804974    -0.231775      54.42
 H      -0.944361    -2.721337    -0.094422      23.38
 C      -0.015999     0.638956    -0.097758      80.38
 H      -0.421516     1.608226     0.070559      20.50
 C       1.341170     0.479617    -0.503867      13.36
 O       2.300068     1.511112    -0.572662     220.67
 C       1.793740     2.794608    -0.166471     111.65
 H       2.674487     3.611427    -0.327516      24.29
 H       1.017015     3.148278    -0.828476      27.54
 H       1.568111     2.842997     0.960223      26.62
 C       1.838853    -0.814555    -0.716266      22.74
 O       3.248265    -0.858677    -0.856813     129.43
 C       1.035428    -1.968200    -0.572659      66.81
 H       1.407469    -3.005034    -0.719303      24.43
 C      -0.807279    -0.573291     0.076768      51.56
 C      -2.278962    -0.516018     0.628043      79.03
 H      -2.464102    -1.510029     1.187512      24.42
 O      -2.453723     0.575061     1.471187     299.45
 H      -1.969220     0.270392     2.280579      27.85
 C      -3.323944    -0.513310    -0.543565      86.48
 H      -3.144044     0.336033    -1.265814      26.49
 O      -3.155040    -1.810354    -1.322427     222.31
 H      -2.683477    -1.495177    -2.133137      27.98
 C      -4.853004    -0.396138    -0.079961      95.98
 O      -5.281476     0.799490     0.693987     249.09
 H      -4.473371     0.973071     1.188210      31.92
 H      -4.937953    -1.285167     0.666743      27.19
 H      -5.528825    -0.486420    -0.982353      27.25
55
name = lig-etoh-Waterframe_102
 C       5.457478    -1.561536     1.871251      65.64
 H       5.382867    -0.470199     1.691452      23.25
 C       5.348669    -3.927455     1.301928      59.18
 H       5.281886    -4.689378     0.574659      20.67
 C       5.539685    -4.309215     2.595171      -6.69
 O       5.699284    -5.641001     3.104048     268.61
 C       4.627890    -6.492558     2.621714     135.89
 H       4.249688    -6.230893     1.636759      30.84
 H       3.748736    -6.363434     3.232090      25.60
 H       4.830223    -7.584562     2.630369      28.92
 C       5.543012    -3.282511     3.630443     -22.77
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 O       5.462130    -3.589958     4.985913     133.24
 H       5.132512    -4.600191     5.301959      17.66
 C       5.557770    -1.915227     3.226631      57.19
 H       5.626272    -1.081198     3.902083      23.95
 C       5.369826    -2.532695     0.894426      12.35
 C       5.356100    -2.243609    -0.704899      96.35
 H       5.799470    -3.083288    -1.116364      27.43
 O       6.144374    -1.130906    -1.098719     254.40
 H       5.831431    -0.183092    -0.868693      22.98
 C       3.908829    -2.142904    -1.355783      91.71
 H       3.341885    -2.995397    -0.983456      27.36
 C       3.848757    -2.154411    -2.883089      93.69
 O       4.014578    -3.534572    -3.454191     272.69
 H       4.780431    -3.600257    -3.997027      30.36
 H       4.491685    -1.410560    -3.452407      24.70
 H       2.805278    -1.735094    -3.074145      27.41
 C      -0.296252    -1.833372    -0.250509      47.80
 H      -0.865951    -2.731455    -0.048144      22.89
 C      -0.007946     0.601576    -0.100081      71.72
 H      -0.373143     1.504830     0.231491      19.43
 C       1.306409     0.490268    -0.517684      23.10
 O       2.247680     1.516042    -0.585516     232.67
 C       1.808665     2.801209    -0.182522     120.94
 H       2.758248     3.405831    -0.491713      23.12
 H       0.979190     3.172984    -0.752127      28.29
 H       1.712561     2.861132     0.959839      26.11
 C       1.893230    -0.805382    -0.740707      29.14
 O       3.243991    -0.914474    -0.890132     176.34
 C       1.091326    -1.940835    -0.644045      58.21
 H       1.554179    -2.969051    -0.685928      24.41
 C      -0.860653    -0.564187     0.042812      75.01
 C      -2.302761    -0.554453     0.569278      76.84
 H      -2.499445    -1.458092     1.169182      25.64
 O      -2.434567     0.619224     1.483339     282.65
 H      -2.020158     0.496888     2.396380      27.74
 C      -3.338740    -0.480228    -0.585998     101.75
 H      -3.149222     0.267318    -1.241462      27.45
 O      -3.182418    -1.764664    -1.314132     249.88
 H      -3.004233    -1.509820    -2.292861      25.76
 C      -4.833709    -0.420452    -0.094264      96.32
 O      -5.305707     0.801908     0.671781     252.45
 H      -4.587442     1.124454     1.221989      32.60
 H      -5.082178    -1.384611     0.469464      28.17
 H      -5.519372    -0.470387    -0.939666      27.98
55
name = lig-etoh-Waterframe_103
 C       5.467236    -1.556034     1.870254      32.70
 H       5.263174    -0.474396     1.623955      22.34
 C       5.383698    -3.914111     1.270419      40.98
 H       5.235304    -4.609801     0.473329      26.87
 C       5.555044    -4.327985     2.686861      20.96
 O       5.681635    -5.656412     3.154253     230.51
 C       4.575027    -6.514752     2.656939     104.67
 H       4.365865    -6.289467     1.597516      27.64
 H       3.745914    -6.388530     3.382356      25.35
 H       5.028765    -7.521432     2.736885      26.90
 C       5.505053    -3.312486     3.654389       2.71
 O       5.433455    -3.569450     4.996800     151.67
 H       5.186765    -4.609488     5.055583      19.00
 C       5.545611    -1.931847     3.233001      50.97
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 H       5.653864    -1.194103     3.983005      23.38
 C       5.273139    -2.560330     0.875707     -27.13
 C       5.344031    -2.255082    -0.701848      75.53
 H       5.814686    -3.126285    -1.208875      23.28
 O       6.167598    -1.129145    -1.045986     233.13
 H       5.626654    -0.334120    -0.807007      25.42
 C       3.898494    -2.153322    -1.293713      91.05
 H       3.371184    -3.041000    -0.941704      27.14
 C       3.867983    -2.118471    -2.905234      97.59
 O       4.008737    -3.458496    -3.426651     275.65
 H       4.882403    -3.449496    -3.794663      29.33
 H       4.677877    -1.451439    -3.269703      24.36
 H       2.832774    -1.896463    -3.266742      27.97
 C      -0.271328    -1.851887    -0.269157      65.78
 H      -0.775529    -2.734564    -0.104196      25.01
 C      -0.064445     0.547137    -0.080046      69.54
 H      -0.404227     1.467040     0.266617      20.95
 C       1.327231     0.455470    -0.518200      18.08
 O       2.195955     1.490985    -0.608389     224.89
 C       1.866491     2.871156    -0.201139     122.83
 H       2.654538     3.526196    -0.504199      25.20
 H       0.866429     3.146491    -0.486228      27.62
 H       1.644151     2.916527     0.875763      27.48
 C       1.917772    -0.846176    -0.762861      28.29
 O       3.305071    -0.934562    -0.929298     202.19
 C       1.068205    -1.935597    -0.682632      66.76
 H       1.579239    -2.924708    -0.777200      24.97
 C      -0.871991    -0.591069    -0.002759      53.62
 C      -2.279070    -0.530693     0.544991      73.95
 H      -2.501211    -1.434344     1.061907      27.30
 O      -2.451079     0.687214     1.476641     261.30
 H      -2.127551     0.285590     2.388697      25.53
 C      -3.384303    -0.454782    -0.609174     101.34
 H      -3.109785     0.397990    -1.169626      27.78
 O      -3.216526    -1.709246    -1.284666     245.69
 H      -3.447563    -1.478088    -2.242819      25.24
 C      -4.846032    -0.427385    -0.091459     109.25
 O      -5.306000     0.773196     0.615395     259.27
 H      -4.584020     1.044963     1.190498      32.10
 H      -5.091341    -1.309814     0.476652      29.74
 H      -5.390485    -0.407718    -1.000650      29.12
55
name = lig-etoh-Waterframe_104
 C       5.418264    -1.567467     1.888061      25.05
 H       5.499619    -0.506839     1.531825      21.52
 C       5.414281    -3.933256     1.290151      41.70
 H       5.388139    -4.757856     0.541817      23.32
 C       5.539222    -4.299939     2.687921      19.53
 O       5.625239    -5.633082     3.166423     252.79
 C       4.575897    -6.566968     2.721439      97.38
 H       4.333329    -6.343497     1.652083      28.39
 H       3.610773    -6.468561     3.330480      24.67
 H       5.028800    -7.552147     2.844086      25.60
 C       5.483208    -3.287307     3.659523      10.23
 O       5.409211    -3.558903     5.002419     187.02
 H       5.190004    -4.530485     5.246161      19.49
 C       5.536212    -1.953789     3.242776      70.88
 H       5.548256    -1.294494     4.086798      24.64
 C       5.257989    -2.599473     0.825940     -11.47
 C       5.290437    -2.269499    -0.654997      79.71
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 H       5.810377    -3.188737    -1.201209      22.44
 O       6.189111    -1.149753    -0.987640     220.68
 H       5.790824    -0.259021    -0.858532      24.63
 C       3.912249    -2.196433    -1.335141      83.59
 H       3.339591    -3.053830    -0.935687      25.93
 C       3.859842    -2.101227    -2.866105     105.83
 O       4.044939    -3.418732    -3.422667     287.60
 H       4.921132    -3.380727    -3.836663      28.83
 H       4.653335    -1.448451    -3.163371      24.46
 H       2.967843    -1.577319    -3.239466      27.93
 C      -0.264185    -1.873562    -0.295959      74.10
 H      -0.821223    -2.754787    -0.210807      25.43
 C      -0.034466     0.519001    -0.091113      71.18
 H      -0.487088     1.479130     0.167713      20.17
 C       1.300087     0.388951    -0.481704      13.34
 O       2.194811     1.516140    -0.636340     195.47
 C       1.846408     2.906703    -0.173029     120.91
 H       2.527249     3.557512    -0.565930      26.83
 H       0.914642     3.238875    -0.738645      25.34
 H       2.000833     2.932460     0.880966      27.32
 C       1.917660    -0.842786    -0.772138      20.01
 O       3.340816    -0.888911    -0.926531     152.56
 C       1.061117    -1.987421    -0.703315      63.10
 H       1.340061    -3.019503    -0.920258      24.19
 C      -0.856877    -0.648508    -0.020792      49.93
 C      -2.299816    -0.453468     0.542676      86.62
 H      -2.488174    -1.347283     1.135526      27.34
 O      -2.477885     0.692749     1.436382     274.35
 H      -2.183912     0.390369     2.416503      25.82
 C      -3.380790    -0.413626    -0.531328      94.80
 H      -3.266579     0.509986    -1.304773      25.72
 O      -3.278082    -1.668366    -1.263880     198.34
 H      -3.301135    -1.464947    -2.266593      24.72
 C      -4.880202    -0.404454    -0.118206     114.52
 O      -5.293036     0.752092     0.557662     253.06
 H      -4.554568     0.914879     1.155023      31.29
 H      -4.994958    -1.271060     0.495392      29.85
 H      -5.488486    -0.533856    -1.017376      28.70
55
name = lig-etoh-Waterframe_105
 C       5.362004    -1.634171     1.852370      51.28
 H       5.618612    -0.595873     1.656742      22.00
 C       5.426859    -3.983180     1.317662      55.54
 H       5.579955    -4.881312     0.643405      19.80
 C       5.479124    -4.281588     2.637692      16.87
 O       5.558259    -5.590660     3.164047     217.41
 C       4.595248    -6.613526     2.773170     113.84
 H       4.296256    -6.550563     1.703535      28.00
 H       3.649516    -6.500862     3.386590      25.19
 H       4.938340    -7.620825     2.943917      27.10
 C       5.464973    -3.292644     3.662953      10.05
 O       5.388304    -3.543570     5.032577     237.26
 H       5.110282    -4.448011     5.191338      22.81
 C       5.502432    -1.930873     3.247470      37.08
 H       5.496428    -1.076244     3.958741      22.31
 C       5.315105    -2.604554     0.897717      23.78
 C       5.281533    -2.278435    -0.644773      88.10
 H       5.796188    -3.220256    -1.105497      23.24
 O       6.213131    -1.201347    -0.937191     251.43
 H       5.845607    -0.312921    -0.798986      25.08
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 C       3.891428    -2.175830    -1.356421      75.31
 H       3.229138    -2.988938    -0.996295      24.39
 C       3.894658    -2.056038    -2.830081      99.81
 O       4.088423    -3.408360    -3.442399     265.71
 H       4.864709    -3.300452    -4.080120      28.00
 H       4.689062    -1.441409    -3.164577      23.12
 H       2.954185    -1.583104    -3.089840      27.25
 C      -0.308767    -1.919234    -0.327856      45.80
 H      -0.952935    -2.824686    -0.314651      23.35
 C      -0.016966     0.480061    -0.118364      62.71
 H      -0.403920     1.545528     0.059317      20.48
 C       1.344313     0.439435    -0.450439       9.01
 O       2.198046     1.539608    -0.655189     210.73
 C       1.838216     2.887609    -0.184566     117.50
 H       2.639650     3.381472    -0.702370      23.51
 H       0.722816     3.269270    -0.408213      24.46
 H       1.883317     3.036726     0.907577      26.99
 C       1.934457    -0.894433    -0.755622      12.88
 O       3.303624    -0.845240    -0.898680     138.94
 C       1.094025    -2.043385    -0.730978      62.81
 H       1.430577    -2.992408    -1.061679      23.74
 C      -0.855439    -0.619847     0.012205      41.21
 C      -2.314199    -0.433938     0.574250      81.17
 H      -2.564765    -1.352783     1.196027      24.45
 O      -2.509927     0.700221     1.391089     298.16
 H      -2.027159     0.613734     2.322856      26.29
 C      -3.419741    -0.372784    -0.525497      88.62
 H      -3.176024     0.550940    -1.317466      24.17
 O      -3.329972    -1.647696    -1.270594     212.55
 H      -2.829533    -1.361649    -2.094638      26.75
 C      -4.884307    -0.435509    -0.132411     105.51
 O      -5.294463     0.784147     0.527164     251.30
 H      -4.630971     1.036702     1.174057      30.72
 H      -5.027753    -1.340014     0.530614      27.25
 H      -5.583693    -0.617443    -1.015602      26.25
55
name = lig-etoh-Waterframe_106
 C       5.365936    -1.639236     1.892975      64.79
 H       5.316054    -0.640637     1.494496      23.68
 C       5.431256    -3.999719     1.281873      59.41
 H       5.488497    -4.785582     0.459952      27.48
 C       5.395232    -4.300180     2.703318       2.02
 O       5.520627    -5.587018     3.159552     204.23
 C       4.571288    -6.652561     2.812075     110.47
 H       4.379100    -6.660768     1.736267      30.69
 H       3.717269    -6.488287     3.458066      26.80
 H       5.166177    -7.503648     3.133816      26.19
 C       5.426847    -3.243392     3.690442      12.93
 O       5.360209    -3.541423     5.038403     163.93
 H       5.107690    -4.415554     5.142034      23.50
 C       5.438146    -1.922313     3.231738      58.81
 H       5.542078    -1.033624     3.927407      22.20
 C       5.358946    -2.679291     0.884969       7.86
 C       5.323819    -2.317868    -0.610795      87.45
 H       5.688148    -3.164998    -1.175847      25.14
 O       6.238457    -1.260495    -0.910596     240.69
 H       5.794637    -0.445633    -0.652663      27.91
 C       3.898736    -2.085617    -1.267605      78.98
 H       3.297770    -2.982237    -1.008635      26.45
 C       3.949056    -2.029602    -2.865900      93.48
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 O       4.101041    -3.382678    -3.470795     240.53
 H       4.998971    -3.182490    -4.007150      24.62
 H       4.724670    -1.318622    -3.193693      23.51
 H       2.949827    -1.821511    -3.232873      27.27
 C      -0.319879    -1.909328    -0.365308      53.22
 H      -0.997930    -2.851818    -0.357064      22.39
 C       0.021266     0.518323    -0.139011      71.36
 H      -0.456523     1.553921     0.109795      20.46
 C       1.401922     0.421498    -0.457115      18.11
 O       2.185443     1.531199    -0.649195     231.92
 C       1.835111     2.859771    -0.186727     109.81
 H       2.520367     3.653546    -0.716169      24.16
 H       0.747320     3.123001    -0.506978      26.07
 H       1.989583     2.915168     0.936697      26.61
 C       1.901388    -0.870289    -0.685712      21.33
 O       3.266623    -0.862439    -0.879624     178.11
 C       1.053559    -2.046720    -0.741895      67.20
 H       1.508399    -2.936234    -1.062598      26.18
 C      -0.861878    -0.656276     0.047750      48.70
 C      -2.333058    -0.484364     0.592432      72.50
 H      -2.580032    -1.441072     1.170422      24.99
 O      -2.531536     0.761906     1.370090     294.00
 H      -1.899703     0.588469     2.177297      26.81
 C      -3.438964    -0.398033    -0.586445      92.61
 H      -3.240554     0.542958    -1.147722      27.17
 O      -3.333913    -1.621262    -1.305723     218.98
 H      -2.650007    -1.541647    -2.025371      27.31
 C      -4.889327    -0.437680    -0.080569     100.56
 O      -5.333364     0.837051     0.503005     244.10
 H      -4.627610     1.086207     1.108487      30.56
 H      -5.065500    -1.341220     0.617650      26.99
 H      -5.501142    -0.477456    -1.051544      26.06
55
name = lig-etoh-Waterframe_107
 C       5.368465    -1.637493     1.833942      40.54
 H       5.073903    -0.640811     1.551866      20.38
 C       5.415442    -4.033285     1.311285      74.88
 H       5.313900    -4.833611     0.557220      28.44
 C       5.321878    -4.282839     2.713158       8.68
 O       5.517155    -5.613845     3.179000     202.45
 C       4.574876    -6.671573     2.871309     117.11
 H       4.362327    -6.783313     1.800794      28.09
 H       3.604761    -6.654418     3.337289      27.11
 H       5.086470    -7.607818     3.222612      25.05
 C       5.358617    -3.256972     3.689868       8.20
 O       5.327879    -3.538694     5.036846     166.83
 H       5.169052    -4.457283     5.235041      24.29
 C       5.382412    -1.886632     3.250808      37.16
 H       5.456372    -1.141155     4.101189      21.91
 C       5.380005    -2.696141     0.866486       7.45
 C       5.349610    -2.362330    -0.599873      99.35
 H       5.621461    -3.182801    -1.170106      27.13
 O       6.272764    -1.297944    -0.896625     241.03
 H       5.998188    -0.394667    -0.662753      26.78
 C       3.947571    -2.052147    -1.242096      91.27
 H       3.382164    -2.932652    -0.895390      27.17
 C       3.949171    -2.035341    -2.867770      89.17
 O       4.128712    -3.338889    -3.488065     265.88
 H       5.107172    -3.478764    -3.812605      27.45
 H       4.678140    -1.256962    -3.277987      23.76
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 H       2.981998    -1.565299    -3.216426      28.20
 C      -0.327853    -1.882799    -0.382645      70.27
 H      -0.950558    -2.860927    -0.362001      19.81
 C      -0.010443     0.508552    -0.108408      68.65
 H      -0.416373     1.534914     0.165283      16.95
 C       1.323789     0.430054    -0.448645      34.96
 O       2.237381     1.506738    -0.656251     234.44
 C       1.799233     2.834666    -0.175222     114.32
 H       2.473139     3.677871    -0.695356      22.96
 H       0.802001     3.019307    -0.465518      27.89
 H       2.016989     2.857776     0.919140      25.13
 C       1.867762    -0.883942    -0.629864      30.62
 O       3.257152    -0.886709    -0.841419     206.85
 C       1.011484    -1.964678    -0.732536      70.28
 H       1.333670    -2.964046    -0.957884      23.30
 C      -0.827683    -0.638753     0.050301      59.96
 C      -2.351384    -0.513806     0.543845      75.40
 H      -2.593419    -1.308724     1.272361      23.19
 O      -2.520242     0.783565     1.348037     286.35
 H      -2.088842     0.707381     2.277495      26.16
 C      -3.408116    -0.439771    -0.571001     107.12
 H      -3.337361     0.358900    -1.156471      28.02
 O      -3.319303    -1.629629    -1.362848     256.83
 H      -2.710708    -1.503767    -2.148565      27.14
 C      -4.913208    -0.369353    -0.047548      99.41
 O      -5.366546     0.877568     0.487249     279.42
 H      -4.662230     1.187643     1.066243      31.18
 H      -5.117598    -1.238720     0.649298      27.60
 H      -5.555125    -0.626263    -0.924183      27.08
55
name = lig-etoh-Waterframe_108
 C       5.327256    -1.634393     1.829563      40.28
 H       5.255374    -0.591389     1.502957      21.75
 C       5.356463    -4.042871     1.362518      69.16
 H       5.330745    -4.939805     0.793532      25.31
 C       5.285112    -4.317463     2.693423       1.04
 O       5.513744    -5.643432     3.221205     249.39
 C       4.569880    -6.718898     2.909975     104.43
 H       4.503337    -6.797549     1.806137      29.68
 H       3.591799    -6.500041     3.382675      25.89
 H       4.963284    -7.713105     3.284077      26.43
 C       5.277668    -3.270228     3.672822       1.48
 O       5.295063    -3.530085     5.042414     157.21
 H       5.160804    -4.546738     5.213321      16.58
 C       5.333273    -1.919304     3.243763      51.64
 H       5.219328    -1.080149     3.948205      26.01
 C       5.377458    -2.681249     0.893267      16.24
 C       5.351310    -2.331565    -0.635038      85.03
 H       5.764521    -3.244706    -1.125252      24.26
 O       6.359616    -1.326275    -0.906526     198.93
 H       5.915191    -0.456168    -0.698404      27.40
 C       3.960113    -2.127818    -1.290965      89.27
 H       3.336397    -2.962095    -0.995272      26.84
 C       3.946042    -2.004213    -2.830077      95.62
 O       4.100609    -3.332675    -3.448958     258.77
 H       5.045047    -3.168332    -3.871311      24.63
 H       4.842832    -1.387013    -3.171468      22.94
 H       2.910632    -1.611140    -3.062830      26.78
 C      -0.372496    -1.837957    -0.360940      38.65
 H      -0.991725    -2.765740    -0.385511      22.22
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 C      -0.081137     0.536085    -0.031670      68.32
 H      -0.530452     1.488205     0.214496      19.80
 C       1.298654     0.444515    -0.444769      16.90
 O       2.268786     1.468429    -0.651838     210.07
 C       1.773798     2.795775    -0.157910     118.99
 H       2.510838     3.442589    -0.718937      24.68
 H       0.805446     3.010815    -0.322338      29.07
 H       1.810128     2.936840     0.922831      27.52
 C       1.892204    -0.859728    -0.624495      21.62
 O       3.262498    -0.876629    -0.769411     160.77
 C       0.997512    -1.952200    -0.715301      64.74
 H       1.407375    -2.964037    -0.923542      23.04
 C      -0.889760    -0.616205     0.037491      51.27
 C      -2.302557    -0.460157     0.549814      92.16
 H      -2.530073    -1.301900     1.187692      26.16
 O      -2.511690     0.780145     1.303729     281.07
 H      -2.296991     0.496246     2.246730      27.14
 C      -3.426370    -0.457846    -0.547759      90.79
 H      -3.175330     0.406342    -1.208931      26.00
 O      -3.297741    -1.677062    -1.414218     220.18
 H      -3.075153    -1.209782    -2.293968      25.10
 C      -4.926891    -0.361545    -0.032374     107.01
 O      -5.389624     0.928944     0.471010     259.54
 H      -4.706571     1.327172     1.010017      32.53
 H      -5.030632    -1.048460     0.787698      29.57
 H      -5.588590    -0.603279    -0.826043      28.71
55
name = lig-etoh-Waterframe_109
 C       5.287710    -1.641796     1.873720      51.23
 H       5.540183    -0.637963     1.509120      20.24
 C       5.283203    -4.029838     1.346223      30.90
 H       5.455978    -4.773641     0.601086      19.54
 C       5.280722    -4.385976     2.776627       5.60
 O       5.519017    -5.663498     3.270260     311.18
 C       4.557382    -6.741994     2.918851      95.51
 H       4.471315    -6.869105     1.817247      28.31
 H       3.575241    -6.417961     3.365997      26.27
 H       5.006446    -7.598773     3.468884      25.92
 C       5.210064    -3.284934     3.688689      10.04
 O       5.251863    -3.526282     5.033864     166.90
 H       5.100958    -4.610633     5.210510      15.06
 C       5.249960    -1.958607     3.194287      65.89
 H       5.144219    -1.147242     3.877872      24.41
 C       5.324630    -2.681180     0.887927      13.97
 C       5.390552    -2.347076    -0.638458      79.91
 H       5.816235    -3.306764    -1.197312      22.42
 O       6.417228    -1.326980    -0.930703     186.86
 H       6.025021    -0.395547    -0.790798      24.41
 C       3.927638    -2.177216    -1.303690      77.38
 H       3.376639    -3.098548    -1.090777      26.14
 C       3.939466    -1.984645    -2.774926     107.92
 O       4.069635    -3.315111    -3.398180     266.34
 H       4.831141    -3.359263    -4.070063      26.60
 H       4.702850    -1.236536    -3.076901      25.35
 H       2.999901    -1.567346    -3.188728      26.86
 C      -0.389294    -1.831446    -0.346710      36.34
 H      -1.060271    -2.642734    -0.411102      22.88
 C      -0.072056     0.594212     0.015574      74.56
 H      -0.507589     1.488856     0.266350      20.48
 C       1.301294     0.428284    -0.419258      15.88
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 O       2.215790     1.454935    -0.593004     210.31
 C       1.788132     2.754446    -0.153861     124.59
 H       2.381972     3.525277    -0.574379      27.24
 H       0.794214     2.964129    -0.613001      26.09
 H       1.933830     2.803236     0.920406      27.42
 C       1.868648    -0.830699    -0.646841      19.72
 O       3.309134    -0.894109    -0.701500     122.16
 C       0.998831    -1.965027    -0.672019      48.85
 H       1.451535    -2.974127    -0.925467      22.70
 C      -0.944811    -0.558075     0.017436      62.05
 C      -2.325642    -0.443872     0.558805      94.47
 H      -2.461403    -1.311671     1.197470      27.55
 O      -2.513821     0.758439     1.289660     286.90
 H      -2.287673     0.557530     2.234111      29.12
 C      -3.453379    -0.462550    -0.573919      78.07
 H      -3.181352     0.571352    -1.201748      24.70
 O      -3.278367    -1.670581    -1.440753     188.82
 H      -3.459016    -1.433612    -2.398587      25.83
 C      -4.902125    -0.366050     0.010753     106.96
 O      -5.408993     0.987735     0.435194     224.21
 H      -4.670118     1.394796     0.890606      32.44
 H      -4.975377    -1.072607     0.816187      30.34
 H      -5.577137    -0.649022    -0.757522      29.28
55
name = lig-etoh-Waterframe_110
 C       5.289245    -1.662488     1.819719      40.27
 H       5.480590    -0.586508     1.660628      21.89
 C       5.239996    -4.035002     1.353828      46.05
 H       5.417435    -4.748339     0.542180      22.07
 C       5.278713    -4.384362     2.753315      12.35
 O       5.525688    -5.681575     3.300914     326.78
 C       4.563063    -6.720053     2.952690     111.18
 H       4.525670    -7.011378     1.887843      28.92
 H       3.493764    -6.580487     3.282364      29.45
 H       4.893850    -7.616218     3.470260      26.13
 C       5.158863    -3.349299     3.689205       1.29
 O       5.190904    -3.526780     5.046791     137.98
 H       5.123797    -4.606511     5.340930      19.01
 C       5.141744    -1.979198     3.232424      41.69
 H       5.256307    -1.269125     4.013998      22.85
 C       5.251336    -2.689780     0.879557      21.09
 C       5.422631    -2.386794    -0.623285      70.89
 H       5.807802    -3.312848    -1.221539      23.52
 O       6.423986    -1.327141    -0.962385     145.77
 H       6.112057    -0.367184    -0.762902      23.53
 C       3.928840    -2.143554    -1.227888      70.72
 H       3.373974    -3.059307    -0.903542      26.06
 C       3.924136    -1.953123    -2.804375     101.83
 O       4.034139    -3.308419    -3.369660     260.27
 H       4.932039    -3.390372    -3.838180      26.54
 H       4.731510    -1.310080    -3.086950      26.69
 H       2.981286    -1.518442    -3.098492      28.43
 C      -0.386991    -1.799721    -0.346187      45.66
 H      -0.982514    -2.638277    -0.413564      22.95
 C      -0.036917     0.600037     0.016801      69.37
 H      -0.283697     1.539457     0.306612      21.78
 C       1.278948     0.433059    -0.367889      16.53
 O       2.184669     1.457432    -0.532375     221.94
 C       1.803193     2.758992    -0.155151     124.74
 H       2.516767     3.426910    -0.500412      26.34
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 H       0.652771     3.007279    -0.520166      25.05
 H       1.686633     2.802984     0.966139      27.48
 C       1.858314    -0.881545    -0.658336      12.64
 O       3.323713    -0.964982    -0.656694     136.95
 C       0.989580    -1.960294    -0.617920      57.21
 H       1.306189    -3.014296    -0.857310      23.26
 C      -0.878775    -0.511932    -0.013508      44.09
 C      -2.398820    -0.490110     0.518960      76.43
 H      -2.593919    -1.313127     1.244707      26.18
 O      -2.546583     0.761625     1.327394     285.95
 H      -2.095799     0.658838     2.183492      29.96
 C      -3.446015    -0.438577    -0.609776      86.76
 H      -3.425250     0.515821    -1.350105      24.83
 O      -3.290935    -1.636709    -1.409102     209.08
 H      -3.396547    -1.365652    -2.368369      26.05
 C      -4.893092    -0.356534     0.039943      98.93
 O      -5.395849     1.000230     0.384417     217.91
 H      -4.675558     1.491266     0.786415      31.35
 H      -4.970611    -1.047332     0.915604      29.18
 H      -5.607670    -0.765212    -0.712785      28.18
55
name = lig-etoh-Waterframe_111
 C       5.266346    -1.669810     1.888174      41.64
 H       5.250602    -0.635180     1.487457      20.62
 C       5.233216    -4.062818     1.347069      49.86
 H       5.212289    -5.015625     0.737009      21.37
 C       5.262139    -4.388793     2.685399       9.83
 O       5.512423    -5.680000     3.289732     237.98
 C       4.567298    -6.750671     2.982956     116.49
 H       4.704554    -6.911082     1.909879      28.95
 H       3.560702    -6.386754     3.245639      28.72
 H       4.877938    -7.616454     3.520171      25.41
 C       5.115830    -3.352810     3.686442       2.86
 O       5.123329    -3.546704     5.078612     180.54
 H       5.068388    -4.580384     5.304535      20.38
 C       5.080687    -2.027638     3.243647      60.86
 H       5.232589    -1.254624     3.990592      25.38
 C       5.232810    -2.705775     0.876293      25.01
 C       5.395598    -2.375525    -0.624730      94.70
 H       5.777628    -3.274356    -1.082483      24.22
 O       6.395943    -1.352752    -0.986506     196.20
 H       5.936135    -0.505725    -0.625466      26.98
 C       3.974255    -2.097716    -1.191753      79.11
 H       3.374057    -3.006408    -0.909503      24.94
 C       3.909283    -1.960516    -2.782199     101.38
 O       4.013533    -3.310984    -3.369378     276.36
 H       4.983583    -3.308913    -3.532710      26.96
 H       4.743757    -1.425075    -3.167617      25.56
 H       2.955327    -1.545395    -3.055629      28.29
 C      -0.373409    -1.755191    -0.354732      34.84
 H      -1.015535    -2.606553    -0.329652      22.25
 C      -0.011676     0.604228     0.009179      69.02
 H      -0.380871     1.550157     0.358208      21.62
 C       1.351923     0.377618    -0.354415      15.39
 O       2.200834     1.452420    -0.484254     193.70
 C       1.763216     2.803776    -0.097627     112.62
 H       2.611156     3.368916    -0.437695      25.67
 H       0.803784     3.241502    -0.715654      24.91
 H       1.623365     2.958834     1.012595      26.52
 C       1.898855    -0.907746    -0.613849      22.95
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 O       3.273891    -1.005263    -0.606611     177.80
 C       0.981374    -1.995514    -0.592237      57.29
 H       1.328015    -3.024741    -0.730795      22.58
 C      -0.917400    -0.540265     0.008925      57.76
 C      -2.371013    -0.437250     0.476947      78.15
 H      -2.659500    -1.412060     0.992182      25.73
 O      -2.595669     0.759930     1.366610     307.66
 H      -2.054555     0.493907     2.101501      29.95
 C      -3.497877    -0.391843    -0.616822      98.23
 H      -3.277298     0.444335    -1.243257      28.42
 O      -3.325504    -1.609256    -1.369870     226.78
 H      -3.007830    -1.259060    -2.254557      26.42
 C      -4.902295    -0.348405     0.045655     103.41
 O      -5.363945     0.982832     0.319687     234.13
 H      -4.684978     1.464254     0.796632      30.22
 H      -4.849266    -0.875081     1.056095      27.37
 H      -5.690172    -0.775887    -0.682516      26.30
55
name = lig-etoh-Waterframe_112
 C       5.185661    -1.734631     1.903083      51.39
 H       5.136362    -0.659984     1.643618      20.57
 C       5.233140    -4.111711     1.306993      55.92
 H       5.145592    -4.927971     0.504155      20.75
 C       5.229409    -4.397114     2.754126      23.35
 O       5.512267    -5.650201     3.256677     428.49
 C       4.587412    -6.755277     2.970525     113.01
 H       4.569897    -7.081493     1.904310      29.26
 H       3.565278    -6.447557     3.201653      28.71
 H       4.846220    -7.567448     3.631202      25.91
 C       5.092411    -3.369070     3.706669      10.82
 O       5.049324    -3.584272     5.070882     268.31
 H       5.004688    -4.510209     5.286840      29.63
 C       5.085077    -2.019657     3.254077      55.22
 H       4.914339    -1.194895     3.998810      20.49
 C       5.275563    -2.723369     0.924719      34.09
 C       5.347527    -2.365184    -0.606642     101.91
 H       5.629688    -3.233969    -1.083745      24.74
 O       6.317875    -1.380382    -0.979540     248.63
 H       6.093517    -0.398203    -0.736381      22.66
 C       3.969208    -2.118625    -1.242141      80.96
 H       3.482012    -3.100143    -1.075090      22.72
 C       3.904167    -1.992153    -2.723403     102.71
 O       4.011503    -3.315255    -3.366775     275.92
 H       4.905070    -3.532771    -3.696681      28.15
 H       4.604014    -1.257244    -3.164518      24.21
 H       2.937974    -1.574225    -3.072579      27.06
 C      -0.393558    -1.794728    -0.348888      61.71
 H      -1.096733    -2.678117    -0.296324      19.37
 C      -0.009108     0.528731    -0.004135      55.75
 H      -0.374131     1.580012     0.263818      19.93
 C       1.368954     0.373411    -0.332174      13.42
 O       2.247231     1.476846    -0.423579     215.38
 C       1.756737     2.857280    -0.068460     107.98
 H       2.664219     3.536294    -0.250968      24.51
 H       1.002521     3.138616    -0.764945      26.39
 H       1.534016     2.924114     1.009143      25.87
 C       1.900295    -0.953600    -0.530565      26.43
 O       3.262183    -0.985154    -0.541796     163.87
 C       1.010689    -2.019831    -0.584871      58.25
 H       1.368373    -3.019231    -0.644432      21.84
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 C      -0.928519    -0.486916     0.035118      59.83
 C      -2.371353    -0.355113     0.450999      87.44
 H      -2.511039    -1.313209     1.025774      23.60
 O      -2.619712     0.709611     1.400121     320.86
 H      -2.287038     0.539470     2.270651      29.67
 C      -3.500190    -0.330138    -0.605302     102.26
 H      -3.415650     0.490041    -1.190125      29.21
 O      -3.367338    -1.583172    -1.366197     229.69
 H      -2.756262    -1.502729    -2.132427      27.14
 C      -4.896806    -0.333610     0.048426     110.26
 O      -5.339481     0.996117     0.255442     264.77
 H      -4.737980     1.353319     0.915963      29.97
 H      -4.800752    -0.941082     0.997389      27.81
 H      -5.681643    -0.918363    -0.540891      26.79
55
name = lig-etoh-Waterframe_113
 C       5.102896    -1.751761     1.908320      41.58
 H       5.106246    -0.693358     1.632745      21.27
 C       5.235193    -4.104958     1.343347      50.18
 H       5.328135    -4.823549     0.500625      21.35
 C       5.200231    -4.395760     2.726509      13.45
 O       5.516052    -5.671092     3.225219     316.15
 C       4.578178    -6.747371     2.953189     119.66
 H       4.666077    -7.227883     1.947190      27.35
 H       3.548562    -6.530984     3.219816      28.00
 H       4.927468    -7.539960     3.663900      25.29
 C       5.086892    -3.362921     3.731391      13.28
 O       4.968845    -3.624335     5.060833     215.43
 H       5.014728    -4.550801     5.321128      23.00
 C       5.076524    -2.022647     3.298885      50.52
 H       4.738709    -1.210758     4.017150      20.70
 C       5.305038    -2.783344     0.923030      32.35
 C       5.293405    -2.372765    -0.567405     100.26
 H       5.680285    -3.242678    -1.131301      22.98
 O       6.271681    -1.390398    -0.973344     236.30
 H       5.938580    -0.423838    -0.754898      22.52
 C       3.905545    -2.175637    -1.214639      81.86
 H       3.296940    -3.034794    -0.953400      24.38
 C       3.897518    -1.982911    -2.766738      90.90
 O       4.011924    -3.338647    -3.366073     270.88
 H       4.832526    -3.265723    -3.895883      27.82
 H       4.697441    -1.235634    -3.103231      22.47
 H       2.807011    -1.728337    -2.934154      25.83
 C      -0.418247    -1.823651    -0.305563      46.15
 H      -1.077327    -2.777144    -0.365620      20.09
 C       0.030071     0.541853    -0.020101      73.71
 H      -0.304191     1.655843     0.143517      19.99
 C       1.352408     0.400153    -0.292455      14.30
 O       2.301078     1.509276    -0.348575     208.46
 C       1.789539     2.851651    -0.052519     117.92
 H       2.690693     3.600461    -0.081292      24.10
 H       1.025615     3.125848    -0.629361      28.92
 H       1.239328     2.856444     0.878464      27.02
 C       1.882825    -0.919853    -0.442866       9.86
 O       3.313805    -0.998014    -0.509102     140.16
 C       0.968860    -2.045616    -0.551860      56.53
 H       1.348566    -3.019277    -0.689656      22.97
 C      -0.886835    -0.546975    -0.012784      56.10
 C      -2.378433    -0.342020     0.507094      83.34
 H      -2.604901    -1.273327     1.034789      25.78
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 O      -2.645715     0.708870     1.439184     302.22
 H      -2.372288     0.370033     2.299993      28.42
 C      -3.472409    -0.312664    -0.639562      90.59
 H      -3.561885     0.580376    -1.349407      26.46
 O      -3.416442    -1.564221    -1.358240     226.39
 H      -2.737131    -1.426827    -2.055755      27.39
 C      -4.868337    -0.369134     0.064234     105.58
 O      -5.324678     1.017507     0.224303     247.44
 H      -4.890394     1.414100     0.979771      30.75
 H      -4.844111    -0.855652     1.032985      28.89
 H      -5.562361    -0.835952    -0.633799      28.04
55
name = lig-etoh-Waterframe_114
 C       5.072764    -1.748137     1.922835      50.84
 H       5.000465    -0.766192     1.500523      23.07
 C       5.275618    -4.097261     1.366981      45.43
 H       5.491338    -5.009970     0.852319      19.82
 C       5.201748    -4.394838     2.715150      12.09
 O       5.508411    -5.705684     3.189491     315.24
 C       4.580243    -6.792242     2.962694     116.83
 H       4.743684    -7.065170     1.903472      30.69
 H       3.548219    -6.454902     3.130081      28.53
 H       4.927476    -7.607502     3.676714      26.55
 C       5.081050    -3.387402     3.713806      -4.87
 O       4.891054    -3.656201     5.069602       5.74
 H       5.074594    -4.708397     5.309949      15.83
 C       5.018516    -2.033825     3.302041      60.23
 H       4.969594    -1.223590     4.081944      22.43
 C       5.259502    -2.734508     0.929232      26.32
 C       5.280868    -2.457479    -0.569746      82.19
 H       5.707364    -3.424117    -1.094035      21.50
 O       6.225245    -1.372000    -0.956704     225.14
 H       5.784621    -0.481173    -0.676629      24.74
 C       3.838454    -2.205074    -1.129550      86.78
 H       3.197047    -3.042264    -0.887810      24.69
 C       3.826585    -2.010636    -2.754708      91.68
 O       4.043471    -3.338393    -3.393004     265.50
 H       4.821000    -3.175448    -3.938624      28.70
 H       4.657233    -1.340914    -3.161587      23.04
 H       2.869298    -1.502407    -3.124555      25.43
 C      -0.402992    -1.877178    -0.274449      32.17
 H      -1.172887    -2.724374    -0.318816      18.79
 C       0.004189     0.598619    -0.042601      71.17
 H      -0.523628     1.603856     0.167727      18.40
 C       1.437476     0.446328    -0.250442       9.65
 O       2.337786     1.504013    -0.273112     217.68
 C       1.773954     2.811214    -0.013208     111.42
 H       2.673590     3.539824     0.072646      24.86
 H       1.160080     3.218214    -0.894386      26.02
 H       1.316572     2.844541     0.978927      26.41
 C       1.903362    -0.911826    -0.394474      20.61
 O       3.318194    -1.020867    -0.505808     177.80
 C       0.965557    -2.002530    -0.491292      59.76
 H       1.281541    -2.991812    -0.774252      22.95
 C      -0.899510    -0.560690    -0.016339      63.17
 C      -2.367170    -0.397614     0.507184      74.11
 H      -2.672685    -1.327422     0.946895      25.77
 O      -2.655520     0.736476     1.483098     282.22
 H      -2.207805     0.423988     2.320072      26.91
 C      -3.488129    -0.344164    -0.614443      84.63
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 H      -3.277443     0.602523    -1.393819      23.99
 O      -3.435518    -1.551150    -1.370409     223.69
 H      -2.922160    -1.373503    -2.195635      26.30
 C      -4.836291    -0.333230     0.061621     114.98
 O      -5.326570     1.015961     0.215348     279.45
 H      -4.969584     1.484366     0.966884      31.08
 H      -4.848710    -0.867586     0.982489      29.36
 H      -5.525157    -0.778601    -0.599682      28.53
55
name = lig-etoh-Waterframe_115
 C       5.060585    -1.714603     1.909700      46.78
 H       4.931537    -0.667184     1.707270      21.80
 C       5.349144    -4.095679     1.384031      38.08
 H       5.564490    -4.870736     0.674865      23.69
 C       5.230055    -4.424828     2.772110      22.56
 O       5.519473    -5.719003     3.180121     285.25
 C       4.592532    -6.820186     2.933272     114.03
 H       4.588144    -7.208338     1.904082      29.63
 H       3.524295    -6.540484     3.135354      29.09
 H       4.801018    -7.696001     3.601731      26.18
 C       5.036892    -3.414982     3.735213       6.12
 O       4.836751    -3.670234     5.050721      24.84
 H       4.997032    -4.751904     5.407921      18.40
 C       4.985048    -2.055791     3.283803      58.07
 H       5.135271    -1.291527     4.040309      26.78
 C       5.183963    -2.747021     0.939763      20.84
 C       5.279282    -2.503976    -0.582783      77.90
 H       5.657553    -3.479568    -1.121095      24.77
 O       6.152691    -1.380972    -0.929610     253.73
 H       5.810508    -0.460925    -0.663593      25.41
 C       3.799794    -2.235868    -1.138334      83.15
 H       3.265682    -3.158130    -0.860716      25.72
 C       3.772127    -2.049037    -2.699477     103.36
 O       4.060663    -3.320342    -3.429143     275.25
 H       4.953884    -3.300564    -3.792406      29.46
 H       4.627789    -1.377341    -2.864418      23.69
 H       2.875451    -1.618132    -3.145445      27.89
 C      -0.405587    -1.832674    -0.235069      49.16
 H      -1.000362    -2.755021    -0.247273      22.46
 C      -0.023959     0.567720    -0.068442      51.13
 H      -0.407011     1.588170     0.221216      17.64
 C       1.416528     0.446208    -0.194073      26.65
 O       2.371128     1.476807    -0.201270     208.99
 C       1.795755     2.803781     0.043009     106.10
 H       2.690839     3.401028     0.167993      24.65
 H       1.135808     3.171387    -0.949343      25.29
 H       1.129424     2.844978     0.952111      26.86
 C       1.925281    -0.887909    -0.376964      23.14
 O       3.281269    -1.035958    -0.504491     187.78
 C       1.016755    -1.964796    -0.441894      54.82
 H       1.418833    -2.955833    -0.746908      22.22
 C      -0.901554    -0.510028     0.032126      50.59
 C      -2.367225    -0.446931     0.490922      81.36
 H      -2.477104    -1.342105     1.115945      24.65
 O      -2.631002     0.719012     1.483714     266.30
 H      -2.092208     0.634165     2.326605      26.60
 C      -3.441114    -0.360085    -0.567225      85.77
 H      -3.248210     0.624441    -1.210688      25.40
 O      -3.425025    -1.571359    -1.420870     197.36
 H      -3.226837    -1.282744    -2.353507      25.31
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 C      -4.854228    -0.261797     0.041834     112.33
 O      -5.350540     1.029064     0.224343     268.43
 H      -4.858460     1.428346     0.945228      30.88
 H      -4.756483    -0.853965     0.956507      28.84
 H      -5.569105    -0.805986    -0.560491      28.57
55
name = lig-etoh-Waterframe_116
 C       5.029207    -1.702767     1.923724      47.15
 H       5.034395    -0.634667     1.682306      20.66
 C       5.406892    -4.070339     1.414744      43.18
 H       5.573182    -4.724232     0.572716      21.12
 C       5.271935    -4.459800     2.756283      30.61
 O       5.546314    -5.778256     3.201000     273.01
 C       4.559867    -6.844370     2.886293     111.98
 H       4.660831    -7.214502     1.857958      29.84
 H       3.554164    -6.503460     3.221553      26.07
 H       4.974778    -7.584227     3.567813      25.44
 C       4.978717    -3.439584     3.735240      10.60
 O       4.789807    -3.666169     5.066346      97.33
 H       4.960159    -4.644457     5.357583      22.00
 C       5.016346    -2.094289     3.269086      52.20
 H       4.958598    -1.327754     3.999904      22.28
 C       5.144814    -2.787521     0.935755      28.10
 C       5.208197    -2.460938    -0.572843     105.60
 H       5.694298    -3.279556    -1.107751      25.01
 O       6.105223    -1.420709    -0.912783     278.35
 H       5.692798    -0.562333    -0.639147      26.08
 C       3.791602    -2.316168    -1.175211      79.54
 H       3.182652    -3.168219    -0.786256      22.71
 C       3.786834    -2.084847    -2.657042     109.94
 O       4.053724    -3.306631    -3.438857     296.51
 H       4.976639    -3.195993    -3.695273      27.97
 H       4.471277    -1.289059    -2.841571      23.49
 H       2.787029    -1.829659    -2.892696      27.75
 C      -0.325988    -1.752698    -0.192213      45.91
 H      -0.916407    -2.610642    -0.140376      22.68
 C       0.010931     0.579381    -0.046938      78.43
 H      -0.303887     1.587202     0.180785      17.31
 C       1.357036     0.391238    -0.160595      30.10
 O       2.353893     1.443367    -0.119525     206.36
 C       1.844330     2.799619     0.091927     118.29
 H       2.586037     3.479519     0.287652      25.88
 H       1.160402     3.170770    -0.836393      25.23
 H       1.101167     2.802663     0.925259      26.80
 C       1.898160    -0.861863    -0.375392      23.93
 O       3.273224    -1.051929    -0.510881     162.50
 C       1.022849    -1.942790    -0.409574      56.15
 H       1.455796    -2.976021    -0.541320      20.31
 C      -0.904218    -0.529511     0.063604      71.45
 C      -2.324440    -0.448990     0.581251      84.25
 H      -2.501399    -1.409855     1.180474      24.44
 O      -2.604076     0.691944     1.419956     282.67
 H      -2.073153     0.378453     2.243069      25.10
 C      -3.418493    -0.367418    -0.575422      86.58
 H      -3.241269     0.484658    -1.132995      27.59
 O      -3.398276    -1.577458    -1.474329     205.91
 H      -3.339979    -1.191000    -2.382698      24.59
 C      -4.867877    -0.280936     0.034433      94.12
 O      -5.379249     1.087111     0.261578     253.29
 H      -4.761870     1.485912     0.879838      31.35
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 H      -4.899989    -0.718100     1.077103      27.38
 H      -5.580616    -0.772186    -0.704680      26.77
55
name = lig-etoh-Waterframe_117
 C       5.012556    -1.771255     1.916249      53.30
 H       5.061856    -0.731576     1.546575      20.23
 C       5.424939    -4.072558     1.387646      47.10
 H       5.653152    -4.988550     0.794183      19.94
 C       5.314439    -4.484942     2.757804      -0.10
 O       5.571539    -5.820801     3.207930     273.71
 C       4.581469    -6.856347     2.880696      98.68
 H       4.602023    -7.026713     1.787406      27.05
 H       3.541484    -6.572352     3.126787      27.85
 H       4.859722    -7.729167     3.444373      23.00
 C       4.966179    -3.486361     3.690187      13.42
 O       4.746188    -3.647579     5.085050     277.78
 H       4.902445    -4.532183     5.375725      27.22
 C       5.028237    -2.102138     3.288962      51.29
 H       4.772292    -1.395980     4.040447      22.74
 C       5.145448    -2.725481     0.963821      32.54
 C       5.153670    -2.485442    -0.538570     107.17
 H       5.526380    -3.354274    -0.954291      24.13
 O       6.070639    -1.418891    -0.901663     267.16
 H       5.783097    -0.504225    -0.726797      25.04
 C       3.796131    -2.350728    -1.121239      77.63
 H       3.144028    -3.248341    -0.910485      22.43
 C       3.751179    -2.109431    -2.660297     106.68
 O       4.048384    -3.288219    -3.415064     280.70
 H       4.856756    -3.241206    -4.014629      25.70
 H       4.263224    -1.275367    -3.088738      24.15
 H       2.696022    -1.841624    -2.834114      25.65
 C      -0.307489    -1.765208    -0.134227      52.19
 H      -0.948231    -2.575619    -0.029067      23.32
 C      -0.024170     0.618189     0.030969      70.32
 H      -0.383088     1.586619     0.154772      20.40
 C       1.398630     0.420211    -0.159031       9.27
 O       2.314313     1.418830    -0.039038     233.23
 C       1.838740     2.780662     0.145911     126.79
 H       2.681879     3.389040     0.349703      26.68
 H       1.412680     3.162263    -0.742995      28.97
 H       1.266054     2.818229     1.070601      27.25
 C       1.925831    -0.915549    -0.400004      25.02
 O       3.278874    -1.062980    -0.536080     144.18
 C       1.046772    -1.961873    -0.387346      66.70
 H       1.312591    -3.051025    -0.373066      21.86
 C      -0.862541    -0.495109     0.090928      46.28
 C      -2.325590    -0.472658     0.593599      83.12
 H      -2.612924    -1.424316     1.143067      25.07
 O      -2.554212     0.660981     1.378190     272.77
 H      -2.334989     0.523798     2.392797      26.24
 C      -3.426087    -0.409275    -0.582148      91.09
 H      -3.219880     0.412911    -1.144423      28.08
 O      -3.370595    -1.551868    -1.483644     230.96
 H      -3.102968    -1.290886    -2.408792      25.34
 C      -4.876964    -0.272173     0.045391      92.90
 O      -5.386370     1.129603     0.289741     238.05
 H      -4.745022     1.641748     0.789615      30.85
 H      -5.016905    -0.926410     0.970407      27.58
 H      -5.633727    -0.703558    -0.721140      26.35
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name = lig-etoh-Waterframe_118
 C       5.018251    -1.774603     1.960428      41.84
 H       4.859097    -0.704669     1.686100      20.66
 C       5.410963    -4.135409     1.407754      32.40
 H       5.709168    -4.878840     0.585909      17.50
 C       5.341536    -4.504821     2.754010       9.10
 O       5.593669    -5.827959     3.206442     307.11
 C       4.606163    -6.853080     2.849181     105.92
 H       4.581986    -6.978246     1.740428      27.97
 H       3.621623    -6.535920     3.204305      27.32
 H       4.816054    -7.820945     3.251031      23.21
 C       5.000752    -3.478887     3.730481      13.17
 O       4.710208    -3.623514     5.051889      58.21
 H       4.853019    -4.688524     5.411345      18.72
 C       4.973083    -2.136732     3.308336      50.28
 H       4.835759    -1.378636     4.096344      23.51
 C       5.198130    -2.812426     0.961002      29.66
 C       5.178766    -2.530633    -0.488928      93.62
 H       5.558368    -3.436668    -0.956842      22.65
 O       6.064002    -1.415003    -0.915431     221.44
 H       5.671918    -0.550023    -0.740263      25.03
 C       3.780064    -2.293041    -1.111918      87.90
 H       3.192751    -3.189413    -0.831351      23.03
 C       3.664445    -2.099827    -2.697427      90.34
 O       4.025972    -3.324644    -3.396182     265.29
 H       4.782758    -3.101575    -4.051980      24.43
 H       4.351825    -1.245385    -2.958296      23.03
 H       2.557495    -1.926364    -2.944184      24.22
 C      -0.347591    -1.804337    -0.064509      50.38
 H      -0.958800    -2.704670     0.054436      22.06
 C       0.011733     0.640074     0.097765      64.87
 H      -0.353891     1.573345     0.317246      21.18
 C       1.381708     0.407829    -0.171282       7.67
 O       2.323442     1.421480     0.026885     213.13
 C       1.864503     2.769417     0.231111     129.12
 H       2.883812     3.225344     0.371953      24.00
 H       1.356305     3.144656    -0.554336      29.91
 H       1.149268     2.943210     1.049764      27.05
 C       1.944290    -0.908227    -0.414247       6.61
 O       3.300837    -1.080247    -0.569900     154.54
 C       1.026366    -2.054157    -0.350186      48.19
 H       1.455692    -3.062164    -0.436059      22.33
 C      -0.856596    -0.510738     0.131028      46.97
 C      -2.346429    -0.523671     0.518616      90.28
 H      -2.435355    -1.413747     1.147047      26.19
 O      -2.540281     0.697737     1.376899     261.00
 H      -2.339256     0.406375     2.382035      25.94
 C      -3.434601    -0.412714    -0.576025      83.01
 H      -3.254146     0.600822    -1.169426      25.85
 O      -3.350471    -1.551881    -1.455923     244.48
 H      -2.853677    -1.240995    -2.247955      25.99
 C      -4.900712    -0.226891     0.025322     104.05
 O      -5.369440     1.116205     0.306473     249.59
 H      -4.677309     1.636945     0.721868      30.63
 H      -4.910671    -0.907167     0.917073      28.35
 H      -5.632052    -0.556826    -0.752937      26.88
55
name = lig-etoh-Waterframe_119
 C       5.021471    -1.805085     1.978628      50.67
 H       4.777091    -0.754600     1.739297      23.58
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 C       5.408785    -4.196928     1.410554      45.44
 H       5.599775    -4.920430     0.558122      21.95
 C       5.341764    -4.521008     2.802180      17.33
 O       5.624359    -5.827015     3.208099     297.81
 C       4.608974    -6.826056     2.784579     109.71
 H       4.544791    -6.889703     1.674038      29.82
 H       3.677007    -6.541712     3.276812      29.33
 H       5.097114    -7.682599     3.257079      24.84
 C       5.061041    -3.485896     3.745241       3.13
 O       4.687251    -3.652982     5.044146     -44.36
 H       4.823810    -4.752617     5.332544      19.04
 C       4.910713    -2.149082     3.317822      49.80
 H       4.900783    -1.342796     4.115480      22.97
 C       5.242828    -2.861648     1.029814      13.79
 C       5.239536    -2.540033    -0.537020      74.24
 H       5.711468    -3.393547    -1.178134      23.07
 O       6.072557    -1.436036    -0.931612     225.48
 H       5.635016    -0.625785    -0.664565      27.73
 C       3.766762    -2.281781    -1.159861      86.32
 H       3.170050    -3.047513    -0.708297      25.86
 C       3.605878    -2.116043    -2.692081      93.12
 O       3.985268    -3.365822    -3.387590     258.95
 H       4.942098    -3.234270    -3.788677      24.69
 H       4.316876    -1.243413    -2.956261      23.48
 H       2.546024    -1.780562    -2.988042      26.41
 C      -0.327417    -1.875778    -0.012122      44.64
 H      -1.083024    -2.734386     0.106884      21.73
 C       0.030071     0.569222     0.138138      64.53
 H      -0.208902     1.476865     0.524204      23.61
 C       1.383317     0.377471    -0.160862       1.30
 O       2.349552     1.403025     0.074900     199.65
 C       1.900363     2.776895     0.311806     107.79
 H       2.784523     3.580828     0.544359      24.24
 H       1.358771     3.168534    -0.605978      26.40
 H       1.271935     2.845096     1.239850      25.88
 C       1.854635    -0.951846    -0.410680       9.55
 O       3.297811    -1.036327    -0.576380     146.50
 C       1.026936    -2.052922    -0.308359      70.84
 H       1.384324    -3.033756    -0.517279      24.59
 C      -0.868249    -0.561857     0.149513      39.55
 C      -2.341142    -0.475267     0.506407      90.81
 H      -2.593041    -1.372176     1.056654      27.16
 O      -2.557586     0.726795     1.380680     284.57
 H      -2.094185     0.352527     2.250922      26.11
 C      -3.448765    -0.352240    -0.568917      80.06
 H      -3.186703     0.663800    -1.263702      25.32
 O      -3.338510    -1.558817    -1.414157     216.08
 H      -2.886772    -1.313044    -2.257936      26.44
 C      -4.898060    -0.218790    -0.015353     118.17
 O      -5.333412     1.097963     0.316552     267.25
 H      -4.610511     1.534261     0.772357      30.58
 H      -5.020878    -0.771921     0.895122      29.15
 H      -5.555380    -0.631251    -0.737855      29.29
55
name = lig-etoh-Waterframe_120
 C       5.009963    -1.860308     1.963901      54.06
 H       4.948625    -0.865911     1.524280      24.90
 C       5.413115    -4.214737     1.439214      40.36
 H       5.466604    -5.128114     0.854319      20.74
 C       5.358748    -4.516226     2.807682      16.94
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 O       5.635607    -5.820990     3.211873     281.66
 C       4.657431    -6.786271     2.762141     119.55
 H       4.499061    -6.810786     1.667109      28.89
 H       3.644326    -6.711596     3.209549      27.77
 H       5.034628    -7.816765     3.061817      27.86
 C       5.075384    -3.500641     3.748573       6.22
 O       4.689037    -3.728553     5.064533       0.59
 H       4.811427    -4.612576     5.455393      16.80
 C       4.912378    -2.146748     3.326545      50.85
 H       4.668545    -1.369953     4.125336      22.24
 C       5.259539    -2.848159     0.991644     -10.97
 C       5.252569    -2.526209    -0.611309      74.47
 H       5.643282    -3.540124    -1.089220      21.31
 O       6.096736    -1.445894    -0.940149     206.05
 H       5.872057    -0.548901    -0.663901      28.15
 C       3.770152    -2.306043    -1.148358      70.14
 H       3.171037    -3.151803    -0.859094      26.64
 C       3.623392    -2.144759    -2.677521     102.27
 O       3.925708    -3.391659    -3.371750     239.83
 H       4.905971    -3.388124    -3.703522      25.11
 H       4.251355    -1.356437    -3.170553      25.31
 H       2.580232    -1.906978    -2.923910      28.12
 C      -0.349488    -1.899338     0.026796      51.69
 H      -0.998299    -2.866641     0.053524      22.80
 C       0.013713     0.469517     0.170871      66.26
 H      -0.352941     1.382819     0.570392      24.62
 C       1.406294     0.370984    -0.102285      -1.35
 O       2.394611     1.374116     0.101719     183.81
 C       1.901684     2.788500     0.395028      90.33
 H       2.908504     3.411924     0.548053      23.70
 H       1.256552     3.199316    -0.551875      24.32
 H       1.279884     2.714603     1.310503      25.76
 C       1.887448    -0.942664    -0.402096      10.57
 O       3.232631    -0.976361    -0.574761     121.34
 C       1.006024    -2.071759    -0.286730      67.19
 H       1.319613    -3.058486    -0.482175      26.93
 C      -0.866284    -0.630485     0.158291      45.33
 C      -2.366751    -0.374949     0.551089      90.49
 H      -2.759317    -1.272049     1.040476      27.68
 O      -2.561335     0.725893     1.395123     310.38
 H      -2.085916     0.713645     2.297337      28.66
 C      -3.419178    -0.290041    -0.616018      89.30
 H      -3.264725     0.586345    -1.343049      27.31
 O      -3.337589    -1.558433    -1.367099     198.57
 H      -3.126670    -1.352485    -2.315157      27.19
 C      -4.877963    -0.253777    -0.036241     107.72
 O      -5.294256     1.112588     0.304912     258.27
 H      -4.632905     1.459625     0.907840      30.99
 H      -4.933316    -0.945561     0.785535      29.57
 H      -5.543838    -0.609808    -0.783594      29.30
55
name = lig-etoh-Waterframe_121
 C       5.021964    -1.882586     1.901177      33.42
 H       4.994262    -0.826636     1.643428      19.25
 C       5.410050    -4.185062     1.444351      53.83
 H       5.529533    -4.986050     0.763502      20.21
 C       5.392323    -4.475278     2.805734      13.60
 O       5.622738    -5.830487     3.229567     254.34
 C       4.684065    -6.801750     2.731905     109.60
 H       4.594637    -6.626329     1.657491      24.69
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 H       3.714232    -6.590507     3.248539      22.20
 H       5.096925    -7.854675     2.851595      24.08
 C       5.029221    -3.502789     3.799828      16.03
 O       4.707693    -3.739371     5.074999      25.98
 H       4.897026    -4.899422     5.373201      14.55
 C       4.940307    -2.174149     3.318065      46.41
 H       4.547337    -1.405030     4.015613      24.35
 C       5.255542    -2.902048     0.887418      29.72
 C       5.184651    -2.509986    -0.570086     100.26
 H       5.597836    -3.373824    -1.150471      22.33
 O       6.155675    -1.451403    -0.970786     187.59
 H       5.810148    -0.583050    -0.674826      24.72
 C       3.801666    -2.280572    -1.128345      79.36
 H       3.199710    -3.151203    -0.833333      24.41
 C       3.653835    -2.166764    -2.694623     105.39
 O       3.863088    -3.453100    -3.347302     238.88
 H       4.726323    -3.260793    -3.900358      24.17
 H       4.261866    -1.363487    -3.079844      25.66
 H       2.622444    -2.032055    -2.796045      27.51
 C      -0.373451    -1.957218     0.022127      46.19
 H      -1.007927    -2.894614     0.060382      21.11
 C       0.014826     0.435500     0.198256      62.94
 H      -0.533817     1.401205     0.396062      20.94
 C       1.400942     0.358825    -0.018722      11.49
 O       2.403800     1.366320     0.110001     209.08
 C       1.910673     2.715418     0.458851     112.04
 H       2.845722     3.256923     0.598397      24.68
 H       1.216457     3.233883    -0.345046      25.17
 H       1.331210     2.806234     1.368404      27.28
 C       1.888511    -0.927102    -0.355050      12.17
 O       3.233192    -1.003113    -0.604024     139.45
 C       1.007854    -2.075602    -0.287278      58.52
 H       1.413141    -3.058817    -0.390395      23.86
 C      -0.924148    -0.649379     0.206059      54.51
 C      -2.384328    -0.363516     0.572527      81.00
 H      -2.647544    -1.287810     1.172063      25.25
 O      -2.576234     0.812568     1.421307     296.99
 H      -2.159542     0.464509     2.298470      27.43
 C      -3.402551    -0.259547    -0.669586     102.23
 H      -3.270861     0.509309    -1.291286      28.65
 O      -3.333089    -1.557150    -1.338089     234.20
 H      -3.219993    -1.283767    -2.289120      26.78
 C      -4.839614    -0.249253    -0.071541      96.93
 O      -5.255329     1.101612     0.295888     275.06
 H      -4.685095     1.426245     0.993459      31.49
 H      -4.855370    -1.014292     0.736400      28.91
 H      -5.575254    -0.478700    -0.876038      27.42
55
name = lig-etoh-Waterframe_122
 C       5.057467    -1.896820     1.879762      55.69
 H       4.884528    -0.853482     1.667881      21.72
 C       5.428619    -4.177743     1.375612      30.57
 H       5.706239    -4.906974     0.651464      18.52
 C       5.408643    -4.475996     2.833838      -4.22
 O       5.627639    -5.811865     3.259505     252.85
 C       4.686761    -6.793528     2.659593      96.46
 H       4.495167    -6.608307     1.604339      25.08
 H       3.711769    -6.759854     3.201596      23.13
 H       5.205241    -7.740078     2.904381      21.84
 C       4.997464    -3.506857     3.778453       5.11
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 O       4.742191    -3.765947     5.112502     146.31
 H       4.819009    -4.709560     5.424620      29.67
 C       4.943717    -2.192976     3.232342      53.17
 H       4.768919    -1.366241     3.891759      23.61
 C       5.214684    -2.866306     0.909022      34.20
 C       5.205277    -2.511058    -0.569844     103.59
 H       5.477078    -3.299026    -1.177340      24.52
 O       6.160192    -1.441454    -0.976183     222.71
 H       5.801450    -0.537241    -0.758897      24.77
 C       3.799279    -2.241012    -1.137193      99.49
 H       3.209862    -3.079892    -0.677092      23.79
 C       3.637009    -2.189739    -2.663914     102.63
 O       3.842634    -3.507136    -3.346371     255.39
 H       4.556242    -3.430340    -4.075618      25.69
 H       4.283433    -1.446675    -3.075036      25.77
 H       2.637404    -1.795172    -2.857460      26.83
 C      -0.390544    -1.974569     0.001340      41.56
 H      -1.021550    -2.829651     0.077582      20.88
 C      -0.036093     0.461220     0.212084      63.21
 H      -0.352534     1.585204     0.270291      20.39
 C       1.387758     0.329992     0.049619      -1.70
 O       2.344913     1.358782     0.112837     211.93
 C       1.932805     2.655704     0.525002     128.95
 H       2.705818     3.266991     0.622180      28.24
 H       1.366762     3.062430    -0.285470      27.46
 H       1.470770     2.591828     1.494961      27.79
 C       1.849877    -0.970309    -0.286040      13.73
 O       3.278725    -1.055886    -0.637620     157.76
 C       1.008755    -2.056966    -0.281961      68.09
 H       1.479093    -3.045125    -0.387392      23.24
 C      -0.914686    -0.654828     0.251460      39.70
 C      -2.400563    -0.387687     0.552371      74.94
 H      -2.821349    -1.237603     1.185872      24.02
 O      -2.575099     0.887220     1.453394     255.52
 H      -2.359227     0.532772     2.356108      26.95
 C      -3.396193    -0.296137    -0.628592     104.48
 H      -3.118282     0.520125    -1.249385      27.39
 O      -3.310798    -1.550990    -1.356799     220.37
 H      -3.043976    -1.407442    -2.309948      26.57
 C      -4.813781    -0.183663    -0.134541     101.25
 O      -5.226594     1.074801     0.306281     269.60
 H      -4.624459     1.392292     0.980792      30.95
 H      -4.996351    -0.923266     0.723909      27.76
 H      -5.533644    -0.569262    -0.957542      26.76
55
name = lig-etoh-Waterframe_123
 C       5.053998    -1.833928     1.887809      48.89
 H       4.904854    -0.845742     1.468527      20.48
 C       5.472733    -4.180730     1.383298      40.55
 H       5.760059    -5.013271     0.723448      20.63
 C       5.391117    -4.511140     2.751909      -1.73
 O       5.613606    -5.777932     3.257844     227.78
 C       4.702618    -6.782175     2.623716     105.95
 H       4.565961    -6.672933     1.540657      29.11
 H       3.741942    -6.862330     3.129985      26.84
 H       5.185001    -7.736115     2.739686      23.93
 C       5.003060    -3.529290     3.724839      -1.27
 O       4.779058    -3.709950     5.112720     188.32
 H       4.916157    -4.753321     5.363000      19.37
 C       4.930875    -2.187427     3.230604      59.94
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 H       4.966494    -1.389133     3.912207      26.34
 C       5.204235    -2.852161     0.918428      16.49
 C       5.266560    -2.497926    -0.637609      96.49
 H       5.636030    -3.406016    -1.057443      25.08
 O       6.123614    -1.418082    -0.958336     230.55
 H       5.770009    -0.482047    -0.764249      23.91
 C       3.775081    -2.292383    -1.133204      84.46
 H       3.219664    -3.201756    -0.786445      24.42
 C       3.635350    -2.211302    -2.679482     101.75
 O       3.804349    -3.537070    -3.346183     258.88
 H       4.673300    -3.402520    -3.868473      25.39
 H       4.463454    -1.621275    -3.076010      23.78
 H       2.616857    -1.798305    -3.020406      25.74
 C      -0.394823    -1.911677     0.002432      27.31
 H      -0.974012    -2.759283     0.008192      21.20
 C      -0.022235     0.509609     0.215257      67.81
 H      -0.501192     1.562922     0.398429      16.45
 C       1.339906     0.294442     0.078780      28.27
 O       2.299801     1.299190     0.101596     214.55
 C       1.929141     2.628076     0.584209     120.01
 H       2.848088     3.175197     0.667627      24.18
 H       1.204287     3.065818    -0.013302      27.54
 H       1.361128     2.510960     1.548209      26.24
 C       1.917974    -0.991714    -0.240817      16.72
 O       3.245184    -1.024138    -0.615111     190.51
 C       0.973208    -2.097409    -0.262692      48.64
 H       1.342486    -3.127103    -0.543409      20.10
 C      -0.900221    -0.639419     0.276419      58.80
 C      -2.412957    -0.390644     0.611871      80.02
 H      -2.820111    -1.229618     1.219696      23.32
 O      -2.575695     0.903918     1.439439     290.12
 H      -2.329253     0.731041     2.350686      28.91
 C      -3.346613    -0.328769    -0.604946      84.85
 H      -3.027488     0.616300    -1.318509      22.99
 O      -3.270727    -1.566329    -1.398012     213.71
 H      -2.810872    -1.296677    -2.245033      25.42
 C      -4.844066    -0.182687    -0.178166      95.61
 O      -5.223054     1.099494     0.322045     271.36
 H      -4.465554     1.358935     0.858799      29.81
 H      -4.979493    -1.000931     0.603540      27.69
 H      -5.465148    -0.395653    -1.117832      26.15
55
name = lig-etoh-Waterframe_124
 C       5.016001    -1.798427     1.853362      34.91
 H       5.030836    -0.713783     1.634970      20.71
 C       5.511166    -4.157243     1.381105      65.74
 H       5.666511    -4.998698     0.641024      24.39
 C       5.332275    -4.497573     2.722250       7.87
 O       5.574300    -5.790842     3.212129     315.28
 C       4.747980    -6.814434     2.599610     107.36
 H       4.660783    -6.485250     1.539232      32.11
 H       3.779586    -6.690127     3.074210      27.98
 H       5.224226    -7.752612     2.694123      25.24
 C       5.022428    -3.501870     3.682577       4.91
 O       4.840014    -3.658631     5.039596      32.92
 H       4.884124    -4.723124     5.389083      15.70
 C       4.939981    -2.146031     3.288638      39.53
 H       4.865134    -1.455979     4.117682      21.65
 C       5.252160    -2.857030     0.886580      -2.76
 C       5.255680    -2.510862    -0.619774      74.49
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 H       5.831801    -3.354998    -1.195522      23.28
 O       6.103894    -1.381262    -0.958351     180.08
 H       5.635285    -0.512474    -0.644531      21.88
 C       3.772909    -2.372869    -1.168153      69.47
 H       3.138704    -3.176812    -0.758224      24.91
 C       3.671434    -2.241002    -2.730164      99.79
 O       3.778719    -3.543681    -3.341280     277.20
 H       4.715118    -3.598126    -3.683248      26.41
 H       4.463750    -1.496077    -3.049843      24.03
 H       2.624721    -1.806332    -3.006867      25.84
 C      -0.394475    -1.857937     0.021110      50.65
 H      -1.069725    -2.666830    -0.050626      20.27
 C      -0.046764     0.500563     0.242423      63.75
 H      -0.464300     1.496891     0.554499      14.72
 C       1.340693     0.265553     0.043518      27.77
 O       2.282664     1.263200     0.083140     217.07
 C       1.874701     2.579079     0.647610     102.94
 H       2.938099     3.127938     0.764831      22.21
 H       1.190515     3.212643     0.021126      25.99
 H       1.535975     2.527890     1.758732      25.18
 C       1.875927    -1.046356    -0.209505      32.94
 O       3.216637    -1.002741    -0.570874     147.52
 C       1.001380    -2.108129    -0.261237      76.86
 H       1.155902    -3.155445    -0.633767      21.87
 C      -0.926116    -0.560438     0.299907      64.80
 C      -2.379271    -0.380908     0.716656      90.15
 H      -2.622541    -1.207357     1.355897      25.58
 O      -2.586569     0.884251     1.382146     332.17
 H      -2.152883     0.655055     2.188835      29.94
 C      -3.327601    -0.328674    -0.609031      76.17
 H      -3.021348     0.649740    -1.326739      22.53
 O      -3.202685    -1.557791    -1.427595     219.39
 H      -2.732378    -1.310690    -2.278255      25.33
 C      -4.855395    -0.218854    -0.239370     104.69
 O      -5.214693     1.121588     0.344326     243.95
 H      -4.446059     1.507560     0.766590      30.32
 H      -5.170843    -1.053222     0.379642      28.83
 H      -5.467030    -0.230390    -1.135132      27.36
55
name = lig-etoh-Waterframe_125
 C       5.003589    -1.816152     1.908618      57.82
 H       4.995079    -0.740249     1.615997      22.85
 C       5.500966    -4.124285     1.332888      38.84
 H       5.658949    -4.918577     0.536125      22.06
 C       5.291661    -4.479229     2.737092      11.87
 O       5.564004    -5.798182     3.173181     304.24
 C       4.769149    -6.809618     2.548397     117.92
 H       4.612429    -6.690238     1.426798      29.08
 H       3.742534    -6.877798     2.984442      27.15
 H       5.214094    -7.759843     2.775345      24.39
 C       5.042289    -3.437603     3.660884      16.52
 O       4.902524    -3.647462     4.978326     155.38
 H       4.970009    -4.668483     5.280509      20.60
 C       4.961873    -2.096061     3.232507      53.90
 H       4.673644    -1.355349     4.018854      19.38
 C       5.307161    -2.793680     0.900247      34.37
 C       5.234209    -2.526308    -0.586538      82.02
 H       5.629615    -3.423674    -1.275986      22.90
 O       6.072947    -1.356443    -0.963801     224.82
 H       5.771873    -0.410176    -0.626805      20.91
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 C       3.781855    -2.357870    -1.182415      83.02
 H       3.165739    -3.160909    -0.803422      24.57
 C       3.691579    -2.234753    -2.719484     103.80
 O       3.779024    -3.560651    -3.344751     261.64
 H       4.629339    -3.696382    -3.815674      26.75
 H       4.417152    -1.501635    -3.191620      24.85
 H       2.663644    -1.859556    -2.945590      26.51
 C      -0.406879    -1.825666     0.038159      25.68
 H      -1.144248    -2.659513    -0.035537      20.40
 C      -0.025505     0.522050     0.291848      76.65
 H      -0.229422     1.519971     0.525747      15.68
 C       1.315543     0.253670     0.003873      23.99
 O       2.274971     1.286176     0.071274     211.07
 C       1.880597     2.529872     0.722701      88.26
 H       2.907371     3.213475     0.722961      22.28
 H       1.154819     3.086679    -0.015141      24.38
 H       1.492126     2.330808     1.775350      25.46
 C       1.835100    -1.040240    -0.224076      23.75
 O       3.231576    -1.074968    -0.551889     153.43
 C       0.917130    -2.124924    -0.262667      47.07
 H       1.331732    -3.114733    -0.553143      19.72
 C      -0.932341    -0.567085     0.313283      67.25
 C      -2.373684    -0.382447     0.698144      93.87
 H      -2.681561    -1.167919     1.371605      27.30
 O      -2.585719     0.859424     1.357053     310.86
 H      -2.184541     0.868510     2.206943      32.11
 C      -3.338204    -0.356808    -0.590287      95.06
 H      -2.989102     0.571281    -1.089658      25.85
 O      -3.117666    -1.516985    -1.427433     240.35
 H      -2.830142    -1.296149    -2.371976      24.21
 C      -4.854777    -0.184497    -0.302761     115.68
 O      -5.211910     1.085125     0.351989     262.27
 H      -4.448815     1.518920     0.733049      30.86
 H      -5.260581    -0.965202     0.298951      29.79
 H      -5.352670    -0.227105    -1.236638      29.14
55
name = lig-etoh-Waterframe_126
 C       5.043808    -1.772552     1.856202      44.86
 H       4.738688    -0.775170     1.480342      22.85
 C       5.445307    -4.095827     1.336219      51.92
 H       5.698041    -4.892310     0.610973      23.25
 C       5.310864    -4.443047     2.657035      20.93
 O       5.555169    -5.769325     3.139186     343.89
 C       4.741940    -6.849689     2.488918     128.49
 H       4.775533    -6.852107     1.372719      28.89
 H       3.716805    -6.901073     2.941605      27.76
 H       5.355903    -7.731355     2.773903      25.89
 C       5.075536    -3.418504     3.634661      29.77
 O       4.957224    -3.657748     4.984345     109.38
 H       5.108711    -4.584610     5.197904      19.66
 C       4.947294    -2.073931     3.221022      60.08
 H       4.685546    -1.164120     3.856484      23.09
 C       5.327246    -2.764107     0.934371      40.67
 C       5.212386    -2.458153    -0.593687     100.96
 H       5.660962    -3.393636    -0.996444      23.89
 O       6.066697    -1.375981    -0.991957     236.55
 H       5.672201    -0.485649    -0.631240      25.96
 C       3.790846    -2.286843    -1.130216      97.58
 H       3.285475    -3.219094    -0.951359      26.77
 C       3.679312    -2.217142    -2.705621     103.67
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 O       3.784259    -3.588324    -3.358783     257.77
 H       4.569587    -3.383770    -3.882736      27.07
 H       4.476781    -1.597929    -3.150511      26.36
 H       2.709383    -1.894311    -2.927935      27.70
 C      -0.479023    -1.878243     0.039837      38.18
 H      -1.199356    -2.789548     0.081284      19.75
 C      -0.001633     0.539896     0.328207      63.77
 H      -0.366847     1.474207     0.476311      16.43
 C       1.345124     0.299750    -0.008879      20.48
 O       2.288370     1.302281     0.054782     238.12
 C       1.900722     2.493595     0.742007     108.26
 H       2.799518     3.193339     0.883366      23.56
 H       0.993674     3.010642     0.282268      25.85
 H       1.460053     2.306269     1.690607      28.19
 C       1.838558    -1.038950    -0.305270      25.70
 O       3.219825    -1.179416    -0.541938     200.91
 C       0.892294    -2.098402    -0.269274      56.94
 H       1.187516    -3.143241    -0.350617      21.55
 C      -0.906917    -0.565942     0.328009      78.25
 C      -2.416911    -0.420537     0.649555      84.27
 H      -2.777611    -1.281805     1.291237      26.29
 O      -2.600356     0.891159     1.345940     297.86
 H      -2.281947     0.745215     2.243109      31.65
 C      -3.310167    -0.340976    -0.564588     107.56
 H      -3.033998     0.480063    -1.048506      29.77
 O      -3.041359    -1.479311    -1.413251     238.00
 H      -2.970388    -1.074470    -2.330904      24.10
 C      -4.847612    -0.144001    -0.343312     114.41
 O      -5.226832     1.028721     0.334746     281.71
 H      -4.401813     1.356914     0.715046      30.61
 H      -5.209827    -1.026888     0.248883      29.30
 H      -5.266155    -0.175634    -1.363231      28.86
55
name = lig-etoh-Waterframe_127
 C       5.062276    -1.691111     1.802141      45.95
 H       4.716005    -0.707341     1.484412      21.66
 C       5.412895    -4.083049     1.300690      56.19
 H       5.616798    -4.863220     0.591559      23.38
 C       5.348456    -4.420789     2.656315      18.52
 O       5.516916    -5.730429     3.083148     277.68
 C       4.773314    -6.891110     2.452295     114.96
 H       4.802031    -6.725901     1.388000      28.08
 H       3.713005    -6.821423     2.773455      27.48
 H       5.300017    -7.818539     2.825717      25.28
 C       5.108631    -3.399013     3.637342       5.19
 O       5.017474    -3.662387     4.994818     113.06
 H       5.117650    -4.570489     5.323567      22.00
 C       4.928422    -2.040098     3.195627      49.98
 H       4.803017    -1.322382     4.075209      24.86
 C       5.289220    -2.732033     0.877413      33.49
 C       5.253730    -2.427968    -0.571784     112.69
 H       5.637936    -3.222220    -1.120634      26.66
 O       6.083646    -1.387390    -1.034583     271.80
 H       5.728522    -0.462807    -0.751671      25.35
 C       3.794537    -2.341163    -1.142907      85.05
 H       3.255867    -3.230661    -0.747278      26.89
 C       3.655654    -2.215850    -2.690131     109.65
 O       3.806560    -3.553577    -3.370177     266.22
 H       4.648459    -3.531682    -3.864943      27.12
 H       4.414578    -1.527207    -3.024523      26.85
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 H       2.740916    -1.760414    -2.953731      28.66
 C      -0.496825    -1.908616     0.044414      49.34
 H      -1.204456    -2.819725     0.178926      20.82
 C      -0.015406     0.501107     0.326996      50.27
 H      -0.494972     1.412359     0.534723      18.06
 C       1.392210     0.308682    -0.016918      11.25
 O       2.340085     1.322102     0.024211     221.20
 C       1.868853     2.501555     0.793503     121.80
 H       2.706913     3.088609     0.851518      27.11
 H       1.167923     3.076978     0.220590      27.05
 H       1.668518     2.172554     1.744047      29.36
 C       1.800980    -1.028989    -0.388276      24.48
 O       3.163190    -1.197327    -0.498919     176.95
 C       0.878566    -2.089828    -0.266280      54.38
 H       1.193376    -3.098563    -0.343676      24.24
 C      -0.926688    -0.601683     0.339714      44.41
 C      -2.421672    -0.400950     0.654783      82.18
 H      -2.751129    -1.295103     1.312086      24.01
 O      -2.632036     0.901205     1.350681     304.47
 H      -2.371002     0.606878     2.250558      29.04
 C      -3.285667    -0.267143    -0.600200      93.06
 H      -2.944056     0.650269    -1.172818      26.69
 O      -2.992399    -1.443422    -1.406715     205.53
 H      -2.895508    -1.223737    -2.389485      24.77
 C      -4.815519    -0.202617    -0.382561     102.60
 O      -5.243682     0.996916     0.319691     239.60
 H      -4.520710     1.344826     0.868477      29.62
 H      -5.243669    -1.192654     0.063556      27.88
 H      -5.320657    -0.144630    -1.419025      26.71
55
name = lig-etoh-Waterframe_128
 C       5.032189    -1.645266     1.843212      52.86
 H       5.024295    -0.613175     1.531142      21.96
 C       5.401418    -4.044246     1.253233      55.60
 H       5.455102    -4.782555     0.500132      24.01
 C       5.353817    -4.396695     2.660774      20.89
 O       5.491867    -5.744297     3.059097     332.37
 C       4.806860    -6.825644     2.409054     137.17
 H       4.882868    -6.876290     1.335092      29.52
 H       3.751394    -6.887835     2.687371      28.40
 H       5.256598    -7.791605     2.785954      25.69
 C       5.138396    -3.388560     3.637294       6.83
 O       5.082729    -3.611543     4.992666     132.28
 H       5.029017    -4.685453     5.304264      20.98
 C       4.956152    -2.045022     3.170073      56.90
 H       4.819541    -1.326881     3.990845      25.37
 C       5.237864    -2.698275     0.847774      20.82
 C       5.279303    -2.455042    -0.657769      91.28
 H       5.653573    -3.311902    -1.178348      26.07
 O       6.130997    -1.346640    -1.084609     263.72
 H       5.852393    -0.413513    -0.814553      23.99
 C       3.753496    -2.424056    -1.141035      68.72
 H       3.258910    -3.342183    -0.708653      25.17
 C       3.660265    -2.221987    -2.672464     107.54
 O       3.811134    -3.485189    -3.362810     276.76
 H       4.718062    -3.498676    -3.731465      26.79
 H       4.419990    -1.516484    -2.973519      25.60
 H       2.619312    -1.861435    -2.945249      26.98
 C      -0.462717    -1.913016     0.069254      41.23
 H      -1.132234    -2.798134     0.133666      22.29
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 C      -0.014952     0.428032     0.289479      70.51
 H      -0.299113     1.451995     0.661240      19.25
 C       1.337732     0.284563    -0.034086      11.49
 O       2.373780     1.343693    -0.002097     197.83
 C       1.911450     2.520378     0.810535     115.89
 H       2.731687     3.101911     0.858731      26.52
 H       1.084219     3.008225     0.334913      26.93
 H       1.502061     2.231235     1.814744      27.26
 C       1.744197    -0.999606    -0.410389      14.13
 O       3.135004    -1.166362    -0.470168     115.58
 C       0.853187    -2.121425    -0.278891      54.75
 H       1.322934    -3.036100    -0.491742      23.20
 C      -0.954376    -0.636140     0.344602      45.92
 C      -2.400059    -0.323542     0.671966      85.43
 H      -2.853365    -1.155763     1.272319      23.61
 O      -2.664978     0.869416     1.389601     314.29
 H      -2.349584     0.885558     2.332078      29.44
 C      -3.264771    -0.225700    -0.690152      76.79
 H      -2.892618     0.858219    -1.200031      23.98
 O      -2.959214    -1.430580    -1.423181     221.59
 H      -2.688714    -1.223365    -2.368731      25.37
 C      -4.785753    -0.248425    -0.436868      97.98
 O      -5.281065     0.950582     0.302663     233.98
 H      -4.611746     1.214549     0.959507      29.85
 H      -5.085758    -1.198298     0.111892      27.36
 H      -5.284234    -0.195443    -1.466576      25.89
55
name = lig-etoh-Waterframe_129
 C       5.030497    -1.673495     1.830641      49.69
 H       5.177587    -0.619718     1.680027      23.68
 C       5.368845    -3.988226     1.267418      67.11
 H       5.389835    -4.765558     0.531215      25.10
 C       5.329912    -4.389466     2.590831      15.32
 O       5.501236    -5.747105     3.069367     325.57
 C       4.809914    -6.781687     2.342589     127.42
 H       5.022702    -6.813205     1.262156      30.28
 H       3.755263    -6.793247     2.601249      29.23
 H       5.353387    -7.627418     2.801093      26.57
 C       5.159650    -3.394800     3.614841      15.64
 O       5.145624    -3.538437     4.984123     180.90
 H       5.058227    -4.609075     5.277741      17.16
 C       5.005206    -2.047835     3.204889      48.90
 H       4.833701    -1.224481     3.831611      21.49
 C       5.221345    -2.650471     0.854438      24.61
 C       5.251679    -2.445823    -0.738995      73.84
 H       5.809238    -3.374564    -1.099723      23.15
 O       6.174510    -1.325378    -1.142978     211.16
 H       5.736581    -0.546468    -0.746527      25.35
 C       3.729950    -2.388915    -1.119987      80.39
 H       3.228934    -3.347830    -0.857512      25.94
 C       3.619261    -2.215990    -2.633583     100.16
 O       3.805878    -3.455416    -3.339929     260.73
 H       4.642693    -3.246240    -3.905599      23.34
 H       4.332673    -1.440136    -2.970590      24.97
 H       2.522259    -1.848096    -2.887798      25.64
 C      -0.477159    -1.959348     0.095965      33.60
 H      -1.124294    -2.786823     0.099245      19.83
 C      -0.025637     0.432561     0.269238      67.89
 H      -0.386135     1.476035     0.689805      19.20
 C       1.316685     0.296778    -0.081893      12.69
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 O       2.318251     1.332671     0.004692     203.49
 C       1.958986     2.517972     0.784771     102.52
 H       2.785836     3.263620     0.946256      24.94
 H       1.119825     3.059772     0.295270      25.83
 H       1.553068     2.230499     1.886429      25.48
 C       1.759002    -1.033272    -0.378326      21.21
 O       3.144512    -1.171235    -0.492122     137.11
 C       0.899378    -2.118080    -0.333180      67.12
 H       1.161428    -3.147853    -0.569422      24.18
 C      -0.943711    -0.614986     0.358848      61.97
 C      -2.430884    -0.299725     0.659408      85.15
 H      -2.846448    -1.175668     1.106130      26.80
 O      -2.700560     0.898955     1.437017     318.31
 H      -2.157630     0.688439     2.306091      27.08
 C      -3.221199    -0.203861    -0.706026      87.99
 H      -2.982769     0.723730    -1.436502      25.61
 O      -2.919229    -1.417085    -1.470361     212.93
 H      -2.566168    -1.103551    -2.344162      25.72
 C      -4.758908    -0.231794    -0.471896     110.97
 O      -5.325026     0.870139     0.263946     250.92
 H      -4.629108     1.063977     0.926059      31.09
 H      -4.885172    -1.135682     0.086644      29.45
 H      -5.315314    -0.369315    -1.404666      27.29
55
name = lig-etoh-Waterframe_130
 C       5.081104    -1.682987     1.842248      57.60
 H       4.957878    -0.631989     1.569239      21.39
 C       5.315254    -3.975671     1.253804      37.63
 H       5.460632    -4.766068     0.487644      22.84
 C       5.300902    -4.397173     2.618796      37.33
 O       5.523280    -5.679017     3.060988     467.14
 C       4.842237    -6.779967     2.294105     131.99
 H       5.036734    -6.586915     1.206365      30.81
 H       3.747450    -6.699774     2.383953      29.94
 H       5.140225    -7.754027     2.656547      26.15
 C       5.169433    -3.362375     3.605264      22.11
 O       5.207753    -3.494219     4.971180     219.63
 H       5.174713    -4.436016     5.319890      23.15
 C       5.052846    -2.024602     3.192780      54.43
 H       4.972644    -1.355992     4.003749      24.14
 C       5.243875    -2.628160     0.794325      48.69
 C       5.253073    -2.407212    -0.671635      92.41
 H       5.628988    -3.354379    -1.299353      22.32
 O       6.145226    -1.350124    -1.181634     236.23
 H       5.893361    -0.465170    -0.867545      25.88
 C       3.751686    -2.301799    -1.154061      96.51
 H       3.235839    -3.156716    -0.705487      23.36
 C       3.511818    -2.157443    -2.623234      99.13
 O       3.805545    -3.442498    -3.321331     258.70
 H       4.516036    -3.309835    -4.047019      25.72
 H       4.202632    -1.357369    -3.000087      23.93
 H       2.450214    -1.777560    -2.820226      24.68
 C      -0.471878    -1.939254     0.091760      24.13
 H      -1.107251    -2.738480     0.119089      20.28
 C      -0.043017     0.507422     0.272193      60.79
 H      -0.545442     1.546845     0.498863      17.28
 C       1.331754     0.308217    -0.106206      12.52
 O       2.247145     1.299922     0.012864     190.38
 C       1.948793     2.523557     0.761794      86.40
 H       3.040485     3.086293     0.748112      22.88
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 H       1.226679     3.191755     0.204598      24.18
 H       1.748469     2.162351     1.865131      23.35
 C       1.837695    -1.057987    -0.334983      16.35
 O       3.185372    -1.188672    -0.534403     182.56
 C       0.847106    -2.132838    -0.360361      62.67
 H       1.209074    -3.172156    -0.614116      21.41
 C      -0.931151    -0.632529     0.373506      52.70
 C      -2.454392    -0.316907     0.586308      81.95
 H      -2.862176    -1.167201     1.101906      26.02
 O      -2.703584     0.913299     1.482309     271.98
 H      -2.293098     0.605615     2.432783      25.63
 C      -3.206357    -0.182661    -0.745739     104.88
 H      -2.858007     0.655007    -1.259785      28.31
 O      -2.879674    -1.391912    -1.513897     224.25
 H      -2.624679    -1.181588    -2.458613      24.49
 C      -4.732569    -0.269720    -0.486083     116.58
 O      -5.356760     0.800266     0.221993     251.91
 H      -4.802025     1.166104     0.945326      30.43
 H      -4.882695    -1.175726     0.053711      29.47
 H      -5.268405    -0.360852    -1.399610      27.79
55
name = lig-etoh-Waterframe_131
 C       5.131457    -1.621520     1.809997      49.19
 H       4.785650    -0.625540     1.495379      21.48
 C       5.285163    -4.004865     1.234157      53.13
 H       5.494325    -4.789876     0.441479      22.60
 C       5.268336    -4.338309     2.635012      27.64
 O       5.536967    -5.672367     3.045159     387.34
 C       4.865216    -6.720856     2.234360     126.24
 H       5.182809    -6.690032     1.140196      28.00
 H       3.765140    -6.597251     2.330217      27.35
 H       5.174209    -7.696051     2.551540      25.85
 C       5.186797    -3.337961     3.605489      17.00
 O       5.273274    -3.476501     4.978910     183.46
 H       5.193693    -4.398884     5.153904      28.48
 C       5.106545    -1.999137     3.171023      60.42
 H       5.086497    -1.277854     4.000826      25.18
 C       5.282934    -2.674797     0.835505      37.31
 C       5.239459    -2.348249    -0.673313      99.72
 H       5.563175    -3.336160    -1.174449      22.27
 O       6.105254    -1.384998    -1.209935     262.53
 H       5.906663    -0.491220    -0.910720      27.81
 C       3.778201    -2.268990    -1.159458      89.93
 H       3.371804    -3.208411    -0.784810      25.56
 C       3.443317    -2.107915    -2.690957     102.91
 O       3.757849    -3.418429    -3.303183     245.72
 H       4.688607    -3.201869    -3.706428      24.38
 H       4.081320    -1.306881    -3.129420      25.44
 H       2.403644    -1.987856    -2.820340      27.13
 C      -0.468134    -1.886614     0.070584      42.80
 H      -1.138355    -2.711378     0.131633      22.34
 C      -0.061075     0.501357     0.247649      67.80
 H      -0.353135     1.562150     0.352938      21.43
 C       1.285109     0.261630    -0.052423      15.76
 O       2.230802     1.284986    -0.014844     209.50
 C       1.985800     2.512827     0.721434     105.60
 H       3.075321     3.001067     0.654500      22.91
 H       1.183038     3.200591     0.356665      25.14
 H       1.645003     2.468194     1.752577      26.81
 C       1.798035    -1.057516    -0.305834      16.54
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 O       3.212607    -1.106816    -0.540008     154.59
 C       0.868288    -2.105769    -0.355454      62.75
 H       1.229811    -3.159777    -0.608881      23.21
 C      -0.934201    -0.574512     0.373435      50.95
 C      -2.415666    -0.339350     0.594101      75.65
 H      -2.928715    -1.183160     1.140507      26.60
 O      -2.691079     0.875388     1.471255     258.69
 H      -2.438247     0.636284     2.479413      26.29
 C      -3.190891    -0.172868    -0.785261     102.01
 H      -2.927189     0.736884    -1.159380      30.07
 O      -2.849765    -1.366023    -1.546121     213.89
 H      -2.844404    -1.114537    -2.515880      24.47
 C      -4.715296    -0.328932    -0.507788     106.60
 O      -5.403048     0.771222     0.185946     217.56
 H      -4.801523     1.128588     0.886771      29.73
 H      -4.912555    -1.322499     0.013185      28.29
 H      -5.171324    -0.317548    -1.489629      27.52
55
name = lig-etoh-Waterframe_132
 C       5.154938    -1.612008     1.779846      51.57
 H       5.024691    -0.546294     1.500379      22.08
 C       5.297899    -4.028536     1.260337      47.15
 H       5.368691    -4.877659     0.516198      20.70
 C       5.266046    -4.334960     2.595385      40.59
 O       5.533857    -5.682307     3.017764     399.81
 C       4.904523    -6.654105     2.174179     147.20
 H       5.235389    -6.658498     1.109991      30.19
 H       3.787383    -6.586934     2.231130      25.72
 H       5.253570    -7.513064     2.720207      25.92
 C       5.224129    -3.273381     3.614573      23.45
 O       5.334276    -3.496081     4.979389     194.39
 H       5.207533    -4.488150     5.268661      27.36
 C       5.167456    -1.931930     3.143119      57.22
 H       5.065930    -1.035087     3.834461      22.52
 C       5.288329    -2.647346     0.872115      38.42
 C       5.218760    -2.393174    -0.710244      93.65
 H       5.653215    -3.263556    -1.077826      23.73
 O       6.103274    -1.383269    -1.236301     244.65
 H       5.782458    -0.548857    -0.870112      26.65
 C       3.759372    -2.224827    -1.179733      78.18
 H       3.227335    -3.148405    -0.901620      25.16
 C       3.418481    -2.119645    -2.716305     110.93
 O       3.729685    -3.372664    -3.312749     246.08
 H       4.721308    -3.431128    -3.558004      24.70
 H       3.817861    -1.268738    -3.282463      27.02
 H       2.388460    -2.003652    -2.795756      28.28
 C      -0.460931    -1.827209     0.048805      49.08
 H      -1.168788    -2.716261     0.087368      23.32
 C      -0.053639     0.506561     0.213238      74.04
 H      -0.315753     1.482171     0.437574      26.17
 C       1.275853     0.236396     0.028226      16.84
 O       2.233788     1.273772    -0.050735     209.03
 C       2.011024     2.533380     0.688590     117.89
 H       2.885501     3.203610     0.710502      25.30
 H       1.324433     3.096881     0.062611      25.82
 H       1.801073     2.312336     1.653136      28.65
 C       1.784776    -1.010739    -0.305320      25.69
 O       3.166358    -0.991674    -0.508568     137.54
 C       0.900110    -2.087984    -0.316330      63.32
 H       1.165223    -3.150742    -0.558241      23.95
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 C      -0.963354    -0.554160     0.352386      46.54
 C      -2.397490    -0.331342     0.654101      80.76
 H      -2.771469    -1.352876     1.089907      25.38
 O      -2.689741     0.819197     1.408302     302.60
 H      -2.263892     0.563685     2.333895      25.32
 C      -3.189334    -0.197907    -0.723101      88.93
 H      -3.048969     0.803575    -1.344303      26.36
 O      -2.828756    -1.320140    -1.581935     186.64
 H      -2.836367    -1.057514    -2.539944      24.15
 C      -4.728837    -0.339918    -0.557100      97.45
 O      -5.430564     0.732925     0.152137     224.95
 H      -4.743709     1.055266     0.793184      29.43
 H      -4.920678    -1.379233    -0.025559      27.05
 H      -5.197926    -0.463074    -1.579709      26.59
55
name = lig-etoh-Waterframe_133
 C       5.189683    -1.613186     1.771754      53.86
 H       5.376654    -0.576533     1.442130      22.62
 C       5.314355    -3.971719     1.262712      45.57
 H       5.259413    -4.759029     0.492481      21.43
 C       5.317427    -4.325030     2.645915      26.48
 O       5.515550    -5.626566     2.992517     334.76
 C       4.943092    -6.654979     2.151512     135.72
 H       5.337383    -6.630217     1.149429      27.17
 H       3.843724    -6.556926     2.069277      26.60
 H       5.128154    -7.668271     2.562944      25.10
 C       5.278431    -3.242201     3.605588       6.44
 O       5.389329    -3.515222     4.966247     197.17
 H       5.200840    -4.573627     5.237391      23.30
 C       5.214984    -1.867404     3.150851      48.17
 H       5.119589    -1.037492     3.940230      22.14
 C       5.255557    -2.641829     0.774802      35.95
 C       5.220282    -2.462615    -0.710703      86.13
 H       5.500946    -3.337083    -1.221924      24.08
 O       6.099951    -1.376072    -1.234325     219.50
 H       5.847716    -0.458836    -0.948214      23.66
 C       3.691305    -2.148916    -1.206326      76.53
 H       3.060299    -2.926974    -0.737204      24.70
 C       3.396056    -2.103798    -2.701218     108.27
 O       3.708118    -3.379342    -3.346050     245.38
 H       4.665870    -3.329464    -3.739063      24.10
 H       3.905253    -1.279025    -3.214521      26.67
 H       2.292077    -2.028551    -2.750894      26.72
 C      -0.445005    -1.822756     0.028491      51.89
 H      -1.167621    -2.748978     0.028741      23.44
 C      -0.078326     0.555742     0.236407      70.24
 H      -0.437239     1.450364     0.557050      26.21
 C       1.330954     0.329071     0.063710       1.73
 O       2.285215     1.282579    -0.076813     203.77
 C       2.014391     2.549337     0.615810     123.05
 H       2.895530     3.038704     0.611559      27.37
 H       1.179876     3.101344     0.153957      26.60
 H       1.680768     2.298381     1.613928      28.25
 C       1.811440    -0.985342    -0.298498      16.08
 O       3.142070    -0.947099    -0.506551     143.07
 C       0.879006    -2.073099    -0.258882      71.01
 H       1.214020    -3.082093    -0.474861      25.53
 C      -0.941531    -0.558610     0.304560      39.41
 C      -2.426045    -0.376689     0.603265      91.88
 H      -2.775832    -1.260849     1.206649      26.07
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 O      -2.689815     0.774441     1.387770     314.84
 H      -2.230582     0.792712     2.277429      28.56
 C      -3.243476    -0.232129    -0.686990      83.10
 H      -2.825033     0.860114    -1.174687      25.36
 O      -2.811091    -1.286967    -1.596234     192.57
 H      -2.654885    -0.971216    -2.519467      25.48
 C      -4.762309    -0.371347    -0.588534     109.16
 O      -5.430590     0.683078     0.114599     236.09
 H      -4.836938     1.138224     0.765090      29.41
 H      -4.965308    -1.311204     0.001359      27.34
 H      -5.232885    -0.443738    -1.630634      26.51
55
name = lig-etoh-Waterframe_134
 C       5.272085    -1.593792     1.737912      46.33
 H       5.402671    -0.541748     1.452470      21.69
 C       5.302775    -3.913989     1.253024      57.66
 H       5.295902    -4.712726     0.553683      22.89
 C       5.382791    -4.223223     2.616480      21.69
 O       5.503243    -5.608492     3.024002     273.90
 C       4.951856    -6.674317     2.103680     120.07
 H       5.477150    -6.615750     1.181729      29.33
 H       3.902545    -6.453751     1.930918      28.46
 H       5.159200    -7.684523     2.578666      26.24
 C       5.339445    -3.244168     3.613750       6.74
 O       5.437076    -3.517724     4.947948     208.65
 H       5.169164    -4.554380     5.074859      25.08
 C       5.256399    -1.897067     3.166221      45.99
 H       5.328548    -1.105020     3.958928      23.91
 C       5.228457    -2.650111     0.751646      35.74
 C       5.156968    -2.401735    -0.767363      88.55
 H       5.398454    -3.358082    -1.343719      22.99
 O       6.106220    -1.420715    -1.222566     221.36
 H       5.718575    -0.538703    -0.862973      24.68
 C       3.647119    -2.123833    -1.144443      92.17
 H       3.175698    -3.065772    -0.748781      25.11
 C       3.369125    -2.080151    -2.690977      95.47
 O       3.703867    -3.396571    -3.383337     251.12
 H       4.482001    -3.111330    -3.986327      24.55
 H       3.996504    -1.271415    -3.095880      25.43
 H       2.240955    -1.870372    -2.952940      25.64
 C      -0.458831    -1.866966     0.017659      47.41
 H      -1.190559    -2.770340     0.014528      19.68
 C      -0.060022     0.598713     0.308909      64.74
 H      -0.496836     1.534121     0.602390      20.29
 C       1.315367     0.385967     0.014819      11.06
 O       2.354401     1.344293    -0.086825     230.60
 C       1.993753     2.555784     0.548674     119.23
 H       2.871987     3.119116     0.538364      25.94
 H       1.199585     3.200147     0.087533      25.89
 H       1.680583     2.461965     1.708648      25.94
 C       1.756552    -0.918389    -0.238900      15.41
 O       3.186261    -0.953019    -0.555784     142.05
 C       0.933063    -2.037774    -0.219795      63.77
 H       1.266294    -3.026155    -0.374578      25.02
 C      -0.927815    -0.550694     0.252166      52.26
 C      -2.443359    -0.459904     0.583681      93.10
 H      -2.805209    -1.294311     1.123758      29.08
 O      -2.712362     0.799136     1.382599     290.15
 H      -2.273348     0.580242     2.243585      29.80
 C      -3.260825    -0.256666    -0.721796      95.11
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 H      -3.042207     0.843136    -0.963522      27.57
 O      -2.794584    -1.277726    -1.597336     223.43
 H      -2.621817    -0.892482    -2.491078      25.51
 C      -4.790865    -0.413884    -0.577154     115.89
 O      -5.454758     0.674492     0.080724     237.13
 H      -4.797145     1.073992     0.714366      30.35
 H      -5.012397    -1.360819    -0.180393      30.16
 H      -5.200631    -0.422984    -1.618544      27.57
55
name = lig-etoh-Waterframe_135
 C       5.354842    -1.587117     1.756334      54.29
 H       5.240674    -0.534285     1.524648      18.50
 C       5.283196    -3.943448     1.219954      37.65
 H       5.334649    -4.765506     0.573330      20.92
 C       5.436573    -4.231867     2.567982      10.07
 O       5.487092    -5.599334     3.056256     213.94
 C       4.981877    -6.625684     2.070938     115.87
 H       5.556309    -6.682633     1.146627      29.06
 H       3.930463    -6.518528     1.813295      29.38
 H       5.099912    -7.532631     2.734220      26.07
 C       5.400632    -3.226095     3.603727      14.31
 O       5.473253    -3.524897     4.938659     254.00
 H       5.290400    -4.466566     5.252851      25.71
 C       5.337495    -1.926641     3.112186      74.23
 H       5.451432    -1.111717     3.793848      28.27
 C       5.225527    -2.554421     0.772213      48.66
 C       5.076315    -2.339977    -0.808511     102.52
 H       5.434166    -3.369917    -1.290227      22.29
 O       6.088417    -1.457060    -1.203633     253.40
 H       5.855559    -0.475106    -0.891751      24.12
 C       3.636321    -2.203709    -1.147009      91.86
 H       3.159421    -3.107277    -0.721301      22.06
 C       3.369740    -2.082710    -2.704308      98.19
 O       3.700755    -3.353439    -3.408217     263.27
 H       4.496170    -3.269121    -4.031642      25.85
 H       4.034836    -1.299992    -3.097352      24.21
 H       2.294259    -1.702784    -2.962719      24.52
 C      -0.430800    -1.863230     0.012003      27.48
 H      -1.090895    -2.738141     0.004181      20.40
 C      -0.048640     0.587529     0.366258      76.22
 H      -0.423239     1.637429     0.635384      17.73
 C       1.291468     0.448217    -0.056355      15.22
 O       2.361674     1.391287    -0.085622     185.67
 C       1.994774     2.672340     0.521811      96.50
 H       2.841019     3.434983     0.515210      23.97
 H       1.217376     3.050388    -0.179673      23.91
 H       1.741093     2.392939     1.675091      23.28
 C       1.802906    -0.869601    -0.216824      14.02
 O       3.158177    -0.945500    -0.574890     146.90
 C       0.950729    -2.019473    -0.180688      54.51
 H       1.437912    -2.931278    -0.312329      21.74
 C      -0.946207    -0.563405     0.251573      48.66
 C      -2.445139    -0.441579     0.588101      92.54
 H      -2.729230    -1.372940     1.035133      27.70
 O      -2.731964     0.778325     1.378537     310.40
 H      -2.483903     0.564793     2.283015      30.46
 C      -3.281110    -0.265406    -0.716940     105.79
 H      -3.192333     0.611129    -1.175711      30.68
 O      -2.775128    -1.272034    -1.627595     216.54
 H      -2.727088    -0.987430    -2.585705      24.06
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 C      -4.821216    -0.464066    -0.602246     109.89
 O      -5.479359     0.685787     0.066202     225.53
 H      -4.817615     0.991846     0.752338      30.11
 H      -5.099106    -1.393886    -0.154000      29.74
 H      -5.176237    -0.460013    -1.616557      28.41
55
name = lig-etoh-Waterframe_136
 C       5.378910    -1.552775     1.751403      55.06
 H       5.240839    -0.505770     1.544937      20.87
 C       5.283200    -3.925419     1.169733      47.63
 H       5.228564    -4.653794     0.380212      20.00
 C       5.455431    -4.312836     2.579301      24.04
 O       5.458881    -5.576996     3.029191     385.59
 C       5.023147    -6.574573     2.109444     125.49
 H       5.707505    -6.726626     1.239085      28.43
 H       4.002697    -6.363494     1.756794      30.41
 H       5.017998    -7.555995     2.616987      27.09
 C       5.466861    -3.279250     3.547364      16.23
 O       5.513119    -3.508403     4.952747     293.95
 H       5.327416    -4.436768     5.056455      31.26
 C       5.468181    -1.901773     3.117292      48.75
 H       5.424767    -1.125837     3.818520      24.57
 C       5.228926    -2.575901     0.755384      42.26
 C       5.089866    -2.371771    -0.705469      98.27
 H       5.396039    -3.359297    -1.210008      23.11
 O       6.065800    -1.432928    -1.220712     221.14
 H       5.851038    -0.435293    -0.931963      21.99
 C       3.600499    -2.240175    -1.234763      82.88
 H       3.064038    -3.029180    -0.736992      23.45
 C       3.423004    -2.085599    -2.733908     113.47
 O       3.677843    -3.306996    -3.429521     282.97
 H       4.595594    -3.181610    -3.779205      26.14
 H       4.091151    -1.281007    -3.061987      24.78
 H       2.354960    -1.901651    -2.858880      26.47
 C      -0.392071    -1.820832     0.023611      40.60
 H      -0.974970    -2.665032    -0.021587      22.77
 C      -0.059247     0.551018     0.356566      75.06
 H      -0.502378     1.575861     0.767900      18.84
 C       1.323296     0.477002    -0.075320      14.99
 O       2.340043     1.445857    -0.079433     210.82
 C       1.984797     2.780419     0.475453     102.45
 H       2.939137     3.465290     0.397470      22.68
 H       1.057295     3.200754     0.048146      25.08
 H       1.547661     2.740264     1.509126      26.04
 C       1.833087    -0.868088    -0.259356      22.64
 O       3.115977    -0.950913    -0.577698     143.50
 C       0.997474    -1.963070    -0.148614      69.05
 H       1.352044    -2.959480    -0.225832      23.42
 C      -0.934498    -0.544971     0.306749      46.00
 C      -2.435320    -0.363821     0.566892      93.20
 H      -2.797447    -1.304731     1.131728      25.19
 O      -2.768010     0.723197     1.386567     325.67
 H      -2.510236     0.641407     2.285297      31.70
 C      -3.312134    -0.287925    -0.749603      96.20
 H      -3.098933     0.701559    -1.202379      28.08
 O      -2.757404    -1.296626    -1.662812     200.29
 H      -2.843930    -0.939099    -2.598217      24.46
 C      -4.857405    -0.480470    -0.619483     103.64
 O      -5.487995     0.680804     0.049606     212.11
 H      -4.904295     0.974182     0.806104      30.49
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 H      -5.137998    -1.399629     0.007126      27.56
 H      -5.285804    -0.542146    -1.601880      28.00
55
name = lig-etoh-Waterframe_137
 C       5.363786    -1.541530     1.745810      55.18
 H       5.395506    -0.515178     1.429547      22.02
 C       5.302583    -3.933910     1.192959      65.05
 H       5.115222    -4.677857     0.390597      20.41
 C       5.435175    -4.286910     2.508186      17.72
 O       5.452147    -5.597169     3.029498     288.67
 C       5.033016    -6.590251     2.118603     121.56
 H       5.817885    -6.590368     1.299142      28.56
 H       4.113518    -6.213173     1.618973      29.64
 H       4.939921    -7.511631     2.662829      27.05
 C       5.551952    -3.271463     3.532024       6.90
 O       5.551710    -3.499935     4.906369     269.19
 H       5.311429    -4.417099     5.170281      23.44
 C       5.587838    -1.906895     3.128443      46.29
 H       5.502892    -1.234258     3.957506      23.13
 C       5.249601    -2.607121     0.817829      40.91
 C       5.119512    -2.425075    -0.680985      87.31
 H       5.484737    -3.307400    -1.113877      24.02
 O       6.026633    -1.396102    -1.247381     197.84
 H       5.593904    -0.517223    -0.919150      23.09
 C       3.629006    -2.191599    -1.215496      81.56
 H       3.047478    -3.081486    -0.995409      25.09
 C       3.436731    -2.059236    -2.741700     111.21
 O       3.690758    -3.293597    -3.459703     272.92
 H       4.597002    -3.288659    -3.841899      25.62
 H       3.974511    -1.193768    -3.158471      25.54
 H       2.444587    -1.820948    -2.944197      28.46
 C      -0.375549    -1.775669     0.063774      53.59
 H      -0.968901    -2.609066     0.014276      24.37
 C      -0.020463     0.584006     0.318715      67.22
 H      -0.508994     1.541110     0.753019      20.21
 C       1.320183     0.457421    -0.031198      16.43
 O       2.282359     1.533099    -0.061322     214.16
 C       1.913069     2.863208     0.441539     114.65
 H       2.914860     3.456143     0.258416      23.69
 H       1.228392     3.430166    -0.190418      26.64
 H       1.845139     2.858921     1.445429      28.93
 C       1.800669    -0.817179    -0.325260      22.09
 O       3.166688    -0.985453    -0.618264     167.52
 C       0.990015    -1.946311    -0.127976      60.77
 H       1.315989    -2.981996    -0.193650      23.58
 C      -0.915755    -0.526315     0.350409      43.39
 C      -2.448928    -0.384686     0.556280      75.96
 H      -2.801417    -1.380263     1.079722      23.82
 O      -2.831219     0.735441     1.411657     311.95
 H      -2.338702     0.485212     2.173325      28.96
 C      -3.305811    -0.298681    -0.809372      79.30
 H      -3.126233     0.880855    -1.123560      25.30
 O      -2.753961    -1.309461    -1.677334     207.49
 H      -2.752344    -0.988945    -2.639375      23.93
 C      -4.874667    -0.457835    -0.586917      97.65
 O      -5.498330     0.674850     0.022994     229.53
 H      -4.871445     0.894233     0.777696      29.97
 H      -5.028160    -1.481341     0.009241      26.61
 H      -5.416196    -0.635920    -1.532967      27.16
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name = lig-etoh-Waterframe_138
 C       5.385601    -1.572665     1.794826      66.35
 H       5.484379    -0.558039     1.436054      21.84
 C       5.300233    -3.982243     1.207259      50.14
 H       5.153633    -4.854763     0.491591      21.85
 C       5.435403    -4.270271     2.566554      12.10
 O       5.457134    -5.586307     3.061844     199.40
 C       5.030383    -6.609313     2.060726     118.76
 H       5.815802    -6.893822     1.307853      26.06
 H       4.059850    -6.423522     1.533912      27.55
 H       4.874518    -7.490350     2.635211      27.70
 C       5.621423    -3.244242     3.513042      22.60
 O       5.598330    -3.501524     4.847723     195.67
 H       5.290363    -4.414801     5.162814      22.28
 C       5.652458    -1.919826     3.118029      51.56
 H       5.807689    -1.139344     3.908011      24.34
 C       5.269139    -2.575292     0.841167      12.07
 C       5.149397    -2.432003    -0.744149     100.90
 H       5.484797    -3.317312    -1.168453      25.59
 O       5.950509    -1.386157    -1.247140     256.34
 H       5.691312    -0.435204    -1.066898      24.30
 C       3.706640    -2.187547    -1.203212      86.46
 H       3.109384    -3.056154    -0.872958      26.77
 C       3.445437    -1.993740    -2.780466      99.02
 O       3.721067    -3.308317    -3.478519     261.14
 H       4.539332    -3.222767    -4.010577      26.28
 H       4.105416    -1.225087    -3.231929      25.05
 H       2.396912    -1.764891    -2.904510      27.79
 C      -0.402515    -1.774891     0.133459      53.51
 H      -1.065503    -2.646766     0.182922      24.45
 C      -0.049577     0.650026     0.319680      65.58
 H      -0.263500     1.694508     0.524177      21.85
 C       1.339750     0.518456     0.018301       8.50
 O       2.194400     1.580621    -0.053435     216.19
 C       1.912233     2.951160     0.382569     107.08
 H       2.856854     3.460698     0.164341      24.74
 H       1.072090     3.377109    -0.204571      27.12
 H       1.727524     2.984574     1.439032      28.74
 C       1.833089    -0.832543    -0.378020      11.74
 O       3.205792    -0.977332    -0.638891     154.98
 C       0.966113    -1.939908    -0.144885      62.43
 H       1.481100    -2.908992    -0.278087      25.46
 C      -0.923632    -0.470887     0.357308      34.00
 C      -2.482703    -0.440774     0.527279      73.86
 H      -2.764663    -1.417329     0.963213      26.77
 O      -2.877361     0.731475     1.437645     268.48
 H      -2.434641     0.652609     2.298627      29.49
 C      -3.283962    -0.262219    -0.807236      89.95
 H      -3.146452     0.742219    -1.452083      26.55
 O      -2.752327    -1.297614    -1.680802     181.14
 H      -2.661570    -1.029070    -2.648581      24.73
 C      -4.845900    -0.483636    -0.575540      99.36
 O      -5.494035     0.679221     0.019652     207.36
 H      -4.927320     0.944248     0.811155      30.34
 H      -4.994598    -1.351572     0.127059      27.94
 H      -5.352001    -0.640652    -1.574765      27.60
55
name = lig-etoh-Waterframe_139
 C       5.455129    -1.590134     1.785983      40.70
 H       5.448173    -0.509680     1.569374      24.26
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 C       5.287284    -3.956398     1.240602      61.33
 H       5.263474    -4.758823     0.438092      22.61
 C       5.454385    -4.300008     2.611247      28.62
 O       5.443064    -5.600376     3.053273     293.31
 C       5.021027    -6.667790     2.044521     112.81
 H       5.820184    -6.917374     1.340802      28.05
 H       4.089247    -6.330610     1.537932      27.77
 H       4.864042    -7.505449     2.713009      27.86
 C       5.647256    -3.248665     3.527364       5.22
 O       5.662374    -3.507948     4.856476      64.76
 H       5.352447    -4.482741     4.916868      22.62
 C       5.702755    -1.886975     3.124890      38.29
 H       6.068476    -1.046054     3.815962      20.13
 C       5.270105    -2.658187     0.757223      17.80
 C       5.148464    -2.376075    -0.745732      84.47
 H       5.496788    -3.323085    -1.274010      23.48
 O       5.949404    -1.373109    -1.280952     232.42
 H       5.572744    -0.513483    -0.969215      24.96
 C       3.728233    -2.216881    -1.272132      74.78
 H       3.180595    -3.028430    -0.751116      24.67
 C       3.504716    -2.012045    -2.798989     101.58
 O       3.735948    -3.300340    -3.483625     272.19
 H       4.583696    -3.136435    -3.957009      26.08
 H       4.188355    -1.201407    -3.149367      24.54
 H       2.398817    -1.735388    -2.923661      26.51
 C      -0.414012    -1.750472     0.213945      37.65
 H      -1.084165    -2.696656     0.382962      22.14
 C      -0.056104     0.710559     0.320471      66.48
 H      -0.462302     1.646333     0.467674      20.36
 C       1.321632     0.508610     0.019874       9.67
 O       2.165348     1.607114    -0.059847     227.17
 C       1.895152     3.010313     0.319766     109.02
 H       2.716244     3.610288     0.099966      25.82
 H       0.980388     3.389384    -0.174234      27.61
 H       1.506918     3.144463     1.433976      27.15
 C       1.847815    -0.804527    -0.341931      20.09
 O       3.215440    -0.917228    -0.625324     121.72
 C       0.975728    -1.898115    -0.198678      56.21
 H       1.308479    -2.967174    -0.323809      24.12
 C      -0.966757    -0.440663     0.347750      64.74
 C      -2.468752    -0.379922     0.542089      84.03
 H      -2.816872    -1.294747     0.905545      30.72
 O      -2.929454     0.686586     1.426039     271.58
 H      -2.537650     0.557683     2.334219      29.78
 C      -3.281160    -0.238559    -0.823563     101.27
 H      -3.099100     0.751337    -1.216806      29.99
 O      -2.750512    -1.304805    -1.673750     210.57
 H      -2.704030    -0.870193    -2.576137      25.36
 C      -4.780162    -0.486762    -0.556704     111.74
 O      -5.483701     0.694459     0.018409     202.60
 H      -4.917465     0.925504     0.825308      30.80
 H      -4.964185    -1.323146     0.038013      30.42
 H      -5.274010    -0.708423    -1.551190      28.56
55
name = lig-etoh-Waterframe_140
 C       5.523397    -1.625824     1.688731      53.38
 H       5.441362    -0.563526     1.373485      23.51
 C       5.292564    -3.957821     1.243646      63.38
 H       5.257008    -4.770110     0.503354      21.85
 C       5.465649    -4.294144     2.562343       3.00
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 O       5.426589    -5.660740     3.028208     268.84
 C       5.013577    -6.691189     2.095111     118.69
 H       5.795883    -6.801667     1.373399      29.15
 H       4.141465    -6.319871     1.535636      29.56
 H       4.776226    -7.603811     2.699592      25.72
 C       5.650708    -3.238028     3.563172      -3.14
 O       5.739479    -3.535289     4.903780     131.53
 H       5.502994    -4.489825     5.313781      20.42
 C       5.759992    -1.891467     3.089673      44.12
 H       5.991696    -1.104818     3.886182      22.53
 C       5.283740    -2.623604     0.761224      35.52
 C       5.133284    -2.389125    -0.762416      83.53
 H       5.559506    -3.371249    -1.296253      22.99
 O       5.993222    -1.318697    -1.307624     170.78
 H       5.707416    -0.438575    -0.985919      25.44
 C       3.675038    -2.184213    -1.271982      79.11
 H       3.039353    -3.071630    -1.028559      24.82
 C       3.554678    -2.067754    -2.770826     108.43
 O       3.754316    -3.274633    -3.486935     282.27
 H       4.643999    -3.311324    -3.924098      25.97
 H       4.195407    -1.253785    -3.138764      25.41
 H       2.502053    -1.667799    -3.080821      26.32
 C      -0.360956    -1.675431     0.258909      46.38
 H      -0.993937    -2.660027     0.418138      21.94
 C      -0.102900     0.670174     0.301523      61.56
 H      -0.501676     1.554606     0.604095      21.95
 C       1.263106     0.540229    -0.004292      11.55
 O       2.212180     1.633056    -0.073975     184.72
 C       1.778443     3.031174     0.267965     107.54
 H       2.650912     3.571006     0.058720      25.88
 H       1.057497     3.427041    -0.463609      26.23
 H       1.760232     3.088113     1.474480      24.31
 C       1.836859    -0.758206    -0.266155      15.40
 O       3.210824    -0.866196    -0.622346      96.06
 C       0.915682    -1.858090    -0.214518      59.38
 H       1.238803    -2.918966    -0.415893      23.46
 C      -0.949185    -0.427951     0.359905      57.59
 C      -2.468105    -0.309119     0.549960      87.38
 H      -2.731087    -1.296295     0.979204      27.54
 O      -2.989182     0.657298     1.418131     286.55
 H      -2.542658     0.339063     2.290478      26.70
 C      -3.239618    -0.220634    -0.778710     108.16
 H      -3.128148     0.726636    -1.113569      31.53
 O      -2.765303    -1.276637    -1.666754     221.88
 H      -2.666300    -1.028140    -2.639824      24.72
 C      -4.753895    -0.453232    -0.553832     112.78
 O      -5.453319     0.687267     0.008975     205.63
 H      -4.879110     0.928032     0.809341      30.33
 H      -4.830466    -1.348373     0.023882      30.28
 H      -5.273306    -0.633928    -1.507018      28.91
55
name = lig-etoh-Waterframe_141
 C       5.589301    -1.600368     1.666252      52.28
 H       5.647224    -0.579168     1.227177      22.39
 C       5.305224    -3.984298     1.177731      59.99
 H       5.113838    -4.796408     0.518405      21.58
 C       5.465341    -4.314723     2.577164      -0.30
 O       5.423462    -5.665005     3.030801     239.31
 C       4.994382    -6.677937     2.111514     125.26
 H       5.756962    -6.993541     1.395571      28.33
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 H       4.066278    -6.487742     1.582999      29.75
 H       4.812402    -7.654221     2.677150      25.77
 C       5.646842    -3.289650     3.569766       3.51
 O       5.835384    -3.527729     4.971756     224.34
 H       5.449651    -4.506047     5.199463      19.59
 C       5.787643    -1.959766     3.040360      51.38
 H       5.786253    -1.119621     3.747307      25.64
 C       5.305863    -2.612831     0.745248      22.09
 C       5.134127    -2.381714    -0.782844      85.50
 H       5.523528    -3.336093    -1.309683      23.04
 O       6.019487    -1.284075    -1.300839     202.26
 H       5.705977    -0.396386    -1.060459      25.93
 C       3.624585    -2.123424    -1.216370      87.15
 H       2.957626    -2.938249    -0.873551      24.76
 C       3.581953    -2.009857    -2.797271     100.32
 O       3.765589    -3.316524    -3.470333     263.77
 H       4.642174    -3.124810    -3.999604      23.83
 H       4.367263    -1.358515    -3.140133      23.85
 H       2.515190    -1.716712    -3.004924      26.01
 C      -0.369073    -1.667972     0.265435      45.51
 H      -1.038337    -2.580168     0.332628      21.54
 C      -0.119462     0.704190     0.289655      58.81
 H      -0.417037     1.632726     0.632758      20.89
 C       1.289195     0.611360    -0.037539      11.12
 O       2.222453     1.633525    -0.087816     206.84
 C       1.756617     2.999874     0.201209     111.95
 H       2.671154     3.557700    -0.019748      24.24
 H       0.834692     3.308219    -0.313981      26.97
 H       1.328231     3.152975     1.274534      26.36
 C       1.802467    -0.726390    -0.237397      20.41
 O       3.164477    -0.862907    -0.632325     141.60
 C       0.944515    -1.805609    -0.198068      67.50
 H       1.314395    -2.810655    -0.461775      22.80
 C      -0.956820    -0.413587     0.408500      61.31
 C      -2.452867    -0.368224     0.545447      69.94
 H      -2.706475    -1.429097     0.978137      25.65
 O      -3.033177     0.662262     1.455373     253.88
 H      -2.679681     0.618643     2.433433      27.20
 C      -3.210337    -0.189153    -0.775170     103.19
 H      -3.043608     0.782815    -1.317854      27.48
 O      -2.777456    -1.252296    -1.651834     229.54
 H      -2.697656    -0.892219    -2.588533      25.14
 C      -4.746642    -0.427291    -0.567745     104.03
 O      -5.417226     0.681613     0.014110     206.15
 H      -4.890954     0.995016     0.818798      30.02
 H      -4.896639    -1.353179     0.126469      28.29
 H      -5.177549    -0.593167    -1.538254      28.85
55
name = lig-etoh-Waterframe_142
 C       5.643372    -1.612031     1.676868      45.43
 H       5.876634    -0.543117     1.521997      22.48
 C       5.302745    -3.996319     1.174232      84.93
 H       5.042027    -4.711780     0.453258      24.75
 C       5.452467    -4.352484     2.566692       0.06
 O       5.427077    -5.633548     3.043975     210.88
 C       4.962642    -6.733646     2.103421     107.75
 H       5.756521    -6.934679     1.328594      26.92
 H       4.023862    -6.422977     1.641771      28.37
 H       4.871403    -7.494057     2.917699      24.93
 C       5.677294    -3.332865     3.561787       6.74
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 O       5.909699    -3.510197     4.956691     209.10
 H       5.502494    -4.425478     5.254097      22.11
 C       5.759822    -2.005930     3.021131      37.18
 H       5.867974    -1.225902     3.728097      24.44
 C       5.353886    -2.676848     0.684677     -19.06
 C       5.133767    -2.310362    -0.775380      90.68
 H       5.363477    -3.149570    -1.387210      26.09
 O       5.998716    -1.277566    -1.270976     256.99
 H       5.526250    -0.460954    -1.066580      30.24
 C       3.641437    -2.070154    -1.193767      91.12
 H       3.146874    -2.915482    -0.713312      26.16
 C       3.560393    -1.965074    -2.791558     100.85
 O       3.785418    -3.349050    -3.429006     249.62
 H       4.580973    -3.236070    -4.110132      25.08
 H       4.311286    -1.252768    -3.108343      24.96
 H       2.646295    -1.511557    -3.120507      27.91
 C      -0.414167    -1.701463     0.229910      48.95
 H      -1.012763    -2.570450     0.232127      21.95
 C      -0.049635     0.813851     0.297426     143.46
 H      -0.525058     1.746754     0.512653      19.99
 C       1.288820     0.621591    -0.039140      11.70
 O       2.204757     1.638080    -0.096695     242.96
 C       1.727567     2.955119     0.152142     114.69
 H       2.481226     3.810968    -0.007393      24.32
 H       0.952473     3.126217    -0.645196      27.03
 H       1.390360     3.040689     1.120879      29.68
 C       1.804286    -0.672738    -0.281427      29.47
 O       3.110225    -0.849299    -0.637283     172.40
 C       0.968336    -1.790299    -0.142755      58.01
 H       1.342853    -2.767821    -0.396531      24.25
 C      -0.946210    -0.399620     0.462582     124.19
 C      -2.455894    -0.411790     0.618225      58.76
 H      -2.894522    -1.442345     0.900211      28.16
 O      -3.069477     0.675856     1.480777     241.95
 H      -2.503579     0.539123     2.373391      24.01
 C      -3.226145    -0.189485    -0.796552      84.63
 H      -2.914276     0.922368    -1.213920      25.45
 O      -2.775479    -1.248471    -1.652265     232.89
 H      -2.703607    -0.862937    -2.571835      25.32
 C      -4.716350    -0.400285    -0.580976     102.96
 O      -5.412776     0.724510     0.027278     213.31
 H      -4.785050     0.893539     0.813985      29.48
 H      -4.944136    -1.416051     0.016060      27.74
 H      -5.172513    -0.604626    -1.537930      28.65
55
name = lig-etoh-Waterframe_143
 C       5.676446    -1.719989     1.675527      59.00
 H       5.778495    -0.668003     1.426544      28.72
 C       5.276824    -4.006415     1.187122      84.37
 H       5.087532    -4.808468     0.500742      26.16
 C       5.449680    -4.343136     2.544194       8.44
 O       5.426460    -5.648355     3.034878     184.78
 C       4.949103    -6.745376     2.165265     109.18
 H       5.693033    -6.935326     1.323878      25.77
 H       3.977983    -6.479195     1.701111      27.35
 H       4.805805    -7.675048     2.740176      25.29
 C       5.716811    -3.343859     3.520629      12.44
 O       5.956224    -3.507605     4.876067     191.17
 H       5.619663    -4.288887     5.347130      25.33
 C       5.731963    -2.031670     3.069893      27.72
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 H       6.078266    -1.344333     3.784937      17.69
 C       5.431399    -2.641405     0.709144      16.03
 C       5.120243    -2.272850    -0.793683      97.27
 H       5.331959    -3.110544    -1.375068      26.95
 O       5.951915    -1.245022    -1.220921     236.28
 H       5.711356    -0.300897    -1.065239      27.38
 C       3.667263    -2.047610    -1.204513      87.33
 H       3.150092    -2.959242    -0.925789      27.88
 C       3.552278    -1.971934    -2.764049     109.69
 O       3.779055    -3.320769    -3.368265     254.23
 H       4.709127    -3.306812    -3.841650      25.00
 H       4.371246    -1.307701    -3.100467      24.82
 H       2.635161    -1.627161    -3.115681      28.96
 C      -0.407644    -1.670277     0.187115      70.29
 H      -0.973282    -2.512226     0.226237      25.53
 C      -0.095671     0.776717     0.343809      79.59
 H      -0.450071     1.827374     0.517500      18.80
 C       1.280728     0.638596    -0.019886      16.66
 O       2.248151     1.637992    -0.114215     215.75
 C       1.662269     2.956343     0.074159     104.66
 H       2.639824     3.612439     0.004729      24.23
 H       0.951122     3.202495    -0.739519      28.37
 H       1.266758     3.026472     1.021581      30.79
 C       1.758654    -0.698759    -0.330942      25.93
 O       3.122158    -0.785623    -0.642542     161.56
 C       0.939948    -1.807721    -0.089309      63.50
 H       1.352683    -2.759117    -0.260976      26.16
 C      -0.892424    -0.369924     0.490796      27.78
 C      -2.526408    -0.365408     0.635981      76.81
 H      -2.727151    -1.324342     1.115283      23.97
 O      -3.049539     0.648028     1.498711     285.92
 H      -2.543058     0.515391     2.436574      25.45
 C      -3.197615    -0.212869    -0.742935      86.92
 H      -3.001188     0.902035    -1.124331      26.00
 O      -2.762070    -1.251288    -1.669119     230.53
 H      -2.677347    -1.063329    -2.639065      25.05
 C      -4.743777    -0.372500    -0.627175      99.61
 O      -5.394854     0.772871     0.047655     196.42
 H      -4.864812     0.962256     0.892104      30.20
 H      -4.823147    -1.304601    -0.019401      28.75
 H      -5.249995    -0.441849    -1.605411      28.01
55
name = lig-etoh-Waterframe_144
 C       5.700980    -1.725345     1.731193      52.85
 H       5.677004    -0.758969     1.289820      28.15
 C       5.260665    -4.007268     1.167702      83.65
 H       5.090678    -4.862380     0.477410      24.19
 C       5.449358    -4.363275     2.519543       1.33
 O       5.424082    -5.704400     3.034645     224.80
 C       4.930476    -6.738763     2.203929     122.94
 H       5.633445    -6.959866     1.368997      27.97
 H       3.929653    -6.516923     1.772176      28.13
 H       4.892547    -7.641655     2.773854      26.08
 C       5.724285    -3.359279     3.493447       6.08
 O       6.004041    -3.523100     4.812430     190.57
 H       5.604151    -4.352419     5.035407      26.88
 C       5.769279    -2.019463     3.094363      41.27
 H       6.059317    -1.237368     3.797587      18.52
 C       5.427541    -2.700080     0.714950       9.63
 C       5.113611    -2.276089    -0.751242      81.22
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 H       5.546945    -3.154616    -1.325974      22.95
 O       5.968858    -1.174149    -1.201546     178.71
 H       5.600749    -0.275665    -0.850821      25.18
 C       3.640083    -2.033003    -1.228243      78.65
 H       2.947138    -2.808803    -0.913769      26.87
 C       3.587108    -1.990485    -2.746794     113.04
 O       3.770485    -3.287785    -3.293843     264.05
 H       4.745708    -3.281723    -3.581323      25.23
 H       4.319931    -1.260780    -3.222456      25.01
 H       2.553528    -1.751680    -2.924392      28.22
 C      -0.410259    -1.612131     0.196602      62.73
 H      -1.074673    -2.434349     0.294996      23.35
 C      -0.095379     0.731540     0.395594      96.15
 H      -0.560914     1.766275     0.727004      18.06
 C       1.275533     0.583761    -0.017516      22.43
 O       2.245889     1.617794    -0.134362     215.98
 C       1.667703     2.983220    -0.006056     102.96
 H       2.587543     3.668291     0.048565      24.62
 H       0.971127     3.310612    -0.773081      28.58
 H       1.017488     3.164498     0.932608      27.07
 C       1.731479    -0.696133    -0.332780      25.81
 O       3.153622    -0.747259    -0.652859     142.72
 C       0.954852    -1.852020    -0.093483      55.58
 H       1.297158    -2.845699    -0.117386      25.09
 C      -0.972969    -0.369567     0.473025      43.08
 C      -2.474837    -0.338451     0.653999      87.51
 H      -2.684980    -1.292502     1.053652      25.83
 O      -3.022996     0.648068     1.526100     302.52
 H      -2.625498     0.456611     2.487601      26.15
 C      -3.211415    -0.215357    -0.740109      91.45
 H      -2.919438     0.712196    -1.154062      28.69
 O      -2.741630    -1.279492    -1.647829     249.45
 H      -2.708798    -0.818064    -2.519512      25.53
 C      -4.769391    -0.317990    -0.624499     112.18
 O      -5.380008     0.816378     0.054314     211.76
 H      -4.849129     0.974845     0.902513      29.97
 H      -5.102679    -1.195149    -0.170128      30.58
 H      -5.219380    -0.344249    -1.664347      28.32
55
name = lig-etoh-Waterframe_145
 C       5.677081    -1.680221     1.703684      36.48
 H       5.786587    -0.613058     1.545429      22.42
 C       5.259107    -4.080899     1.143901      68.59
 H       4.976278    -4.812248     0.320740      23.03
 C       5.452930    -4.416441     2.525395       2.42
 O       5.436096    -5.703731     3.054328     254.29
 C       4.909803    -6.781086     2.196383     114.94
 H       5.552256    -6.927058     1.348192      27.60
 H       3.882515    -6.524515     1.873949      29.20
 H       4.915660    -7.522723     2.944476      25.80
 C       5.729154    -3.340534     3.452463      -6.03
 O       6.032869    -3.611053     4.788102     227.14
 H       5.739828    -4.448842     5.121128      20.00
 C       5.849394    -1.977392     3.059425      40.33
 H       5.854848    -1.186230     3.875859      26.13
 C       5.366841    -2.713911     0.756478      14.30
 C       5.161252    -2.296318    -0.693013      75.13
 H       5.515916    -3.163118    -1.438001      23.86
 O       5.987639    -1.121776    -1.165527     140.82
 H       5.511970    -0.253748    -0.830392      23.91
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 C       3.647652    -2.004661    -1.190369      82.31
 H       3.022821    -2.822908    -0.790808      26.22
 C       3.561605    -1.955558    -2.731387     105.92
 O       3.789856    -3.305635    -3.230703     263.13
 H       4.663754    -3.414808    -3.725038      26.15
 H       4.141673    -1.117279    -3.216286      26.38
 H       2.505758    -1.636721    -2.983049      27.29
 C      -0.425670    -1.637634     0.236956      32.80
 H      -1.083609    -2.569974     0.325464      21.56
 C      -0.077388     0.731222     0.449162      76.38
 H      -0.498540     1.777531     0.786848      18.35
 C       1.231894     0.572326    -0.010982      23.41
 O       2.163676     1.610514    -0.144664     217.77
 C       1.694398     3.020693    -0.072707     106.84
 H       2.482061     3.739274     0.037689      25.93
 H       1.248073     3.156678    -1.035681      28.23
 H       1.048836     3.111506     0.960225      24.78
 C       1.817112    -0.740994    -0.314468      21.86
 O       3.149243    -0.744225    -0.668052     152.53
 C       0.935148    -1.854967    -0.113822      64.69
 H       1.267722    -2.884572    -0.118810      25.06
 C      -0.992088    -0.358821     0.419634      78.06
 C      -2.450221    -0.368158     0.655389      75.92
 H      -2.824633    -1.369676     0.927460      28.51
 O      -3.002858     0.679337     1.560957     306.61
 H      -2.539257     0.443794     2.422698      29.93
 C      -3.227544    -0.219258    -0.742775      99.96
 H      -2.982812     0.674531    -1.162616      29.37
 O      -2.745567    -1.286561    -1.580272     249.00
 H      -2.601858    -0.975734    -2.524022      24.69
 C      -4.795813    -0.255856    -0.615659     116.50
 O      -5.373869     0.866561     0.053001     225.71
 H      -4.719441     1.018973     0.810160      28.73
 H      -5.199093    -1.204155    -0.258372      30.41
 H      -5.110900    -0.187912    -1.701358      28.88
55
name = lig-etoh-Waterframe_146
 C       5.641441    -1.635346     1.680294      55.05
 H       5.786030    -0.593338     1.302518      23.04
 C       5.256856    -4.106422     1.157365      63.55
 H       4.964193    -4.894479     0.389892      20.70
 C       5.461708    -4.417742     2.498149       0.27
 O       5.452286    -5.681187     3.066917     259.55
 C       4.897030    -6.806110     2.229317     117.82
 H       5.493499    -7.039377     1.355706      28.56
 H       3.862560    -6.602306     1.908015      29.82
 H       4.880790    -7.753463     2.792765      25.73
 C       5.758637    -3.356173     3.448217      -5.35
 O       6.054629    -3.703284     4.775666     262.52
 H       5.710404    -4.540250     5.150470      20.13
 C       5.883425    -2.008562     3.029395      51.84
 H       5.944046    -1.206944     3.853502      24.77
 C       5.320049    -2.658419     0.792084      10.70
 C       5.186048    -2.249845    -0.713724      92.76
 H       5.487282    -3.164950    -1.365918      23.84
 O       6.000931    -1.132913    -1.101307     215.31
 H       5.633038    -0.169481    -0.957356      22.70
 C       3.725278    -2.003933    -1.132482      90.54
 H       3.176821    -2.914665    -0.797095      25.05
 C       3.516243    -1.919486    -2.700582      97.15
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 O       3.814867    -3.338469    -3.199906     259.63
 H       4.506956    -3.173384    -3.889252      26.52
 H       4.318984    -1.284441    -3.081556      25.54
 H       2.437118    -1.723353    -3.001558      25.49
 C      -0.412399    -1.691262     0.258070      42.12
 H      -1.063755    -2.675661     0.330803      20.32
 C      -0.100922     0.739158     0.472733      68.22
 H      -0.393978     1.797906     0.657097      17.99
 C       1.241207     0.565654    -0.004305      16.79
 O       2.102916     1.621062    -0.141562     215.79
 C       1.718446     3.002976    -0.134074     118.26
 H       2.621913     3.456054    -0.000203      25.99
 H       1.145979     3.310941    -1.039085      27.52
 H       0.865025     3.304545     0.651064      25.00
 C       1.799899    -0.755356    -0.251969      27.58
 O       3.144632    -0.760364    -0.673050     150.08
 C       0.928243    -1.830846    -0.123240      65.73
 H       1.306253    -2.871138    -0.307841      23.55
 C      -0.930470    -0.400190     0.410832      57.29
 C      -2.545016    -0.364074     0.619496      67.23
 H      -2.751611    -1.395880     1.150036      25.15
 O      -2.960199     0.681899     1.572011     306.21
 H      -2.500944     0.581786     2.400425      32.16
 C      -3.237074    -0.187305    -0.720330     100.07
 H      -3.010328     0.852331    -1.153818      26.32
 O      -2.770909    -1.312303    -1.505875     228.16
 H      -2.586683    -1.139958    -2.466184      25.12
 C      -4.802124    -0.215589    -0.664417     104.96
 O      -5.361236     0.916046     0.068400     214.42
 H      -4.722726     1.285471     0.744448      28.24
 H      -5.094719    -1.247782    -0.172643      28.22
 H      -5.183312    -0.139442    -1.692988      28.17
55
name = lig-etoh-Waterframe_147
 C       5.617320    -1.651380     1.696181      60.22
 H       5.696998    -0.638901     1.216475      26.13
 C       5.240235    -3.998356     1.159180      87.12
 H       5.066246    -4.855219     0.474401      26.48
 C       5.480209    -4.384949     2.492465     -45.38
 O       5.451839    -5.715258     3.053263     270.29
 C       4.899000    -6.816541     2.264779     113.26
 H       5.551000    -6.934959     1.364866      30.59
 H       3.887004    -6.579476     1.901511      28.98
 H       4.956995    -7.738414     2.943606      26.04
 C       5.803305    -3.411445     3.467138      -6.94
 O       6.078661    -3.760910     4.760829     219.67
 H       5.531361    -4.569893     4.949459      24.83
 C       5.873269    -2.049998     3.036479      29.45
 H       6.305732    -1.311921     3.768747      18.64
 C       5.294581    -2.658613     0.751943      12.44
 C       5.177917    -2.195621    -0.715615     100.55
 H       5.585626    -3.001071    -1.263283      25.18
 O       6.065747    -1.153044    -1.059003     249.68
 H       5.532187    -0.290443    -0.894640      26.96
 C       3.737891    -2.034884    -1.153485      98.33
 H       3.184063    -2.880626    -0.694456      26.61
 C       3.555202    -1.999436    -2.635250     108.55
 O       3.830154    -3.322121    -3.203985     267.74
 H       4.552092    -3.233984    -3.867470      27.51
 H       4.203922    -1.278077    -3.101575      26.72
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 H       2.503851    -1.592623    -2.848357      27.00
 C      -0.380311    -1.725488     0.253456      33.66
 H      -1.112952    -2.626050     0.281826      21.18
 C      -0.096284     0.712683     0.417454      76.82
 H      -0.594197     1.615621     0.540215      20.04
 C       1.229079     0.563247     0.040798      20.91
 O       2.087572     1.616876    -0.144664     231.09
 C       1.688857     3.003532    -0.193399     127.65
 H       2.624638     3.488930    -0.020737      26.23
 H       1.311189     3.391136    -1.196720      26.83
 H       1.134439     3.341885     0.653132      29.18
 C       1.752404    -0.703397    -0.196753      23.14
 O       3.134223    -0.775765    -0.632094     124.84
 C       0.961493    -1.866863    -0.123872      62.90
 H       1.371138    -2.868278    -0.482935      23.89
 C      -0.987126    -0.452452     0.474647      96.15
 C      -2.527493    -0.331381     0.669585      65.43
 H      -2.911554    -1.383479     1.064133      26.94
 O      -2.926065     0.695461     1.542453     303.72
 H      -2.446559     0.484816     2.332677      32.03
 C      -3.277922    -0.144109    -0.716394      93.35
 H      -2.735762     0.841433    -1.210886      25.79
 O      -2.805545    -1.353134    -1.446682     208.71
 H      -2.722181    -0.966470    -2.350728      26.52
 C      -4.778751    -0.173670    -0.679861     112.99
 O      -5.367893     0.959146     0.070344     192.79
 H      -4.612990     1.331732     0.605541      31.17
 H      -5.146322    -1.157782    -0.129111      28.25
 H      -5.268313    -0.251760    -1.624054      28.60
55
name = lig-etoh-Waterframe_148
 C       5.598863    -1.717848     1.731421      48.76
 H       5.727541    -0.618271     1.678591      25.48
 C       5.220221    -3.956950     1.157260      79.67
 H       5.062101    -4.638413     0.343097      27.48
 C       5.483138    -4.390191     2.508554      -2.78
 O       5.449041    -5.714550     3.022543     268.15
 C       4.925768    -6.796949     2.268297     117.31
 H       5.575062    -7.061230     1.370284      28.51
 H       3.879993    -6.658058     1.986702      27.48
 H       4.983551    -7.645619     3.042831      25.93
 C       5.838875    -3.421430     3.460091       1.92
 O       6.101902    -3.796626     4.747357     192.25
 H       5.665573    -4.660714     5.192836      22.01
 C       5.890929    -2.071818     3.057516      27.68
 H       6.382685    -1.387126     3.724051      16.45
 C       5.294025    -2.614337     0.726909      20.36
 C       5.200067    -2.233481    -0.697503      93.43
 H       5.490800    -3.026908    -1.300008      27.46
 O       6.122240    -1.129807    -1.023526     214.03
 H       5.777443    -0.181316    -0.892239      24.51
 C       3.685608    -2.048898    -1.126720      84.71
 H       3.187555    -2.931941    -0.704324      26.44
 C       3.599075    -2.048658    -2.638456     115.15
 O       3.831590    -3.311919    -3.236144     285.09
 H       4.704670    -3.317025    -3.649531      28.59
 H       4.171903    -1.239906    -3.053248      27.00
 H       2.534033    -1.835431    -2.843086      28.51
 C      -0.407163    -1.745939     0.249522      67.58
 H      -0.973583    -2.676240     0.200580      23.70
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 C      -0.213489     0.635549     0.355756      84.88
 H      -0.600473     1.577827     0.441853      21.37
 C       1.200060     0.604922     0.089867      19.31
 O       2.111833     1.615159    -0.159114     217.62
 C       1.706306     3.040137    -0.209778     101.57
 H       2.658566     3.685095    -0.152719      24.49
 H       1.171753     3.177304    -1.205256      26.25
 H       1.079869     3.223239     0.561040      29.74
 C       1.793800    -0.745264    -0.197302      21.52
 O       3.117314    -0.775581    -0.566382     168.29
 C       0.978327    -1.882315    -0.115275      59.54
 H       1.358306    -2.897014    -0.441851      23.55
 C      -0.990728    -0.496850     0.539421      28.57
 C      -2.497713    -0.349007     0.681423      81.81
 H      -2.957563    -1.266192     0.978798      25.14
 O      -2.892163     0.743233     1.531965     306.49
 H      -2.556357     0.575590     2.447096      29.22
 C      -3.213195    -0.156549    -0.698744      90.54
 H      -2.881740     0.761750    -1.344622      26.43
 O      -2.860444    -1.350679    -1.422913     225.78
 H      -2.691786    -1.213171    -2.398148      25.66
 C      -4.806587    -0.134765    -0.638322     109.32
 O      -5.372921     1.002249     0.046791     190.91
 H      -4.619231     1.343651     0.599970      32.38
 H      -5.037828    -1.056543    -0.088346      30.30
 H      -5.164447    -0.165681    -1.663559      28.59
55
name = lig-etoh-Waterframe_149
 C       5.620032    -1.677346     1.824626      57.32
 H       5.691787    -0.614646     1.547007      22.89
 C       5.211119    -3.997428     1.146296      79.53
 H       4.969752    -4.727938     0.427895      25.89
 C       5.455097    -4.405515     2.452174     -15.20
 O       5.464442    -5.663912     2.991804     264.56
 C       4.942645    -6.814836     2.260340     130.72
 H       5.521863    -7.141785     1.365788      30.73
 H       3.910952    -6.665818     1.963491      28.59
 H       4.990796    -7.699287     2.926206      26.47
 C       5.835071    -3.464392     3.482792      -4.71
 O       6.159463    -3.795007     4.774521     236.59
 H       5.702928    -4.712837     5.144727      16.69
 C       5.939958    -2.121277     3.110735      64.29
 H       6.128140    -1.351163     3.799268      28.83
 C       5.322042    -2.598882     0.791937       1.03
 C       5.197932    -2.219280    -0.700978      87.90
 H       5.524983    -3.098142    -1.337127      24.34
 O       6.166843    -1.121879    -1.003721     222.04
 H       5.704711    -0.248091    -0.808820      27.39
 C       3.692437    -2.039123    -1.057839      85.40
 H       3.136836    -2.907190    -0.721951      26.27
 C       3.548156    -2.016369    -2.670935     101.69
 O       3.856429    -3.352814    -3.274798     271.57
 H       4.740262    -3.272185    -3.657600      27.77
 H       4.279435    -1.285700    -3.061294      24.72
 H       2.537595    -1.894208    -2.964229      28.32
 C      -0.405563    -1.808590     0.246072      57.52
 H      -0.977608    -2.660474     0.258439      24.06
 C      -0.234943     0.652891     0.312146      92.36
 H      -0.726591     1.604728     0.402179      21.28
 C       1.183601     0.537873     0.076759       8.48
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 O       2.145933     1.630695    -0.159067     185.72
 C       1.690189     3.022565    -0.225772     103.77
 H       2.655982     3.715829    -0.267672      24.00
 H       0.978172     3.195602    -1.045624      27.50
 H       0.982539     3.314909     0.582728      27.27
 C       1.779714    -0.746717    -0.183346      24.07
 O       3.141455    -0.802525    -0.517366     179.42
 C       0.941256    -1.871338    -0.095120      59.28
 H       1.295771    -2.890336    -0.265363      23.95
 C      -0.992701    -0.577302     0.555691      32.32
 C      -2.501802    -0.378235     0.675503      87.04
 H      -2.848701    -1.236305     1.144716      24.65
 O      -2.876160     0.813778     1.522768     274.73
 H      -2.514437     0.622150     2.469410      28.01
 C      -3.177604    -0.161950    -0.720518      99.95
 H      -2.866739     0.729412    -1.164055      29.85
 O      -2.914912    -1.372975    -1.433757     242.38
 H      -2.576530    -1.110601    -2.353634      25.64
 C      -4.774225    -0.126285    -0.580721     111.04
 O      -5.373183     1.062416     0.028075     170.92
 H      -4.756275     1.291903     0.769663      32.99
 H      -5.156345    -0.989571    -0.148665      30.65
 H      -5.139847    -0.093354    -1.648675      27.60
55
name = lig-etoh-Waterframe_150
 C       5.662713    -1.643332     1.845845      45.56
 H       5.711464    -0.624533     1.497946      21.57
 C       5.204715    -4.018726     1.117440      81.41
 H       4.905859    -4.793250     0.462297      23.92
 C       5.452543    -4.387494     2.462063       1.67
 O       5.478630    -5.687863     2.957018     212.46
 C       4.941913    -6.849274     2.228901     123.38
 H       5.572519    -6.933135     1.362127      30.52
 H       3.926863    -6.615433     1.899405      29.31
 H       5.001363    -7.621549     2.950632      26.23
 C       5.827297    -3.490724     3.497931      -7.05
 O       6.220531    -3.796142     4.803542     251.81
 H       5.738494    -4.680496     5.093989      17.77
 C       5.958540    -2.114880     3.192795      34.64
 H       5.984739    -1.497399     4.069974      26.74
 C       5.359516    -2.635467     0.869290      22.04
 C       5.207651    -2.181814    -0.642585      78.71
 H       5.645541    -3.096700    -1.271143      22.58
 O       6.150210    -1.138253    -0.993735     213.51
 H       5.721389    -0.258409    -0.829717      26.23
 C       3.715771    -2.022833    -1.100634      89.46
 H       3.239610    -2.880740    -0.625154      26.66
 C       3.498044    -2.010999    -2.675817      97.98
 O       3.873179    -3.377667    -3.276459     239.73
 H       4.658771    -3.263291    -3.917030      24.94
 H       4.182785    -1.229352    -3.159093      26.06
 H       2.552561    -1.596024    -2.946672      27.98
 C      -0.440474    -1.860218     0.279276      42.07
 H      -0.999948    -2.723515     0.368845      22.65
 C      -0.171325     0.624731     0.306278      66.43
 H      -0.754241     1.589470     0.399558      21.03
 C       1.196172     0.544045     0.002570       4.11
 O       2.130070     1.612423    -0.137801     203.30
 C       1.596014     2.978781    -0.229129     108.84
 H       2.579821     3.604861    -0.366151      24.75
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 H       1.058137     3.195413    -1.115931      28.26
 H       1.322083     3.355158     0.868182      25.24
 C       1.741136    -0.752036    -0.163684      11.45
 O       3.164687    -0.827214    -0.461252     126.85
 C       0.937926    -1.907436    -0.074349      62.33
 H       1.409858    -2.839344    -0.192877      25.32
 C      -0.987664    -0.540790     0.495388      53.73
 C      -2.510095    -0.376692     0.716182      74.85
 H      -2.979542    -1.279798     1.241450      27.16
 O      -2.860335     0.859094     1.488881     258.19
 H      -2.324190     0.637437     2.377168      26.94
 C      -3.220242    -0.185544    -0.661152     104.56
 H      -2.753918     0.631819    -1.073554      29.79
 O      -2.948835    -1.386686    -1.479404     216.55
 H      -2.588453    -1.080204    -2.380515      26.00
 C      -4.731127    -0.097860    -0.577151     109.49
 O      -5.354350     1.108794     0.038802     172.76
 H      -4.952612     1.135067     0.931395      32.50
 H      -5.153281    -0.974127    -0.080527      29.64
 H      -5.175747    -0.120844    -1.631820      28.05
55
name = lig-etoh-Waterframe_151
 C       5.732357    -1.696960     1.889525      61.30
 H       5.825669    -0.650099     1.719253      30.04
 C       5.213181    -4.011631     1.179967      72.68
 H       4.949045    -4.631604     0.324054      23.19
 C       5.471850    -4.424026     2.512862      16.49
 O       5.483599    -5.748871     2.947240     234.25
 C       4.947477    -6.818143     2.170370     124.11
 H       5.563105    -7.110786     1.312519      26.36
 H       3.880478    -6.705993     1.862315      26.55
 H       4.990847    -7.658510     2.804577      24.75
 C       5.855485    -3.441337     3.519720      -1.77
 O       6.256181    -3.822130     4.799878     236.97
 H       5.922815    -4.612964     5.278517      25.07
 C       5.900334    -2.072601     3.226645      44.65
 H       6.167509    -1.443592     4.115136      18.84
 C       5.376827    -2.618316     0.861371      16.02
 C       5.241423    -2.184499    -0.568895      63.97
 H       5.546454    -3.109180    -1.206456      23.05
 O       6.105346    -1.141894    -0.991139     169.10
 H       5.817552    -0.224937    -0.894031      24.98
 C       3.748982    -2.024564    -1.145075      78.70
 H       3.291012    -2.969989    -0.793808      26.04
 C       3.531242    -2.011887    -2.676315     104.97
 O       3.818910    -3.345367    -3.240612     238.81
 H       4.666853    -3.215546    -3.847776      22.99
 H       4.248430    -1.246560    -3.118360      26.15
 H       2.461201    -1.832969    -2.836622      27.34
 C      -0.455501    -1.828312     0.323602      51.92
 H      -1.037148    -2.753489     0.466668      23.64
 C      -0.140303     0.586978     0.314608      67.48
 H      -0.512023     1.681495     0.450897      22.77
 C       1.224413     0.559032    -0.070976      11.17
 O       2.072516     1.577910    -0.122874     222.88
 C       1.599709     2.948549    -0.202114     114.53
 H       2.488325     3.462772    -0.509515      26.77
 H       0.740492     3.044890    -0.856903      28.14
 H       1.057586     3.296409     0.822430      25.97
 C       1.766946    -0.795294    -0.183316      11.45
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 O       3.146064    -0.836880    -0.407661     118.27
 C       0.943240    -1.963139    -0.031197      62.19
 H       1.423638    -2.879695    -0.167671      26.67
 C      -0.990375    -0.532549     0.418143      44.84
 C      -2.516358    -0.340905     0.751402      78.10
 H      -2.946112    -1.334895     1.308188      27.38
 O      -2.816447     0.856658     1.453333     269.09
 H      -2.408910     0.904122     2.427032      28.39
 C      -3.228104    -0.225739    -0.608135      92.61
 H      -2.797855     0.691710    -1.162167      28.20
 O      -2.981695    -1.379069    -1.493955     197.50
 H      -2.777298    -1.146536    -2.462913      25.26
 C      -4.768919    -0.056502    -0.585077     107.80
 O      -5.317052     1.113022     0.060200     184.00
 H      -5.109095     1.087408     1.006316      31.45
 H      -5.061481    -1.000379     0.046266      28.36
 H      -5.131845    -0.111408    -1.647513      28.71
55
name = lig-etoh-Waterframe_152
 C       5.781713    -1.712996     1.912542      40.93
 H       5.952407    -0.679164     1.654136      29.34
 C       5.241497    -3.948625     1.266942      80.07
 H       5.040929    -4.739738     0.475758      26.05
 C       5.501248    -4.443765     2.552043      17.08
 O       5.485818    -5.789426     2.964859     165.28
 C       4.940186    -6.833123     2.088783     111.96
 H       5.543984    -7.060590     1.165233      26.03
 H       3.892497    -6.534555     1.775632      26.00
 H       4.923092    -7.690159     2.749292      25.84
 C       5.863198    -3.474342     3.576908       0.60
 O       6.306686    -3.823656     4.797684     204.39
 H       5.836019    -4.643739     5.098349      23.96
 C       5.855859    -2.083605     3.262906      41.82
 H       6.325638    -1.221387     3.841967      16.59
 C       5.392844    -2.588590     0.906256      42.48
 C       5.216721    -2.212765    -0.594566      94.92
 H       5.607787    -3.043927    -1.115919      26.18
 O       6.104999    -1.134119    -1.005777     207.90
 H       5.591992    -0.338065    -0.824063      28.40
 C       3.787955    -2.047905    -1.081114      77.36
 H       3.171395    -2.940102    -0.859639      26.76
 C       3.599612    -1.994787    -2.645082     102.84
 O       3.752569    -3.297835    -3.202443     254.42
 H       4.710709    -3.439997    -3.592217      24.80
 H       4.106394    -1.206902    -3.231990      26.69
 H       2.483179    -1.862104    -2.802158      27.87
 C      -0.398403    -1.792743     0.334420      47.31
 H      -1.125762    -2.686729     0.526198      23.07
 C      -0.119738     0.612407     0.291916      72.72
 H      -0.594899     1.615966     0.588549      21.06
 C       1.188482     0.418404    -0.086375      13.63
 O       2.065136     1.569377    -0.121260     214.07
 C       1.553649     2.907850    -0.167512     124.37
 H       2.228094     3.582079    -0.521425      28.86
 H       0.682784     2.886667    -0.875043      27.72
 H       1.297469     3.309767     0.839124      28.16
 C       1.776689    -0.846269    -0.224850      28.18
 O       3.143083    -0.882449    -0.397888     140.93
 C       0.944654    -1.967051     0.024212      64.41
 H       1.256047    -2.999899    -0.039486      25.70
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 C      -1.011300    -0.534561     0.409470      52.73
 C      -2.467131    -0.343223     0.739603      82.94
 H      -2.770520    -1.238327     1.384256      28.78
 O      -2.790164     0.881811     1.430285     260.54
 H      -2.391139     0.685363     2.405457      27.84
 C      -3.241230    -0.214964    -0.653796      82.27
 H      -2.808910     0.836737    -1.120020      27.29
 O      -3.023549    -1.382464    -1.454198     218.60
 H      -2.847825    -1.002806    -2.360596      26.76
 C      -4.791531    -0.079279    -0.543064     107.44
 O      -5.297088     1.115920     0.069660     179.80
 H      -5.034913     1.072148     1.004590      30.75
 H      -5.374432    -1.018919    -0.121266      28.73
 H      -5.199702    -0.034498    -1.541739      30.19
55
name = lig-etoh-Waterframe_153
 C       5.784705    -1.659045     1.903732      54.97
 H       6.070881    -0.646849     1.567815      27.47
 C       5.272076    -3.941522     1.327395      72.01
 H       4.997635    -4.746831     0.559971      23.93
 C       5.528376    -4.410416     2.616054      14.16
 O       5.487880    -5.807220     2.978561     207.86
 C       4.912413    -6.824461     2.010333     108.63
 H       5.634369    -6.865163     1.152072      26.87
 H       3.925835    -6.442383     1.652628      25.12
 H       4.817300    -7.749900     2.623653      25.03
 C       5.852213    -3.483673     3.609593      -6.45
 O       6.361410    -3.833047     4.829924     246.22
 H       5.943596    -4.745786     5.279657      20.31
 C       5.888131    -2.112745     3.249826      32.93
 H       6.233256    -1.441238     4.118477      18.45
 C       5.396831    -2.594660     0.928700      17.88
 C       5.247815    -2.264433    -0.607459      91.59
 H       5.591653    -3.092101    -1.140086      26.40
 O       6.087382    -1.127547    -1.015137     225.13
 H       5.680650    -0.225350    -0.907994      26.43
 C       3.767551    -2.073325    -1.030789      87.15
 H       3.270199    -2.986086    -0.635067      25.17
 C       3.605134    -1.943136    -2.594855     100.18
 O       3.709394    -3.298582    -3.173894     260.86
 H       4.642099    -3.369009    -3.645031      25.34
 H       4.223437    -1.236044    -3.113150      25.82
 H       2.552653    -1.521391    -2.682712      26.83
 C      -0.407684    -1.766815     0.341953      66.69
 H      -0.991569    -2.774722     0.512063      22.02
 C      -0.193528     0.595236     0.271240      63.41
 H      -0.525261     1.616367     0.508828      18.57
 C       1.194714     0.413692    -0.063070       9.59
 O       2.102747     1.505856    -0.130372     197.47
 C       1.469977     2.870676    -0.136229     112.99
 H       2.232824     3.493795    -0.593124      27.01
 H       0.570975     2.969602    -0.830452      26.78
 H       1.346984     3.179270     0.819846      29.37
 C       1.776984    -0.922986    -0.258296      21.46
 O       3.178700    -0.937064    -0.414558     192.60
 C       0.955523    -1.995104     0.063352      48.93
 H       1.355530    -3.053692     0.091852      22.05
 C      -0.954654    -0.486849     0.441919      39.82
 C      -2.447498    -0.354920     0.669138      86.67
 H      -2.833104    -1.158335     1.182107      27.34
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 O      -2.755944     0.895981     1.442585     275.09
 H      -2.370720     0.713525     2.408009      26.99
 C      -3.296130    -0.203613    -0.628988      90.62
 H      -2.868984     0.702303    -1.204825      26.13
 O      -3.052043    -1.374436    -1.422900     237.32
 H      -2.725235    -1.245312    -2.356449      25.97
 C      -4.839706    -0.115035    -0.542909     114.45
 O      -5.293430     1.127144     0.097322     177.57
 H      -4.802486     1.241883     0.935396      30.82
 H      -5.265747    -1.025627    -0.087128      30.13
 H      -5.137764     0.005384    -1.549128      29.44
55
name = lig-etoh-Waterframe_154
 C       5.770888    -1.622320     1.913879      45.98
 H       6.021941    -0.545542     1.702435      21.25
 C       5.280454    -3.976359     1.340479      65.95
 H       4.932316    -4.634936     0.509617      21.32
 C       5.518546    -4.446649     2.652871      16.37
 O       5.470374    -5.805229     2.981319     248.49
 C       4.909078    -6.716694     1.953422     121.17
 H       5.629635    -6.953835     1.143154      26.40
 H       3.947574    -6.465949     1.524228      27.65
 H       4.807831    -7.743783     2.422863      24.61
 C       5.864859    -3.475494     3.649941     -11.08
 O       6.419456    -3.829205     4.885055     224.79
 H       5.983024    -4.686302     5.346516      15.90
 C       5.964642    -2.119413     3.246502      32.37
 H       6.077876    -1.540743     4.173050      23.96
 C       5.420220    -2.606645     0.912818      -1.93
 C       5.292662    -2.258913    -0.570407      95.16
 H       5.630061    -3.122149    -1.210816      25.75
 O       6.086268    -1.149485    -1.029945     243.04
 H       5.612334    -0.251663    -0.878695      24.55
 C       3.768560    -2.138399    -1.019578      88.66
 H       3.294719    -3.081145    -0.707475      25.12
 C       3.594286    -1.922337    -2.511558     108.24
 O       3.674063    -3.282236    -3.160589     269.34
 H       4.390085    -3.175065    -3.884383      26.12
 H       4.488017    -1.393829    -2.742022      24.39
 H       2.619205    -1.461063    -2.802095      25.59
 C      -0.403710    -1.818615     0.356109      40.76
 H      -1.135564    -2.667918     0.537120      20.47
 C      -0.120889     0.652096     0.234012      99.18
 H      -0.602795     1.591760     0.279835      17.69
 C       1.228045     0.429419    -0.037728      18.53
 O       2.106305     1.442011    -0.155686     192.37
 C       1.463846     2.814847    -0.125788     101.72
 H       2.348412     3.416650    -0.583695      23.58
 H       0.458040     2.810231    -0.652495      23.85
 H       1.180955     3.099194     0.870532      27.63
 C       1.780271    -0.893179    -0.233950      19.89
 O       3.192289    -0.955021    -0.411280     185.78
 C       0.962332    -2.040347     0.082682      36.52
 H       1.459825    -3.080065     0.134715      18.77
 C      -0.990515    -0.539037     0.468158      52.28
 C      -2.495203    -0.315660     0.644560      86.29
 H      -2.876022    -1.224883     1.078254      24.43
 O      -2.724296     0.881021     1.460953     299.16
 H      -2.324137     0.782555     2.399555      29.62
 C      -3.315235    -0.190911    -0.651475     105.23
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 H      -3.064319     0.652239    -1.190653      28.78
 O      -3.073982    -1.421155    -1.406522     256.08
 H      -2.642674    -1.114096    -2.258453      25.35
 C      -4.857495    -0.098701    -0.536150     118.63
 O      -5.301182     1.126737     0.138129     198.75
 H      -4.518451     1.361030     0.675144      32.09
 H      -5.170900    -0.936839    -0.012960      31.29
 H      -5.242529    -0.161901    -1.571080      29.08
55
name = lig-etoh-Waterframe_155
 C       5.760508    -1.672159     1.954210      59.35
 H       5.775461    -0.570294     1.749966      23.36
 C       5.272954    -3.967200     1.310890      61.30
 H       5.007301    -4.726165     0.600354      22.06
 C       5.496328    -4.457649     2.641478       4.27
 O       5.427579    -5.808465     2.964405     350.96
 C       4.929908    -6.641510     1.899058     136.87
 H       5.643639    -6.717358     1.080606      31.13
 H       4.032954    -6.220890     1.507918      25.98
 H       4.750837    -7.565216     2.520684      24.03
 C       5.927537    -3.506462     3.667397       8.74
 O       6.455199    -3.795414     4.921794     283.60
 H       6.076508    -4.652856     5.175691      25.74
 C       6.008788    -2.111000     3.278321      48.18
 H       6.209904    -1.273075     3.884448      26.97
 C       5.480475    -2.596554     0.958035      28.97
 C       5.282975    -2.261902    -0.558660      89.06
 H       5.786491    -3.184190    -1.110648      23.21
 O       6.093528    -1.167023    -1.040794     229.94
 H       5.575910    -0.320177    -0.750658      24.20
 C       3.768004    -2.208752    -0.984405      77.64
 H       3.192169    -3.085077    -0.691825      24.99
 C       3.645255    -1.973936    -2.468128     110.96
 O       3.638431    -3.234303    -3.173163     280.63
 H       4.360872    -3.253318    -3.874329      27.08
 H       4.499990    -1.318756    -2.809921      23.65
 H       2.797404    -1.375527    -2.784131      27.04
 C      -0.434014    -1.876167     0.394237      33.02
 H      -1.054738    -2.720587     0.537411      18.18
 C      -0.130302     0.589263     0.221998      66.44
 H      -0.560999     1.523171     0.138345      17.82
 C       1.246147     0.391885    -0.025944      12.32
 O       2.128174     1.460092    -0.191015     230.79
 C       1.518634     2.713775    -0.111034     109.00
 H       2.168297     3.654088    -0.505897      24.67
 H       0.721703     2.706280    -0.894999      25.74
 H       1.256441     3.028016     0.991712      26.59
 C       1.782405    -0.905839    -0.136305      27.37
 O       3.168529    -0.951642    -0.372809     154.88
 C       0.985357    -2.016656     0.080229      66.28
 H       1.368868    -3.083129     0.064576      21.40
 C      -0.967937    -0.533899     0.423904      77.85
 C      -2.525121    -0.292406     0.676646      60.50
 H      -2.963394    -1.243849     1.260796      24.88
 O      -2.717438     0.866920     1.473212     267.67
 H      -2.286135     0.599553     2.322398      29.27
 C      -3.334895    -0.170854    -0.722331     102.71
 H      -2.964115     0.652870    -1.258842      28.35
 O      -3.081821    -1.452976    -1.399193     238.61
 H      -2.710011    -1.189410    -2.296979      26.01
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 C      -4.862870    -0.093599    -0.494998     114.46
 O      -5.291890     1.124493     0.167101     193.86
 H      -4.492486     1.528355     0.519857      34.36
 H      -5.236854    -0.918933     0.131328      29.66
 H      -5.466963    -0.188430    -1.476791      27.93
55
name = lig-etoh-Waterframe_156
 C       5.749684    -1.728008     2.001973      62.26
 H       5.679442    -0.671452     1.730222      28.71
 C       5.291187    -3.957587     1.323576      74.45
 H       5.113816    -4.607442     0.522122      24.77
 C       5.512325    -4.383754     2.635755      12.92
 O       5.398757    -5.774934     2.957088     198.05
 C       4.928591    -6.587061     1.862854     123.23
 H       5.679537    -6.679189     1.087590      28.03
 H       4.030759    -6.156232     1.447752      26.49
 H       4.666016    -7.620746     2.192778      25.51
 C       6.021500    -3.476294     3.641375       7.06
 O       6.460479    -3.777525     4.919715     117.39
 H       6.258277    -4.692270     5.294464      27.02
 C       6.025088    -2.108201     3.306298      41.11
 H       6.461311    -1.430286     4.010357      18.12
 C       5.494571    -2.627948     0.957688      29.93
 C       5.281588    -2.308914    -0.510957      76.12
 H       5.661326    -3.243501    -1.096410      24.82
 O       6.075728    -1.183502    -1.031569     206.25
 H       5.800042    -0.211647    -0.840794      24.56
 C       3.767158    -2.200836    -0.925696      75.67
 H       3.259223    -3.088964    -0.545098      25.55
 C       3.712231    -1.982856    -2.492567     102.00
 O       3.609836    -3.218907    -3.225320     267.99
 H       4.539213    -3.304005    -3.539778      27.62
 H       4.569467    -1.345748    -2.939424      23.68
 H       2.778321    -1.486328    -2.518208      28.65
 C      -0.421275    -1.864829     0.411358      47.64
 H      -0.915087    -2.740497     0.533626      23.04
 C      -0.151127     0.503601     0.199008      73.06
 H      -0.542961     1.478288     0.206876      22.69
 C       1.243727     0.373126    -0.013710       0.81
 O       2.200763     1.448496    -0.226818     195.38
 C       1.551420     2.721813    -0.136999     110.20
 H       2.433684     3.435772    -0.311743      24.77
 H       0.695437     2.895711    -0.751162      27.02
 H       1.036433     2.822101     0.944373      26.06
 C       1.831015    -0.937944    -0.034210      19.67
 O       3.160351    -0.978607    -0.322043     152.17
 C       0.913042    -2.026621     0.105644      64.61
 H       1.357346    -3.006359    -0.041332      25.34
 C      -1.004096    -0.595612     0.384336      53.38
 C      -2.501761    -0.314137     0.651374      69.43
 H      -2.993491    -1.234651     1.245095      26.11
 O      -2.718269     0.866866     1.499395     269.56
 H      -2.381853     0.729759     2.387763      30.67
 C      -3.341836    -0.203917    -0.728022      93.69
 H      -2.875439     0.637541    -1.384069      26.67
 O      -3.078987    -1.453490    -1.411642     206.08
 H      -2.849612    -1.389382    -2.368734      27.46
 C      -4.886262    -0.096500    -0.442105     108.35
 O      -5.279712     1.156383     0.181234     175.93
 H      -4.544713     1.589602     0.623368      32.06
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 H      -5.102256    -1.033726     0.252238      28.13
 H      -5.464026    -0.129756    -1.434366      27.37
55
name = lig-etoh-Waterframe_157
 C       5.738150    -1.695313     1.993238      57.65
 H       5.855939    -0.652370     1.785924      25.81
 C       5.341114    -3.969605     1.326440      69.47
 H       5.118855    -4.668333     0.571551      24.10
 C       5.564160    -4.369759     2.660511      22.22
 O       5.383333    -5.722013     2.966213     197.81
 C       4.906429    -6.553505     1.804436     116.87
 H       5.710250    -6.662319     1.058428      26.99
 H       4.010680    -6.172134     1.262964      25.47
 H       4.724808    -7.557491     2.164183      26.26
 C       6.073501    -3.473704     3.626847      10.90
 O       6.472274    -3.775161     4.904126     116.41
 H       6.044184    -4.748194     5.168414      24.58
 C       6.071232    -2.116062     3.337845      15.78
 H       6.453680    -1.552338     4.216412      18.05
 C       5.476678    -2.641837     0.975035      33.41
 C       5.265272    -2.296862    -0.468001      89.56
 H       5.543541    -3.114809    -1.078050      25.96
 O       6.088255    -1.237505    -1.020392     222.24
 H       5.552434    -0.395647    -0.786430      26.53
 C       3.822108    -2.153352    -0.889668      87.44
 H       3.299846    -3.093824    -0.645327      26.45
 C       3.692526    -1.970323    -2.465795      99.43
 O       3.621286    -3.229771    -3.278023     265.02
 H       4.518471    -3.486239    -3.551271      27.62
 H       4.578696    -1.336292    -2.796804      24.72
 H       2.747090    -1.490139    -2.699062      28.75
 C      -0.448371    -1.891025     0.408378      42.98
 H      -1.081485    -2.739745     0.565243      22.80
 C      -0.127495     0.489388     0.161308      65.21
 H      -0.647059     1.450866     0.307646      22.82
 C       1.283231     0.349665    -0.001112       6.55
 O       2.201346     1.374931    -0.259345     198.47
 C       1.589773     2.780048    -0.125715     114.46
 H       2.407698     3.420001    -0.097082      28.11
 H       0.931289     2.994001    -0.925973      27.87
 H       1.138721     2.844292     0.881043      27.79
 C       1.804330    -0.957356     0.022050      23.59
 O       3.199186    -1.033061    -0.263247     156.05
 C       0.955677    -2.052561     0.130036      67.31
 H       1.223097    -3.058528     0.026262      26.19
 C      -1.062262    -0.639735     0.385785      46.21
 C      -2.491226    -0.355569     0.623437      85.65
 H      -2.880043    -1.280063     1.052622      29.15
 O      -2.729278     0.874425     1.496507     269.86
 H      -2.383223     0.689696     2.355777      30.77
 C      -3.319255    -0.243198    -0.690229      92.33
 H      -3.070737     0.745188    -1.354364      26.27
 O      -3.085269    -1.477460    -1.427157     212.35
 H      -2.893917    -1.090782    -2.316431      26.65
 C      -4.852206    -0.081999    -0.397987     108.37
 O      -5.277792     1.202558     0.187383     187.03
 H      -4.538404     1.325349     0.796241      30.62
 H      -5.198238    -0.985805     0.279498      28.61
 H      -5.410707    -0.257703    -1.323157      29.28
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name = lig-etoh-Waterframe_158
 C       5.781225    -1.626134     2.025909      58.50
 H       5.965110    -0.618368     1.733481      22.94
 C       5.403491    -3.985135     1.347743      56.31
 H       5.090724    -4.722467     0.629014      18.88
 C       5.624895    -4.414345     2.639364      23.64
 O       5.354577    -5.714888     2.958485     231.23
 C       4.916781    -6.539984     1.778515     114.90
 H       5.759097    -6.574125     1.049405      28.42
 H       3.973643    -6.107362     1.313340      26.77
 H       4.723533    -7.400923     2.349288      25.37
 C       6.075480    -3.483743     3.638065      21.47
 O       6.472207    -3.825915     4.893806     222.96
 H       6.065060    -4.781111     5.314172      20.20
 C       6.114274    -2.104240     3.296887      48.42
 H       6.239313    -1.261691     4.051753      24.25
 C       5.459829    -2.584822     1.028185      20.22
 C       5.271857    -2.301380    -0.486626      97.45
 H       5.590741    -3.191795    -0.928327      24.77
 O       6.091425    -1.275001    -0.984209     229.24
 H       5.733261    -0.324647    -0.843374      26.21
 C       3.799678    -2.159638    -0.926804      85.74
 H       3.303297    -3.110725    -0.647606      24.08
 C       3.659729    -1.966804    -2.451869     104.42
 O       3.645701    -3.246682    -3.272167     261.30
 H       4.485648    -3.273759    -3.782657      26.03
 H       4.476477    -1.348073    -2.807525      25.69
 H       2.766757    -1.399590    -2.786343      26.59
 C      -0.479278    -1.938548     0.388733      50.62
 H      -1.141546    -2.865777     0.552060      22.16
 C      -0.136562     0.476772     0.158010      57.96
 H      -0.505132     1.563724     0.164028      20.55
 C       1.259068     0.333456     0.008540       3.85
 O       2.148857     1.352800    -0.277568     219.96
 C       1.680793     2.787081    -0.099629     118.99
 H       2.464877     3.437159    -0.056353      27.54
 H       1.168296     3.031157    -1.024497      27.20
 H       1.057669     2.905006     0.730693      28.98
 C       1.829244    -1.008028    -0.002211       7.68
 O       3.221014    -1.054593    -0.170524     174.74
 C       0.950790    -2.122933     0.181807      53.26
 H       1.392662    -3.077926     0.174858      22.92
 C      -0.959134    -0.590329     0.386692      43.99
 C      -2.516085    -0.386418     0.631741      85.67
 H      -2.901921    -1.177490     1.153902      29.07
 O      -2.743594     0.832290     1.455340     289.58
 H      -2.323270     0.598798     2.260925      29.43
 C      -3.346122    -0.238188    -0.628645      95.14
 H      -2.947299     0.661768    -1.217301      26.31
 O      -3.097721    -1.454917    -1.449193     206.14
 H      -2.777050    -1.250949    -2.382399      25.40
 C      -4.848422    -0.099112    -0.354216     118.06
 O      -5.238550     1.212581     0.181477     188.48
 H      -4.739944     1.386389     0.983256      30.11
 H      -5.201277    -0.807221     0.365417      30.27
 H      -5.334934    -0.197624    -1.281351      30.85
55
name = lig-etoh-Waterframe_159
 C       5.842376    -1.601061     1.987968      54.97
 H       5.878102    -0.539109     1.777201      21.32
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 C       5.446429    -3.901122     1.348867      50.52
 H       5.141161    -4.517176     0.474467      12.47
 C       5.686832    -4.428094     2.631222      29.05
 O       5.335003    -5.746329     2.944906     330.23
 C       4.934840    -6.531353     1.849379     110.46
 H       5.698657    -6.708465     1.040690      28.61
 H       3.986296    -6.143067     1.366748      28.30
 H       4.700831    -7.538103     2.122477      23.29
 C       6.051025    -3.477120     3.644775       1.55
 O       6.470984    -3.894707     4.922769     322.78
 H       6.154118    -4.842588     5.143974      31.57
 C       6.126831    -2.072549     3.282888      53.45
 H       6.321096    -1.322683     4.121618      24.39
 C       5.450596    -2.550822     1.043754      53.96
 C       5.264067    -2.336539    -0.472185      92.60
 H       5.718670    -3.245945    -0.975584      24.94
 O       6.134817    -1.268572    -0.973256     158.06
 H       5.815986    -0.329419    -0.741380      23.19
 C       3.752296    -2.215728    -0.958201      69.21
 H       3.241638    -3.134855    -0.632358      20.68
 C       3.640385    -1.955493    -2.505132     104.30
 O       3.674780    -3.237790    -3.224913     290.27
 H       4.452644    -3.128115    -3.788208      27.05
 H       4.455706    -1.388670    -2.829531      23.91
 H       2.623467    -1.457433    -2.555363      23.71
 C      -0.419836    -1.942279     0.362260      16.86
 H      -1.167037    -2.850107     0.506959      19.44
 C      -0.099613     0.527595     0.170496      91.44
 H      -0.585724     1.561763    -0.036889      17.11
 C       1.244276     0.266736    -0.012664      12.29
 O       2.110961     1.384974    -0.272896     204.24
 C       1.757423     2.745008    -0.113037     124.51
 H       2.688667     3.285523     0.069201      24.19
 H       1.131239     3.181279    -1.009126      23.97
 H       1.029526     2.903680     0.652780      27.02
 C       1.813475    -1.030667    -0.036196      18.79
 O       3.220150    -1.074993    -0.086468     163.01
 C       0.932135    -2.175442     0.237606      27.34
 H       1.426820    -3.127785     0.353438      15.34
 C      -0.960324    -0.633063     0.405956      67.98
 C      -2.480056    -0.400314     0.680930      78.00
 H      -2.835857    -1.282726     1.296292      24.04
 O      -2.748971     0.769222     1.416567     301.55
 H      -2.330849     0.741938     2.269691      30.64
 C      -3.334504    -0.243475    -0.629610     100.63
 H      -2.996194     0.628522    -1.084288      27.40
 O      -3.129351    -1.421930    -1.445672     247.77
 H      -2.714897    -1.175306    -2.331526      24.59
 C      -4.865897    -0.087838    -0.293948     116.87
 O      -5.207285     1.216026     0.155406     223.68
 H      -4.756056     1.459506     0.960264      30.38
 H      -5.136623    -0.902040     0.310333      30.50
 H      -5.409841    -0.175627    -1.228561      29.36
55
name = lig-etoh-Waterframe_160
 C       5.886772    -1.582248     1.970890      54.09
 H       5.808142    -0.493157     1.816898      21.12
 C       5.457849    -3.856561     1.347325      42.11
 H       5.260621    -4.611359     0.521547      14.21
 C       5.693347    -4.400535     2.617748      12.60
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 O       5.365128    -5.758272     2.966709     311.39
 C       4.916244    -6.592696     1.861953      97.86
 H       5.732958    -6.553369     1.109884      27.25
 H       4.071170    -6.111773     1.360966      30.05
 H       4.723761    -7.594443     2.255812      23.11
 C       6.053099    -3.478103     3.659186      -6.12
 O       6.457121    -3.933913     4.917004     275.07
 H       6.134608    -4.805010     5.121069      33.77
 C       6.129087    -2.087330     3.329164      51.81
 H       6.556743    -1.519865     4.171030      22.86
 C       5.476845    -2.511249     0.985692      57.29
 C       5.261052    -2.331877    -0.473713      88.89
 H       5.682105    -3.253038    -1.093199      22.08
 O       6.172722    -1.245966    -0.975311     133.43
 H       5.677721    -0.453821    -0.629338      24.91
 C       3.783147    -2.239068    -0.927544      68.58
 H       3.202347    -3.155212    -0.782314      21.35
 C       3.605811    -1.951845    -2.485080     101.82
 O       3.695827    -3.206483    -3.175811     285.61
 H       4.531264    -3.395615    -3.641118      27.27
 H       4.306752    -1.210270    -2.812823      23.63
 H       2.583190    -1.534184    -2.751063      24.78
 C      -0.406638    -1.922571     0.373051      59.59
 H      -1.105248    -2.832686     0.519596      18.51
 C      -0.144453     0.476089     0.185373      80.28
 H      -0.585994     1.500550     0.025712      18.11
 C       1.256363     0.300627    -0.070851      11.17
 O       2.124971     1.343995    -0.277380     227.74
 C       1.741816     2.727324    -0.123706     104.68
 H       2.761772     3.321016     0.152075      22.97
 H       1.410302     3.243585    -1.129238      23.34
 H       1.186422     2.880827     0.854854      24.92
 C       1.780871    -1.065034    -0.021889      21.16
 O       3.195869    -1.142203    -0.063059     174.84
 C       1.010883    -2.154238     0.255901      39.23
 H       1.251497    -3.227050     0.434106      17.53
 C      -0.974798    -0.631720     0.411558      48.24
 C      -2.417850    -0.464677     0.707596      67.02
 H      -2.819407    -1.504227     1.197136      22.63
 O      -2.752671     0.761146     1.419713     283.27
 H      -2.323001     0.733136     2.297009      29.53
 C      -3.315422    -0.254365    -0.607574      95.34
 H      -3.067778     0.627971    -1.104975      27.06
 O      -3.166852    -1.393468    -1.444771     244.51
 H      -2.790324    -1.013921    -2.288825      24.87
 C      -4.850027    -0.094923    -0.280741     101.44
 O      -5.213790     1.236592     0.140441     210.46
 H      -4.492267     1.435785     0.758860      29.19
 H      -5.188540    -0.926119     0.450209      28.13
 H      -5.467579    -0.306106    -1.226064      27.57
55
name = lig-etoh-Waterframe_161
 C       5.893597    -1.598279     2.042256      50.55
 H       6.008132    -0.503460     1.817243      27.23
 C       5.456476    -3.906007     1.341859      50.19
 H       5.257911    -4.681149     0.541994      20.02
 C       5.631068    -4.386454     2.630928      24.32
 O       5.426255    -5.716415     2.992357     216.62
 C       4.929210    -6.612287     1.845821     112.33
 H       5.744636    -6.764495     1.134849      27.58
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 H       4.004897    -6.286884     1.420604      29.07
 H       4.747062    -7.540129     2.422401      26.42
 C       6.068899    -3.505509     3.657225      15.01
 O       6.438741    -3.931468     4.890747     152.97
 H       6.073385    -4.863108     5.181187      24.56
 C       6.149176    -2.125937     3.342092      54.21
 H       6.563317    -1.421520     4.017028      21.33
 C       5.550813    -2.503395     0.975790      12.39
 C       5.307818    -2.286311    -0.551513      81.64
 H       5.641031    -3.304130    -0.994793      21.99
 O       6.143487    -1.219342    -0.968788     212.09
 H       5.837693    -0.298885    -0.816785      28.27
 C       3.790574    -2.188806    -0.909484      80.71
 H       3.424745    -3.208469    -0.667529      24.77
 C       3.593999    -1.927351    -2.417112     101.61
 O       3.712396    -3.214850    -3.141044     253.09
 H       4.667622    -3.187338    -3.454069      25.32
 H       4.320303    -1.169153    -2.837572      24.44
 H       2.537148    -1.640559    -2.644265      27.16
 C      -0.393530    -1.928948     0.419636      50.67
 H      -0.995513    -2.800587     0.603396      24.00
 C      -0.139415     0.450788     0.161154      73.02
 H      -0.574436     1.417109     0.292981      22.45
 C       1.202426     0.294704    -0.104789      14.46
 O       2.181396     1.286995    -0.301808     173.16
 C       1.771442     2.739764    -0.096723      97.76
 H       2.835902     3.254834     0.055648      22.00
 H       1.200223     3.087031    -0.997319      25.31
 H       0.926689     2.877681     0.705426      24.75
 C       1.838535    -1.022756    -0.001847       7.74
 O       3.173105    -1.223559    -0.084168     174.88
 C       0.955263    -2.136393     0.264862      45.39
 H       1.526621    -3.141422     0.319643      22.89
 C      -0.953101    -0.661129     0.414273      45.83
 C      -2.448083    -0.503431     0.658894      78.50
 H      -2.866452    -1.396166     1.286869      25.81
 O      -2.739970     0.750578     1.463923     252.72
 H      -2.329584     0.620774     2.379887      28.15
 C      -3.332525    -0.265176    -0.546858      94.58
 H      -2.924468     0.669071    -1.089551      26.33
 O      -3.189829    -1.377010    -1.480452     207.88
 H      -2.875827    -1.176223    -2.404661      26.27
 C      -4.837469    -0.134453    -0.280042     102.01
 O      -5.212359     1.249521     0.137682     163.69
 H      -4.409096     1.677163     0.478788      30.74
 H      -5.172059    -0.739560     0.672843      27.40
 H      -5.364193    -0.416147    -1.274938      27.85
55
name = lig-etoh-Waterframe_162
 C       5.885794    -1.667083     2.053478      57.74
 H       6.215629    -0.615778     1.893233      22.11
 C       5.445977    -3.915134     1.305954      64.60
 H       5.157405    -4.581426     0.485572      22.34
 C       5.562891    -4.381230     2.646645      30.74
 O       5.469136    -5.702618     2.959182     238.78
 C       4.980418    -6.610662     1.922085     122.69
 H       5.634713    -6.901335     1.110351      27.87
 H       4.059113    -6.298181     1.449281      28.08
 H       4.767462    -7.580887     2.460573      27.31
 C       6.063962    -3.508024     3.637219      21.24
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 O       6.427840    -3.924822     4.901411     137.43
 H       6.101062    -4.992696     5.072504      19.43
 C       6.189198    -2.132361     3.332273      47.29
 H       6.439542    -1.454972     4.109380      24.37
 C       5.614933    -2.582010     1.014779      33.31
 C       5.353693    -2.219056    -0.520879      88.07
 H       5.750227    -2.990405    -1.152247      23.36
 O       6.143397    -1.167639    -1.018847     246.65
 H       5.671331    -0.327378    -0.822981      28.29
 C       3.828683    -2.187610    -0.908012      81.51
 H       3.488380    -3.209216    -0.624876      25.18
 C       3.559687    -1.937579    -2.360498     113.83
 O       3.751251    -3.213134    -3.103320     226.75
 H       4.631858    -3.125602    -3.648999      24.58
 H       4.326198    -1.198848    -2.801580      24.20
 H       2.537922    -1.534664    -2.362511      26.45
 C      -0.413621    -2.007713     0.491823      39.65
 H      -1.024714    -2.797763     0.699263      21.62
 C      -0.145981     0.475883     0.144738      69.92
 H      -0.546783     1.407654     0.347840      20.96
 C       1.274114     0.247563    -0.112494       4.61
 O       2.207569     1.289162    -0.316956     198.89
 C       1.760360     2.679397    -0.119153     111.49
 H       2.592304     3.465451     0.030707      25.09
 H       1.261777     2.986793    -0.957841      28.60
 H       1.128262     2.781914     0.828534      26.63
 C       1.782011    -1.028220    -0.001047      37.11
 O       3.186428    -1.219628    -0.082735     180.38
 C       0.990466    -2.079953     0.241634      54.27
 H       1.477522    -3.126854     0.273844      23.87
 C      -0.978438    -0.697646     0.412606      35.09
 C      -2.497768    -0.476521     0.696732      87.62
 H      -2.823702    -1.329533     1.217393      28.52
 O      -2.707563     0.712410     1.505108     259.47
 H      -2.316610     0.516904     2.460240      27.02
 C      -3.340226    -0.291987    -0.583543      86.15
 H      -2.943480     0.780124    -1.000876      25.83
 O      -3.202093    -1.397945    -1.523688     222.28
 H      -2.893197    -0.947541    -2.358425      26.26
 C      -4.824800    -0.103367    -0.221357     115.85
 O      -5.212712     1.257739     0.100477     161.07
 H      -4.423166     1.794402     0.256616      32.84
 H      -5.112552    -0.911027     0.536947      28.48
 H      -5.427019    -0.418454    -1.105577      28.19
55
name = lig-etoh-Waterframe_163
 C       5.943035    -1.708857     2.022671      54.01
 H       6.044917    -0.658374     1.716071      25.16
 C       5.406706    -3.955174     1.295894      58.88
 H       5.116741    -4.617440     0.524864      21.89
 C       5.547162    -4.365955     2.595430      28.15
 O       5.503982    -5.742539     2.925872     236.37
 C       5.008789    -6.635469     2.001133     121.81
 H       5.767664    -6.701450     1.210436      28.34
 H       4.098157    -6.166542     1.550865      27.29
 H       4.766301    -7.586223     2.560787      24.84
 C       6.042118    -3.506545     3.648670       5.87
 O       6.413159    -3.926305     4.906376     164.08
 H       6.178710    -4.957671     5.203248      20.86
 C       6.205744    -2.150554     3.352546      57.18
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 H       6.428839    -1.533387     4.223049      24.25
 C       5.638423    -2.596087     0.973687      29.12
 C       5.407853    -2.214999    -0.459888      87.07
 H       5.725772    -3.033286    -1.028693      24.92
 O       6.141269    -1.046487    -1.072700     213.71
 H       5.718633    -0.226119    -0.730931      27.24
 C       3.894513    -2.236289    -0.842997      66.89
 H       3.415416    -3.209375    -0.662877      25.04
 C       3.556333    -1.966343    -2.339867     104.26
 O       3.761744    -3.189238    -3.080176     245.84
 H       4.614266    -3.134848    -3.687547      25.09
 H       4.237712    -1.131211    -2.707846      23.33
 H       2.563945    -1.654600    -2.533862      26.57
 C      -0.429384    -2.012759     0.532979      33.43
 H      -0.965406    -2.887726     0.751063      20.35
 C      -0.121954     0.420003     0.145561      71.61
 H      -0.510586     1.401581     0.108825      19.07
 C       1.279422     0.313686    -0.083092      12.17
 O       2.231705     1.308158    -0.325174     225.95
 C       1.722021     2.626156    -0.136277     132.79
 H       2.586106     3.202000    -0.093723      25.76
 H       1.094758     2.949922    -0.906455      28.73
 H       1.256535     2.630444     0.819774      28.81
 C       1.824543    -1.049839    -0.053323      13.79
 O       3.202348    -1.140999    -0.052584     162.36
 C       0.942227    -2.164057     0.249626      46.84
 H       1.418101    -3.170284     0.325494      22.07
 C      -0.996161    -0.693486     0.419802      53.16
 C      -2.477642    -0.477255     0.750252      79.97
 H      -2.873071    -1.354469     1.156990      28.63
 O      -2.683298     0.677137     1.537992     264.04
 H      -2.210773     0.525559     2.499013      25.28
 C      -3.350872    -0.284420    -0.607915      86.53
 H      -3.044356     0.620382    -1.240610      25.54
 O      -3.195769    -1.382480    -1.550824     213.41
 H      -2.909926    -1.049991    -2.453974      24.90
 C      -4.842885    -0.099009    -0.203181     118.22
 O      -5.220956     1.273873     0.058203     194.98
 H      -4.388066     1.719610     0.271568      31.65
 H      -5.061568    -0.691878     0.647346      30.30
 H      -5.459377    -0.329199    -1.021119      29.66
55
name = lig-etoh-Waterframe_164
 C       6.023396    -1.708833     1.983546      52.41
 H       5.917271    -0.656998     1.776018      21.33
 C       5.362877    -3.970394     1.258223      54.72
 H       5.142291    -4.715261     0.552026      22.99
 C       5.596888    -4.426756     2.599543      26.24
 O       5.556478    -5.728705     2.984634     292.48
 C       5.009830    -6.657509     1.995968     132.22
 H       5.758170    -6.901679     1.199918      29.77
 H       4.003853    -6.382547     1.539439      27.28
 H       4.849563    -7.630417     2.507334      25.51
 C       6.008557    -3.538562     3.655983      21.17
 O       6.397721    -3.933761     4.914982     202.75
 H       6.089377    -4.831053     5.078735      30.77
 C       6.181398    -2.166213     3.350495      61.97
 H       6.540235    -1.406397     4.102235      25.85
 C       5.647430    -2.583575     0.965727      58.64
 C       5.443418    -2.209955    -0.499042      91.69
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 H       5.891595    -3.091846    -1.019923      24.55
 O       6.114795    -0.971431    -1.074572     197.18
 H       5.770581    -0.122377    -0.698943      24.45
 C       3.883270    -2.216131    -0.781439      63.32
 H       3.526864    -3.173252    -0.368697      20.10
 C       3.597338    -1.974105    -2.317867      98.52
 O       3.765600    -3.179047    -3.093613     253.35
 H       4.761875    -3.111365    -3.415012      25.39
 H       4.217381    -1.160934    -2.697371      21.81
 H       2.559282    -1.806697    -2.397304      25.76
 C      -0.424321    -1.967750     0.531038      16.03
 H      -1.073029    -2.847688     0.806173      18.08
 C      -0.102839     0.389726     0.137518      84.71
 H      -0.637140     1.327176    -0.103210      14.92
 C       1.282831     0.241625    -0.055433      19.96
 O       2.212716     1.284685    -0.342311     213.53
 C       1.708796     2.623116    -0.124905     127.96
 H       2.533852     3.215589    -0.260305      24.25
 H       0.873723     2.872111    -0.847540      25.21
 H       1.233817     2.739834     0.813214      27.64
 C       1.826487    -1.064589    -0.068209      22.34
 O       3.242314    -1.087628    -0.041572     164.68
 C       0.940493    -2.221684     0.252115      38.87
 H       1.335255    -3.187864     0.390174      18.71
 C      -0.963355    -0.708118     0.455732      57.29
 C      -2.438301    -0.498289     0.691587      66.83
 H      -2.884475    -1.443176     1.230179      23.86
 O      -2.678697     0.669561     1.568200     238.68
 H      -2.124998     0.545111     2.483034      24.25
 C      -3.352664    -0.250009    -0.630252      88.31
 H      -3.041958     0.641360    -1.077624      25.74
 O      -3.192047    -1.383377    -1.547445     221.38
 H      -2.909311    -1.089766    -2.460334      24.26
 C      -4.878895    -0.106769    -0.215021     109.11
 O      -5.209994     1.317146     0.014096     205.92
 H      -4.495780     1.756036     0.512004      29.39
 H      -5.078930    -0.552934     0.714942      30.04
 H      -5.486976    -0.556699    -0.980295      29.13
55
name = lig-etoh-Waterframe_165
 C       6.047361    -1.703148     1.988702      56.96
 H       6.182788    -0.642642     1.874512      21.78
 C       5.378239    -3.959884     1.290793      49.73
 H       5.168511    -4.610001     0.446972      22.71
 C       5.663283    -4.429928     2.592895      24.36
 O       5.576850    -5.764909     3.025127     304.90
 C       5.019859    -6.734222     1.989655     113.90
 H       5.693128    -6.887509     1.103463      28.80
 H       4.033274    -6.358535     1.605725      27.26
 H       4.934393    -7.592903     2.621652      24.71
 C       6.004792    -3.516023     3.641055       9.90
 O       6.368447    -3.942011     4.912818     267.81
 H       6.147285    -4.908022     5.163202      31.90
 C       6.148380    -2.167818     3.279260      66.29
 H       6.533744    -1.468452     4.091564      24.48
 C       5.652488    -2.608875     0.958274      50.50
 C       5.443047    -2.151356    -0.554497      97.16
 H       5.916433    -2.888802    -1.336616      21.40
 O       6.097765    -0.982395    -1.038264     229.82
 H       5.526534    -0.217963    -0.702268      24.17
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 C       3.902901    -2.154287    -0.762394      81.51
 H       3.513862    -3.096926    -0.348833      18.98
 C       3.592329    -2.002497    -2.245481     101.96
 O       3.791793    -3.177201    -3.111876     241.57
 H       4.753939    -3.312670    -3.475173      25.06
 H       4.143598    -1.196387    -2.636781      22.99
 H       2.537605    -1.668665    -2.260517      24.14
 C      -0.379316    -1.994986     0.520670      53.83
 H      -1.168106    -2.812821     0.820852      17.04
 C      -0.116407     0.387311     0.106444      65.69
 H      -0.575287     1.432639    -0.042589      13.76
 C       1.281770     0.159922    -0.061108      15.59
 O       2.149789     1.229534    -0.347415     208.97
 C       1.682831     2.638071    -0.119372     102.72
 H       2.433548     3.431253    -0.372059      23.41
 H       0.890957     2.789483    -1.018673      22.15
 H       1.402697     2.845395     0.940710      25.36
 C       1.821801    -1.145723    -0.005967      28.51
 O       3.270468    -1.081088    -0.057355     186.61
 C       0.999833    -2.192772     0.247561      58.87
 H       1.345267    -3.139390     0.340313      21.30
 C      -0.921485    -0.677256     0.465737      82.57
 C      -2.444205    -0.487161     0.632730      59.07
 H      -2.796850    -1.528168     1.174034      21.20
 O      -2.685782     0.663430     1.552600     248.34
 H      -2.169137     0.438521     2.426391      22.64
 C      -3.345463    -0.236710    -0.608945      92.02
 H      -3.046322     0.691474    -0.978289      26.06
 O      -3.190833    -1.383254    -1.529925     237.93
 H      -2.882073    -0.926671    -2.353295      24.99
 C      -4.863061    -0.070754    -0.194880      97.96
 O      -5.209755     1.341426    -0.063167     206.91
 H      -4.632805     1.663708     0.656058      29.81
 H      -5.033100    -0.723801     0.738691      29.29
 H      -5.578346    -0.514508    -0.965268      27.49
55
name = lig-etoh-Waterframe_166
 C       6.012999    -1.695474     1.938811      60.81
 H       6.402971    -0.739149     1.653610      23.56
 C       5.447491    -3.936891     1.314176      59.34
 H       5.120584    -4.653720     0.500049      22.74
 C       5.701071    -4.439667     2.600397      19.51
 O       5.577687    -5.821881     2.980890     343.46
 C       5.042913    -6.777174     2.038828     126.76
 H       5.733164    -6.809320     1.182975      31.35
 H       4.072138    -6.398620     1.744476      29.22
 H       4.914852    -7.712344     2.511606      27.16
 C       6.027295    -3.530287     3.622175      20.04
 O       6.336004    -3.908840     4.899001     163.91
 H       6.127625    -4.998232     5.060754      22.04
 C       6.148526    -2.171214     3.289666      50.55
 H       6.396769    -1.499294     4.149064      21.80
 C       5.684260    -2.585068     0.914459      44.48
 C       5.428063    -2.150727    -0.552575      98.22
 H       5.644292    -3.085808    -1.211597      21.67
 O       6.083294    -0.982597    -0.968773     289.38
 H       5.615968    -0.075794    -0.795002      21.25
 C       3.939786    -2.155495    -0.777433      84.97
 H       3.562309    -3.151778    -0.505063      22.63
 C       3.566108    -1.999537    -2.235984     107.85
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 O       3.779617    -3.193880    -3.101884     238.22
 H       4.674540    -3.019408    -3.554731      24.96
 H       4.155465    -1.178667    -2.603571      25.73
 H       2.462528    -1.810413    -2.486172      24.78
 C      -0.355091    -1.980257     0.510676      43.65
 H      -0.894220    -2.999302     0.700288      19.61
 C      -0.089937     0.405067     0.074245      72.24
 H      -0.432204     1.502707     0.164400      17.69
 C       1.237180     0.173260    -0.080511      19.23
 O       2.115255     1.207195    -0.339046     181.71
 C       1.658522     2.622669    -0.171669      95.92
 H       2.685635     3.136401    -0.450408      21.83
 H       0.649276     2.914811    -0.728988      22.58
 H       1.324334     2.758677     0.933548      24.33
 C       1.909960    -1.111683     0.050289      12.32
 O       3.258708    -1.092076    -0.068231     175.30
 C       1.014076    -2.239534     0.281551      54.63
 H       1.483493    -3.125457     0.354169      24.49
 C      -0.940267    -0.699194     0.423929      62.12
 C      -2.437214    -0.474480     0.654913      86.16
 H      -2.886280    -1.429761     1.047902      26.59
 O      -2.704225     0.636603     1.495815     307.53
 H      -2.310733     0.501457     2.381015      27.65
 C      -3.343752    -0.241086    -0.569338      91.16
 H      -3.044092     0.658940    -1.205737      24.64
 O      -3.183432    -1.340262    -1.512523     217.58
 H      -2.890146    -1.059921    -2.412679      26.12
 C      -4.824357    -0.044325    -0.181810      95.15
 O      -5.212159     1.323409    -0.126249     210.49
 H      -4.753124     1.798868     0.594644      28.98
 H      -5.095610    -0.610717     0.839089      28.46
 H      -5.458507    -0.361562    -1.101119      26.71
55
name = lig-etoh-Waterframe_167
 C       5.993456    -1.708660     1.926777      46.68
 H       6.124490    -0.677728     1.620261      24.62
 C       5.522943    -3.948292     1.281884      47.94
 H       5.121991    -4.757556     0.581072      18.58
 C       5.700059    -4.491133     2.575810      48.37
 O       5.595111    -5.833190     2.943916     426.82
 C       5.047659    -6.783022     2.053129     155.85
 H       5.667515    -6.938049     1.162241      34.89
 H       4.065283    -6.587675     1.676423      30.04
 H       5.039682    -7.760476     2.499078      29.42
 C       6.067018    -3.542424     3.613553      21.44
 O       6.305642    -3.874347     4.891777      63.57
 H       5.992937    -4.884509     5.108092      23.35
 C       6.150708    -2.149151     3.286757      59.71
 H       6.329325    -1.429265     4.068502      24.18
 C       5.705157    -2.595074     0.903849      53.04
 C       5.384914    -2.211585    -0.488653      91.72
 H       5.902398    -2.944147    -1.094703      22.05
 O       6.118957    -0.980985    -0.924874     186.24
 H       5.549915    -0.160287    -0.608838      24.43
 C       3.879173    -2.213312    -0.819129      75.60
 H       3.571750    -3.195602    -0.411233      22.31
 C       3.526026    -1.974020    -2.336351     105.46
 O       3.776806    -3.188388    -3.079408     246.95
 H       4.663216    -3.123403    -3.558416      25.85
 H       4.086252    -1.099570    -2.775495      23.35
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 H       2.377966    -1.779274    -2.270588      24.31
 C      -0.327138    -2.005554     0.481870      44.97
 H      -1.024227    -2.851328     0.662182      19.13
 C      -0.132196     0.380032     0.103740      78.01
 H      -0.586021     1.410957     0.183423      18.47
 C       1.278924     0.186961    -0.096805      16.33
 O       2.104905     1.237362    -0.349831     216.65
 C       1.667824     2.543940    -0.179104     114.88
 H       2.581110     3.242403    -0.505161      24.29
 H       0.912584     2.872183    -0.984740      25.13
 H       1.496254     2.803738     0.908815      25.10
 C       1.867133    -1.070171     0.080914      25.38
 O       3.275769    -1.103300    -0.061281     175.61
 C       1.098384    -2.188717     0.321299      62.14
 H       1.437054    -3.168186     0.540782      23.88
 C      -0.963371    -0.731532     0.355835      53.33
 C      -2.442060    -0.510482     0.675036      99.23
 H      -2.796621    -1.341507     1.140322      28.98
 O      -2.733838     0.646495     1.454897     315.23
 H      -2.330839     0.534196     2.294661      31.45
 C      -3.310253    -0.225610    -0.603921      82.46
 H      -2.986027     0.838223    -1.105234      24.00
 O      -3.182790    -1.341689    -1.501345     212.97
 H      -2.940539    -0.945786    -2.377222      25.62
 C      -4.797854    -0.025604    -0.205180     103.84
 O      -5.229470     1.337004    -0.175223     236.35
 H      -4.698288     1.970070     0.356253      28.07
 H      -5.162704    -0.531278     0.741968      28.81
 H      -5.315178    -0.625340    -1.000567      27.67
55
name = lig-etoh-Waterframe_168
 C       5.981268    -1.705897     1.964488      59.96
 H       5.744963    -0.637616     1.892326      26.41
 C       5.572061    -4.049307     1.238024      67.56
 H       5.298752    -4.638987     0.329602      21.65
 C       5.720230    -4.461939     2.551310      25.67
 O       5.609386    -5.807810     2.930416     202.26
 C       5.043513    -6.834810     1.987798     107.69
 H       5.674791    -6.944826     1.092206      26.56
 H       3.991698    -6.583654     1.748595      27.30
 H       5.098985    -7.646578     2.743537      25.45
 C       6.084960    -3.523970     3.564400      16.42
 O       6.272891    -3.856583     4.925181     128.26
 H       6.139943    -4.771855     5.167449      24.18
 C       6.150236    -2.146679     3.243215      51.98
 H       6.332264    -1.456278     4.012221      23.36
 C       5.688710    -2.672384     0.962658      11.84
 C       5.413063    -2.233653    -0.502221      73.88
 H       5.832486    -2.931713    -1.165994      26.05
 O       6.130866    -1.011159    -0.867553     166.40
 H       5.611234    -0.153561    -0.580338      24.55
 C       3.827510    -2.236198    -0.867587      66.06
 H       3.281357    -3.161281    -0.585044      24.29
 C       3.482699    -1.971989    -2.370787     102.50
 O       3.769005    -3.183011    -3.089671     256.77
 H       4.680236    -3.211497    -3.445347      27.83
 H       3.983858    -1.047571    -2.838838      24.71
 H       2.387472    -1.762202    -2.452674      26.84
 C      -0.323543    -2.028486     0.435476      47.35
 H      -0.921768    -2.830663     0.692863      23.84
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 C      -0.146372     0.351397     0.137294      71.35
 H      -0.647886     1.290174     0.047694      21.05
 C       1.225793     0.229130    -0.074757      11.77
 O       2.161751     1.241518    -0.383989     201.97
 C       1.708370     2.583392    -0.214465     128.87
 H       2.543700     3.247463    -0.422865      25.97
 H       0.929654     2.704305    -0.858117      28.36
 H       1.299329     2.803878     0.754153      28.39
 C       1.886446    -1.046667     0.052615      10.16
 O       3.289911    -1.118393    -0.042984     161.21
 C       1.065315    -2.151396     0.395563      50.26
 H       1.584968    -3.154425     0.586590      22.27
 C      -0.941268    -0.777277     0.319871      51.40
 C      -2.460861    -0.552617     0.643696      85.21
 H      -2.794819    -1.441416     1.197460      26.41
 O      -2.743296     0.686866     1.445491     278.31
 H      -2.276626     0.581041     2.255124      32.19
 C      -3.282644    -0.221633    -0.587508      87.51
 H      -2.799003     0.750313    -1.006261      25.45
 O      -3.171860    -1.343759    -1.528049     197.78
 H      -3.010964    -0.973173    -2.436960      26.10
 C      -4.790532    -0.032379    -0.235963     109.49
 O      -5.269300     1.373933    -0.250010     229.25
 H      -4.527583     1.872854     0.153481      30.18
 H      -4.861075    -0.475566     0.699456      30.74
 H      -5.440780    -0.469009    -0.951882      28.31
55
name = lig-etoh-Waterframe_169
 C       5.901263    -1.708472     1.951146      58.38
 H       5.722914    -0.628761     1.742934      27.19
 C       5.617829    -4.086029     1.166385      61.34
 H       5.512902    -4.833201     0.386030      19.83
 C       5.757579    -4.477949     2.535228      22.28
 O       5.609991    -5.780490     2.909988     281.30
 C       5.052572    -6.829709     1.986954     115.94
 H       5.672412    -7.017305     1.081108      28.14
 H       3.981653    -6.545341     1.730336      26.97
 H       4.998901    -7.825528     2.567209      25.88
 C       6.085502    -3.532970     3.581403      14.95
 O       6.250336    -3.821099     4.927052      80.36
 H       6.084522    -4.797527     5.059419      22.40
 C       6.169862    -2.176386     3.276796      49.03
 H       6.333402    -1.528191     4.108050      23.10
 C       5.652916    -2.692766     0.953971       7.83
 C       5.405525    -2.258183    -0.540183      69.59
 H       5.699180    -3.086321    -1.194106      24.96
 O       6.123021    -1.061512    -0.807536     196.97
 H       5.644043    -0.168401    -0.685116      24.88
 C       3.814558    -2.181702    -0.896199      73.00
 H       3.374027    -3.180377    -0.691016      24.73
 C       3.447804    -1.958478    -2.373551     106.73
 O       3.758658    -3.195382    -3.134019     253.14
 H       4.635999    -3.029052    -3.472696      28.12
 H       4.096742    -1.122373    -2.759302      25.23
 H       2.442003    -1.862865    -2.599784      27.52
 C      -0.356460    -2.079467     0.428485      46.41
 H      -0.806208    -2.970072     0.663423      22.99
 C      -0.147415     0.377647     0.124186      57.31
 H      -0.590859     1.305808     0.042662      21.27
 C       1.267305     0.238964    -0.055805      10.45
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 O       2.213019     1.234813    -0.403440     159.97
 C       1.704347     2.664418    -0.255642     121.26
 H       2.521605     3.254207    -0.407034      27.53
 H       0.925129     2.868471    -0.925866      27.96
 H       1.267836     2.719612     0.702192      28.49
 C       1.883880    -1.031319     0.025669      16.56
 O       3.270776    -1.133559    -0.030897     182.06
 C       1.062682    -2.125305     0.430453      41.23
 H       1.638753    -3.151360     0.586096      22.17
 C      -0.966833    -0.802107     0.340809      32.22
 C      -2.444363    -0.552935     0.637820      76.74
 H      -2.956903    -1.529169     1.145449      23.08
 O      -2.713811     0.691409     1.432190     269.14
 H      -2.255808     0.601975     2.292282      28.82
 C      -3.283232    -0.254272    -0.621976      92.87
 H      -2.848085     0.562802    -1.092292      27.13
 O      -3.151366    -1.337935    -1.577382     212.66
 H      -3.031400    -1.003002    -2.505095      25.46
 C      -4.801763     0.004652    -0.270960     105.25
 O      -5.266752     1.380497    -0.316119     248.27
 H      -4.667779     2.034098     0.132787      29.00
 H      -4.947219    -0.340587     0.732461      30.00
 H      -5.441076    -0.530143    -0.942465      28.45
55
name = lig-etoh-Waterframe_170
 C       5.799617    -1.769279     1.945645      44.06
 H       5.958168    -0.738408     1.568382      21.65
 C       5.677119    -4.072831     1.187598      62.96
 H       5.576372    -4.852879     0.485270      21.27
 C       5.798068    -4.497713     2.492912       9.47
 O       5.599823    -5.831538     2.905297     260.20
 C       5.051711    -6.773621     2.007194     122.08
 H       5.707245    -6.905932     1.123543      27.91
 H       4.071731    -6.447290     1.547915      28.42
 H       4.962559    -7.781485     2.541343      24.98
 C       6.066575    -3.555545     3.589777       3.24
 O       6.232039    -3.821300     4.910552     173.39
 H       5.932633    -4.822811     5.226564      18.40
 C       6.162924    -2.168916     3.269388      45.86
 H       6.345215    -1.480908     4.124317      24.39
 C       5.599510    -2.679074     0.851723       4.48
 C       5.307305    -2.277806    -0.545534      97.99
 H       5.855656    -3.035694    -1.227902      22.42
 O       6.137495    -1.100329    -0.790882     245.87
 H       5.488435    -0.343454    -0.718282      27.36
 C       3.829508    -2.151206    -0.886071      89.46
 H       3.547558    -3.137255    -0.497359      24.02
 C       3.457956    -1.952467    -2.400465     109.89
 O       3.769209    -3.183254    -3.184520     263.20
 H       4.588796    -3.139734    -3.678424      28.83
 H       4.003287    -1.122693    -2.830462      25.71
 H       2.440510    -1.671749    -2.405391      26.07
 C      -0.348648    -2.100149     0.467702      43.68
 H      -0.995455    -2.993043     0.583590      17.62
 C      -0.119607     0.366197     0.092956      50.17
 H      -0.556705     1.317278     0.154104      17.96
 C       1.324140     0.248526    -0.069325       7.87
 O       2.200586     1.292254    -0.414814     195.94
 C       1.696193     2.673725    -0.287178     112.75
 H       2.552539     3.317576    -0.362004      25.52
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 H       1.050558     3.032641    -1.214428      24.54
 H       1.370214     2.855111     0.767850      26.42
 C       1.840400    -1.053970     0.047022      33.44
 O       3.247740    -1.140779    -0.033313     213.42
 C       1.074511    -2.123348     0.391973      47.95
 H       1.537122    -3.167934     0.591301      21.37
 C      -0.971620    -0.777058     0.387709      41.64
 C      -2.460872    -0.518779     0.630206      74.70
 H      -2.911501    -1.472414     1.209445      21.00
 O      -2.660924     0.659000     1.404605     286.07
 H      -2.250837     0.463352     2.337121      25.26
 C      -3.303014    -0.263692    -0.704905      88.24
 H      -3.014216     0.641387    -1.124297      26.68
 O      -3.137995    -1.359443    -1.629362     246.11
 H      -2.929805    -0.912558    -2.494280      23.66
 C      -4.803494     0.048739    -0.274316      98.05
 O      -5.248330     1.395135    -0.402956     229.78
 H      -4.843493     2.035430     0.250180      27.96
 H      -5.173918    -0.340845     0.763428      28.68
 H      -5.368199    -0.601273    -0.990241      27.99
55
name = lig-etoh-Waterframe_171
 C       5.760383    -1.818299     1.901313      60.61
 H       5.933977    -0.743539     1.756108      23.39
 C       5.704001    -4.053712     1.186496      58.50
 H       5.511399    -4.699929     0.366310      15.46
 C       5.839088    -4.511224     2.550931      15.21
 O       5.604732    -5.855856     2.937688     342.23
 C       5.044423    -6.730272     1.948375     131.82
 H       5.796209    -6.931946     1.191925      30.81
 H       4.102325    -6.342687     1.576496      30.32
 H       4.836473    -7.594839     2.593480      26.12
 C       6.032108    -3.554404     3.550295      14.06
 O       6.210382    -3.853048     4.922011     200.86
 H       6.013202    -4.948442     5.105741      19.13
 C       6.094851    -2.195307     3.195302      51.57
 H       6.366956    -1.367281     3.930951      21.88
 C       5.552228    -2.730800     0.873170      31.58
 C       5.313600    -2.263205    -0.569853     101.38
 H       5.588885    -3.142102    -1.317301      24.07
 O       6.120788    -1.097666    -0.807827     263.40
 H       5.667598    -0.213658    -0.737008      26.68
 C       3.834166    -2.188338    -0.871301      80.13
 H       3.297432    -3.123724    -0.649122      23.96
 C       3.516648    -1.953110    -2.413998     106.09
 O       3.751343    -3.148560    -3.222411     255.48
 H       4.653067    -3.067555    -3.595241      28.20
 H       3.998558    -1.106733    -2.838010      26.01
 H       2.389505    -1.795436    -2.453986      25.27
 C      -0.359811    -2.008456     0.510785      13.23
 H      -1.040194    -2.962531     0.609714      20.34
 C      -0.071564     0.335608     0.091598      59.23
 H      -0.542359     1.332923     0.159812      15.85
 C       1.276163     0.267662    -0.099856      25.46
 O       2.148315     1.350147    -0.418631     231.79
 C       1.745920     2.700098    -0.312878      97.57
 H       2.737190     3.266002    -0.375665      21.03
 H       0.868707     2.914053    -1.186540      22.04
 H       1.048272     2.975083     0.596657      23.45
 C       1.876219    -1.042549     0.062530      23.58
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 O       3.241341    -1.126843    -0.044950     206.86
 C       1.005927    -2.224640     0.345130      66.21
 H       1.590602    -3.135667     0.455653      17.91
 C      -0.897323    -0.761783     0.406838      56.58
 C      -2.468755    -0.507679     0.572866      85.27
 H      -2.856331    -1.365786     1.071980      26.96
 O      -2.615232     0.646007     1.394367     292.79
 H      -2.194324     0.422775     2.353444      24.23
 C      -3.325307    -0.238880    -0.699115      81.84
 H      -2.961823     0.737861    -1.192522      22.99
 O      -3.132799    -1.356215    -1.656661     239.81
 H      -2.847658    -1.087487    -2.584186      22.43
 C      -4.828062     0.014965    -0.303786      88.62
 O      -5.226865     1.429776    -0.497345     180.43
 H      -4.832836     1.890468     0.293357      28.69
 H      -4.953762    -0.409688     0.808369      28.61
 H      -5.516994    -0.422415    -1.097084      26.96
55
name = lig-etoh-Waterframe_172
 C       5.772486    -1.778302     1.865210      60.45
 H       5.548221    -0.725769     1.660073      23.80
 C       5.680943    -4.129737     1.201632      49.93
 H       5.519475    -4.860061     0.394885      16.47
 C       5.837942    -4.534408     2.551504      16.95
 O       5.633643    -5.826097     2.977265     271.37
 C       5.029437    -6.717368     1.910511     120.25
 H       5.718180    -7.064635     1.138903      30.38
 H       4.210807    -6.217547     1.430056      29.62
 H       4.682933    -7.603848     2.364324      28.03
 C       6.021271    -3.561420     3.600296       8.83
 O       6.194919    -3.885158     4.893534     221.34
 H       5.938472    -4.849805     5.112870      25.49
 C       6.011670    -2.230455     3.141241      64.89
 H       6.299850    -1.450303     3.922036      23.02
 C       5.538215    -2.746680     0.884188      31.68
 C       5.329847    -2.284188    -0.559143     100.38
 H       5.758476    -3.032998    -1.258406      25.98
 O       6.106775    -1.079076    -0.860544     200.02
 H       5.612661    -0.244390    -0.688886      26.76
 C       3.783437    -2.201994    -0.907552      81.15
 H       3.332407    -3.205426    -0.699215      23.58
 C       3.533422    -1.937979    -2.396007     102.16
 O       3.759201    -3.106698    -3.248228     248.83
 H       4.718776    -3.118492    -3.520352      27.14
 H       4.093677    -1.081429    -2.750092      24.53
 H       2.380674    -1.833476    -2.595615      24.65
 C      -0.361963    -2.008523     0.536753      38.48
 H      -1.104158    -2.899215     0.816359      17.42
 C      -0.094967     0.389905     0.119113      65.29
 H      -0.600500     1.418804    -0.044374      15.94
 C       1.296831     0.240103    -0.121068      12.68
 O       2.102144     1.329485    -0.402127     208.29
 C       1.698706     2.750965    -0.353741      96.40
 H       2.637878     3.449818    -0.435857      23.53
 H       1.163233     3.048566    -1.317255      24.16
 H       1.199727     2.953430     0.660965      23.92
 C       1.843450    -1.075185     0.058613      21.29
 O       3.261814    -1.108296    -0.070203     198.28
 C       1.049653    -2.205956     0.279628      73.59
 H       1.346747    -3.191038     0.342543      21.99
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 C      -0.919521    -0.706741     0.378808      53.70
 C      -2.402011    -0.522947     0.521587      90.09
 H      -2.828961    -1.386280     0.892505      26.44
 O      -2.596982     0.667283     1.401237     248.21
 H      -2.082067     0.437580     2.327967      25.56
 C      -3.315419    -0.213473    -0.723959      80.32
 H      -2.869881     0.769511    -1.278615      22.86
 O      -3.137610    -1.341935    -1.614376     222.82
 H      -2.957744    -0.940674    -2.522182      22.60
 C      -4.843397    -0.006570    -0.399858     100.85
 O      -5.182419     1.434392    -0.538635     169.26
 H      -4.745081     2.044242     0.127095      28.16
 H      -5.061442    -0.262288     0.678943      29.67
 H      -5.543574    -0.688392    -0.977963      28.39
55
name = lig-etoh-Waterframe_173
 C       5.742633    -1.758341     1.824317      47.03
 H       5.447492    -0.750897     1.566732      27.36
 C       5.628049    -4.172366     1.217989      59.46
 H       5.576644    -5.017630     0.477849      20.74
 C       5.804346    -4.522763     2.538048      21.26
 O       5.647622    -5.868938     2.958943     229.16
 C       5.011463    -6.709362     1.905060     117.41
 H       5.834456    -6.972439     1.192327      28.98
 H       4.310935    -6.084685     1.346507      28.47
 H       4.561899    -7.536562     2.391895      27.65
 C       6.004786    -3.584672     3.556777      11.01
 O       6.191359    -3.897035     4.891699     239.33
 H       5.841040    -4.788739     5.181729      24.19
 C       5.971229    -2.208925     3.209717      33.06
 H       6.026676    -1.518602     4.069458      19.71
 C       5.573479    -2.765494     0.850537       4.03
 C       5.330425    -2.320787    -0.566255      73.07
 H       5.852258    -2.998250    -1.134097      25.33
 O       6.076269    -1.064280    -0.920456     139.96
 H       5.502879    -0.330340    -0.666067      29.24
 C       3.796842    -2.212099    -0.934939      84.79
 H       3.407987    -3.155086    -0.499348      24.71
 C       3.506358    -1.915950    -2.410229     105.93
 O       3.796920    -3.079838    -3.253894     255.06
 H       4.725692    -3.130617    -3.687041      25.33
 H       4.161340    -1.052742    -2.685391      25.28
 H       2.431571    -1.475645    -2.498188      25.65
 C      -0.336289    -1.984566     0.524143      39.74
 H      -0.942802    -2.866226     0.873215      19.82
 C      -0.110183     0.467159     0.100156      83.91
 H      -0.577611     1.501178    -0.163951      17.43
 C       1.244024     0.232625    -0.087841      11.97
 O       2.123174     1.306185    -0.397356     156.34
 C       1.643911     2.785681    -0.400745     113.63
 H       2.670282     3.245649    -0.343476      24.61
 H       1.037773     3.060848    -1.143883      28.31
 H       1.141530     3.029941     0.514860      27.40
 C       1.869291    -1.067372    -0.004752      21.35
 O       3.261638    -1.119854    -0.116022     188.51
 C       1.009981    -2.175879     0.256861      59.93
 H       1.423946    -3.135050     0.255879      23.14
 C      -0.938265    -0.706919     0.332901      65.70
 C      -2.400640    -0.470533     0.526133      81.95
 H      -2.814536    -1.468515     0.986838      25.16
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 O      -2.596277     0.670178     1.398456     245.08
 H      -2.111602     0.457658     2.329960      27.49
 C      -3.272460    -0.198480    -0.755214      93.45
 H      -2.983675     0.795846    -1.279443      25.12
 O      -3.137442    -1.320561    -1.563187     221.77
 H      -3.068385    -1.051228    -2.537894      23.46
 C      -4.813333     0.037816    -0.422833     106.69
 O      -5.164158     1.423447    -0.598646     205.58
 H      -4.476399     1.869498    -0.009570      30.47
 H      -5.055465    -0.227323     0.539375      32.32
 H      -5.381019    -0.547151    -1.154023      29.90
55
name = lig-etoh-Waterframe_174
 C       5.693991    -1.823656     1.894682      40.44
 H       5.710101    -0.776917     1.652436      19.98
 C       5.587842    -4.120663     1.186363      60.10
 H       5.538400    -4.846741     0.309028      22.80
 C       5.750881    -4.570967     2.544917       8.48
 O       5.644355    -5.914745     2.911905     325.77
 C       5.020399    -6.691594     1.911275     123.12
 H       5.809984    -7.167122     1.237603      25.59
 H       4.191966    -6.149842     1.363560      27.11
 H       4.536007    -7.514849     2.468442      24.76
 C       5.985578    -3.555902     3.541316      -3.78
 O       6.194614    -3.883838     4.884356     266.97
 H       5.844970    -4.960076     5.150704      17.10
 C       5.915819    -2.155956     3.232975      48.97
 H       5.800519    -1.485522     4.040585      21.25
 C       5.625081    -2.789085     0.849468      29.85
 C       5.355609    -2.330413    -0.626514      90.75
 H       5.614383    -3.139156    -1.317819      26.18
 O       6.010579    -1.082381    -0.962351     225.04
 H       5.582869    -0.253720    -0.741997      25.78
 C       3.849630    -2.245298    -0.915276      82.03
 H       3.303083    -3.172489    -0.696365      26.52
 C       3.535409    -1.878916    -2.427514     103.68
 O       3.807655    -3.065951    -3.248822     260.52
 H       4.625852    -2.764880    -3.763036      25.67
 H       4.265970    -1.075066    -2.721834      25.36
 H       2.485716    -1.636383    -2.614707      25.39
 C      -0.356627    -1.930492     0.486195      37.16
 H      -0.918694    -2.764586     0.723898      20.42
 C      -0.148926     0.443939     0.039777      84.25
 H      -0.582577     1.477453    -0.033841      15.76
 C       1.245992     0.286388    -0.065048      17.56
 O       2.135900     1.325422    -0.398323     210.06
 C       1.625338     2.731171    -0.397805     128.58
 H       2.533874     3.321725    -0.524042      24.61
 H       0.965338     2.910701    -1.209464      27.38
 H       1.070482     2.965453     0.444122      29.75
 C       1.853421    -1.025498    -0.071957      20.55
 O       3.252137    -1.126684    -0.170385     180.81
 C       1.038781    -2.142883     0.239128      52.14
 H       1.549988    -3.106779     0.321304      21.58
 C      -0.915619    -0.670020     0.295996      50.70
 C      -2.451401    -0.417618     0.557129      65.40
 H      -2.927254    -1.398341     1.118080      23.40
 O      -2.615181     0.683829     1.396146     273.42
 H      -2.235793     0.440219     2.313985      26.48
 C      -3.258643    -0.138572    -0.723044     110.36
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 H      -2.836502     0.657606    -1.247853      26.42
 O      -3.120969    -1.344478    -1.557089     215.50
 H      -2.958079    -1.099649    -2.528711      23.54
 C      -4.755966     0.069107    -0.449827     107.71
 O      -5.138565     1.440952    -0.647158     224.46
 H      -4.448843     2.027471    -0.181471      30.22
 H      -5.034195    -0.387271     0.480191      30.85
 H      -5.274144    -0.367282    -1.268965      28.46
55
name = lig-etoh-Waterframe_175
 C       5.680514    -1.835885     1.923094      53.33
 H       5.817898    -0.795270     1.686816      23.78
 C       5.579866    -4.120839     1.171191      50.23
 H       5.393034    -4.810950     0.314683      20.98
 C       5.708743    -4.543687     2.510090       7.03
 O       5.648449    -5.898842     2.881345     326.30
 C       4.992996    -6.775435     1.910142     114.14
 H       5.650623    -7.214409     1.122544      26.52
 H       4.201162    -6.203366     1.324504      26.64
 H       4.533210    -7.615910     2.519703      24.47
 C       5.939488    -3.565917     3.586916      14.93
 O       6.196440    -3.872714     4.855456     196.39
 H       5.934008    -4.892389     5.156008      21.32
 C       5.834233    -2.193163     3.258956      60.10
 H       5.856315    -1.407349     3.958673      22.50
 C       5.651886    -2.733394     0.841793      11.81
 C       5.336060    -2.327814    -0.634487      84.16
 H       5.751011    -3.084792    -1.463630      22.28
 O       5.979033    -1.126335    -1.017126     261.37
 H       5.435249    -0.387752    -0.736169      28.47
 C       3.808741    -2.230457    -0.949612      84.58
 H       3.383115    -3.217821    -0.778154      25.22
 C       3.598126    -1.882167    -2.422889     111.79
 O       3.824683    -3.038790    -3.250983     245.41
 H       4.668654    -3.043568    -3.865225      24.99
 H       4.145271    -0.987882    -2.782528      24.40
 H       2.591202    -1.671164    -2.520417      26.41
 C      -0.348949    -1.928642     0.416095      31.96
 H      -1.010796    -2.679830     0.589061      19.25
 C      -0.124185     0.454905    -0.022345      91.52
 H      -0.650155     1.370312     0.055380      14.96
 C       1.291356     0.331745    -0.107605      14.56
 O       2.142587     1.373265    -0.384438     217.84
 C       1.604574     2.653282    -0.413003     119.00
 H       2.295271     3.436294    -0.583229      26.18
 H       0.889158     2.701822    -1.412585      22.78
 H       1.133789     2.882794     0.562402      27.50
 C       1.833003    -0.982412    -0.103219      28.63
 O       3.243274    -1.111717    -0.207184     195.18
 C       1.065438    -2.081046     0.227510      50.28
 H       1.436957    -3.121594     0.454582      20.21
 C      -0.995527    -0.651384     0.299870      56.79
 C      -2.454111    -0.423459     0.580787      82.89
 H      -2.925761    -1.355641     0.994509      22.50
 O      -2.652704     0.750270     1.425118     293.46
 H      -2.260532     0.510338     2.287817      27.33
 C      -3.220437    -0.131116    -0.711048     104.37
 H      -2.763887     0.662868    -1.178301      26.70
 O      -3.085793    -1.374616    -1.553427     212.72
 H      -2.807313    -0.944889    -2.408282      24.03
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 C      -4.713615     0.104469    -0.534815      94.90
 O      -5.116998     1.505139    -0.665563     226.18
 H      -4.563896     2.247727    -0.254437      28.58
 H      -5.135299    -0.349984     0.493338      27.81
 H      -5.239900    -0.501049    -1.275915      27.50
55
name = lig-etoh-Waterframe_176
 C       5.713635    -1.776591     1.875199      41.03
 H       5.645283    -0.702438     1.691585      21.21
 C       5.578130    -4.099926     1.155444      58.48
 H       5.358996    -4.910354     0.489382      20.06
 C       5.687735    -4.494564     2.486367       9.32
 O       5.647273    -5.868869     2.844860     208.09
 C       4.947935    -6.867325     1.898259     108.56
 H       5.727777    -7.154083     1.231513      28.53
 H       4.101166    -6.325717     1.445964      27.57
 H       4.537541    -7.675952     2.572192      25.63
 C       5.848901    -3.601448     3.564016       0.91
 O       6.215556    -3.890754     4.877340     236.62
 H       5.844718    -4.738670     5.126336      25.67
 C       5.761599    -2.248982     3.274647      47.69
 H       6.042233    -1.552588     4.065137      21.30
 C       5.615459    -2.716523     0.822196      22.53
 C       5.304190    -2.328409    -0.611600      89.44
 H       5.849178    -3.229297    -1.155661      24.56
 O       5.971274    -1.135876    -1.067313     244.42
 H       5.485434    -0.347161    -0.773118      28.39
 C       3.790615    -2.210169    -0.991701      84.23
 H       3.262307    -3.086456    -0.611648      23.63
 C       3.612077    -1.884837    -2.450327     107.50
 O       3.847625    -3.054228    -3.286945     258.24
 H       4.853935    -3.067662    -3.585465      26.25
 H       4.228110    -1.007938    -2.705005      22.66
 H       2.585443    -1.624838    -2.530691      26.76
 C      -0.381177    -1.910288     0.337974      36.95
 H      -0.891551    -2.861674     0.571477      19.63
 C      -0.127831     0.481127    -0.026583      63.09
 H      -0.483342     1.444726    -0.075113      14.04
 C       1.273474     0.332428    -0.195585      22.69
 O       2.208428     1.385871    -0.365125     203.69
 C       1.531657     2.664498    -0.461943     110.96
 H       2.379566     3.313803    -0.620029      22.76
 H       0.508526     2.728849    -1.180334      21.57
 H       0.963544     2.908673     0.550397      24.85
 C       1.886162    -0.956862    -0.106440      21.72
 O       3.235805    -1.084086    -0.224973     218.24
 C       0.990466    -2.047864     0.235210      52.43
 H       1.562227    -3.033594     0.356495      17.26
 C      -0.955755    -0.657033     0.299753      50.24
 C      -2.457426    -0.420978     0.603117      84.62
 H      -2.812679    -1.264658     1.048382      24.39
 O      -2.686764     0.806304     1.455926     303.26
 H      -2.238053     0.647371     2.266778      28.04
 C      -3.183240    -0.176794    -0.731440      83.72
 H      -2.769070     0.752460    -1.240557      22.66
 O      -3.021050    -1.351932    -1.542360     235.92
 H      -2.813263    -1.174266    -2.499636      23.22
 C      -4.711699     0.173838    -0.587659      85.77
 O      -5.130242     1.574926    -0.708639     226.47
 H      -4.432779     1.995569    -0.106156      28.53
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 H      -5.043519    -0.124840     0.530090      27.47
 H      -5.258633    -0.344839    -1.421735      27.28
55
name = lig-etoh-Waterframe_177
 C       5.728740    -1.750752     1.898457      56.08
 H       5.585117    -0.680003     1.660384      21.57
 C       5.563851    -4.064293     1.153912      41.97
 H       5.462510    -4.749595     0.352597      20.43
 C       5.657544    -4.547931     2.480759      14.74
 O       5.617819    -5.870803     2.802207     221.64
 C       4.944647    -6.862488     1.935278     127.28
 H       5.610021    -7.297427     1.216698      28.02
 H       4.059031    -6.559718     1.415119      28.80
 H       4.716916    -7.703088     2.619698      26.15
 C       5.782638    -3.603016     3.563676      -4.33
 O       6.218013    -3.928534     4.876881     293.21
 H       5.822363    -4.792428     5.225106      24.75
 C       5.751754    -2.222157     3.188337      54.48
 H       5.961860    -1.643376     4.134763      21.61
 C       5.531294    -2.692201     0.845438      31.56
 C       5.293150    -2.328971    -0.595572     106.19
 H       5.561620    -3.153260    -1.254141      26.56
 O       5.984261    -1.137591    -1.097992     259.62
 H       5.611078    -0.277512    -0.818464      27.17
 C       3.792547    -2.215775    -0.959819      77.17
 H       3.196222    -3.126672    -0.748462      22.12
 C       3.580641    -1.892663    -2.500000      98.73
 O       3.877463    -3.080922    -3.308111     259.16
 H       4.859817    -2.965897    -3.634345      25.88
 H       4.331155    -1.151712    -2.759150      20.91
 H       2.530154    -1.583786    -2.820806      23.61
 C      -0.402895    -1.932432     0.304185      67.64
 H      -1.054937    -2.892220     0.585773      18.74
 C      -0.108991     0.498277    -0.010178      52.65
 H      -0.581555     1.435880    -0.132334      16.27
 C       1.288066     0.299397    -0.268365      14.43
 O       2.196737     1.386917    -0.365453     174.48
 C       1.449219     2.724119    -0.463232     103.14
 H       2.184164     3.478916    -0.848957      25.34
 H       0.772984     2.714298    -1.363096      24.47
 H       1.127612     3.026879     0.596829      23.89
 C       1.846645    -0.971768    -0.087323      21.87
 O       3.261719    -1.037243    -0.231305     214.71
 C       1.027464    -2.012339     0.192777      61.18
 H       1.401371    -3.072779     0.282315      19.92
 C      -0.926743    -0.591204     0.295437      54.42
 C      -2.429593    -0.367182     0.627203      75.81
 H      -2.824219    -1.214636     1.186743      23.96
 O      -2.706608     0.821522     1.443169     320.84
 H      -2.255112     0.654980     2.239163      29.30
 C      -3.199842    -0.154845    -0.777606      64.54
 H      -2.573132     0.727015    -1.330592      21.93
 O      -2.951408    -1.357768    -1.538419     212.16
 H      -2.911025    -1.026753    -2.486210      23.14
 C      -4.737362     0.229944    -0.610909     100.31
 O      -5.098479     1.625532    -0.751166     246.69
 H      -4.655511     2.226089    -0.038324      26.23
 H      -5.099288    -0.238724     0.319339      29.31
 H      -5.343224    -0.313409    -1.401739      27.66
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name = lig-etoh-Waterframe_178
 C       5.677574    -1.734830     1.876916      55.80
 H       5.749244    -0.630705     1.709623      22.46
 C       5.528131    -4.049940     1.155204      23.92
 H       5.557213    -4.649040     0.271918      16.62
 C       5.610579    -4.557453     2.471855      26.37
 O       5.581888    -5.922971     2.773436     313.79
 C       4.963058    -6.875680     1.971788     136.26
 H       5.610127    -7.245905     1.143060      28.47
 H       4.043652    -6.493526     1.542331      29.26
 H       4.750924    -7.648820     2.699000      25.11
 C       5.769513    -3.610827     3.549757      13.12
 O       6.191653    -3.942875     4.824803     312.85
 H       5.756303    -4.950210     5.165250      18.16
 C       5.807299    -2.228716     3.217554      55.74
 H       5.738879    -1.345604     3.949413      20.88
 C       5.475480    -2.659966     0.881729      34.89
 C       5.250846    -2.296174    -0.640081     123.96
 H       5.624193    -3.021499    -1.262348      27.25
 O       6.021420    -1.149324    -1.108703     252.82
 H       5.478337    -0.391332    -0.775377      27.31
 C       3.739187    -2.171244    -0.968654      78.98
 H       3.314348    -3.158961    -0.673191      21.75
 C       3.593473    -1.919780    -2.545653      96.54
 O       3.906859    -3.117197    -3.306027     282.61
 H       4.653740    -3.107611    -3.988521      26.89
 H       4.235249    -1.096401    -2.848519      22.44
 H       2.486738    -1.522301    -2.779994      22.80
 C      -0.373888    -1.868614     0.314556      20.00
 H      -1.174282    -2.741335     0.468654      19.05
 C      -0.070407     0.509493    -0.015710      79.65
 H      -0.590866     1.485083    -0.011271      18.39
 C       1.279025     0.337587    -0.268327      19.16
 O       2.111754     1.442214    -0.395863     216.29
 C       1.465688     2.758648    -0.502414     126.46
 H       2.228128     3.532292    -0.817967      25.32
 H       0.680249     2.656483    -1.105074      26.86
 H       0.965935     3.078707     0.412455      25.78
 C       1.878412    -0.954077    -0.107616      16.43
 O       3.256408    -1.017031    -0.223911     199.18
 C       0.985526    -2.109348     0.144128      60.73
 H       1.464715    -3.092021     0.244656      17.85
 C      -0.945021    -0.590681     0.311671      65.74
 C      -2.417973    -0.287744     0.593561      74.84
 H      -2.870533    -1.304898     1.074067      24.12
 O      -2.705022     0.830091     1.410466     321.29
 H      -2.326835     0.656918     2.259329      29.38
 C      -3.197538    -0.102828    -0.758603      72.69
 H      -2.709899     0.798405    -1.331373      23.53
 O      -2.917317    -1.364480    -1.547947     220.31
 H      -2.880326    -1.054932    -2.503339      23.29
 C      -4.753125     0.245173    -0.635718     103.12
 O      -5.054586     1.675591    -0.796566     265.46
 H      -4.929593     2.341935    -0.032349      25.03
 H      -5.137235    -0.135026     0.220959      31.02
 H      -5.276655    -0.207106    -1.505445      28.23
55
name = lig-etoh-Waterframe_179
 C       5.622108    -1.733618     1.911328      54.95
 H       5.779082    -0.654027     1.699554      24.21
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 C       5.471496    -4.041353     1.145315      41.90
 H       5.476657    -4.849007     0.386396      18.10
 C       5.562613    -4.535759     2.446965      17.47
 O       5.597841    -5.914101     2.816503     305.76
 C       4.928750    -6.922859     1.958752     127.33
 H       5.658680    -7.175186     1.114374      29.91
 H       3.984509    -6.449695     1.621605      26.90
 H       4.699355    -7.805951     2.519138      24.87
 C       5.806438    -3.596982     3.518214       1.53
 O       6.141393    -3.968727     4.770973     309.86
 H       5.657836    -4.911242     5.089795      22.74
 C       5.840862    -2.201610     3.229240      45.69
 H       5.900279    -1.505272     4.141348      19.95
 C       5.442348    -2.648469     0.810870      24.23
 C       5.247135    -2.277925    -0.668274     107.41
 H       5.669925    -3.165740    -1.132338      24.10
 O       6.028944    -1.139586    -1.080268     258.32
 H       5.612960    -0.236633    -0.868058      25.76
 C       3.755649    -2.126749    -1.041589      84.89
 H       3.210943    -2.979287    -0.610666      22.36
 C       3.606098    -1.924367    -2.567607     101.30
 O       3.898688    -3.172647    -3.298862     275.65
 H       4.710805    -2.963668    -3.829025      26.85
 H       4.245692    -1.086272    -2.841774      23.17
 H       2.485757    -1.782072    -2.741117      23.65
 C      -0.386881    -1.831503     0.344516      54.80
 H      -1.007759    -2.763442     0.440605      18.55
 C      -0.122646     0.507530     0.002761      63.31
 H      -0.398751     1.598048     0.123342      17.36
 C       1.266941     0.371650    -0.202666       6.77
 O       2.058525     1.523889    -0.443833     247.14
 C       1.448952     2.777114    -0.536790     121.66
 H       2.326637     3.424011    -0.825782      24.16
 H       0.620327     2.845437    -1.233122      25.83
 H       1.080168     3.074790     0.402653      26.99
 C       1.843708    -0.970859    -0.140987       9.02
 O       3.225273    -1.027150    -0.227040     199.07
 C       1.009589    -2.118344     0.081685      59.94
 H       1.383449    -3.113233     0.167025      18.49
 C      -0.923631    -0.538822     0.309437      56.28
 C      -2.438881    -0.285409     0.513286      74.03
 H      -2.907471    -1.280143     0.976924      24.13
 O      -2.692543     0.860697     1.392138     301.25
 H      -2.321692     0.627040     2.264123      26.48
 C      -3.191277    -0.058561    -0.763730      88.90
 H      -2.876989     0.781993    -1.296382      25.91
 O      -2.927648    -1.326670    -1.532215     241.96
 H      -2.755251    -1.152400    -2.492339      23.78
 C      -4.735103     0.281804    -0.669337      99.70
 O      -5.026288     1.721838    -0.864804     260.21
 H      -4.770683     2.096179     0.033694      26.45
 H      -5.219652    -0.039770     0.266359      28.95
 H      -5.153636    -0.165912    -1.560587      28.33
55
name = lig-etoh-Waterframe_180
 C       5.596877    -1.749630     1.908285      55.49
 H       5.554342    -0.683712     1.690046      23.52
 C       5.397370    -4.055365     1.110083      55.64
 H       5.220955    -4.821002     0.284390      14.03
 C       5.542757    -4.514613     2.456744      21.10
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 O       5.607852    -5.883649     2.874058     257.40
 C       4.898042    -6.910136     1.929424     120.57
 H       5.541413    -7.138613     1.015169      28.87
 H       3.918697    -6.572075     1.462371      25.99
 H       4.805241    -7.817021     2.498448      24.66
 C       5.839729    -3.581291     3.454818      -9.26
 O       6.087291    -3.999880     4.756561     242.80
 H       5.774164    -4.854161     5.052998      25.54
 C       5.852145    -2.200128     3.225644      61.98
 H       6.237577    -1.693902     4.098872      22.92
 C       5.423403    -2.656152     0.813963      33.22
 C       5.264081    -2.266112    -0.639884      81.60
 H       5.610931    -3.140852    -1.373151      22.75
 O       6.051863    -1.116874    -1.057076     203.04
 H       5.579369    -0.227559    -0.786861      24.74
 C       3.798889    -2.122281    -1.072838      84.67
 H       3.279983    -3.086328    -0.954470      22.94
 C       3.557839    -1.942136    -2.567879     108.13
 O       3.906193    -3.190749    -3.284583     250.33
 H       4.836615    -3.218646    -3.564548      27.48
 H       4.167287    -1.161240    -3.028507      24.66
 H       2.561850    -1.703525    -2.838330      26.13
 C      -0.366767    -1.868547     0.346417      15.46
 H      -0.997780    -2.657609     0.569514      17.17
 C      -0.098823     0.600698     0.045375      69.09
 H      -0.677221     1.589973     0.117029      15.91
 C       1.243449     0.368969    -0.134381      10.15
 O       2.050630     1.502176    -0.498219     185.83
 C       1.413110     2.856887    -0.552827     108.23
 H       2.253592     3.516177    -0.852248      25.46
 H       0.733645     3.062461    -1.535697      22.62
 H       1.171991     3.236776     0.437346      25.90
 C       1.803325    -0.938774    -0.180415      25.21
 O       3.200888    -1.025493    -0.266192     193.70
 C       0.982604    -2.023639     0.047716      54.62
 H       1.332115    -3.009026     0.078454      19.86
 C      -0.972947    -0.543032     0.308739      79.89
 C      -2.449859    -0.299654     0.501442      84.17
 H      -2.890814    -1.150604     0.973104      24.78
 O      -2.678372     0.883144     1.373379     281.12
 H      -2.222507     0.600688     2.237026      27.13
 C      -3.206023    -0.025126    -0.848131      95.10
 H      -2.703274     0.735759    -1.348012      26.62
 O      -2.969297    -1.272421    -1.498349     265.64
 H      -2.777194    -0.968807    -2.415840      24.04
 C      -4.715509     0.325993    -0.736823      97.46
 O      -4.981189     1.728526    -0.914182     276.26
 H      -4.706435     2.341098    -0.151955      25.26
 H      -5.256889    -0.122451     0.261151      27.11
 H      -5.210025    -0.261930    -1.505545      28.25
55
name = lig-etoh-Waterframe_181
 C       5.595780    -1.749688     1.872755      48.94
 H       5.448808    -0.704704     1.705813      24.68
 C       5.317166    -4.083703     1.105584      58.14
 H       5.036613    -4.690551     0.194374      19.08
 C       5.544196    -4.541372     2.407642      19.84
 O       5.544850    -5.865515     2.859506     308.56
 C       4.921060    -6.846230     1.912202     131.63
 H       5.623763    -6.985852     1.083190      32.32
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 H       3.873882    -6.490391     1.695667      28.36
 H       4.865185    -7.687187     2.601223      26.07
 C       5.849100    -3.616013     3.470068       7.15
 O       6.062166    -3.994453     4.752224     183.69
 H       5.781454    -4.865450     4.942931      25.17
 C       5.889622    -2.223408     3.190110      55.48
 H       6.232220    -1.474776     3.826908      22.07
 C       5.406187    -2.706212     0.871455      17.52
 C       5.267119    -2.233497    -0.643703      52.67
 H       5.763432    -3.089108    -1.315663      24.12
 O       6.075427    -1.089901    -1.026561     183.61
 H       5.538922    -0.267935    -0.667874      25.46
 C       3.777038    -2.132620    -1.081552      81.72
 H       3.401417    -3.119724    -0.769512      23.09
 C       3.552523    -1.927580    -2.630657     109.31
 O       3.898741    -3.220636    -3.251130     248.84
 H       4.809526    -3.203971    -3.585641      28.17
 H       4.177463    -1.137265    -3.084218      25.85
 H       2.540172    -1.738589    -2.769908      27.72
 C      -0.439806    -1.828313     0.341420      16.08
 H      -0.962084    -2.654072     0.609069      21.08
 C      -0.178546     0.594412     0.134503      72.50
 H      -0.571580     1.643909    -0.033463      17.34
 C       1.236379     0.461990    -0.131222      13.56
 O       2.050654     1.475262    -0.546949     185.27
 C       1.469801     2.947549    -0.595761      88.61
 H       2.337843     3.548684    -0.776676      23.29
 H       0.450121     2.867655    -1.288000      22.12
 H       0.835394     3.236476     0.325097      24.79
 C       1.812602    -0.858944    -0.209164      16.50
 O       3.180450    -1.034683    -0.336155     194.79
 C       0.945733    -1.981404     0.041066      49.73
 H       1.481694    -2.898123     0.025919      20.60
 C      -0.957890    -0.556212     0.301166      47.10
 C      -2.484957    -0.263009     0.535961      82.75
 H      -2.934658    -1.104352     0.924715      26.89
 O      -2.656577     0.886643     1.354108     293.72
 H      -2.179617     0.733478     2.268463      28.36
 C      -3.187552     0.002308    -0.859132      82.02
 H      -2.596407     0.830713    -1.425464      24.04
 O      -3.030752    -1.244901    -1.520059     243.85
 H      -2.908815    -1.160361    -2.502150      25.04
 C      -4.703649     0.353235    -0.789148      96.33
 O      -4.949808     1.746989    -0.986050     250.68
 H      -4.816871     2.295409    -0.149081      26.02
 H      -5.014924    -0.014526     0.307301      27.66
 H      -5.289120    -0.069996    -1.621455      28.10
55
name = lig-etoh-Waterframe_182
 C       5.612598    -1.786082     1.858942      58.89
 H       5.635733    -0.743160     1.633129      20.62
 C       5.248073    -4.101063     1.107246      56.63
 H       5.010559    -4.867269     0.345192      22.12
 C       5.559113    -4.562847     2.398361      11.86
 O       5.459349    -5.849320     2.818365     278.43
 C       4.960402    -6.768700     1.962638     133.17
 H       5.505064    -6.909422     1.054447      30.49
 H       3.943333    -6.467262     1.633192      30.01
 H       4.878662    -7.781282     2.421949      26.25
 C       5.844692    -3.613304     3.463147       0.90
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 O       6.061307    -3.986126     4.769796     257.74
 H       5.752479    -4.912051     5.057043      21.99
 C       5.933632    -2.226802     3.122102      55.59
 H       6.012330    -1.511745     3.917117      23.59
 C       5.364555    -2.692886     0.818771      27.42
 C       5.275875    -2.224716    -0.637119      96.36
 H       5.718592    -3.075200    -1.150940      24.03
 O       6.067621    -1.059400    -0.969719     224.79
 H       5.695202    -0.127216    -0.719978      23.09
 C       3.756518    -2.137994    -1.099368      82.54
 H       3.234443    -3.010531    -0.693433      24.05
 C       3.566723    -1.953228    -2.640952     103.42
 O       3.889307    -3.240994    -3.240309     273.16
 H       4.631929    -3.055318    -3.834834      28.07
 H       4.224507    -1.102383    -2.973188      24.70
 H       2.494472    -1.802360    -2.844700      25.66
 C      -0.455885    -1.821518     0.324188      22.32
 H      -1.081488    -2.695317     0.494883      18.88
 C      -0.150952     0.587542     0.165807      66.38
 H      -0.676734     1.552392     0.095621      18.47
 C       1.193085     0.509769    -0.165107      12.44
 O       2.051487     1.560276    -0.582429     212.47
 C       1.474090     2.910083    -0.610544     108.43
 H       2.218819     3.623425    -0.861641      25.49
 H       0.847153     2.991166    -1.569056      24.05
 H       1.131522     3.118305     0.481426      24.24
 C       1.761002    -0.824195    -0.202876      14.19
 O       3.171470    -1.010076    -0.409224     182.51
 C       0.953888    -1.921473     0.042072      60.35
 H       1.361625    -2.947541     0.084684      21.47
 C      -1.039879    -0.509042     0.336570      59.56
 C      -2.492748    -0.237105     0.530313      84.16
 H      -3.023567    -1.156100     0.961736      24.82
 O      -2.652912     0.924099     1.356101     272.40
 H      -2.168808     0.658570     2.273242      26.63
 C      -3.156897     0.020672    -0.848933      78.63
 H      -2.675562     0.966223    -1.448260      22.83
 O      -3.093544    -1.280200    -1.564640     203.90
 H      -2.966926    -1.001644    -2.541272      23.17
 C      -4.667116     0.394438    -0.807727     102.96
 O      -4.941871     1.809986    -1.053710     255.41
 H      -4.850390     2.199486    -0.155729      26.63
 H      -5.158995     0.102979     0.105711      31.02
 H      -5.176863    -0.222537    -1.597655      29.65
55
name = lig-etoh-Waterframe_183
 C       5.654794    -1.812148     1.793657      55.69
 H       5.805846    -0.784523     1.581673      19.84
 C       5.216221    -4.085549     1.110541      52.83
 H       5.008920    -4.832361     0.375589      21.72
 C       5.553021    -4.493947     2.421558       7.17
 O       5.426059    -5.825613     2.862509     241.62
 C       4.909270    -6.789675     1.890820     115.55
 H       5.573609    -6.815769     1.028495      29.03
 H       3.921045    -6.562924     1.539121      31.83
 H       4.922115    -7.780391     2.442506      24.09
 C       5.848268    -3.608188     3.439640       8.43
 O       6.071717    -3.966189     4.788753     257.48
 H       5.713344    -4.960862     5.129609      19.89
 C       5.944284    -2.263057     3.142189      44.87
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 H       5.968714    -1.662144     4.089070      22.04
 C       5.315130    -2.702459     0.762944      28.43
 C       5.230199    -2.229174    -0.642438     106.32
 H       5.630798    -2.881887    -1.310114      25.27
 O       6.063734    -1.034928    -0.918489     221.63
 H       5.450376    -0.237271    -0.691968      24.73
 C       3.725241    -2.129300    -1.103614      81.64
 H       3.218119    -3.092990    -0.918090      23.00
 C       3.563423    -2.001678    -2.588647     104.99
 O       3.909816    -3.224210    -3.283503     277.59
 H       4.607348    -3.216132    -3.961525      27.43
 H       4.245122    -1.208387    -2.986795      24.05
 H       2.516695    -1.605958    -2.933252      23.92
 C      -0.457439    -1.769688     0.294711      -0.42
 H      -1.115590    -2.727271     0.293819      19.22
 C      -0.163295     0.642856     0.157338      61.27
 H      -0.609133     1.583600     0.319970      18.92
 C       1.208350     0.495987    -0.228582      -5.23
 O       2.053544     1.626974    -0.603824     246.58
 C       1.499536     2.878352    -0.641695     130.77
 H       2.376104     3.517022    -0.763294      24.56
 H       0.743294     3.107482    -1.286115      27.60
 H       1.029892     3.242319     0.322048      25.79
 C       1.772365    -0.811162    -0.208703      16.28
 O       3.135540    -0.912479    -0.465673     161.03
 C       0.897144    -1.906238     0.074327      57.40
 H       1.356947    -2.949981     0.094315      20.29
 C      -1.025805    -0.525226     0.385847      68.81
 C      -2.512936    -0.218338     0.498614      82.31
 H      -3.067292    -1.144853     1.044402      24.86
 O      -2.669982     0.976362     1.382669     241.09
 H      -2.224213     0.637617     2.308419      25.29
 C      -3.192744     0.012747    -0.843909      86.73
 H      -2.521187     0.727232    -1.434059      23.91
 O      -3.132383    -1.280675    -1.600680     197.96
 H      -2.902515    -1.007281    -2.561978      23.00
 C      -4.670443     0.437587    -0.815926     106.33
 O      -4.938525     1.854691    -1.110719     266.69
 H      -4.780354     2.499604    -0.394692      25.35
 H      -5.177585     0.150919     0.009519      31.47
 H      -5.052788    -0.186716    -1.671854      28.64
55
name = lig-etoh-Waterframe_184
 C       5.730361    -1.831680     1.798718      52.44
 H       5.757612    -0.766714     1.569048      25.14
 C       5.213096    -4.066888     1.111591      43.48
 H       4.947937    -4.718556     0.332826      17.32
 C       5.490078    -4.505764     2.420782      20.46
 O       5.393197    -5.808547     2.901278     206.67
 C       4.866430    -6.827163     1.801387     108.69
 H       5.667143    -6.863962     1.027057      30.43
 H       3.857037    -6.587076     1.542025      29.38
 H       4.889055    -7.753860     2.431685      25.76
 C       5.871336    -3.612783     3.511461      11.86
 O       6.079150    -3.945787     4.786799     166.10
 H       5.725465    -4.987855     4.960383      23.97
 C       5.904357    -2.260513     3.136693      51.63
 H       6.223459    -1.435963     3.890029      20.09
 C       5.315933    -2.729967     0.780770      46.34
 C       5.171313    -2.223559    -0.712625     104.74
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 H       5.585094    -2.971701    -1.405729      23.83
 O       5.995695    -1.014583    -0.860637     219.15
 H       5.451995    -0.160458    -0.695346      24.20
 C       3.689835    -2.103557    -1.093720      80.81
 H       3.224412    -3.004467    -0.625602      20.66
 C       3.605131    -1.964478    -2.639628      99.27
 O       3.908417    -3.233122    -3.331900     255.80
 H       4.816648    -3.044819    -3.729699      24.96
 H       4.347776    -1.222252    -2.931079      23.80
 H       2.480224    -1.711844    -2.830274      24.27
 C      -0.484643    -1.756190     0.262340      68.38
 H      -1.144591    -2.749342     0.274761      18.42
 C      -0.171725     0.673948     0.147077      60.55
 H      -0.466376     1.637352     0.342170      20.07
 C       1.194199     0.516059    -0.275092       6.91
 O       2.049596     1.551891    -0.607676     213.06
 C       1.490657     2.986007    -0.626976     105.49
 H       2.425015     3.593547    -0.827527      23.96
 H       0.693142     3.006877    -1.341164      26.17
 H       1.066012     3.187593     0.317368      26.75
 C       1.766344    -0.813167    -0.225520      18.38
 O       3.108061    -0.841989    -0.525376     171.97
 C       0.927772    -1.905622     0.089074      53.28
 H       1.381452    -2.957353     0.045674      20.82
 C      -0.972479    -0.435206     0.391564      51.15
 C      -2.524733    -0.202171     0.549181      74.25
 H      -3.047971    -1.114080     1.032376      25.38
 O      -2.702936     1.006073     1.394141     242.08
 H      -2.289926     0.728991     2.341817      23.97
 C      -3.205247    -0.011558    -0.874598      84.44
 H      -2.642610     0.695097    -1.379541      27.10
 O      -3.155767    -1.257907    -1.594592     239.15
 H      -2.908672    -1.117724    -2.562878      24.70
 C      -4.698537     0.511964    -0.844898     101.81
 O      -4.929726     1.888978    -1.189399     243.95
 H      -4.702935     2.422474    -0.389688      26.64
 H      -5.142425     0.153496     0.138709      29.14
 H      -5.241330     0.133961    -1.730168      28.59
55
name = lig-etoh-Waterframe_185
 C       5.765979    -1.837154     1.800653      55.11
 H       5.806414    -0.748485     1.606110      23.62
 C       5.208975    -4.095417     1.118574      42.57
 H       4.885038    -4.815189     0.395276      14.06
 C       5.433811    -4.529187     2.485249      12.77
 O       5.322888    -5.860275     2.856542     253.48
 C       4.882117    -6.826137     1.835322      95.44
 H       5.527109    -6.912494     0.891886      28.75
 H       3.917509    -6.504845     1.384228      30.58
 H       4.765527    -7.825619     2.267014      25.47
 C       5.844266    -3.578997     3.478564       0.98
 O       6.091612    -3.964981     4.803238     167.25
 H       5.833185    -4.975881     5.101506      23.47
 C       5.907666    -2.205913     3.123000      66.06
 H       6.380251    -1.410713     3.788068      22.08
 C       5.371128    -2.689227     0.781375      46.28
 C       5.148223    -2.197862    -0.675506      95.73
 H       5.617046    -3.075831    -1.340128      21.95
 O       5.901082    -1.001961    -0.835556     234.80
 H       5.394206    -0.150464    -0.695657      24.61
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 C       3.675481    -2.043006    -1.091127      86.10
 H       3.070382    -2.854988    -0.638402      20.15
 C       3.605404    -1.945570    -2.670975     101.20
 O       3.918111    -3.210533    -3.357422     255.89
 H       4.873241    -3.220071    -3.758341      25.36
 H       4.214718    -1.126557    -2.965109      25.03
 H       2.597745    -1.676815    -3.058141      25.57
 C      -0.446430    -1.723556     0.244783      48.54
 H      -1.208818    -2.567032     0.423590      17.93
 C      -0.116548     0.735470     0.134039      71.32
 H      -0.594286     1.685983     0.171862      17.76
 C       1.150391     0.505814    -0.272630      21.72
 O       2.044823     1.517251    -0.612736     179.33
 C       1.484260     3.011518    -0.596187      93.01
 H       2.289132     3.768845    -0.950116      23.86
 H       0.801055     3.040083    -1.544491      22.85
 H       1.201633     3.238665     0.394118      25.00
 C       1.719822    -0.785706    -0.256466      19.11
 O       3.113984    -0.820403    -0.591554     195.60
 C       0.950960    -1.914414     0.067372      53.86
 H       1.351260    -2.951946     0.065780      19.36
 C      -1.021759    -0.393919     0.364438      76.61
 C      -2.497792    -0.173453     0.598033      85.35
 H      -2.884333    -1.021265     1.068258      26.43
 O      -2.758332     1.018064     1.391182     250.19
 H      -2.298242     0.770317     2.302656      25.92
 C      -3.222650     0.032417    -0.896225      75.86
 H      -2.732685     0.804239    -1.395413      26.21
 O      -3.171449    -1.259856    -1.551572     245.39
 H      -2.989372    -0.937553    -2.479149      23.90
 C      -4.740954     0.543775    -0.914259      94.33
 O      -4.885594     1.953893    -1.228854     232.18
 H      -4.845708     2.464442    -0.356792      24.49
 H      -5.305747     0.387017     0.184752      27.59
 H      -5.314021    -0.157866    -1.540705      29.74
55
name = lig-etoh-Waterframe_186
 C       5.759623    -1.780230     1.781063      34.64
 H       5.929141    -0.722018     1.536574      20.61
 C       5.212089    -4.083565     1.169507      38.25
 H       4.903389    -4.823954     0.407147      17.96
 C       5.384244    -4.524345     2.469039      13.28
 O       5.259235    -5.936068     2.817523     296.65
 C       4.866325    -6.812172     1.829880     131.29
 H       5.706282    -6.862010     1.067274      30.06
 H       3.863873    -6.466047     1.402514      27.43
 H       4.725657    -7.752772     2.318593      23.75
 C       5.783142    -3.580491     3.481792      -3.59
 O       6.114447    -3.974582     4.808463     251.81
 H       5.784740    -4.871651     5.028899      28.23
 C       5.978178    -2.202536     3.143139      49.37
 H       6.263197    -1.595701     4.009399      21.48
 C       5.400738    -2.739051     0.786128      21.35
 C       5.138415    -2.185912    -0.560568      92.03
 H       5.597537    -2.892112    -1.393742      24.09
 O       5.838405    -0.976654    -0.858878     201.66
 H       5.227191    -0.245310    -0.695723      26.74
 C       3.645350    -2.014064    -1.140162      86.30
 H       3.091834    -2.949992    -0.971158      24.70
 C       3.583945    -1.929746    -2.704550     108.14
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 O       3.933473    -3.176850    -3.346557     243.65
 H       4.780575    -3.091647    -3.968207      25.60
 H       4.300156    -1.203494    -3.048592      25.01
 H       2.612898    -1.672123    -2.993137      26.93
 C      -0.447583    -1.632060     0.284724      23.47
 H      -0.993162    -2.523072     0.495967      21.34
 C      -0.210966     0.755170     0.136253      84.39
 H      -0.608698     1.797794    -0.039980      15.88
 C       1.183429     0.534157    -0.257591       6.86
 O       2.047634     1.593559    -0.623353     211.06
 C       1.520840     2.933426    -0.622379     108.80
 H       2.478486     3.504202    -0.803951      22.64
 H       0.452272     3.160108    -1.160406      23.03
 H       1.074451     3.299140     0.337460      26.15
 C       1.745835    -0.797634    -0.308811      17.36
 O       3.088149    -0.788060    -0.633325     197.61
 C       0.916193    -1.898935     0.018330      56.31
 H       1.366143    -2.869735     0.133529      19.69
 C      -0.988374    -0.380145     0.308336      67.11
 C      -2.507167    -0.126858     0.550225      85.72
 H      -2.900267    -0.977115     1.021540      27.92
 O      -2.809786     1.025547     1.401042     243.92
 H      -2.310294     0.875222     2.278904      28.48
 C      -3.282611     0.096077    -0.823842      82.38
 H      -2.618258     0.800937    -1.461303      23.69
 O      -3.169346    -1.229569    -1.507796     208.15
 H      -3.040269    -1.150418    -2.486926      25.67
 C      -4.780581     0.549881    -0.897540      97.97
 O      -4.827050     2.008247    -1.270943     188.20
 H      -4.935901     2.532552    -0.390761      24.51
 H      -5.252692     0.506478     0.177493      28.72
 H      -5.279949    -0.075647    -1.646178      30.07
55
name = lig-etoh-Waterframe_187
 C       5.766481    -1.777370     1.843440      49.90
 H       5.858651    -0.726840     1.498107      20.08
 C       5.197847    -4.077264     1.167638      47.89
 H       4.962918    -4.769912     0.297145      20.51
 C       5.362683    -4.566866     2.486370      12.24
 O       5.230358    -5.887593     2.860899     232.19
 C       4.827270    -6.843326     1.763010     126.58
 H       5.639938    -6.983874     1.058103      28.53
 H       3.871700    -6.592932     1.215419      27.73
 H       4.710117    -7.750371     2.301440      25.40
 C       5.745524    -3.617385     3.525977      12.68
 O       6.118611    -3.969314     4.766804     256.70
 H       5.846426    -4.820065     5.017679      25.25
 C       6.021198    -2.261697     3.146044      56.26
 H       6.175652    -1.599821     3.945159      25.37
 C       5.402434    -2.719875     0.869352      28.31
 C       5.098735    -2.196538    -0.604943      85.41
 H       5.530536    -2.980125    -1.227408      24.14
 O       5.797013    -0.942221    -0.888007     214.36
 H       5.371504    -0.101724    -0.697880      24.80
 C       3.659496    -2.057385    -1.204697      78.53
 H       3.041059    -2.893756    -0.861671      24.67
 C       3.602876    -1.876715    -2.731011     108.07
 O       3.941054    -3.163948    -3.333203     253.75
 H       4.750687    -2.854755    -3.887614      24.02
 H       4.350028    -1.115373    -3.081709      24.47
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 H       2.591497    -1.608797    -2.912129      26.24
 C      -0.438901    -1.643682     0.345795      29.13
 H      -1.044181    -2.437560     0.559587      21.31
 C      -0.172193     0.779839     0.048283      66.83
 H      -0.724677     1.822593     0.048288      18.34
 C       1.166473     0.585668    -0.227757      15.32
 O       2.031379     1.627681    -0.625423     203.17
 C       1.523512     2.909227    -0.583257     118.90
 H       2.303521     3.568733    -0.959186      26.04
 H       0.772544     3.026910    -1.475015      24.13
 H       1.370712     3.114802     0.538425      25.44
 C       1.735476    -0.739036    -0.339866      21.08
 O       3.061986    -0.789648    -0.664740     151.97
 C       0.908758    -1.831562    -0.030002      68.49
 H       1.247506    -2.807551     0.102216      22.88
 C      -1.046264    -0.307863     0.283310      58.08
 C      -2.561640    -0.094770     0.492395      79.23
 H      -3.017770    -1.072400     0.923980      25.03
 O      -2.843090     1.042968     1.410972     234.54
 H      -2.324410     0.807691     2.228438      27.71
 C      -3.303085     0.104918    -0.803201      81.54
 H      -2.726712     0.975199    -1.452723      22.90
 O      -3.173134    -1.204699    -1.444240     232.89
 H      -2.962291    -0.941615    -2.391391      24.98
 C      -4.766988     0.624034    -0.829836     112.21
 O      -4.781536     2.028545    -1.305200     247.85
 H      -4.754252     2.570141    -0.414520      24.66
 H      -5.318839     0.349043     0.012818      31.71
 H      -5.292093     0.221133    -1.688681      30.30
55
name = lig-etoh-Waterframe_188
 C       5.775172    -1.816628     1.910274      69.30
 H       5.840709    -0.719776     1.787103      32.73
 C       5.188471    -4.072686     1.162713      48.92
 H       4.969400    -4.782758     0.303714      16.61
 C       5.365862    -4.553501     2.493184      20.51
 O       5.183481    -5.865550     2.876994     236.88
 C       4.810777    -6.884496     1.737899     114.82
 H       5.593269    -6.972823     1.025318      28.35
 H       3.934141    -6.508789     1.197463      27.20
 H       4.607088    -7.827248     2.249259      23.91
 C       5.748828    -3.645988     3.478380      27.81
 O       6.121159    -3.978645     4.771189     217.14
 H       5.907010    -4.944551     5.091506      17.91
 C       6.004818    -2.312368     3.174888      80.51
 H       6.328277    -1.603358     3.879911      25.22
 C       5.329359    -2.643619     0.875116      10.15
 C       5.083024    -2.189585    -0.656647      79.51
 H       5.575379    -2.902139    -1.205059      24.16
 O       5.798661    -0.954229    -0.940083     215.42
 H       5.292460    -0.173257    -0.693489      30.07
 C       3.653870    -2.071543    -1.190797      87.94
 H       3.038826    -2.910419    -0.864705      23.21
 C       3.619262    -1.845110    -2.711656      98.40
 O       3.948796    -3.129813    -3.336778     264.72
 H       4.807380    -3.273227    -3.843910      25.19
 H       4.292059    -0.970011    -2.984730      23.53
 H       2.600782    -1.536392    -3.119445      25.51
 C      -0.494921    -1.582886     0.378387      32.69
 H      -1.091324    -2.417424     0.616777      20.85
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 C      -0.195013     0.808517    -0.036471      86.80
 H      -0.558849     1.913869     0.107314      21.33
 C       1.181349     0.626530    -0.249653      23.01
 O       2.062646     1.573226    -0.624968     211.10
 C       1.546699     2.980259    -0.576675     123.26
 H       2.278443     3.652306    -0.879404      28.72
 H       0.643056     3.038197    -1.134797      27.48
 H       1.142637     3.344674     0.440891      28.16
 C       1.691438    -0.663763    -0.345003      14.40
 O       3.067051    -0.806982    -0.695538     153.00
 C       0.881847    -1.774208    -0.032922      59.22
 H       1.305840    -2.729707    -0.088127      22.57
 C      -1.077261    -0.313623     0.289691      56.27
 C      -2.605800    -0.062661     0.509328      72.83
 H      -3.030711    -1.087926     0.975683      24.63
 O      -2.856394     1.045772     1.411070     247.48
 H      -2.407112     0.782107     2.220657      28.36
 C      -3.315571     0.133209    -0.830345      87.32
 H      -2.760752     0.910662    -1.481121      25.12
 O      -3.176167    -1.165205    -1.414333     243.07
 H      -2.915566    -0.990511    -2.380786      24.96
 C      -4.759362     0.690645    -0.833956     110.23
 O      -4.741616     2.049414    -1.276896     296.48
 H      -4.707031     2.731447    -0.512173      25.08
 H      -5.367188     0.547156    -0.009596      31.17
 H      -5.194992     0.036370    -1.637355      29.93
55
name = lig-etoh-Waterframe_189
 C       5.740493    -1.805620     1.911837      54.15
 H       5.911598    -0.732594     1.870994      29.18
 C       5.180067    -4.000143     1.149858      57.62
 H       4.912553    -4.743638     0.381937      16.70
 C       5.356133    -4.538306     2.419815      17.98
 O       5.125348    -5.924227     2.837817     238.08
 C       4.806393    -6.850077     1.767825     116.46
 H       5.698648    -6.931881     1.151710      29.47
 H       3.923032    -6.460532     1.296926      29.44
 H       4.545372    -7.837989     2.266692      25.32
 C       5.814453    -3.677716     3.508824       0.45
 O       6.125760    -3.998772     4.798335     108.51
 H       5.777522    -5.069001     5.021165      21.30
 C       5.979668    -2.322380     3.220876      49.45
 H       6.504787    -1.816368     4.052984      19.61
 C       5.224893    -2.642404     0.815735      49.14
 C       5.118869    -2.165616    -0.631834      89.20
 H       5.561801    -2.927927    -1.308185      24.52
 O       5.818427    -0.989775    -0.999658     217.48
 H       5.251469    -0.234179    -0.784746      27.78
 C       3.591776    -2.043376    -1.165835      83.37
 H       3.104015    -2.998649    -0.967863      25.04
 C       3.646154    -1.859344    -2.708272      96.63
 O       3.933490    -3.130308    -3.341606     255.28
 H       4.848689    -2.968946    -3.767446      24.14
 H       4.521152    -1.163431    -2.903904      23.04
 H       2.570879    -1.578620    -3.092758      24.68
 C      -0.525233    -1.535634     0.364679      51.29
 H      -1.095740    -2.461090     0.636088      21.08
 C      -0.259352     0.816840    -0.058141      65.64
 H      -0.648721     1.853676    -0.014624      22.86
 C       1.145792     0.631214    -0.307669     -19.21
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 O       2.115959     1.640438    -0.610291     196.14
 C       1.535617     3.040520    -0.566259     108.53
 H       2.403628     3.583076    -0.859295      26.09
 H       0.694153     3.117696    -1.149237      28.04
 H       1.279796     3.283647     0.483210      27.87
 C       1.702310    -0.707893    -0.346583       4.33
 O       3.049157    -0.799865    -0.690705     169.14
 C       0.817299    -1.717353    -0.004614      63.73
 H       1.232725    -2.708409    -0.147114      23.96
 C      -1.081277    -0.252936     0.303467      46.86
 C      -2.594673    -0.049109     0.558350      78.39
 H      -3.071307    -0.958865     1.021603      26.22
 O      -2.860458     1.056389     1.423076     260.86
 H      -2.484715     0.870608     2.260237      29.33
 C      -3.295847     0.185989    -0.834167      92.29
 H      -2.709031     0.793336    -1.401020      28.80
 O      -3.186328    -1.151357    -1.432419     232.81
 H      -2.977755    -1.108865    -2.417741      26.70
 C      -4.759319     0.703190    -0.867604      98.49
 O      -4.712207     2.103775    -1.275487     282.70
 H      -4.940642     2.504404    -0.350244      23.99
 H      -5.228421     0.723344     0.187610      27.95
 H      -5.349871     0.091873    -1.635866      28.96
55
name = lig-etoh-Waterframe_190
 C       5.667972    -1.782661     1.903680      64.80
 H       5.922580    -0.796455     1.571053      29.40
 C       5.121834    -3.995504     1.104789      61.73
 H       4.831649    -4.625590     0.295798      15.26
 C       5.365324    -4.560650     2.453272      28.98
 O       5.094805    -5.913800     2.794443     287.77
 C       4.790416    -6.810262     1.793634     121.55
 H       5.638796    -7.014439     1.056030      29.60
 H       3.962459    -6.589757     1.114180      31.18
 H       4.582572    -7.819614     2.305613      25.48
 C       5.852961    -3.726428     3.511513      -2.59
 O       6.121960    -4.044473     4.813747     106.83
 H       5.889017    -5.018534     5.180510      20.63
 C       5.974940    -2.329276     3.208231      43.65
 H       6.425792    -1.660539     4.037873      20.25
 C       5.223204    -2.577632     0.855676      37.59
 C       5.078895    -2.173031    -0.630614      72.78
 H       5.480084    -3.125728    -1.232635      20.90
 O       5.852050    -1.007432    -1.039948     231.24
 H       5.476872    -0.108823    -0.896561      28.86
 C       3.605932    -2.031165    -1.175912      85.96
 H       2.952279    -2.845198    -0.803189      23.06
 C       3.657031    -1.898563    -2.682819     111.19
 O       3.936859    -3.139210    -3.347030     266.22
 H       4.732928    -3.007549    -3.971162      24.69
 H       4.408959    -1.170444    -2.991042      24.06
 H       2.722435    -1.337434    -3.015653      24.93
 C      -0.543748    -1.506877     0.339761      51.62
 H      -1.254251    -2.404665     0.594592      20.05
 C      -0.245348     0.865766    -0.065940      64.16
 H      -0.745914     1.750127    -0.174974      21.61
 C       1.122982     0.623923    -0.379498      -0.03
 O       2.088201     1.734589    -0.581314     193.34
 C       1.576782     3.047286    -0.534024     117.99
 H       2.402098     3.761724    -0.915480      25.04
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 H       0.861293     3.222953    -1.359263      25.66
 H       1.418519     3.283241     0.493221      26.60
 C       1.674863    -0.677538    -0.342982      20.87
 O       3.009694    -0.795454    -0.647579     149.42
 C       0.794979    -1.743838     0.010233      57.35
 H       1.014337    -2.836890     0.069938      21.33
 C      -1.115152    -0.214539     0.336118      53.69
 C      -2.584079    -0.036022     0.580424      85.50
 H      -2.943741    -0.935623     0.948967      28.05
 O      -2.869806     1.109923     1.461833     257.75
 H      -2.454991     0.878978     2.257020      29.29
 C      -3.255671     0.178849    -0.845177      80.66
 H      -2.696410     0.912569    -1.348181      27.03
 O      -3.209160    -1.164721    -1.460515     257.17
 H      -3.018254    -0.852612    -2.393924      25.55
 C      -4.728857     0.718540    -0.888654      96.00
 O      -4.715793     2.162168    -1.261223     267.93
 H      -4.928882     2.722357    -0.427159      24.72
 H      -5.157816     0.456189     0.237952      26.91
 H      -5.497781     0.232995    -1.529629      29.10
55
name = lig-etoh-Waterframe_191
 C       5.627220    -1.747657     1.927748      59.40
 H       5.861676    -0.713640     1.742614      17.87
 C       5.059708    -4.012647     1.148971      39.25
 H       4.774458    -4.622772     0.343032      21.56
 C       5.357097    -4.562605     2.420946      25.42
 O       5.094607    -5.831332     2.787570     258.08
 C       4.763784    -6.870694     1.717171     105.42
 H       5.703617    -6.986472     1.075046      27.48
 H       3.848072    -6.530647     1.160044      28.44
 H       4.549332    -7.764613     2.349849      23.60
 C       5.847649    -3.705065     3.482512      18.48
 O       6.138051    -4.069323     4.825808     265.86
 H       5.836549    -5.049941     4.933839      23.81
 C       5.972788    -2.326916     3.143238      43.43
 H       6.195404    -1.520443     3.931153      25.53
 C       5.237889    -2.614290     0.886637      20.65
 C       5.005200    -2.158012    -0.608101      83.98
 H       5.540447    -3.015352    -1.206628      22.20
 O       5.902126    -1.048757    -1.073910     211.74
 H       5.395438    -0.209561    -0.871429      27.70
 C       3.618020    -2.021875    -1.135701      84.02
 H       2.994680    -2.897571    -0.819909      24.16
 C       3.652416    -1.861677    -2.694372     106.64
 O       3.924901    -3.168908    -3.361217     262.54
 H       4.715343    -3.169277    -3.956911      26.97
 H       4.432286    -1.176472    -2.869717      25.11
 H       2.675145    -1.610114    -3.044304      26.89
 C      -0.591499    -1.473425     0.330600      54.34
 H      -1.288605    -2.381891     0.542880      21.64
 C      -0.243420     0.895599    -0.068907      72.88
 H      -0.534922     1.853714    -0.212969      21.88
 C       1.114870     0.709405    -0.413484       7.20
 O       2.036315     1.719804    -0.559624     228.60
 C       1.639211     3.107905    -0.528984     112.08
 H       2.604278     3.759868    -0.728077      22.96
 H       0.590995     3.266242    -1.108152      23.15
 H       1.119902     3.480220     0.354440      25.73
 C       1.616360    -0.680239    -0.342822       3.21
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 O       3.004097    -0.771234    -0.596446     147.15
 C       0.771096    -1.776776     0.022165      58.09
 H       1.269594    -2.797876     0.210045      20.52
 C      -1.070006    -0.184469     0.341998      42.33
 C      -2.600113     0.009331     0.564738      79.71
 H      -2.974587    -0.884281     1.015373      27.27
 O      -2.874018     1.151215     1.500680     260.75
 H      -2.405189     0.923584     2.266307      29.15
 C      -3.262346     0.150611    -0.846185      75.50
 H      -2.607232     0.908294    -1.484661      23.89
 O      -3.223345    -1.132818    -1.498988     237.03
 H      -3.010924    -1.097899    -2.483127      24.67
 C      -4.696947     0.753825    -0.855630      98.88
 O      -4.737358     2.197751    -1.242341     277.03
 H      -4.725307     2.665301    -0.352507      25.45
 H      -5.262861     0.669722     0.158989      27.47
 H      -5.154767     0.224248    -1.673234      29.55
55
name = lig-etoh-Waterframe_192
 C       5.612289    -1.744718     1.899396      56.93
 H       5.598836    -0.649641     1.957139      17.59
 C       5.022819    -3.993439     1.181645      37.41
 H       4.704419    -4.713517     0.450836      21.79
 C       5.354042    -4.503377     2.412937      26.50
 O       5.090322    -5.834764     2.767648     251.12
 C       4.749402    -6.879050     1.696696     110.14
 H       5.609906    -7.008945     1.001972      26.63
 H       3.822252    -6.534114     1.157014      27.06
 H       4.547669    -7.786292     2.223016      23.94
 C       5.834677    -3.637285     3.467702      14.84
 O       6.145652    -4.068422     4.756160     170.32
 H       5.837798    -5.139395     4.970418      23.12
 C       5.953320    -2.299581     3.156196      39.44
 H       6.203353    -1.725371     4.068989      21.94
 C       5.218146    -2.644744     0.858736      37.29
 C       5.061263    -2.170620    -0.567592      88.80
 H       5.293686    -3.020602    -1.203872      26.00
 O       5.895701    -1.097217    -1.059606     190.62
 H       5.470471    -0.191359    -0.886870      26.39
 C       3.571111    -1.995505    -1.110010      73.37
 H       3.098342    -2.978452    -0.906515      25.65
 C       3.626020    -1.861847    -2.709331     105.44
 O       3.906383    -3.201098    -3.358097     269.69
 H       4.781195    -3.013028    -3.697139      27.24
 H       4.358487    -1.144781    -3.008784      26.13
 H       2.667910    -1.611501    -3.056284      27.84
 C      -0.586221    -1.508421     0.330570      61.68
 H      -1.312685    -2.300399     0.606981      20.91
 C      -0.229349     0.951873    -0.077152      72.70
 H      -0.640437     1.958958     0.029092      21.25
 C       1.087477     0.690150    -0.371795       8.23
 O       2.020721     1.700419    -0.540446     194.27
 C       1.595934     3.176930    -0.490623      97.81
 H       2.617754     3.650890    -0.742264      24.62
 H       0.980154     3.364427    -1.502670      23.66
 H       1.309356     3.354271     0.591211      24.88
 C       1.586807    -0.663572    -0.356801      15.18
 O       3.000682    -0.758844    -0.543912     157.32
 C       0.769624    -1.722988     0.032033      53.88
 H       1.301994    -2.722026     0.184868      22.61
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 C      -1.076432    -0.135240     0.320748      48.45
 C      -2.574043     0.061607     0.557938      73.55
 H      -3.065582    -0.854205     1.075986      23.64
 O      -2.868682     1.173362     1.497979     268.49
 H      -2.391567     0.949348     2.278243      27.47
 C      -3.267293     0.195391    -0.844819      59.02
 H      -2.564460     0.889348    -1.565614      23.57
 O      -3.250383    -1.131495    -1.509892     216.34
 H      -2.916801    -0.891403    -2.442872      24.67
 C      -4.684883     0.806502    -0.865654     114.68
 O      -4.739118     2.209003    -1.216368     305.78
 H      -4.832739     2.586546    -0.312310      26.32
 H      -5.302849     0.627930    -0.048797      30.39
 H      -5.109739     0.276125    -1.691169      30.49
55
name = lig-etoh-Waterframe_193
 C       5.600684    -1.762970     1.902024      58.41
 H       5.442726    -0.695761     1.597578      34.76
 C       5.014712    -3.977508     1.154892      42.54
 H       4.641933    -4.674614     0.359442      17.50
 C       5.329178    -4.497491     2.459251      17.41
 O       5.092047    -5.886664     2.731823     268.15
 C       4.742855    -6.815664     1.714364     118.57
 H       5.507164    -6.940159     0.978905      29.20
 H       3.838189    -6.590010     1.109728      29.84
 H       4.613332    -7.732599     2.198721      26.12
 C       5.809656    -3.654580     3.455462      22.29
 O       6.150617    -4.062988     4.672314     135.78
 H       5.919700    -5.110795     4.863921      25.45
 C       5.918037    -2.242350     3.222108      56.00
 H       6.278594    -1.621500     3.999508      18.78
 C       5.206557    -2.582945     0.852279      34.18
 C       5.049087    -2.213839    -0.613582      80.47
 H       5.370210    -3.047398    -1.132473      22.51
 O       5.885986    -1.135081    -1.007448     181.84
 H       5.513948    -0.199646    -0.842428      28.48
 C       3.574329    -1.959920    -1.127133      82.15
 H       2.906038    -2.757829    -0.786662      23.43
 C       3.554016    -1.901684    -2.690455     106.32
 O       3.909624    -3.170902    -3.318741     275.44
 H       4.763319    -3.192816    -3.762388      27.21
 H       4.275755    -1.185024    -3.120133      24.13
 H       2.592325    -1.476137    -3.008247      26.16
 C      -0.591552    -1.455706     0.341884      52.85
 H      -1.153790    -2.282759     0.646950      22.30
 C      -0.287249     0.963639    -0.031513      75.68
 H      -0.718570     2.035689     0.173037      18.57
 C       1.089182     0.682776    -0.311411      14.04
 O       2.033987     1.721873    -0.532415     195.77
 C       1.630928     3.121243    -0.486923     121.15
 H       2.538585     3.666275    -0.546264      27.13
 H       0.818875     3.407097    -1.249411      25.89
 H       1.173497     3.483154     0.522819      27.30
 C       1.617805    -0.618421    -0.369087      21.62
 O       2.979774    -0.778885    -0.498389     179.89
 C       0.778489    -1.680349     0.040430      54.12
 H       1.081820    -2.735121     0.066726      23.50
 C      -1.091157    -0.161405     0.286077      36.65
 C      -2.553924     0.102784     0.562072      77.03
 H      -2.951087    -0.951888     0.951511      23.80
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 O      -2.847085     1.197490     1.461518     279.52
 H      -2.415992     0.930305     2.291219      28.25
 C      -3.253023     0.271428    -0.837178      71.91
 H      -2.646389     1.020697    -1.436462      25.37
 O      -3.275552    -1.107874    -1.494105     201.97
 H      -2.978453    -0.881185    -2.443189      26.14
 C      -4.714005     0.799907    -0.942108     110.44
 O      -4.733582     2.239853    -1.168857     291.91
 H      -5.017935     2.714443    -0.392950      27.65
 H      -5.182452     0.481800    -0.072906      30.98
 H      -5.314359     0.351234    -1.767019      30.20
55
name = lig-etoh-Waterframe_194
 C       5.571751    -1.729236     1.920957      56.04
 H       5.807619    -0.647011     1.669841      27.69
 C       5.036667    -3.962153     1.149894      49.98
 H       4.688476    -4.602959     0.275606      13.80
 C       5.244436    -4.550862     2.374517      44.50
 O       5.114713    -5.877276     2.739783     293.00
 C       4.737798    -6.776408     1.681074     127.52
 H       5.555867    -6.803707     0.994028      31.94
 H       3.759599    -6.475439     1.299507      30.94
 H       4.638572    -7.718126     2.218263      25.92
 C       5.774600    -3.615009     3.427512       8.10
 O       6.179374    -4.099308     4.669128     133.32
 H       5.906290    -5.082364     4.697216      28.80
 C       5.860069    -2.202742     3.210313      62.93
 H       6.233810    -1.509566     3.894943      20.81
 C       5.173534    -2.625880     0.876550      43.28
 C       4.975317    -2.233937    -0.654336      76.02
 H       5.446399    -3.044154    -1.201055      21.56
 O       5.905666    -1.144699    -0.966575     188.34
 H       5.380698    -0.290736    -0.740296      28.79
 C       3.554112    -1.976084    -1.137549      81.13
 H       2.968296    -2.843982    -0.816076      23.90
 C       3.505243    -1.887406    -2.683645     103.28
 O       3.887506    -3.154530    -3.262102     249.96
 H       4.665206    -2.989553    -3.823693      26.36
 H       4.311530    -1.104750    -2.895042      24.91
 H       2.409704    -1.766767    -3.031635      24.78
 C      -0.559782    -1.416939     0.351978      40.06
 H      -1.145742    -2.222527     0.612950      21.70
 C      -0.276966     0.919115     0.040797      71.45
 H      -0.667094     2.047477     0.010641      19.60
 C       1.080975     0.776937    -0.259575       1.78
 O       2.048562     1.738628    -0.517476     244.51
 C       1.637995     3.080041    -0.455942     133.01
 H       2.442278     3.679859    -0.571592      27.23
 H       0.923120     3.260566    -1.149703      29.37
 H       1.095070     3.267728     0.500244      27.31
 C       1.629580    -0.623867    -0.332345       2.37
 O       3.019453    -0.764495    -0.480428     158.12
 C       0.759419    -1.659076     0.025506      61.63
 H       1.102433    -2.657978     0.001660      23.16
 C      -1.133002    -0.139966     0.273130      50.90
 C      -2.589821     0.081576     0.527660      77.16
 H      -3.050292    -0.807964     1.027889      24.46
 O      -2.808005     1.214197     1.423066     268.59
 H      -2.446343     0.947716     2.316701      28.48
 C      -3.272967     0.325396    -0.882821      95.60
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 H      -2.664999     0.933774    -1.420486      27.35
 O      -3.271758    -1.032762    -1.469249     230.26
 H      -3.148673    -1.019783    -2.462389      27.40
 C      -4.753289     0.792160    -0.972944      89.70
 O      -4.751621     2.283601    -1.137626     298.43
 H      -4.923683     2.539240    -0.204308      26.66
 H      -5.282241     0.557187     0.031109      28.09
 H      -5.174689     0.312223    -1.939255      28.35
55
name = lig-etoh-Waterframe_195
 C       5.543106    -1.682923     1.869355      56.90
 H       6.000628    -0.689193     1.810736      21.19
 C       5.016115    -4.021710     1.094437      55.22
 H       4.790370    -4.700314     0.222859      13.70
 C       5.235806    -4.502120     2.399763      20.22
 O       5.142669    -5.824927     2.766973     260.21
 C       4.730224    -6.761256     1.663716      89.83
 H       5.422531    -6.740064     0.775043      27.87
 H       3.761130    -6.436310     1.259771      31.52
 H       4.661754    -7.834435     2.066549      24.22
 C       5.707420    -3.610540     3.402843       2.52
 O       6.195906    -4.152162     4.654852     256.55
 H       5.920606    -5.053380     4.845829      28.93
 C       5.800774    -2.226596     3.161485      41.51
 H       6.157368    -1.645865     4.007920      22.73
 C       5.135316    -2.593090     0.868100      20.62
 C       4.988035    -2.235086    -0.608716      65.95
 H       5.216159    -3.153227    -1.321201      21.36
 O       5.885679    -1.137872    -0.934061     178.36
 H       5.515322    -0.183839    -0.745175      27.85
 C       3.497361    -2.030554    -1.115963      81.10
 H       3.010971    -2.976950    -0.857031      23.15
 C       3.440922    -1.855982    -2.635842     104.06
 O       3.881279    -3.151478    -3.235262     240.76
 H       4.692446    -2.944823    -3.747219      26.23
 H       4.027274    -0.956673    -3.017777      25.17
 H       2.384889    -1.573595    -3.051428      24.84
 C      -0.593501    -1.422205     0.359886      27.95
 H      -1.267115    -2.247167     0.535557      19.43
 C      -0.215169     0.972718     0.073676      75.73
 H      -0.768625     1.973925    -0.074473      19.11
 C       1.143502     0.726529    -0.221695      21.87
 O       2.082790     1.717861    -0.493311     198.43
 C       1.577605     3.097907    -0.414449     117.87
 H       2.447126     3.735744    -0.555769      26.21
 H       0.994443     3.257851    -1.286783      26.62
 H       1.251378     3.224587     0.589537      26.88
 C       1.624549    -0.552461    -0.254070      18.79
 O       3.066075    -0.746365    -0.491772     136.46
 C       0.793501    -1.660126    -0.010615      62.30
 H       1.196724    -2.613704     0.051294      22.44
 C      -1.146536    -0.146650     0.306890      55.14
 C      -2.673197     0.081557     0.491940      80.48
 H      -3.149594    -0.747463     0.899030      27.23
 O      -2.776544     1.244397     1.385469     258.08
 H      -2.363700     0.890620     2.265906      27.21
 C      -3.313912     0.319926    -0.926925      99.23
 H      -2.732305     0.981808    -1.522815      25.87
 O      -3.254497    -0.984906    -1.462103     252.51
 H      -3.174936    -0.716670    -2.419803      26.21
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 C      -4.739401     0.855579    -0.977928      92.40
 O      -4.801146     2.295806    -1.091157     300.41
 H      -4.741532     2.673519    -0.155707      26.04
 H      -5.601804     0.465724    -0.194923      26.81
 H      -5.178187     0.367316    -1.925736      28.36
55
name = lig-etoh-Waterframe_196
 C       5.540670    -1.698700     1.852990      64.24
 H       5.718851    -0.707880     1.488154      27.21
 C       4.989186    -4.004551     1.078640      29.93
 H       4.855908    -4.739245     0.284003      12.41
 C       5.248430    -4.464356     2.399099      21.30
 O       5.155750    -5.819059     2.754096     241.21
 C       4.718288    -6.714652     1.654541     114.54
 H       5.472643    -6.633078     0.786346      26.57
 H       3.689016    -6.493712     1.319389      29.01
 H       4.763574    -7.785295     2.115881      22.39
 C       5.655389    -3.655563     3.466320       1.39
 O       6.188603    -4.168320     4.607611     292.73
 H       5.851659    -4.999982     4.789735      33.54
 C       5.754835    -2.286817     3.139452      55.03
 H       6.118454    -1.657904     4.019134      21.83
 C       5.107936    -2.601077     0.816875      36.15
 C       4.975005    -2.195665    -0.586385      83.66
 H       5.490201    -3.113764    -1.162057      18.12
 O       5.864601    -1.138207    -0.925489     215.71
 H       5.376787    -0.219872    -0.788864      26.66
 C       3.493966    -2.014259    -1.064010      87.24
 H       2.815649    -2.789581    -0.691448      21.47
 C       3.363609    -1.835967    -2.604739     101.28
 O       3.870958    -3.110256    -3.240063     243.37
 H       4.773681    -3.086747    -3.632430      27.11
 H       4.102465    -1.092975    -2.952136      23.46
 H       2.293464    -1.665891    -2.845571      25.36
 C      -0.599594    -1.467445     0.325661      22.09
 H      -1.251480    -2.394912     0.455036      18.03
 C      -0.232498     0.970741     0.082440      59.80
 H      -0.520993     2.010676     0.019032      19.30
 C       1.171546     0.741929    -0.175401       7.34
 O       2.122081     1.719590    -0.463502     205.84
 C       1.572334     3.109013    -0.390937     100.03
 H       2.559719     3.752174    -0.460505      22.65
 H       0.640397     3.416623    -1.133712      22.75
 H       1.027721     3.434283     0.507282      25.66
 C       1.716528    -0.613470    -0.186862      17.54
 O       3.037079    -0.751701    -0.503665     194.87
 C       0.776914    -1.648623     0.007996      74.54
 H       1.189810    -2.624126     0.078090      21.01
 C      -1.099580    -0.127491     0.339507      56.31
 C      -2.679091     0.145057     0.459970      79.06
 H      -3.141703    -0.751969     0.810303      26.45
 O      -2.776401     1.271141     1.354225     262.62
 H      -2.247376     0.951687     2.217176      25.00
 C      -3.345957     0.344693    -0.879926      82.83
 H      -2.735987     1.150766    -1.520937      23.19
 O      -3.238645    -0.970914    -1.533558     242.99
 H      -3.080588    -0.883886    -2.511513      26.41
 C      -4.798721     0.909775    -1.009870     101.93
 O      -4.850854     2.319246    -1.046396     292.48
 H      -4.914990     2.751713    -0.115490      25.21
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 H      -5.384367     0.382097    -0.161245      28.04
 H      -5.129164     0.724319    -2.008048      28.88
55
name = lig-etoh-Waterframe_197
 C       5.503058    -1.811613     1.830852      62.40
 H       5.498649    -0.754726     1.665312      25.10
 C       4.981671    -3.963084     1.125348      29.43
 H       4.765151    -4.607235     0.315795      13.97
 C       5.234052    -4.515312     2.359487      28.27
 O       5.146582    -5.823399     2.703277     284.61
 C       4.730359    -6.680040     1.675083     134.91
 H       5.449649    -6.616768     0.810695      29.20
 H       3.684088    -6.510764     1.398469      30.01
 H       4.831070    -7.698106     2.143261      21.43
 C       5.623351    -3.641956     3.453537       2.56
 O       6.169693    -4.182406     4.603762     260.66
 H       5.891154    -5.054045     4.709312      35.64
 C       5.743408    -2.276622     3.160678      52.40
 H       6.120144    -1.492230     3.916989      20.71
 C       5.108594    -2.638826     0.844829      54.73
 C       4.970273    -2.197322    -0.620655      99.53
 H       5.371109    -3.034542    -1.227701      22.18
 O       5.834087    -1.095342    -0.931943     243.53
 H       5.331928    -0.184155    -0.867299      23.56
 C       3.515023    -1.969964    -1.035588      90.66
 H       2.951070    -2.829822    -0.605728      20.57
 C       3.369771    -1.889137    -2.570580     112.43
 O       3.822222    -3.070251    -3.250537     267.01
 H       4.717694    -2.803075    -3.581546      26.95
 H       3.901127    -0.993327    -2.833341      24.85
 H       2.371989    -1.799280    -2.862018      26.88
 C      -0.578121    -1.449319     0.266577      63.44
 H      -1.268763    -2.375797     0.403074      20.44
 C      -0.177690     0.936541     0.085183      66.38
 H      -0.554408     1.878821     0.186925      21.72
 C       1.180990     0.713376    -0.118771      -0.81
 O       2.100985     1.785013    -0.410357     210.94
 C       1.578128     3.137711    -0.354251      91.64
 H       2.480611     3.906666    -0.602151      23.19
 H       0.859764     3.239193    -1.380169      22.12
 H       1.139027     3.255535     0.674708      24.74
 C       1.701089    -0.637909    -0.132913      12.76
 O       3.019805    -0.743020    -0.499712     185.25
 C       0.779371    -1.679557     0.075298      60.28
 H       1.038016    -2.762210     0.013930      20.85
 C      -1.108978    -0.141797     0.326119      53.42
 C      -2.580770     0.174112     0.470408      75.07
 H      -3.054607    -0.730391     1.027165      23.33
 O      -2.808063     1.309961     1.337655     250.71
 H      -2.237341     1.070841     2.215490      23.30
 C      -3.349155     0.415497    -0.927080      67.39
 H      -2.590940     1.177337    -1.499457      22.87
 O      -3.236328    -0.966568    -1.616869     211.40
 H      -2.954193    -0.783898    -2.556790      25.40
 C      -4.836505     0.910055    -1.032255     110.32
 O      -4.910029     2.405853    -0.983018     281.29
 H      -5.127187     2.574661     0.013674      24.00
 H      -5.471957     0.530472    -0.309868      29.78
 H      -5.171033     0.547542    -1.958655      29.92
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name = lig-etoh-Waterframe_198
 C       5.460923    -1.810689     1.909305      59.64
 H       5.529603    -0.732701     1.835435      23.38
 C       4.953027    -4.040831     1.108345      19.46
 H       4.597298    -4.639479     0.323378      13.52
 C       5.234184    -4.501779     2.398924      15.55
 O       5.143166    -5.825936     2.689854     274.22
 C       4.739976    -6.737539     1.665991     108.28
 H       5.288091    -6.651953     0.753091      31.38
 H       3.715125    -6.514549     1.346103      32.88
 H       4.787513    -7.727563     2.035915      23.82
 C       5.644874    -3.636411     3.400260       7.73
 O       6.131182    -4.192762     4.627626     289.50
 H       6.034097    -5.134368     4.712615      31.74
 C       5.742456    -2.250854     3.176174      67.34
 H       6.081713    -1.539851     3.982061      24.11
 C       5.117962    -2.649372     0.800740      61.89
 C       4.987132    -2.198381    -0.642085     111.81
 H       5.170067    -2.960211    -1.283256      25.54
 O       5.808783    -1.038923    -0.943898     280.87
 H       5.357169    -0.130991    -0.796043      24.29
 C       3.525542    -1.992080    -1.021234      85.09
 H       3.052550    -2.929446    -0.654361      19.22
 C       3.337848    -1.903106    -2.530751     115.75
 O       3.807648    -3.033811    -3.272484     260.83
 H       4.663166    -2.918258    -3.818537      26.51
 H       3.746250    -1.014117    -2.921475      25.05
 H       2.303733    -1.783185    -2.746720      25.68
 C      -0.601792    -1.424165     0.236488      68.24
 H      -1.341115    -2.287316     0.327962      21.29
 C      -0.164117     0.903034     0.127754      61.32
 H      -0.576671     1.837272     0.209666      20.47
 C       1.217852     0.713757    -0.075784      18.54
 O       2.089704     1.803078    -0.341395     212.59
 C       1.584173     3.140825    -0.368841     114.87
 H       2.474650     3.825919    -0.460135      24.84
 H       0.773100     3.310038    -1.121013      24.86
 H       1.113622     3.459816     0.606777      25.84
 C       1.646143    -0.622346    -0.108692      10.92
 O       3.020532    -0.719022    -0.471219     167.58
 C       0.801826    -1.737134     0.130559      51.31
 H       1.144277    -2.819963    -0.055467      18.61
 C      -1.074445    -0.140366     0.259669      31.18
 C      -2.548333     0.173318     0.491034      65.22
 H      -3.068092    -0.780188     0.975226      22.43
 O      -2.828715     1.369658     1.325759     243.95
 H      -2.370120     1.152521     2.278271      24.57
 C      -3.291316     0.409717    -0.981199      73.37
 H      -2.773528     1.167259    -1.620520      23.54
 O      -3.243699    -0.906626    -1.678511     239.31
 H      -2.967616    -0.644348    -2.595713      24.76
 C      -4.834243     0.938811    -1.036456      95.94
 O      -4.981598     2.447570    -0.924031     263.29
 H      -5.076243     2.757581     0.074428      23.19
 H      -5.477525     0.540739    -0.316316      28.75
 H      -5.255238     0.537234    -1.985745      28.59
55
name = lig-etoh-Waterframe_199
 C       5.417833    -1.720276     1.923085      50.83
 H       5.601521    -0.682157     1.600008      21.75
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 C       4.926084    -4.053956     1.046158      44.16
 H       4.569352    -4.821396     0.390518      14.87
 C       5.218931    -4.494297     2.368770      24.26
 O       5.152613    -5.873564     2.725028     245.51
 C       4.710319    -6.812654     1.610890     124.14
 H       5.404195    -6.707575     0.816577      33.62
 H       3.647821    -6.606232     1.390697      29.71
 H       4.798989    -7.751082     2.043888      25.35
 C       5.734703    -3.673679     3.455804      17.91
 O       6.081847    -4.170161     4.648454     199.15
 H       6.011242    -5.154395     4.625899      26.38
 C       5.742419    -2.284076     3.228326      47.38
 H       6.006189    -1.685111     4.088194      22.56
 C       5.146774    -2.681584     0.810323       3.52
 C       4.998919    -2.147240    -0.638606      96.40
 H       5.473090    -2.925527    -1.269488      20.39
 O       5.803188    -1.014793    -0.963224     292.51
 H       5.286775    -0.219075    -0.700043      26.78
 C       3.524022    -2.014664    -1.010906      78.94
 H       2.889422    -2.802091    -0.606773      20.45
 C       3.268740    -1.850688    -2.545388      98.54
 O       3.792129    -3.051040    -3.307999     233.92
 H       4.692766    -2.881670    -3.816837      24.96
 H       3.845103    -0.993701    -2.886150      22.04
 H       2.140716    -1.883291    -2.618374      22.61
 C      -0.594872    -1.504821     0.228066      35.03
 H      -1.346394    -2.283317     0.276438      17.25
 C      -0.155060     0.958184     0.182077      57.41
 H      -0.491578     1.995467     0.147434      16.94
 C       1.188928     0.755758    -0.034482      20.18
 O       2.105151     1.766528    -0.266593     220.36
 C       1.556296     3.176961    -0.352847     122.14
 H       2.434638     3.653548    -0.556799      25.16
 H       0.888661     3.326626    -1.046366      28.89
 H       1.095503     3.520870     0.574090      26.48
 C       1.692692    -0.642147    -0.114679      18.46
 O       3.006220    -0.736781    -0.423481     197.53
 C       0.772377    -1.720525     0.133292      38.38
 H       1.270718    -2.759434     0.106430      17.53
 C      -1.068250    -0.122752     0.223700      77.35
 C      -2.599860     0.205702     0.429530      63.79
 H      -3.086118    -0.711949     0.857062      23.38
 O      -2.825248     1.400985     1.297004     262.47
 H      -2.499026     1.082732     2.268222      26.23
 C      -3.280170     0.406140    -1.001209      90.93
 H      -2.725633     1.099687    -1.488224      24.93
 O      -3.252293    -0.814591    -1.718812     290.66
 H      -3.124485    -0.746505    -2.695669      24.87
 C      -4.806354     0.998669    -0.981615      83.00
 O      -5.039695     2.438611    -0.899334     265.92
 H      -4.949103     2.698772     0.096314      26.07
 H      -5.310040     0.370301    -0.132418      26.90
 H      -5.195264     0.935578    -2.075475      26.28
55
name = lig-etoh-Waterframe_200
 C       5.415821    -1.764131     1.883973      58.35
 H       5.588506    -0.685492     1.668273      20.92
 C       4.943730    -4.033260     1.082184      70.28
 H       4.664998    -4.651947     0.187420      19.60
 C       5.233130    -4.560361     2.351002      24.49
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 O       5.138859    -5.926158     2.724994     255.55
 C       4.708562    -6.854169     1.635955     111.93
 H       5.414559    -6.788867     0.779473      29.71
 H       3.654114    -6.675779     1.260817      29.10
 H       4.799059    -7.831656     2.077939      24.63
 C       5.754865    -3.691333     3.401541     -16.38
 O       6.049676    -4.169741     4.709699     164.91
 H       5.911453    -5.192906     4.761357      25.99
 C       5.735182    -2.281818     3.233717      41.06
 H       5.955853    -1.676374     4.051858      20.35
 C       5.165310    -2.614425     0.870268      29.27
 C       5.030882    -2.156377    -0.609598      75.42
 H       5.553451    -3.028691    -1.275347      19.95
 O       5.793613    -0.989192    -0.969040     268.76
 H       5.408406    -0.117853    -0.789156      25.70
 C       3.493758    -1.998854    -1.033318      80.42
 H       3.010361    -2.889211    -0.613690      19.44
 C       3.247303    -1.865799    -2.565355      95.06
 O       3.743164    -3.054113    -3.318827     248.15
 H       4.706735    -2.797220    -3.607145      24.40
 H       3.658415    -0.845031    -2.883926      22.24
 H       2.130801    -1.743716    -2.916899      22.40
 C      -0.634218    -1.483972     0.228621     -12.61
 H      -1.202485    -2.354863     0.292781      15.41
 C      -0.178768     1.018602     0.213645     102.54
 H      -0.639887     2.083700     0.205371      14.67
 C       1.190713     0.701251    -0.006963       7.89
 O       2.109924     1.767817    -0.193042     192.50
 C       1.576297     3.171392    -0.333883     107.42
 H       2.376292     3.784051    -0.590830      25.46
 H       0.911750     3.170458    -1.241597      23.92
 H       1.226237     3.459434     0.655397      24.60
 C       1.661225    -0.601261    -0.095956      20.98
 O       3.038750    -0.786475    -0.376707     204.72
 C       0.806237    -1.676848     0.095705      69.67
 H       1.074684    -2.731422     0.307356      18.57
 C      -1.114261    -0.149040     0.247077     107.37
 C      -2.635527     0.222206     0.334701      86.83
 H      -3.106413    -0.544915     0.844262      27.27
 O      -2.816559     1.388221     1.236479     260.82
 H      -2.482076     0.973847     2.150721      27.74
 C      -3.289380     0.523288    -1.011085      97.32
 H      -2.582208     1.224575    -1.462683      24.29
 O      -3.281551    -0.772930    -1.726428     247.77
 H      -3.185052    -0.505483    -2.677699      23.44
 C      -4.735079     1.044276    -0.953045      95.35
 O      -5.061083     2.420599    -0.841492     268.94
 H      -5.047292     2.752707     0.116891      26.79
 H      -5.475818     0.388739    -0.227525      27.17
 H      -5.174055     0.579923    -1.947054      27.87
55
name = lig-etoh-Waterframe_201
 C       5.491330    -1.786934     1.958156      69.84
 H       5.482164    -0.681258     1.859034      29.06
 C       5.007145    -3.978188     1.135032      43.27
 H       4.772500    -4.561743     0.177823      14.81
 C       5.283186    -4.640295     2.361838      42.01
 O       5.104297    -5.960707     2.686521     278.35
 C       4.733560    -6.879447     1.686366     103.96
 H       5.430412    -6.841399     0.767904      28.87
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 H       3.710222    -6.597387     1.304159      29.62
 H       4.688120    -7.917363     2.129632      23.21
 C       5.706902    -3.716342     3.385858      10.54
 O       6.019455    -4.163330     4.733164     105.32
 H       5.852784    -5.213332     4.939676      26.22
 C       5.723993    -2.307474     3.167612      72.19
 H       5.951884    -1.635510     3.948562      18.29
 C       5.134398    -2.611781     0.843821      40.01
 C       5.026178    -2.147563    -0.596414      59.36
 H       5.341774    -3.074404    -1.280420      21.27
 O       5.818020    -0.985933    -0.967399     228.29
 H       5.294450    -0.176575    -0.815730      26.39
 C       3.485120    -2.010230    -1.050465      74.87
 H       3.028393    -2.957330    -0.731926      20.82
 C       3.236075    -1.881814    -2.592490      99.98
 O       3.694539    -3.012662    -3.289637     236.06
 H       4.634262    -3.020869    -3.710831      25.03
 H       3.823874    -0.986006    -3.012448      23.24
 H       2.082553    -1.836884    -2.774676      23.84
 C      -0.616319    -1.404467     0.228472      28.94
 H      -1.249244    -2.235862     0.337592      20.61
 C      -0.243641     0.922459     0.217798      64.06
 H      -0.636528     2.030840     0.343835      17.31
 C       1.151646     0.772034     0.013051      12.03
 O       2.135725     1.785035    -0.128798     231.91
 C       1.634121     3.098056    -0.329235     110.06
 H       2.489766     3.813386    -0.533341      23.96
 H       0.591909     3.140092    -1.107667      22.27
 H       1.060886     3.540907     0.540830      26.03
 C       1.679109    -0.613879    -0.088169       7.98
 O       3.062733    -0.820697    -0.318742     167.27
 C       0.738611    -1.659728     0.090454      49.88
 H       1.189132    -2.625324     0.145654      20.09
 C      -1.154557    -0.100823     0.273618      50.98
 C      -2.631000     0.222300     0.322865      72.00
 H      -3.230304    -0.620740     0.621562      23.30
 O      -2.803040     1.359283     1.168330     290.22
 H      -2.385204     1.121347     2.087999      28.48
 C      -3.264169     0.629488    -1.009672      84.39
 H      -2.713119     1.443433    -1.725938      22.52
 O      -3.328238    -0.704119    -1.706323     232.37
 H      -3.074472    -0.619674    -2.688758      23.51
 C      -4.747917     1.004019    -0.952696      98.99
 O      -5.060947     2.432365    -0.792551     247.65
 H      -5.148408     2.619047     0.171366      27.91
 H      -5.186996     0.480574    -0.041949      29.06
 H      -5.147136     0.719284    -1.924986      29.64
55
name = lig-etoh-Waterframe_202
 C       5.527017    -1.743712     1.915363      54.02
 H       5.504318    -0.644843     1.898090      27.47
 C       5.079608    -3.996748     1.115930      38.12
 H       4.804756    -4.802766     0.379983      14.91
 C       5.331954    -4.612399     2.378811      31.14
 O       5.101435    -5.967744     2.691170     301.51
 C       4.713738    -6.906248     1.665543     116.04
 H       5.541504    -6.987280     0.887838      26.44
 H       3.728198    -6.635846     1.297824      28.71
 H       4.641890    -7.904595     2.245195      21.08
 C       5.648837    -3.801595     3.480717      33.98
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 O       5.982572    -4.130816     4.715253     144.25
 H       5.863500    -5.226263     4.786440      26.53
 C       5.750032    -2.407640     3.201595      22.64
 H       6.013917    -1.771055     4.085750      19.62
 C       5.137933    -2.603558     0.860001      30.20
 C       4.958241    -2.148510    -0.639847      75.53
 H       5.437632    -2.909538    -1.223607      23.10
 O       5.835952    -1.030024    -0.955153     207.03
 H       5.349234    -0.187948    -0.797504      26.75
 C       3.531699    -2.023171    -1.047135      82.46
 H       2.922164    -2.872437    -0.712393      23.53
 C       3.252449    -1.841460    -2.577324     106.86
 O       3.650499    -3.061503    -3.277658     245.17
 H       4.491628    -2.761542    -3.770827      25.37
 H       3.762209    -0.957411    -3.010683      25.22
 H       2.181455    -1.744887    -2.638196      26.71
 C      -0.659118    -1.375865     0.243596      41.61
 H      -1.412515    -2.170239     0.334618      18.80
 C      -0.218826     0.937316     0.212367      77.16
 H      -0.667694     1.986682     0.367438      18.46
 C       1.162443     0.746269     0.023925      16.24
 O       2.142796     1.777115    -0.063430     200.76
 C       1.605045     3.087709    -0.300314     103.33
 H       2.557024     3.666491    -0.710869      23.16
 H       0.928460     3.073488    -1.348472      23.49
 H       1.198917     3.502107     0.664968      25.22
 C       1.672022    -0.571883    -0.083532      14.13
 O       3.033079    -0.838062    -0.259825     162.78
 C       0.744681    -1.636884     0.079852      51.57
 H       1.027383    -2.631662    -0.080272      21.23
 C      -1.172153    -0.109831     0.271385      51.07
 C      -2.619663     0.251178     0.321761      63.63
 H      -3.217159    -0.723241     0.533813      23.23
 O      -2.808051     1.360591     1.153776     291.74
 H      -2.332610     1.208294     2.032854      29.11
 C      -3.260569     0.644617    -1.084894      83.32
 H      -2.643053     1.506414    -1.696450      23.81
 O      -3.366097    -0.632814    -1.681790     259.14
 H      -2.985449    -0.657859    -2.611679      25.40
 C      -4.785602     1.005104    -0.911966     110.19
 O      -5.053634     2.443318    -0.750510     251.29
 H      -5.093040     2.632950     0.201431      28.70
 H      -5.108420     0.391328    -0.162546      32.13
 H      -5.282309     0.786529    -1.783050      31.02
55
name = lig-etoh-Waterframe_203
 C       5.534045    -1.782732     1.936767      62.60
 H       5.674406    -0.722302     1.766682      26.63
 C       5.144859    -4.079115     1.106460      23.43
 H       4.837750    -4.676268     0.243093      12.80
 C       5.322248    -4.604869     2.378151      27.97
 O       5.126258    -5.943240     2.713242     258.69
 C       4.690569    -6.933265     1.657196     118.03
 H       5.462449    -7.091603     0.902330      27.51
 H       3.817630    -6.708860     1.084751      32.47
 H       4.561083    -7.884731     2.258298      22.69
 C       5.615755    -3.757860     3.480656      25.65
 O       5.950727    -4.167990     4.760660     176.39
 H       5.938915    -5.245408     4.972822      22.15
 C       5.780654    -2.431051     3.215590      52.52
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 H       6.090328    -1.875888     4.183773      24.75
 C       5.171509    -2.609310     0.851052     -29.04
 C       4.988651    -2.186114    -0.630490      81.60
 H       5.312858    -2.966436    -1.207809      25.44
 O       5.827597    -1.072518    -0.942962     234.03
 H       5.548085    -0.145173    -0.784882      29.07
 C       3.501170    -1.986915    -1.030004      87.70
 H       3.046296    -2.947387    -0.696755      23.23
 C       3.243116    -1.799601    -2.516744     106.58
 O       3.613336    -3.089498    -3.272924     239.64
 H       4.480403    -2.982196    -3.812063      24.29
 H       3.759915    -0.947851    -2.913889      25.77
 H       2.261450    -1.605219    -2.723079      27.50
 C      -0.694369    -1.431716     0.253153      34.80
 H      -1.336438    -2.379341     0.257980      15.90
 C      -0.174995     1.019816     0.208101      56.81
 H      -0.519728     2.041636     0.216840      18.82
 C       1.197531     0.724603     0.042264      13.58
 O       2.130362     1.738159    -0.000095     219.57
 C       1.628758     3.096853    -0.330419     117.13
 H       2.561899     3.750664    -0.536334      24.86
 H       0.912652     3.087139    -1.061386      27.97
 H       1.156680     3.615347     0.510277      26.50
 C       1.644439    -0.615827    -0.079201      25.33
 O       3.009374    -0.824796    -0.223082     177.70
 C       0.710339    -1.626836     0.049389      62.40
 H       0.944016    -2.645582    -0.120362      21.79
 C      -1.126590    -0.071449     0.245939      82.32
 C      -2.625043     0.286806     0.269430      73.26
 H      -3.183393    -0.574945     0.828888      25.72
 O      -2.836827     1.407771     1.197229     257.60
 H      -2.387050     1.097498     2.015671      29.29
 C      -3.301883     0.633229    -1.087397     101.22
 H      -2.624910     1.293201    -1.635562      25.61
 O      -3.378548    -0.633169    -1.713507     268.98
 H      -3.097367    -0.498620    -2.672884      25.28
 C      -4.798058     1.059937    -0.888511     108.35
 O      -5.050125     2.448989    -0.686967     285.56
 H      -4.972840     2.735318     0.224635      29.91
 H      -5.274366     0.450257    -0.140160      30.22
 H      -5.342497     0.691559    -1.769166      29.07
55
name = lig-etoh-Waterframe_204
 C       5.548074    -1.870098     1.968567      70.40
 H       5.813452    -0.846112     1.796737      23.11
 C       5.175106    -4.063555     1.054045      57.66
 H       4.984180    -4.698334     0.221581      15.24
 C       5.268279    -4.650242     2.371287      43.97
 O       5.136138    -5.956504     2.700102     263.70
 C       4.698480    -6.932208     1.681412     135.11
 H       5.518507    -7.096219     1.051799      29.65
 H       3.816395    -6.510344     1.175845      29.63
 H       4.411872    -7.829073     2.228632      23.26
 C       5.625438    -3.752865     3.466070     -17.03
 O       5.920708    -4.214521     4.827461     207.01
 H       5.772351    -5.230361     4.899725      23.77
 C       5.808868    -2.338584     3.222137      46.66
 H       6.179628    -1.611796     4.030632      23.90
 C       5.233939    -2.720694     0.863418      20.13
 C       5.020008    -2.201642    -0.569538      73.56
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 H       5.244146    -3.040322    -1.253142      24.56
 O       5.864079    -1.101330    -0.959475     251.87
 H       5.302793    -0.315214    -0.710912      29.87
 C       3.461486    -1.965592    -0.951382      83.79
 H       2.947048    -2.903768    -0.657549      24.41
 C       3.257190    -1.791752    -2.514000     104.64
 O       3.567888    -3.059502    -3.242800     265.26
 H       4.473511    -3.100621    -3.622827      26.80
 H       3.979548    -1.093830    -2.825349      25.61
 H       2.221546    -1.648246    -2.742173      26.43
 C      -0.684085    -1.419544     0.228897      36.09
 H      -1.432357    -2.298633     0.244919      18.46
 C      -0.160449     1.027083     0.184565      58.83
 H      -0.467748     1.993437     0.148849      21.38
 C       1.190362     0.731027     0.072915      11.20
 O       2.149520     1.747793     0.043487     214.67
 C       1.666696     3.105886    -0.322928     120.08
 H       2.561006     3.675888    -0.571228      25.85
 H       0.987447     3.086637    -1.078844      28.67
 H       1.101704     3.515077     0.483832      26.68
 C       1.621618    -0.659066    -0.065745      15.80
 O       3.008779    -0.820252    -0.219029     191.04
 C       0.636406    -1.705159     0.012168      61.55
 H       1.129516    -2.688591    -0.013510      20.98
 C      -1.104781    -0.020915     0.213629      71.96
 C      -2.619526     0.339091     0.308958      74.86
 H      -3.168864    -0.585633     0.644070      26.19
 O      -2.857840     1.469406     1.248341     276.71
 H      -2.537464     1.132870     2.080862      29.59
 C      -3.353531     0.602083    -1.011500      99.36
 H      -2.899693     1.290871    -1.580192      27.68
 O      -3.380842    -0.691881    -1.792871     229.80
 H      -3.324817    -0.541308    -2.798017      24.11
 C      -4.817354     1.093781    -0.869599      88.04
 O      -5.044417     2.495201    -0.635228     267.44
 H      -4.967822     2.609162     0.312941      29.40
 H      -5.269599     0.546692     0.095057      27.48
 H      -5.300062     0.926207    -1.940296      27.31
55
name = lig-etoh-Waterframe_205
 C       5.590844    -1.897313     1.918066      64.83
 H       5.712287    -0.841475     1.702458      26.86
 C       5.171388    -4.163018     1.055521      50.47
 H       5.112713    -4.834180     0.244786      17.42
 C       5.248119    -4.607638     2.386049      37.97
 O       5.139719    -6.008236     2.707455     249.98
 C       4.701979    -6.886738     1.724521     139.15
 H       5.482256    -7.170745     1.066678      30.90
 H       3.839995    -6.403630     1.127023      28.07
 H       4.350304    -7.757746     2.212671      27.17
 C       5.669015    -3.771969     3.532912     -25.05
 O       5.864416    -4.208501     4.795450     120.92
 H       5.770026    -5.134481     4.956363      20.06
 C       5.829854    -2.346215     3.272018      45.65
 H       6.178757    -1.581764     3.977412      21.24
 C       5.310710    -2.741328     0.861906      35.74
 C       4.993928    -2.250571    -0.535802      82.51
 H       5.400614    -3.106113    -1.271169      20.74
 O       5.879866    -1.117347    -0.966519     199.72
 H       5.428995    -0.223809    -0.797908      27.54
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 C       3.485428    -2.000060    -0.880739      78.56
 H       2.851235    -2.818741    -0.539976      23.74
 C       3.321257    -1.826538    -2.497894      99.74
 O       3.520200    -3.028350    -3.188519     283.52
 H       4.405210    -2.924638    -3.556375      26.65
 H       3.957776    -1.004093    -2.871142      24.62
 H       2.244347    -1.408716    -2.708903      24.92
 C      -0.733604    -1.332067     0.171744      51.74
 H      -1.589545    -2.040959     0.326387      19.34
 C      -0.183616     1.007367     0.147810      70.52
 H      -0.563169     1.958493     0.198261      20.95
 C       1.207497     0.701476     0.089327      12.93
 O       2.192860     1.769974     0.064421     187.86
 C       1.696954     3.083963    -0.292028     103.54
 H       2.557851     3.643297    -0.503035      26.76
 H       1.143015     3.023784    -1.422670      23.54
 H       1.197353     3.555992     0.568543      25.28
 C       1.580598    -0.641661    -0.040876      17.46
 O       2.992881    -0.809214    -0.218050     157.74
 C       0.694726    -1.753910    -0.014719      74.96
 H       0.896773    -2.886587     0.082258      20.55
 C      -1.141334    -0.022048     0.200676      40.84
 C      -2.610545     0.351986     0.384011      80.17
 H      -3.038182    -0.538538     0.752548      27.37
 O      -2.872440     1.502875     1.278677     280.10
 H      -2.586182     1.253544     2.125649      30.74
 C      -3.396637     0.581242    -1.015717      80.04
 H      -2.926765     1.407852    -1.606541      25.57
 O      -3.402818    -0.733400    -1.808548     210.27
 H      -3.238919    -0.434542    -2.763340      24.14
 C      -4.853070     1.106291    -0.827769      92.99
 O      -5.009458     2.558971    -0.584053     246.15
 H      -5.136861     2.820977     0.354118      26.33
 H      -5.519909     0.356046    -0.125660      27.61
 H      -5.433065     0.873390    -1.845160      28.24
55
name = lig-etoh-Waterframe_206
 C       5.662257    -1.892770     1.916130      65.63
 H       5.577782    -0.826970     1.676491      31.19
 C       5.184602    -4.221472     1.118645      48.99
 H       5.069488    -4.914880     0.305815      17.03
 C       5.285208    -4.628621     2.454563      22.80
 O       5.163606    -5.984067     2.778253     211.95
 C       4.660265    -6.867012     1.718594     126.77
 H       5.457906    -7.195329     1.021937      29.22
 H       3.846316    -6.454705     1.020754      28.13
 H       4.280611    -7.723639     2.231364      27.26
 C       5.678898    -3.737598     3.513036       4.97
 O       5.814959    -4.182394     4.785725      82.42
 H       5.824707    -5.154101     4.927057      23.57
 C       5.837821    -2.414809     3.246087      64.05
 H       6.071280    -1.873654     4.110822      17.76
 C       5.345406    -2.789067     0.834598       4.55
 C       5.008562    -2.264772    -0.547832      86.91
 H       5.282973    -3.161043    -1.290924      21.37
 O       5.873143    -1.139825    -0.962102     191.90
 H       5.571011    -0.180439    -0.867500      28.47
 C       3.515626    -2.036246    -0.879382      80.81
 H       3.013127    -2.955752    -0.564300      22.47
 C       3.343601    -1.784676    -2.385505      91.50
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 O       3.506375    -3.022869    -3.160005     260.87
 H       4.286033    -3.065806    -3.735325      27.91
 H       4.111585    -1.027754    -2.773854      23.19
 H       2.227298    -1.391622    -2.580455      24.51
 C      -0.723548    -1.334196     0.109472      48.43
 H      -1.403095    -2.142147     0.274056      24.31
 C      -0.180169     1.019058     0.121357      80.46
 H      -0.498911     2.069916     0.242366      21.45
 C       1.178285     0.748738     0.087813       4.03
 O       2.215111     1.726224     0.077772     191.47
 C       1.776651     3.065843    -0.286002     100.62
 H       2.643465     3.662852    -0.325248      25.88
 H       0.927044     3.073740    -1.315807      22.53
 H       1.025885     3.596578     0.401110      24.42
 C       1.640571    -0.696026    -0.039506       7.85
 O       2.982951    -0.781780    -0.207705     154.70
 C       0.605197    -1.685396     0.011695      56.65
 H       0.872138    -2.822232    -0.063054      21.05
 C      -1.174001     0.020914     0.196492      36.46
 C      -2.655194     0.330638     0.422543      79.45
 H      -3.095632    -0.443057     1.017405      25.28
 O      -2.875402     1.514152     1.282162     278.20
 H      -2.446869     1.260047     2.058572      30.90
 C      -3.437602     0.566773    -1.004064      70.41
 H      -2.691409     1.301796    -1.644529      23.63
 O      -3.431340    -0.688562    -1.753420     230.90
 H      -3.061252    -0.576233    -2.673640      26.29
 C      -4.941654     1.090757    -0.802660     100.85
 O      -4.963463     2.585390    -0.550769     231.26
 H      -5.222160     2.881498     0.363051      25.68
 H      -5.497079     0.542296    -0.021031      28.99
 H      -5.360750     1.012878    -1.801266      29.81
55
name = lig-etoh-Waterframe_207
 C       5.699043    -1.928112     1.898394      52.93
 H       5.718491    -0.820640     1.831974      23.25
 C       5.223120    -4.165386     1.175762      56.80
 H       4.924649    -4.892557     0.404728      17.64
 C       5.352907    -4.698263     2.477593      24.16
 O       5.164731    -5.967997     2.846865     249.29
 C       4.615242    -6.871286     1.718068     114.51
 H       5.551981    -7.124471     1.121484      27.35
 H       3.803330    -6.304917     1.241744      27.11
 H       4.219602    -7.742093     2.274728      22.93
 C       5.649408    -3.792022     3.459250      10.05
 O       5.785276    -4.146613     4.826895     187.85
 H       5.749197    -5.187799     4.851676      26.07
 C       5.855001    -2.400822     3.185730      49.25
 H       5.984904    -1.822140     4.050210      25.12
 C       5.358175    -2.841301     0.871288      29.32
 C       5.051543    -2.260411    -0.576202      98.03
 H       5.252588    -3.020187    -1.311931      28.42
 O       5.885510    -1.175612    -0.967190     232.84
 H       5.282797    -0.394675    -0.738765      29.73
 C       3.550765    -2.043658    -0.866923      88.60
 H       3.000715    -2.949643    -0.564855      24.73
 C       3.356571    -1.747508    -2.313568      96.60
 O       3.491673    -3.030804    -3.145621     238.40
 H       4.363266    -2.868547    -3.628610      26.87
 H       4.172790    -1.009922    -2.588392      24.47
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 H       2.299493    -1.411270    -2.513606      26.61
 C      -0.782850    -1.330406     0.093580      52.57
 H      -1.370129    -2.189909     0.069742      24.62
 C      -0.190992     1.075684     0.129281      69.77
 H      -0.493399     2.208625     0.199941      20.46
 C       1.201237     0.696243     0.058081      12.21
 O       2.195404     1.674318     0.079560     190.35
 C       1.795576     3.070951    -0.275958     107.42
 H       2.710761     3.667812    -0.392928      26.39
 H       1.421906     3.034341    -1.321577      26.80
 H       1.141819     3.392439     0.584176      24.84
 C       1.611886    -0.623801    -0.031211      21.85
 O       3.023439    -0.818828    -0.199920     156.81
 C       0.618475    -1.601320     0.017966      52.02
 H       0.925826    -2.662171    -0.190494      20.98
 C      -1.191222     0.016234     0.192183      34.74
 C      -2.729421     0.329320     0.423088      78.25
 H      -3.215463    -0.627372     0.872912      26.00
 O      -2.855537     1.522013     1.271033     281.10
 H      -2.324989     1.336978     2.016243      30.79
 C      -3.456757     0.550468    -0.916821      84.31
 H      -2.916526     1.459585    -1.517731      25.32
 O      -3.465158    -0.640047    -1.668365     227.92
 H      -3.063787    -0.520397    -2.565544      26.74
 C      -4.956895     1.146823    -0.793552     114.45
 O      -4.927336     2.573329    -0.542926     269.12
 H      -5.060541     2.679281     0.438471      26.21
 H      -5.393327     0.692774    -0.018368      31.51
 H      -5.472111     0.966362    -1.665837      31.98
55
name = lig-etoh-Waterframe_208
 C       5.720289    -1.925927     1.876469      55.37
 H       5.950632    -0.867139     1.613885      22.46
 C       5.234003    -4.181959     1.181500      32.07
 H       4.869992    -4.772923     0.294585      16.58
 C       5.415203    -4.717043     2.449212      26.21
 O       5.127567    -6.045361     2.877965     317.15
 C       4.606723    -6.836957     1.818488     103.54
 H       5.361350    -7.093171     0.973115      25.96
 H       3.823664    -6.344860     1.288369      31.47
 H       4.215867    -7.811376     2.255673      22.04
 C       5.668595    -3.781433     3.542609      39.50
 O       5.757418    -4.107193     4.831226     163.85
 H       5.669295    -5.145348     5.170249      24.39
 C       5.858876    -2.431901     3.188181      69.54
 H       6.026282    -1.601869     3.888662      28.25
 C       5.371792    -2.774300     0.852674      21.97
 C       5.094519    -2.353236    -0.564015      87.47
 H       5.375738    -3.104003    -1.189553      27.21
 O       5.874187    -1.182582    -0.961717     248.44
 H       5.448495    -0.297532    -0.688978      30.04
 C       3.549168    -2.040860    -0.812884      85.74
 H       2.959848    -2.919362    -0.476620      23.77
 C       3.345556    -1.770029    -2.337351     106.79
 O       3.501198    -2.974791    -3.128893     256.86
 H       4.443702    -2.912559    -3.558797      25.28
 H       4.004440    -0.988294    -2.722546      25.54
 H       2.429408    -1.318440    -2.500114      28.42
 C      -0.787134    -1.311718     0.095321      24.03
 H      -1.578226    -2.020218    -0.059838      18.15
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 C      -0.210710     1.039064     0.156591      67.24
 H      -0.564570     2.173481     0.120212      22.00
 C       1.159281     0.765973     0.032642      15.62
 O       2.200895     1.655448     0.059660     223.89
 C       1.844600     3.021134    -0.261147     124.42
 H       2.847507     3.585858    -0.175162      25.06
 H       1.408937     3.140141    -1.105251      31.62
 H       1.187076     3.561762     0.460194      26.58
 C       1.623756    -0.589428    -0.038516       9.46
 O       3.057682    -0.859902    -0.159096     159.47
 C       0.644572    -1.584800    -0.018690      62.89
 H       0.948538    -2.589709    -0.138598      23.74
 C      -1.228126     0.033417     0.195918      39.87
 C      -2.731741     0.337306     0.410409      80.68
 H      -3.231233    -0.623249     0.876745      26.51
 O      -2.834036     1.515804     1.253363     282.47
 H      -2.344333     1.346267     2.056923      31.62
 C      -3.524212     0.655422    -0.849731      98.47
 H      -2.966508     1.404611    -1.385333      27.64
 O      -3.490251    -0.625404    -1.596748     226.00
 H      -3.237626    -0.324242    -2.505071      26.62
 C      -4.916398     1.166156    -0.748647     116.97
 O      -4.906921     2.561524    -0.536140     276.10
 H      -4.828039     2.796920     0.438434      26.26
 H      -5.494915     0.636771     0.062517      28.86
 H      -5.510617     0.870854    -1.615623      29.47
55
name = lig-etoh-Waterframe_209
 C       5.760634    -1.903468     1.864265      62.55
 H       6.072348    -0.877117     1.614835      22.58
 C       5.224404    -4.181837     1.124682      49.56
 H       4.958158    -4.935894     0.322918      19.23
 C       5.432255    -4.714986     2.496055      21.04
 O       5.116140    -6.068576     2.886324     336.57
 C       4.567918    -6.852177     1.863208     116.40
 H       5.337227    -7.029649     1.081993      26.63
 H       3.678104    -6.411297     1.450660      28.81
 H       4.291958    -7.845581     2.340060      21.97
 C       5.700783    -3.765874     3.553946      -0.08
 O       5.734073    -4.076161     4.913486      -1.63
 H       5.704683    -5.189355     4.936701      28.70
 C       5.866065    -2.406090     3.204935      35.82
 H       6.181208    -1.743081     4.112122      21.27
 C       5.387755    -2.800701     0.849759      42.99
 C       5.082890    -2.366749    -0.537179      71.19
 H       5.396956    -3.193272    -1.205868      25.64
 O       5.879758    -1.197455    -0.965654     217.85
 H       5.538072    -0.288123    -0.654943      28.97
 C       3.530408    -2.071532    -0.824182      69.91
 H       2.980942    -2.973273    -0.502190      24.43
 C       3.321605    -1.769887    -2.369967     108.93
 O       3.521123    -2.927848    -3.128682     265.82
 H       4.384204    -2.946780    -3.735021      25.36
 H       4.056166    -1.056897    -2.662712      25.19
 H       2.319439    -1.518120    -2.492297      27.62
 C      -0.739520    -1.268861     0.080187      16.91
 H      -1.466929    -2.129950     0.013647      21.21
 C      -0.255339     1.026603     0.172463      69.67
 H      -0.580581     2.119243     0.202411      21.82
 C       1.138813     0.782885     0.025253       5.07
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 O       2.202451     1.683787     0.028528     218.95
 C       1.920795     3.035121    -0.211176     109.22
 H       2.960083     3.578453    -0.169013      23.13
 H       1.335737     3.206336    -1.229406      25.71
 H       1.231479     3.441843     0.517675      25.71
 C       1.659180    -0.617612    -0.062078      -1.91
 O       3.054363    -0.842380    -0.072300     147.01
 C       0.610812    -1.622273    -0.062485      63.17
 H       0.871831    -2.609961    -0.069103      23.62
 C      -1.225413     0.020602     0.192454      47.84
 C      -2.689188     0.366561     0.429780      85.79
 H      -3.159784    -0.444850     1.012345      26.61
 O      -2.815299     1.527367     1.256073     289.99
 H      -2.451082     1.241353     2.137122      29.82
 C      -3.502663     0.706029    -0.850273      99.69
 H      -2.992077     1.357379    -1.402183      28.79
 O      -3.508572    -0.577786    -1.550678     218.25
 H      -3.469832    -0.473102    -2.533324      27.23
 C      -4.949914     1.137698    -0.645666      89.48
 O      -4.907429     2.604037    -0.531178     230.80
 H      -4.774995     2.831157     0.447339      26.95
 H      -5.550514     0.567926     0.276765      26.70
 H      -5.368519     1.060645    -1.744291      26.64
55
name = lig-etoh-Waterframe_210
 C       5.814435    -1.915092     1.913708      65.44
 H       5.979745    -0.857884     1.729826      31.96
 C       5.241194    -4.231657     1.188628      62.95
 H       5.026059    -4.935566     0.358786      19.62
 C       5.377823    -4.690587     2.507347      15.65
 O       5.147963    -5.987031     2.911543     232.23
 C       4.511247    -6.924110     1.866139     115.70
 H       5.208437    -7.044058     1.086209      29.16
 H       3.530357    -6.492233     1.556843      29.03
 H       4.401203    -7.862116     2.425573      26.26
 C       5.710592    -3.757556     3.534554     -35.77
 O       5.719729    -4.071489     4.954878       4.63
 H       5.723078    -5.126532     5.205546      22.87
 C       5.905594    -2.364545     3.217272      20.72
 H       6.245197    -1.769463     4.155038      12.44
 C       5.402978    -2.865806     0.879765       1.97
 C       5.026873    -2.287947    -0.553220      69.55
 H       5.253928    -3.135086    -1.379805      23.48
 O       5.900261    -1.235459    -0.981036     216.07
 H       5.382609    -0.434872    -0.610082      29.47
 C       3.529643    -2.084816    -0.858306      73.25
 H       2.935048    -2.949693    -0.564532      25.43
 C       3.300155    -1.745723    -2.333908     102.92
 O       3.540015    -2.965719    -3.173695     267.61
 H       4.363383    -2.730551    -3.732674      24.48
 H       3.926683    -0.889198    -2.539231      26.57
 H       2.217298    -1.459508    -2.524390      26.14
 C      -0.723094    -1.310547     0.048468      50.42
 H      -1.368504    -2.248645     0.217088      20.21
 C      -0.227392     1.085690     0.167990      54.35
 H      -0.568323     2.070781     0.355356      21.55
 C       1.176350     0.683683     0.021494       3.94
 O       2.205026     1.685027    -0.001404     172.10
 C       1.948135     3.128040    -0.166255     101.25
 H       2.928399     3.692187    -0.221974      25.18
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 H       1.539342     3.240426    -1.394284      24.26
 H       1.384966     3.458150     0.675158      26.42
 C       1.608268    -0.629948    -0.075183      25.02
 O       3.030785    -0.844476    -0.001364     113.84
 C       0.652946    -1.634298    -0.090478      61.14
 H       0.808792    -2.679314    -0.095316      23.18
 C      -1.191281     0.019594     0.191395      54.75
 C      -2.657883     0.398781     0.461910      85.53
 H      -3.130250    -0.462182     0.841614      27.98
 O      -2.786453     1.578177     1.294781     291.80
 H      -2.501612     1.319551     2.251904      28.95
 C      -3.442313     0.652951    -0.852675      87.88
 H      -3.037023     1.521463    -1.474885      26.20
 O      -3.531276    -0.556996    -1.539892     231.58
 H      -3.451318    -0.394656    -2.511724      27.35
 C      -4.952660     1.196744    -0.596361      82.69
 O      -4.938243     2.651770    -0.487864     242.04
 H      -4.848512     2.860626     0.512845      26.56
 H      -5.548947     0.600365     0.271519      27.82
 H      -5.631075     0.872153    -1.538248      27.94
55
name = lig-etoh-Waterframe_211
 C       5.826843    -1.965206     1.915786      60.80
 H       5.839623    -0.916222     1.681059      33.09
 C       5.263546    -4.242805     1.226134      53.63
 H       4.963070    -4.916118     0.443596      15.31
 C       5.315332    -4.657468     2.550725      23.69
 O       5.153683    -5.954089     2.906621     230.38
 C       4.503279    -6.944738     1.936206     120.44
 H       5.003788    -7.097569     1.013162      31.45
 H       3.443484    -6.616038     1.593116      29.51
 H       4.455872    -7.863280     2.478861      27.27
 C       5.698456    -3.739185     3.607098      18.97
 O       5.715772    -4.060734     4.935301     117.16
 H       5.713482    -5.008937     5.110755      21.45
 C       5.975166    -2.412950     3.284128      58.30
 H       6.182802    -1.559355     3.954819      20.73
 C       5.413266    -2.832450     0.900763     -21.63
 C       5.000549    -2.318314    -0.561423      75.76
 H       5.219622    -3.231123    -1.288263      22.05
 O       5.885520    -1.248470    -0.983644     203.60
 H       5.606053    -0.281277    -0.781636      29.59
 C       3.499737    -2.022720    -0.823363      87.34
 H       3.003588    -2.952763    -0.532742      23.14
 C       3.255157    -1.748706    -2.312303      88.45
 O       3.539000    -2.954807    -3.189157     252.28
 H       4.425054    -3.040784    -3.705826      23.99
 H       3.922401    -0.934627    -2.677990      24.05
 H       2.134059    -1.363530    -2.483743      24.41
 C      -0.718258    -1.365277     0.044740      31.95
 H      -1.548778    -2.114963     0.207933      20.53
 C      -0.141355     1.062513     0.158888      64.27
 H      -0.370872     2.026615     0.343938      22.52
 C       1.179856     0.751830     0.016758       8.79
 O       2.237131     1.672192    -0.026526     199.06
 C       1.969519     3.171095    -0.160065     114.62
 H       2.940030     3.544373    -0.061729      25.47
 H       1.220820     3.565635    -1.022639      24.54
 H       1.324965     3.703706     0.564564      26.24
 C       1.630783    -0.653509    -0.076314      11.02
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 O       2.993235    -0.900656     0.012485     161.40
 C       0.642601    -1.672334    -0.099877      48.94
 H       1.071528    -2.723686    -0.185958      20.75
 C      -1.123878     0.044461     0.201181      45.78
 C      -2.623547     0.411787     0.475791      71.86
 H      -3.126248    -0.451913     0.926676      24.63
 O      -2.761704     1.625847     1.334451     269.88
 H      -2.342016     1.355213     2.283497      25.91
 C      -3.487712     0.681568    -0.818478      72.09
 H      -2.813178     1.488962    -1.533061      23.23
 O      -3.539537    -0.583036    -1.585870     220.56
 H      -3.219903    -0.321491    -2.479490      26.56
 C      -4.922912     1.239008    -0.562489     112.56
 O      -4.986909     2.677380    -0.423992     259.36
 H      -4.974385     2.957123     0.574853      25.86
 H      -5.218285     0.903255     0.371186      30.43
 H      -5.596064     0.939356    -1.369717      29.65
55
name = lig-etoh-Waterframe_212
 C       5.807823    -2.002075     1.930479      55.56
 H       5.906539    -0.941644     1.737831      22.81
 C       5.252083    -4.166881     1.215392      52.83
 H       4.933590    -4.903817     0.541284      14.94
 C       5.294387    -4.610068     2.589910      19.48
 O       5.123319    -6.007607     2.895979     271.19
 C       4.506820    -6.917166     2.032785     144.29
 H       5.127095    -7.050631     1.098818      29.45
 H       3.405198    -6.606690     1.920828      28.33
 H       4.526899    -7.831799     2.582005      24.53
 C       5.672023    -3.716642     3.662751       6.26
 O       5.717621    -4.070074     4.947982     159.90
 H       5.733447    -4.981876     5.004019      21.58
 C       6.031955    -2.407634     3.260977      59.39
 H       6.182158    -1.742258     4.072699      23.92
 C       5.386389    -2.826108     0.879443      26.33
 C       5.014636    -2.353126    -0.499382      93.20
 H       5.259085    -3.165966    -1.160056      24.24
 O       5.888287    -1.268501    -1.009494     207.52
 H       5.506689    -0.318191    -0.882675      26.87
 C       3.478630    -2.006428    -0.766012      85.48
 H       2.962957    -2.950192    -0.500089      23.01
 C       3.256714    -1.765744    -2.363953      94.16
 O       3.483579    -2.940943    -3.159623     258.73
 H       4.424073    -2.834180    -3.475277      25.41
 H       3.977784    -0.975111    -2.698474      23.75
 H       2.115778    -1.597343    -2.529980      24.25
 C      -0.751642    -1.320265     0.076229      38.66
 H      -1.505972    -2.099244    -0.023476      19.49
 C      -0.102610     1.048215     0.165318      69.66
 H      -0.415511     2.057574     0.209636      20.64
 C       1.285497     0.751617    -0.007615      11.28
 O       2.258445     1.732395    -0.056436     225.45
 C       1.943143     3.187109    -0.123902     117.01
 H       2.884205     3.598729    -0.227125      27.46
 H       1.524182     3.356264    -1.029692      29.22
 H       1.474111     3.403299     0.898952      24.79
 C       1.608262    -0.628209    -0.063122      16.86
 O       2.980246    -0.959195    -0.005947     185.60
 C       0.644579    -1.692516    -0.095968      58.47
 H       1.010552    -2.816072    -0.210688      19.70
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 C      -1.084906     0.005201     0.211895      33.08
 C      -2.591597     0.440328     0.488847      70.96
 H      -3.010144    -0.393643     1.163897      24.13
 O      -2.723291     1.636450     1.348316     261.54
 H      -2.171828     1.339405     2.241614      25.41
 C      -3.480765     0.721332    -0.802547      74.19
 H      -2.848994     1.482826    -1.483964      23.10
 O      -3.539397    -0.583704    -1.639266     210.75
 H      -3.051053    -0.503441    -2.490649      26.26
 C      -4.875954     1.275760    -0.465087     119.80
 O      -5.031770     2.719389    -0.388778     274.83
 H      -4.971567     3.009220     0.613940      25.26
 H      -5.126385     0.814247     0.413831      30.46
 H      -5.479631     0.971743    -1.224857      30.52
55
name = lig-etoh-Waterframe_213
 C       5.798787    -1.934105     1.947905      49.34
 H       6.081649    -0.891187     1.739928      17.37
 C       5.186248    -4.170342     1.262091      48.88
 H       4.959289    -4.830690     0.456118      19.00
 C       5.297055    -4.625728     2.571055      14.36
 O       5.134903    -5.966839     2.963691     284.74
 C       4.487530    -6.915242     2.111001     128.32
 H       5.004401    -6.998634     1.060907      25.55
 H       3.442962    -6.683167     1.876605      30.38
 H       4.568694    -7.877228     2.604145      21.66
 C       5.647663    -3.722008     3.603195      16.37
 O       5.724225    -4.086907     5.007453     122.35
 H       5.784874    -5.140319     5.259072      17.99
 C       6.031208    -2.408348     3.251939      52.76
 H       6.382797    -1.806764     4.028521      27.16
 C       5.361931    -2.809456     0.904150      12.71
 C       5.022489    -2.329018    -0.487453     102.14
 H       5.163305    -3.126993    -1.099509      25.60
 O       5.894150    -1.294407    -1.033692     255.57
 H       5.304343    -0.469969    -0.880625      27.48
 C       3.492194    -2.107601    -0.800803      76.48
 H       2.900064    -3.009079    -0.535721      22.80
 C       3.236413    -1.801251    -2.336061     107.70
 O       3.457014    -2.951190    -3.126545     273.61
 H       4.322263    -2.877307    -3.627541      26.21
 H       3.863735    -0.916117    -2.605600      24.49
 H       2.244709    -1.398658    -2.497913      26.12
 C      -0.717013    -1.331438     0.075316      23.38
 H      -1.445677    -2.084218    -0.057876      19.35
 C      -0.068551     1.036829     0.162606      71.57
 H      -0.534600     2.074550     0.101159      18.52
 C       1.302901     0.747793    -0.015789       4.98
 O       2.326302     1.773490    -0.095218     213.07
 C       1.948514     3.131262    -0.086969     121.12
 H       2.834890     3.777136    -0.189763      25.75
 H       1.293364     3.332761    -0.880944      28.12
 H       1.371718     3.490913     0.889935      24.93
 C       1.621435    -0.670190    -0.054045      25.04
 O       2.990004    -0.946773    -0.006384     171.52
 C       0.604812    -1.619217    -0.068924      64.15
 H       0.781000    -2.767305    -0.156667      20.77
 C      -1.102958     0.057456     0.237037      54.25
 C      -2.546504     0.459967     0.509742      75.66
 H      -3.074512    -0.478961     0.959460      23.69
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 O      -2.653823     1.632123     1.326878     269.27
 H      -2.257370     1.393382     2.312354      25.66
 C      -3.372433     0.716958    -0.817043      85.43
 H      -3.029747     1.508595    -1.360941      26.68
 O      -3.548336    -0.540184    -1.641686     232.36
 H      -3.046888    -0.379568    -2.475265      26.27
 C      -4.851572     1.282387    -0.370313      91.08
 O      -5.055774     2.740404    -0.364773     267.95
 H      -4.921589     3.188129     0.555648      24.70
 H      -5.332061     0.691762     0.545284      27.67
 H      -5.507503     0.912122    -1.171810      28.64
55
name = lig-etoh-Waterframe_214
 C       5.808936    -1.853968     1.940814      60.12
 H       6.128154    -0.831187     1.646508      22.35
 C       5.101294    -4.177254     1.256795      58.01
 H       4.893727    -4.875528     0.422596      21.28
 C       5.299526    -4.683048     2.570658      26.09
 O       5.152795    -5.906908     3.058822     259.03
 C       4.462036    -6.927057     2.130087     113.35
 H       4.987176    -6.981495     1.119934      25.76
 H       3.448245    -6.668432     2.017764      29.58
 H       4.555774    -7.894054     2.661826      22.57
 C       5.661703    -3.766684     3.642255      16.84
 O       5.731097    -4.055655     4.998866     -66.57
 H       5.829361    -5.193598     5.227709      16.41
 C       5.993087    -2.419587     3.276258      32.28
 H       6.543513    -1.768174     3.931830      26.23
 C       5.339373    -2.755896     0.997806      26.09
 C       5.010968    -2.363973    -0.540222      78.58
 H       5.277667    -3.271185    -1.133913      22.38
 O       5.860967    -1.303069    -1.032873     232.38
 H       5.557905    -0.320175    -0.972391      26.60
 C       3.494078    -2.174260    -0.839766      74.98
 H       3.016615    -3.108413    -0.488245      22.45
 C       3.213698    -1.776960    -2.251007     107.54
 O       3.459088    -2.996949    -3.129153     256.18
 H       4.198878    -2.864488    -3.772731      27.62
 H       3.985437    -1.083514    -2.576739      23.97
 H       2.248214    -1.461731    -2.352341      27.40
 C      -0.766193    -1.255222     0.073229      20.81
 H      -1.450069    -2.056208     0.152790      20.79
 C      -0.078428     1.058065     0.141563      68.37
 H      -0.297816     2.218897     0.200110      17.45
 C       1.283903     0.744868    -0.007674       9.31
 O       2.383535     1.719528    -0.123620     189.61
 C       1.898923     3.129147    -0.071815      98.33
 H       2.866591     3.782724    -0.124240      23.32
 H       0.991196     3.434641    -0.780951      24.50
 H       1.422185     3.395227     0.915285      25.97
 C       1.692790    -0.637160    -0.043070      14.95
 O       3.026312    -0.945960    -0.021867     149.43
 C       0.616492    -1.605897    -0.043034      55.12
 H       0.943495    -2.648903    -0.135743      20.48
 C      -1.078674     0.068747     0.258711      44.89
 C      -2.510790     0.440584     0.472980      85.74
 H      -3.068940    -0.398261     0.920432      23.93
 O      -2.591929     1.636995     1.300142     278.43
 H      -2.351791     1.275429     2.258039      24.58
 C      -3.352231     0.742675    -0.785922      83.65
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 H      -2.923911     1.461420    -1.369555      27.08
 O      -3.540859    -0.445529    -1.603585     246.27
 H      -3.228560    -0.257775    -2.520351      26.32
 C      -4.849868     1.251499    -0.335681      72.06
 O      -5.055279     2.718727    -0.360679     261.15
 H      -5.002890     3.095028     0.557431      26.14
 H      -5.174854     0.926543     0.827548      25.89
 H      -5.526260     0.930299    -1.251246      26.29
55
name = lig-etoh-Waterframe_215
 C       5.815817    -1.874990     1.984294      68.20
 H       6.060450    -0.823845     1.735686      28.86
 C       5.054097    -4.128647     1.286529      49.59
 H       4.685464    -4.822711     0.463719      16.83
 C       5.303805    -4.626531     2.609524      24.37
 O       5.124833    -5.977869     3.104166     281.49
 C       4.469090    -6.898400     2.192892     128.87
 H       5.017847    -6.948137     1.265531      29.76
 H       3.447194    -6.583907     2.156345      30.22
 H       4.542518    -7.886086     2.734159      23.91
 C       5.700928    -3.722093     3.650505       2.27
 O       5.747295    -4.021596     4.963261     -62.64
 H       5.779357    -5.037924     5.192027      19.82
 C       5.971976    -2.394376     3.270966      51.29
 H       6.402107    -1.827010     4.165165      20.26
 C       5.263325    -2.755566     0.966335      33.07
 C       5.017840    -2.400347    -0.523307      76.58
 H       5.492855    -3.276290    -1.186926      21.19
 O       5.851171    -1.302809    -1.047580     192.66
 H       5.444199    -0.371557    -0.805880      26.58
 C       3.513619    -2.178057    -0.790090      88.34
 H       2.946558    -3.069222    -0.480238      22.74
 C       3.239311    -1.820658    -2.260522     103.74
 O       3.442696    -3.025518    -3.136046     268.09
 H       4.234719    -2.739371    -3.618736      26.59
 H       3.910429    -1.005762    -2.522328      24.62
 H       2.216924    -1.538340    -2.402169      26.21
 C      -0.728111    -1.245812     0.092354      36.13
 H      -1.524335    -1.957271     0.293682      20.18
 C      -0.043564     1.118868     0.128042      63.83
 H      -0.418073     2.218012     0.342688      18.37
 C       1.327188     0.745030    -0.004787      16.36
 O       2.339273     1.667821    -0.146118     181.18
 C       1.845669     3.128985    -0.019059      98.64
 H       2.798101     3.742848    -0.330634      24.97
 H       1.222375     3.275771    -1.039371      23.07
 H       1.627131     3.158560     0.981024      26.63
 C       1.679728    -0.615745    -0.033272      19.31
 O       3.092476    -0.979011    -0.053582     158.86
 C       0.685966    -1.592896    -0.022953      59.57
 H       0.947964    -2.583534    -0.063441      22.76
 C      -1.060527     0.114741     0.241082      44.18
 C      -2.520878     0.444586     0.447198      92.21
 H      -2.903965    -0.337226     1.043722      25.04
 O      -2.554482     1.642006     1.281443     289.20
 H      -2.239311     1.340398     2.175833      27.48
 C      -3.418198     0.814084    -0.754949      82.65
 H      -2.778045     1.636221    -1.348040      24.61
 O      -3.527584    -0.366420    -1.568489     234.40
 H      -3.413004    -0.172553    -2.522882      26.75
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 C      -4.816022     1.284360    -0.338675      98.27
 O      -5.042684     2.673554    -0.376340     294.20
 H      -5.082685     3.010722     0.532623      27.74
 H      -4.961602     0.770293     0.694233      28.05
 H      -5.614399     0.640350    -0.937016      27.76
55
name = lig-etoh-Waterframe_216
 C       5.772067    -1.944492     1.969180      38.89
 H       5.971354    -0.877138     1.839609      26.14
 C       5.019264    -4.095683     1.369202      53.63
 H       4.507093    -4.779373     0.622427      19.52
 C       5.279937    -4.603029     2.662247      21.68
 O       5.113013    -5.988209     3.119949     281.05
 C       4.472415    -6.875612     2.276213     132.13
 H       4.911784    -6.952893     1.321795      29.89
 H       3.391357    -6.631440     1.966703      29.29
 H       4.480100    -7.913036     2.713206      24.51
 C       5.719234    -3.676301     3.595495      16.56
 O       5.774947    -3.986436     4.962300     123.54
 H       5.860180    -4.885030     5.136382      19.45
 C       5.980902    -2.345969     3.306650      48.75
 H       6.124639    -1.588699     4.181034      24.79
 C       5.241446    -2.761888     0.956802      20.74
 C       5.065009    -2.397610    -0.484774      63.21
 H       5.245361    -3.376093    -1.139712      22.52
 O       5.836046    -1.291700    -1.043749     196.04
 H       5.311633    -0.490531    -0.657408      28.21
 C       3.513178    -2.159457    -0.771471      86.59
 H       2.921606    -3.017797    -0.438356      24.63
 C       3.249470    -1.908939    -2.300561     105.27
 O       3.453583    -3.001332    -3.148443     260.62
 H       4.342272    -3.132007    -3.560874      26.27
 H       3.806071    -1.023056    -2.610588      26.67
 H       2.140328    -1.550225    -2.431778      26.20
 C      -0.612879    -1.237145     0.142378      42.57
 H      -1.376580    -2.053929     0.162219      21.31
 C      -0.023334     1.137302     0.146594      66.59
 H      -0.380926     2.189175     0.227738      23.71
 C       1.322879     0.764083    -0.003126      16.63
 O       2.300470     1.688590    -0.168744     238.76
 C       1.901371     3.038925    -0.056427     133.02
 H       2.795477     3.700305    -0.150244      26.23
 H       0.892781     3.303030    -0.590411      24.81
 H       1.429127     3.411440     0.807762      28.28
 C       1.727260    -0.654070    -0.041484       8.21
 O       3.121859    -0.978670    -0.064440     151.57
 C       0.684038    -1.608949     0.010942      62.96
 H       0.906141    -2.604833     0.033361      26.29
 C      -1.018614     0.147043     0.159016      29.01
 C      -2.521052     0.501702     0.481666      91.95
 H      -2.993208    -0.394304     0.941530      27.87
 O      -2.537877     1.682679     1.277638     293.65
 H      -2.164831     1.427769     2.096542      32.87
 C      -3.423358     0.868469    -0.766421      74.96
 H      -2.962206     1.923596    -1.297827      25.64
 O      -3.519462    -0.324563    -1.564551     221.34
 H      -3.452667    -0.049785    -2.500867      28.01
 C      -4.807515     1.235608    -0.296772     117.83
 O      -5.045682     2.654135    -0.394362     255.90
 H      -5.119640     3.054804     0.473798      28.50
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 H      -4.910033     0.978213     0.657771      31.17
 H      -5.563825     0.761680    -0.928735      30.04
55
name = lig-etoh-Waterframe_217
 C       5.732705    -1.907748     1.964534      59.14
 H       5.879406    -0.895364     1.599163      20.93
 C       4.949353    -4.139961     1.419526      56.93
 H       4.500847    -4.849661     0.702465      19.05
 C       5.241592    -4.636943     2.676192      28.75
 O       5.120069    -5.882812     3.147744     237.22
 C       4.428998    -6.911635     2.251465     119.84
 H       5.044328    -7.016048     1.351386      26.73
 H       3.318170    -6.560491     2.122101      26.19
 H       4.465853    -7.828673     2.871079      23.52
 C       5.738531    -3.654848     3.683273      -2.85
 O       5.817599    -3.947293     4.971364     -23.42
 H       5.933601    -4.905405     5.130075      17.11
 C       5.947741    -2.297432     3.291542      52.22
 H       6.103326    -1.441948     4.027539      27.65
 C       5.291779    -2.803623     1.016969      40.83
 C       5.015911    -2.395381    -0.494953      83.27
 H       5.347453    -3.267555    -1.077890      23.94
 O       5.806806    -1.300915    -0.997337     223.28
 H       5.517679    -0.332226    -0.822883      25.85
 C       3.528017    -2.159153    -0.808558      83.26
 H       3.034719    -3.038306    -0.386642      26.24
 C       3.246068    -1.909117    -2.312342     101.39
 O       3.478550    -3.050849    -3.195162     235.75
 H       4.459323    -3.044249    -3.431914      24.88
 H       3.886988    -1.098030    -2.689703      27.19
 H       2.063913    -1.789482    -2.401172      26.52
 C      -0.605607    -1.187814     0.174534      46.06
 H      -1.311622    -2.057583     0.112476      21.03
 C      -0.027834     1.118654     0.154310      50.44
 H      -0.215440     2.132145     0.104329      25.73
 C       1.314727     0.692148    -0.006751      11.96
 O       2.314499     1.727066    -0.181197     179.71
 C       1.893433     3.057460    -0.065407     127.08
 H       2.740153     3.634685    -0.340219      28.45
 H       1.235448     3.311557    -0.874319      27.90
 H       1.587116     3.270729     1.040137      26.57
 C       1.775522    -0.642312    -0.045735      26.82
 O       3.108022    -0.929462    -0.059828     147.50
 C       0.772289    -1.647160     0.056309      44.86
 H       0.955125    -2.720223     0.078705      25.89
 C      -1.025341     0.112142     0.114966      35.63
 C      -2.470676     0.568832     0.437107      94.83
 H      -3.054903    -0.304243     0.924294      27.23
 O      -2.534581     1.755051     1.294244     271.39
 H      -2.255056     1.441243     2.139618      31.30
 C      -3.384601     0.891024    -0.746618      80.88
 H      -3.053575     1.724404    -1.468030      26.94
 O      -3.497667    -0.289843    -1.603760     228.73
 H      -3.343211    -0.103105    -2.554814      27.66
 C      -4.857857     1.216722    -0.229227     105.12
 O      -5.067329     2.680816    -0.421163     255.58
 H      -5.112382     3.056227     0.475973      27.88
 H      -5.061954     0.982447     0.774549      29.38
 H      -5.483711     0.756081    -0.904508      30.72
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name = lig-etoh-Waterframe_218
 C       5.704842    -1.832271     1.932216      40.22
 H       5.907783    -0.827596     1.571294      18.95
 C       4.898705    -4.192583     1.400101      56.05
 H       4.568069    -4.865595     0.642018      23.35
 C       5.256165    -4.546709     2.741062      14.92
 O       5.085649    -5.848526     3.162790     269.21
 C       4.426094    -6.905010     2.283522      84.80
 H       4.995151    -7.115674     1.309848      22.90
 H       3.348834    -6.602257     2.034281      28.26
 H       4.467326    -7.756475     2.938234      22.17
 C       5.720022    -3.598848     3.684141       0.76
 O       5.884029    -3.932449     5.050496     -53.52
 H       5.842789    -5.038292     5.243848      23.38
 C       5.889365    -2.263074     3.280789      48.56
 H       6.284072    -1.629135     4.064057      20.60
 C       5.286127    -2.872643     1.011438      -0.56
 C       4.981407    -2.384490    -0.468296      96.66
 H       5.332067    -3.108411    -1.077604      26.39
 O       5.824358    -1.307209    -0.955960     217.29
 H       5.384945    -0.397275    -0.814128      24.28
 C       3.541910    -2.160282    -0.823503      82.25
 H       2.927724    -3.014728    -0.493735      22.73
 C       3.220739    -1.924744    -2.327049      97.94
 O       3.520054    -3.119604    -3.215401     245.77
 H       4.417330    -2.925460    -3.699363      23.58
 H       3.733943    -0.993637    -2.636731      25.02
 H       2.127944    -1.632138    -2.469032      25.53
 C      -0.580934    -1.268909     0.154898      41.91
 H      -1.450055    -1.940576     0.314916      20.23
 C       0.005719     1.063646     0.109375      70.63
 H      -0.255327     2.034394     0.113235      24.59
 C       1.352452     0.719270    -0.022031      12.84
 O       2.342835     1.675534    -0.192286     172.07
 C       1.907107     3.156048    -0.112609     107.87
 H       2.807713     3.657834    -0.260475      26.74
 H       1.210254     3.387503    -0.838572      26.38
 H       1.613804     3.319457     1.029586      23.64
 C       1.764394    -0.664602    -0.024902      19.88
 O       3.132182    -0.889306    -0.080311     158.36
 C       0.791276    -1.617966     0.112245      56.35
 H       1.077853    -2.726112     0.106725      22.05
 C      -1.046873     0.142571     0.154720      33.24
 C      -2.441884     0.618363     0.380417      92.58
 H      -2.850815    -0.207381     1.045359      23.90
 O      -2.523122     1.825957     1.291361     265.02
 H      -2.343233     1.419994     2.195330      26.38
 C      -3.406791     0.880547    -0.770774      90.64
 H      -2.997109     1.667614    -1.244035      28.42
 O      -3.472806    -0.292410    -1.647263     255.43
 H      -3.119555    -0.062535    -2.539899      26.52
 C      -4.878552     1.277662    -0.223756      92.58
 O      -5.105995     2.695458    -0.433639     265.83
 H      -5.137919     3.182378     0.455014      24.99
 H      -5.143516     0.800810     0.878223      27.17
 H      -5.552492     0.651007    -0.834725      28.69
55
name = lig-etoh-Waterframe_219
 C       5.667402    -1.871332     1.906064      54.46
 H       5.933481    -0.850954     1.661116      23.99
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 C       4.945678    -4.159236     1.393558      40.79
 H       4.633224    -4.923272     0.740594      18.14
 C       5.216735    -4.510744     2.729171      13.48
 O       5.027548    -5.861736     3.173918     304.70
 C       4.450272    -6.850281     2.353143     110.95
 H       5.052767    -7.073337     1.384930      27.17
 H       3.466831    -6.661911     2.006061      32.49
 H       4.422760    -7.758155     2.893439      24.71
 C       5.674928    -3.562575     3.719799     -24.94
 O       5.951956    -3.911248     5.096309     102.45
 H       5.799388    -5.036054     5.207245      25.46
 C       5.865379    -2.211266     3.285907      53.27
 H       6.333612    -1.615233     3.994944      20.77
 C       5.215020    -2.826378     0.964936      39.81
 C       5.021658    -2.424593    -0.460333      86.15
 H       5.172403    -3.307960    -1.111854      23.77
 O       5.848888    -1.292541    -0.902451     190.94
 H       5.336537    -0.458817    -0.686805      25.85
 C       3.492146    -2.134867    -0.823995      77.03
 H       2.880973    -2.981241    -0.436464      22.06
 C       3.208125    -1.937043    -2.380391     102.58
 O       3.548683    -3.118772    -3.191195     261.75
 H       4.283045    -3.032716    -3.884340      26.24
 H       3.827975    -1.097310    -2.748327      23.67
 H       2.182118    -1.787738    -2.480524      25.96
 C      -0.647240    -1.274655     0.161114      47.99
 H      -1.246342    -2.160080     0.405452      21.21
 C       0.032479     1.065909     0.041706      64.95
 H      -0.295793     2.071149     0.174900      20.57
 C       1.399175     0.735919    -0.043373      24.87
 O       2.373601     1.692219    -0.210404     169.08
 C       1.977959     3.170264    -0.152108     115.88
 H       2.896585     3.736785    -0.212505      25.07
 H       1.082073     3.459117    -0.730391      23.45
 H       1.404493     3.566498     0.780862      23.53
 C       1.773532    -0.608284     0.004597      12.58
 O       3.160078    -0.897634    -0.131566     189.16
 C       0.719002    -1.614851     0.153365      51.84
 H       1.094805    -2.725762     0.216110      18.83
 C      -0.955295     0.081768     0.189913      36.33
 C      -2.464462     0.621791     0.450619      78.46
 H      -2.939896    -0.207591     0.979060      22.51
 O      -2.504135     1.877375     1.231407     286.59
 H      -2.216634     1.486186     2.198865      22.65
 C      -3.451556     0.871970    -0.790204      81.38
 H      -3.086819     1.755242    -1.237822      25.42
 O      -3.452253    -0.298214    -1.677118     269.41
 H      -3.017104    -0.083798    -2.536752      25.78
 C      -4.867886     1.301425    -0.281956      83.96
 O      -5.163478     2.692277    -0.439318     250.77
 H      -5.099302     3.188325     0.485519      24.49
 H      -4.871047     1.117500     0.965129      24.18
 H      -5.708078     0.803727    -0.938821      25.17
55
name = lig-etoh-Waterframe_220
 C       5.637820    -1.917180     1.939587      59.71
 H       5.877599    -0.932832     1.550045      25.95
 C       5.026161    -4.101034     1.403261      57.23
 H       4.685957    -4.858162     0.713846      13.87
 C       5.147410    -4.547782     2.740052      34.45
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 O       4.982490    -5.810378     3.217637     280.75
 C       4.465694    -6.835438     2.357105     133.55
 H       5.224141    -6.946044     1.563723      30.97
 H       3.505984    -6.562310     2.059903      33.47
 H       4.440911    -7.729088     2.955082      24.26
 C       5.625533    -3.549168     3.788928       5.58
 O       5.988715    -3.880765     5.040761     138.81
 H       5.958564    -4.891835     5.293873      23.29
 C       5.861908    -2.226147     3.296547      72.20
 H       6.205863    -1.374761     3.825971      23.48
 C       5.148182    -2.760159     0.957653      40.10
 C       4.997160    -2.445365    -0.531767      86.33
 H       5.422463    -3.400994    -1.179655      20.40
 O       5.864049    -1.308105    -0.844607     201.48
 H       5.479967    -0.424153    -0.657563      27.46
 C       3.482260    -2.121657    -0.844213      85.79
 H       2.925643    -2.973083    -0.404336      22.12
 C       3.233825    -1.954527    -2.421676     109.81
 O       3.539417    -3.125078    -3.157427     258.51
 H       4.446068    -2.890884    -3.538932      25.09
 H       3.814996    -1.096450    -2.808986      24.69
 H       2.224506    -1.811176    -2.569856      26.83
 C      -0.658038    -1.307307     0.222945      20.74
 H      -1.428954    -2.084696     0.306252      18.36
 C       0.040815     1.082708     0.006048      61.97
 H      -0.278238     2.188822     0.090822      18.79
 C       1.405055     0.774857    -0.069231       3.93
 O       2.408945     1.805087    -0.223610     201.03
 C       1.992694     3.147870    -0.165837     112.37
 H       2.933416     3.755011    -0.432391      24.89
 H       1.499381     3.326862    -1.245004      23.69
 H       1.683348     3.286190     0.850423      24.84
 C       1.771157    -0.627348     0.017727      20.00
 O       3.134370    -0.910272    -0.179109     194.83
 C       0.736041    -1.569792     0.162748      64.66
 H       0.908475    -2.702732     0.304959      20.15
 C      -0.990403     0.082972     0.208383      40.72
 C      -2.491351     0.581824     0.495347      81.68
 H      -3.042164    -0.119307     1.093348      24.27
 O      -2.471992     1.884561     1.148545     269.55
 H      -2.135009     1.735044     2.169422      24.91
 C      -3.427502     0.874053    -0.799339      77.43
 H      -3.035877     1.736079    -1.467236      23.89
 O      -3.446131    -0.293617    -1.673320     255.91
 H      -3.100266    -0.154938    -2.589801      25.38
 C      -4.859062     1.311800    -0.324980      97.85
 O      -5.213430     2.717513    -0.470582     240.43
 H      -5.053171     3.133162     0.488099      24.68
 H      -4.957699     1.029835     0.772233      27.44
 H      -5.666289     0.595977    -0.772625      27.11
55
name = lig-etoh-Waterframe_221
 C       5.604739    -1.871502     1.945901      53.21
 H       5.864941    -0.839508     1.696237      24.08
 C       5.038344    -4.120206     1.411505      65.09
 H       4.764685    -4.808369     0.578718      14.75
 C       5.136266    -4.466353     2.809796      28.63
 O       4.938705    -5.753139     3.296940     241.41
 C       4.499928    -6.827579     2.343333     103.94
 H       5.151140    -7.008209     1.510169      29.53
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 H       3.508716    -6.605183     1.848455      31.21
 H       4.447087    -7.733424     2.992953      24.73
 C       5.573652    -3.558164     3.728373      18.37
 O       6.014307    -3.867798     5.007714     195.58
 H       5.951430    -4.793191     5.124452      24.63
 C       5.843540    -2.260442     3.294629      52.54
 H       6.115813    -1.465837     4.050315      24.37
 C       5.124880    -2.791936     0.987972      13.98
 C       4.966716    -2.386132    -0.546135      95.38
 H       5.456572    -3.253320    -1.222828      21.17
 O       5.892964    -1.330840    -0.820954     217.61
 H       5.420181    -0.494615    -0.701901      28.96
 C       3.512330    -2.158873    -0.926659      90.58
 H       2.901717    -3.004708    -0.599378      23.76
 C       3.217936    -1.933724    -2.389029     109.84
 O       3.558782    -3.145215    -3.147193     239.87
 H       4.525917    -3.209371    -3.430172      25.58
 H       3.804176    -1.063676    -2.732037      25.72
 H       2.161895    -1.626457    -2.594153      26.15
 C      -0.635485    -1.234792     0.293287      32.19
 H      -1.430572    -1.964838     0.287985      19.70
 C      -0.002272     1.087656     0.020200      63.03
 H      -0.323979     2.225506    -0.180492      19.83
 C       1.402472     0.816857    -0.091936       4.27
 O       2.438202     1.798104    -0.236197     214.06
 C       2.052098     3.155101    -0.250168     118.58
 H       3.051460     3.746931    -0.203833      24.16
 H       1.097165     3.507432    -0.986120      23.54
 H       1.516236     3.513449     0.588979      26.49
 C       1.769710    -0.610444    -0.011704       9.53
 O       3.088539    -0.910033    -0.202499     170.39
 C       0.741505    -1.584980     0.175636      55.36
 H       1.131998    -2.615030     0.191365      22.09
 C      -1.078078     0.120249     0.218989      47.98
 C      -2.498128     0.573891     0.454390      96.97
 H      -2.955234    -0.127790     1.169774      26.40
 O      -2.440496     1.903329     1.060671     243.28
 H      -2.193165     1.658411     2.097199      26.21
 C      -3.369826     0.865572    -0.823450      77.22
 H      -2.669700     1.770941    -1.294702      23.66
 O      -3.464409    -0.316414    -1.638230     243.19
 H      -3.242908    -0.099830    -2.578631      25.46
 C      -4.867209     1.272983    -0.322356      96.71
 O      -5.241404     2.717989    -0.522985     232.02
 H      -5.205267     3.178704     0.417046      26.53
 H      -4.993218     1.023355     0.602178      31.87
 H      -5.518210     0.681004    -0.975928      28.79
55
name = lig-etoh-Waterframe_222
 C       5.568367    -1.795870     1.974004      61.01
 H       5.748327    -0.742290     1.724657      24.72
 C       4.986671    -4.158537     1.424408      56.58
 H       4.801013    -5.052859     0.752009      15.77
 C       5.110284    -4.471134     2.762255      21.37
 O       4.879464    -5.742963     3.329408     235.13
 C       4.536643    -6.793983     2.346148     114.35
 H       5.329562    -6.958940     1.633641      28.33
 H       3.479065    -6.590465     1.851832      26.87
 H       4.424392    -7.760323     2.953281      23.78
 C       5.596101    -3.516239     3.708337       0.68
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 O       6.009289    -3.884203     4.976035     138.18
 H       5.948030    -4.794915     5.151728      27.52
 C       5.796199    -2.223813     3.266222      49.73
 H       6.213400    -1.680975     4.199671      21.12
 C       5.154345    -2.801941     0.998012       5.04
 C       5.001916    -2.373093    -0.477760      94.69
 H       5.158206    -3.254988    -1.055648      24.21
 O       5.902316    -1.308232    -0.826833     217.63
 H       5.513300    -0.431640    -0.756779      28.79
 C       3.494010    -2.165246    -0.955937      82.83
 H       2.984726    -3.079571    -0.634913      25.13
 C       3.248067    -1.881617    -2.409392      99.24
 O       3.551382    -3.162740    -3.151179     227.15
 H       4.491119    -3.060117    -3.540749      24.81
 H       3.912587    -1.099973    -2.784522      25.85
 H       2.074018    -1.764100    -2.550815      25.44
 C      -0.620483    -1.157540     0.341826      52.17
 H      -1.232468    -2.019489     0.516148      21.65
 C      -0.037168     1.122851     0.019052      66.40
 H      -0.420200     2.201143    -0.212412      20.43
 C       1.343217     0.794048    -0.087911      16.15
 O       2.412055     1.720443    -0.256533     168.82
 C       2.035165     3.241837    -0.277312     100.96
 H       3.003160     3.822838    -0.393860      25.11
 H       1.446825     3.451147    -1.216793      26.29
 H       1.524471     3.475637     0.661072      25.01
 C       1.720873    -0.548953    -0.063961      10.48
 O       3.075825    -0.925320    -0.220870     143.29
 C       0.753819    -1.563305     0.176158      47.66
 H       1.024885    -2.570089     0.116240      22.09
 C      -1.026743     0.155223     0.208973      47.58
 C      -2.492976     0.598552     0.394244      96.52
 H      -3.022132    -0.191861     1.024229      26.72
 O      -2.426784     1.923264     1.008644     240.71
 H      -2.262152     1.668135     2.047238      26.56
 C      -3.330994     0.851488    -0.788453      87.74
 H      -2.899488     1.737091    -1.437334      24.81
 O      -3.488090    -0.343197    -1.604134     244.85
 H      -3.278364    -0.195737    -2.565385      25.27
 C      -4.840855     1.286641    -0.395074      94.83
 O      -5.244964     2.680016    -0.567806     231.45
 H      -5.321489     3.090457     0.359328      28.10
 H      -5.045944     0.980118     0.648759      29.44
 H      -5.446714     0.840041    -1.111490      29.53
55
name = lig-etoh-Waterframe_223
 C       5.503551    -1.789989     1.957853      50.02
 H       5.624451    -0.759145     1.562158      25.42
 C       4.929476    -4.153048     1.408502      70.11
 H       4.677511    -4.948009     0.636070      18.24
 C       5.094459    -4.529725     2.768036      15.54
 O       4.817046    -5.746263     3.310404     278.14
 C       4.564974    -6.776335     2.381654     100.35
 H       5.437011    -6.814646     1.710109      28.30
 H       3.620155    -6.500612     1.765748      28.16
 H       4.457253    -7.743165     2.959903      23.23
 C       5.625636    -3.541869     3.684240      -1.50
 O       5.988846    -3.895805     4.943955      81.84
 H       5.905358    -4.895143     5.185506      20.02
 C       5.775515    -2.161037     3.328730      51.82
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 H       6.298610    -1.305844     3.891375      20.97
 C       5.199981    -2.756396     1.027704      40.57
 C       4.997943    -2.401432    -0.427526      87.59
 H       5.379961    -3.181247    -0.972236      22.38
 O       5.906889    -1.284534    -0.856867     199.57
 H       5.499769    -0.422352    -0.699446      28.68
 C       3.497756    -2.104113    -0.871414      82.34
 H       2.912682    -2.988613    -0.563537      23.86
 C       3.300952    -1.909702    -2.467923      97.39
 O       3.546595    -3.137292    -3.179286     250.30
 H       4.377025    -2.962005    -3.744955      24.39
 H       3.814320    -1.046994    -2.882701      25.70
 H       2.161338    -1.601478    -2.638599      24.93
 C      -0.576117    -1.190580     0.381748      35.94
 H      -1.341079    -1.864723     0.764357      20.95
 C      -0.032510     1.202608    -0.020047      69.67
 H      -0.329207     2.251037    -0.024796      19.58
 C       1.294859     0.820257    -0.091575      10.88
 O       2.342001     1.716541    -0.283857     199.22
 C       2.027860     3.224144    -0.323879     111.02
 H       3.004576     3.682042    -0.398139      25.36
 H       1.513602     3.409121    -1.143090      27.83
 H       1.576561     3.464408     0.676742      24.07
 C       1.710196    -0.590216    -0.119567      18.36
 O       3.054653    -0.921038    -0.232452     189.36
 C       0.727664    -1.494785     0.159182      65.32
 H       0.884738    -2.500387     0.224060      23.92
 C      -0.989398     0.178654     0.202208      40.36
 C      -2.429547     0.634140     0.373296      83.59
 H      -3.021631    -0.108490     0.992098      23.16
 O      -2.444988     1.938625     1.009235     252.18
 H      -2.265948     1.795841     2.039267      26.42
 C      -3.397137     0.870744    -0.863483      96.18
 H      -3.048736     1.601267    -1.511125      27.76
 O      -3.509248    -0.391659    -1.565397     250.28
 H      -3.141990    -0.295746    -2.488197      25.61
 C      -4.811007     1.303366    -0.496195      95.06
 O      -5.219444     2.656984    -0.591134     245.93
 H      -5.252672     3.083840     0.302901      26.34
 H      -5.210461     0.796220     0.619431      26.35
 H      -5.409361     0.658255    -1.143552      28.73
55
name = lig-etoh-Waterframe_224
 C       5.463069    -1.802202     1.994067      57.22
 H       5.613318    -0.767694     1.642041      22.44
 C       4.906782    -4.093348     1.402819      59.68
 H       4.505158    -4.631267     0.540602      17.13
 C       5.096553    -4.495179     2.751950      19.60
 O       4.766972    -5.737195     3.324964     308.35
 C       4.586903    -6.790093     2.362803      83.85
 H       5.446486    -6.926473     1.646752      29.39
 H       3.744184    -6.662880     1.725788      35.58
 H       4.439114    -7.717825     2.911765      26.11
 C       5.647878    -3.530480     3.665449     -29.45
 O       5.971597    -3.910949     4.940647      -1.89
 H       5.810573    -4.998503     5.127516      25.02
 C       5.759347    -2.115024     3.309354      45.45
 H       6.150787    -1.353190     4.022686      19.68
 C       5.173082    -2.795524     1.039898      35.20
 C       5.006896    -2.374908    -0.440772      78.44
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 H       5.414339    -3.214417    -1.079064      23.46
 O       5.886194    -1.278592    -0.882838     201.44
 H       5.463639    -0.421409    -0.665726      27.29
 C       3.524796    -2.081103    -0.852219      77.83
 H       2.836558    -2.873729    -0.522599      22.70
 C       3.324689    -1.918913    -2.460448     101.41
 O       3.561770    -3.107122    -3.241353     256.50
 H       4.392411    -3.145822    -3.807505      25.70
 H       4.042124    -1.156644    -2.789713      24.69
 H       2.283654    -1.629040    -2.618494      26.11
 C      -0.654494    -1.112829     0.418000      44.53
 H      -1.370193    -1.892000     0.792210      20.78
 C      -0.027171     1.241819    -0.045250      68.34
 H      -0.271817     2.218464     0.051266      21.43
 C       1.332707     0.825672    -0.142773      19.76
 O       2.290881     1.774800    -0.317297     242.77
 C       2.048354     3.108429    -0.345362     139.20
 H       2.996138     3.553640    -0.348061      26.21
 H       1.265138     3.463831    -1.033177      25.31
 H       1.447660     3.625690     0.506601      24.36
 C       1.705649    -0.561393    -0.164782       6.65
 O       3.044731    -0.858564    -0.224277     178.94
 C       0.713844    -1.562269     0.153000      49.29
 H       1.101507    -2.535365     0.360308      20.89
 C      -0.995411     0.199295     0.196429      34.47
 C      -2.423220     0.693959     0.361926      83.85
 H      -2.863882    -0.059059     1.030635      25.14
 O      -2.479614     1.981242     1.039024     268.11
 H      -2.254160     1.704547     2.008814      26.06
 C      -3.403646     0.877019    -0.958569      87.65
 H      -2.951924     1.553794    -1.562897      27.68
 O      -3.525936    -0.466564    -1.540251     254.10
 H      -3.074156    -0.428162    -2.430766      26.20
 C      -4.869488     1.234510    -0.556340      86.22
 O      -5.174123     2.658692    -0.618453     251.88
 H      -5.151433     3.046970     0.268907      27.52
 H      -5.030997     0.838904     0.612859      25.01
 H      -5.530246     0.753019    -1.380508      26.21
55
name = lig-etoh-Waterframe_225
 C       5.463761    -1.771978     1.999693      60.01
 H       5.590913    -0.729556     1.759862      21.36
 C       4.874466    -4.080709     1.403101      40.53
 H       4.429935    -4.849654     0.813037      13.48
 C       5.099355    -4.433300     2.737229      29.09
 O       4.740165    -5.702570     3.311674     264.76
 C       4.585945    -6.848293     2.307367     103.51
 H       5.556930    -6.941501     1.750088      30.99
 H       3.724509    -6.698010     1.760736      33.24
 H       4.469744    -7.693765     2.924862      25.59
 C       5.646435    -3.499348     3.668183      -2.60
 O       5.952446    -3.902551     4.937110      48.19
 H       5.892934    -4.991032     5.188525      24.12
 C       5.744810    -2.176052     3.323444      61.26
 H       5.891151    -1.584278     4.177611      20.84
 C       5.127302    -2.731914     1.003664      26.99
 C       5.008985    -2.329594    -0.475508      80.12
 H       5.120028    -3.326739    -1.145550      21.83
 O       5.855401    -1.284204    -0.894929     241.15
 H       5.512394    -0.348465    -0.746797      24.87
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 C       3.522349    -2.096849    -0.905868      69.80
 H       2.997324    -2.984411    -0.505210      22.53
 C       3.390871    -1.894991    -2.409761     107.24
 O       3.575294    -3.124268    -3.304212     258.27
 H       4.472909    -2.935122    -3.681618      25.37
 H       4.141945    -1.127144    -2.689887      23.06
 H       2.436603    -1.585814    -2.618010      27.29
 C      -0.654190    -1.103693     0.413166      43.53
 H      -1.474597    -1.846894     0.668674      19.10
 C      -0.000355     1.193678    -0.046207      73.45
 H      -0.297116     2.163606    -0.072466      22.52
 C       1.305836     0.828013    -0.219969      21.96
 O       2.330036     1.751189    -0.352696     195.01
 C       1.993516     3.146859    -0.331616     107.67
 H       2.881340     3.701801    -0.564535      25.64
 H       1.324080     3.440449    -1.359671      22.96
 H       1.638461     3.287553     0.738331      23.72
 C       1.647769    -0.560334    -0.166885       7.08
 O       3.077938    -0.773238    -0.224188     135.85
 C       0.687945    -1.547237     0.168783      52.07
 H       1.024622    -2.616112     0.386677      19.88
 C      -1.035310     0.306176     0.176399      35.72
 C      -2.500330     0.749989     0.339939      86.16
 H      -3.019232    -0.010787     0.906478      24.34
 O      -2.516757     2.026213     1.084086     293.99
 H      -2.292411     1.767702     2.019183      27.18
 C      -3.363389     0.807500    -0.966605      86.62
 H      -2.932587     1.522487    -1.753109      24.23
 O      -3.518224    -0.543540    -1.537481     246.68
 H      -3.176227    -0.567153    -2.476948      25.95
 C      -4.902383     1.210827    -0.608707      98.78
 O      -5.111981     2.655983    -0.645787     269.99
 H      -5.159237     2.996698     0.247586      28.05
 H      -5.147582     0.759142     0.302113      29.54
 H      -5.689984     0.751524    -1.325214      27.53
55
name = lig-etoh-Waterframe_226
 C       5.483086    -1.757120     1.985742      57.50
 H       5.599124    -0.717613     1.759610      25.34
 C       4.840870    -4.066336     1.414032      34.59
 H       4.517471    -4.857278     0.781140      15.30
 C       5.085067    -4.447775     2.743265      34.15
 O       4.735969    -5.672462     3.238077     239.30
 C       4.589166    -6.856175     2.327137     100.23
 H       5.491126    -6.881563     1.660511      28.73
 H       3.733733    -6.730777     1.616411      29.18
 H       4.495455    -7.708868     2.955349      23.80
 C       5.612699    -3.573960     3.693701      19.87
 O       5.944465    -3.867525     4.959314     100.13
 H       5.938055    -4.885382     5.082094      21.53
 C       5.719802    -2.204784     3.357669      58.19
 H       5.849740    -1.462355     4.073935      24.26
 C       5.089569    -2.645636     0.971215      20.92
 C       4.923664    -2.314309    -0.500273      90.92
 H       5.462198    -3.187533    -1.058198      20.07
 O       5.869999    -1.288867    -0.923758     195.44
 H       5.415014    -0.377095    -0.819201      26.17
 C       3.526518    -2.076809    -0.901436      81.99
 H       2.886032    -2.912655    -0.550083      21.72
 C       3.428688    -1.872757    -2.423809     104.05
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 O       3.615062    -3.095105    -3.304956     257.43
 H       4.446724    -3.028143    -3.867656      25.43
 H       4.155110    -1.090063    -2.751304      22.73
 H       2.498991    -1.435391    -2.659126      26.84
 C      -0.670239    -1.052597     0.349063      45.67
 H      -1.452505    -1.810246     0.570037      19.87
 C      -0.042402     1.226247    -0.060549      74.79
 H      -0.257190     2.283270    -0.277298      18.96
 C       1.312577     0.792553    -0.282277       3.42
 O       2.412840     1.691191    -0.416709     148.12
 C       1.963906     3.206156    -0.327644      88.44
 H       2.878688     3.776781    -0.558101      24.86
 H       0.837174     3.461620    -0.925677      20.96
 H       1.604579     3.478205     0.687495      25.48
 C       1.679634    -0.566814    -0.146128      18.65
 O       3.070701    -0.762602    -0.261793     159.22
 C       0.641461    -1.468342     0.202620      56.32
 H       0.780926    -2.636764     0.247652      19.94
 C      -1.084627     0.259096     0.191731      42.10
 C      -2.562872     0.781497     0.340781      82.49
 H      -3.112043     0.028474     0.925603      23.66
 O      -2.574619     2.057865     1.104932     308.58
 H      -2.382559     1.787199     2.004387      28.66
 C      -3.419060     0.739518    -0.971209      82.01
 H      -2.979175     1.455573    -1.879481      22.81
 O      -3.479506    -0.629478    -1.533045     235.16
 H      -3.294259    -0.458650    -2.503065      24.28
 C      -4.890204     1.211963    -0.669894     107.84
 O      -5.049506     2.644119    -0.663454     292.67
 H      -5.140043     2.952201     0.236543      29.00
 H      -5.230046     0.808414     0.199558      31.07
 H      -5.471343     0.734404    -1.489983      28.59
55
name = lig-etoh-Waterframe_227
 C       5.497659    -1.775448     2.012180      60.64
 H       5.731385    -0.747027     1.784184      24.64
 C       4.838454    -3.966467     1.390251      59.16
 H       4.580202    -4.568808     0.535941      17.12
 C       5.051163    -4.481688     2.697982      34.17
 O       4.730423    -5.719985     3.177185     265.05
 C       4.600130    -6.801932     2.338541     109.55
 H       5.463986    -6.937316     1.684101      28.24
 H       3.602591    -6.787347     1.674636      29.01
 H       4.535511    -7.703320     2.972175      23.88
 C       5.577222    -3.543403     3.706472       0.69
 O       5.941417    -3.867278     5.009302     157.01
 H       5.933676    -4.770243     5.303972      24.95
 C       5.674753    -2.183793     3.305511      57.96
 H       6.057481    -1.458802     4.026335      21.59
 C       5.050020    -2.685467     1.023849      51.32
 C       4.967741    -2.322502    -0.480382      89.10
 H       5.203954    -3.233801    -1.026066      24.07
 O       5.875776    -1.268939    -0.954016     215.47
 H       5.537050    -0.292661    -0.851721      23.18
 C       3.472822    -2.034422    -0.927425      82.31
 H       2.755790    -2.812384    -0.619694      21.99
 C       3.445827    -1.828057    -2.526542      99.64
 O       3.652098    -3.051999    -3.256430     264.52
 H       4.450345    -2.946515    -3.844034      26.47
 H       4.288964    -1.144339    -2.763560      22.54
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 H       2.377844    -1.470063    -2.756236      24.52
 C      -0.748476    -1.039727     0.292563      48.47
 H      -1.409943    -1.855854     0.519220      22.70
 C      -0.069252     1.228776    -0.114578      58.12
 H      -0.405148     2.360158    -0.243587      16.80
 C       1.313538     0.810039    -0.281571      -0.19
 O       2.411474     1.724656    -0.487206     176.25
 C       1.933721     3.183627    -0.290903     104.50
 H       2.753379     3.802722    -0.751426      24.58
 H       1.064919     3.403735    -0.982022      24.40
 H       1.824340     3.404346     0.728128      26.56
 C       1.717471    -0.563068    -0.120262      17.11
 O       3.049451    -0.823636    -0.317663     188.66
 C       0.647044    -1.431585     0.197563      52.44
 H       0.835826    -2.577478     0.205981      18.95
 C      -1.122502     0.315089     0.194198      35.04
 C      -2.582261     0.746683     0.378521      78.84
 H      -3.039080     0.014066     1.094327      21.91
 O      -2.648853     2.057420     1.080202     338.89
 H      -2.469678     1.799612     1.949892      28.65
 C      -3.487543     0.715122    -0.967434      78.19
 H      -2.947693     1.425737    -1.753617      22.50
 O      -3.427703    -0.688455    -1.520173     232.91
 H      -3.334174    -0.580263    -2.517602      24.33
 C      -4.871298     1.196260    -0.758570     100.72
 O      -4.991535     2.644509    -0.685009     290.05
 H      -4.976408     2.921102     0.238037      28.79
 H      -5.334337     0.733537     0.289727      26.37
 H      -5.426398     0.953789    -1.632068      28.28
55
name = lig-etoh-Waterframe_228
 C       5.494617    -1.746041     1.992508      61.90
 H       5.840125    -0.762506     1.690723      25.90
 C       4.820895    -3.997168     1.362734      54.13
 H       4.496520    -4.721585     0.583053      16.13
 C       5.033632    -4.432044     2.698299      24.33
 O       4.739788    -5.734739     3.183855     270.70
 C       4.582563    -6.841333     2.279009     103.41
 H       5.409998    -6.902173     1.598161      29.39
 H       3.557261    -6.720117     1.744489      28.31
 H       4.567156    -7.724845     2.986949      23.68
 C       5.507028    -3.536303     3.686171      -6.77
 O       5.928394    -3.855809     5.035408     181.15
 H       5.835378    -4.778637     5.272336      26.89
 C       5.680007    -2.186229     3.330708      49.46
 H       6.248982    -1.549498     4.089904      21.64
 C       5.070807    -2.616256     1.038814      43.63
 C       4.970595    -2.316438    -0.459397      88.36
 H       5.176545    -3.146060    -1.015847      23.83
 O       5.883121    -1.272621    -0.972078     211.56
 H       5.487902    -0.339678    -0.736585      25.19
 C       3.446753    -2.024414    -1.024434      81.86
 H       2.907337    -2.945842    -0.777384      22.58
 C       3.443812    -1.772328    -2.566745      99.55
 O       3.690581    -3.047200    -3.217301     275.56
 H       4.573627    -2.930081    -3.652596      25.32
 H       4.161597    -0.985582    -2.842105      24.10
 H       2.418226    -1.321387    -2.981823      24.17
 C      -0.745140    -1.061876     0.262782      39.48
 H      -1.508957    -1.764088     0.480964      22.43
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 C      -0.060056     1.215919    -0.168544      68.30
 H      -0.369199     2.380709    -0.124176      17.64
 C       1.305098     0.876688    -0.233302       7.54
 O       2.316538     1.801877    -0.540918     236.09
 C       1.974443     3.117434    -0.315023     134.69
 H       2.797148     3.761135    -0.751253      24.87
 H       1.151014     3.336899    -0.762767      30.33
 H       1.911097     3.258335     0.725870      28.82
 C       1.662003    -0.505799    -0.114724       9.71
 O       3.028608    -0.850129    -0.345822     165.33
 C       0.628235    -1.440574     0.150702      54.51
 H       0.947583    -2.470314     0.325360      21.04
 C      -1.123349     0.358473     0.161764      29.93
 C      -2.607600     0.699414     0.417774      80.07
 H      -3.024125    -0.110178     1.082690      22.53
 O      -2.731142     2.027722     1.030191     339.86
 H      -2.520829     1.937358     1.909712      30.86
 C      -3.418949     0.670752    -0.938226      88.30
 H      -2.934185     1.343253    -1.596539      25.59
 O      -3.390058    -0.708820    -1.488128     254.92
 H      -3.214526    -0.623466    -2.477824      25.27
 C      -4.928432     1.207287    -0.834167      88.18
 O      -4.928166     2.654912    -0.704685     283.49
 H      -4.815123     2.947297     0.218546      27.77
 H      -5.533077     0.499351     0.082374      25.56
 H      -5.554936     0.944662    -1.665108      28.18
55
name = lig-etoh-Waterframe_229
 C       5.519722    -1.677610     2.019771      47.50
 H       5.864950    -0.685442     1.699732      21.77
 C       4.810373    -4.034736     1.383934      33.18
 H       4.420727    -4.859358     0.712941      15.29
 C       4.985467    -4.436927     2.712949      27.53
 O       4.776707    -5.704321     3.212786     233.56
 C       4.547887    -6.882482     2.214488     110.92
 H       5.288954    -6.891973     1.443689      30.72
 H       3.628822    -6.823367     1.668747      31.45
 H       4.571036    -7.847154     2.803698      24.64
 C       5.467623    -3.512423     3.738542      26.27
 O       5.878397    -3.842822     4.978476     122.45
 H       5.777551    -4.832563     5.157441      22.80
 C       5.733257    -2.189800     3.355182      39.29
 H       6.204534    -1.489624     4.159467      24.36
 C       5.068532    -2.622110     0.964813      -8.80
 C       4.922598    -2.272482    -0.524374      90.49
 H       5.428554    -3.146646    -0.950607      21.20
 O       5.877532    -1.293662    -0.959115     199.82
 H       5.529528    -0.334710    -0.749097      26.52
 C       3.489507    -2.030441    -1.103556      78.62
 H       2.851717    -2.901061    -0.905305      24.21
 C       3.434652    -1.711319    -2.578970      99.42
 O       3.743596    -3.050047    -3.200301     265.09
 H       4.614299    -3.142799    -3.646173      25.66
 H       4.205560    -1.014032    -2.857168      24.76
 H       2.358271    -1.417305    -2.893123      25.14
 C      -0.718965    -1.030832     0.249134      53.40
 H      -1.472857    -1.756480     0.492746      22.27
 C      -0.088025     1.269234    -0.152371      69.18
 H      -0.296470     2.394086    -0.238668      18.74
 C       1.282473     0.904019    -0.202038       7.61
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 O       2.239139     1.775784    -0.606445     229.66
 C       2.020633     3.165811    -0.323230     123.63
 H       2.922688     3.732180    -0.662402      25.45
 H       1.029879     3.577787    -0.656520      25.33
 H       1.935117     3.386619     0.785007      27.48
 C       1.610796    -0.462434    -0.155035       4.24
 O       2.962777    -0.816537    -0.327648     128.93
 C       0.606242    -1.454643     0.101712      59.48
 H       0.879555    -2.418127     0.323396      23.32
 C      -1.080818     0.262663     0.127035      31.49
 C      -2.610637     0.661082     0.422219      83.83
 H      -3.035542    -0.117896     1.089310      24.70
 O      -2.820784     1.984677     0.976806     325.42
 H      -2.537640     1.924062     1.837473      31.77
 C      -3.386234     0.634415    -0.920540      95.83
 H      -2.871228     1.232143    -1.547168      27.55
 O      -3.354197    -0.710852    -1.442667     280.85
 H      -3.087823    -0.538789    -2.391130      26.40
 C      -4.950436     1.186611    -0.879765      95.00
 O      -4.879943     2.647712    -0.739426     274.46
 H      -4.906443     2.865417     0.225150      27.16
 H      -5.561727     0.814569    -0.026805      28.37
 H      -5.345439     0.956087    -1.901357      28.69
55
name = lig-etoh-Waterframe_230
 C       5.528224    -1.730717     1.997944      50.77
 H       5.757632    -0.662582     1.852642      19.64
 C       4.806684    -3.975223     1.408164      47.23
 H       4.443192    -4.661356     0.592206      16.87
 C       4.953543    -4.421629     2.762485      19.61
 O       4.798128    -5.762140     3.200658     255.91
 C       4.524426    -6.850809     2.178074     111.61
 H       5.332373    -6.770165     1.448794      28.93
 H       3.582283    -6.750319     1.788753      32.26
 H       4.637860    -7.787741     2.766999      24.50
 C       5.444408    -3.466445     3.698759      19.36
 O       5.816114    -3.863927     4.944717     141.13
 H       5.805525    -4.895581     5.236343      20.63
 C       5.776196    -2.140712     3.314426      46.00
 H       6.082633    -1.440214     4.146048      23.75
 C       5.048321    -2.659726     1.007481      17.94
 C       4.918895    -2.271635    -0.584678      72.12
 H       5.180344    -3.301249    -1.173328      21.51
 O       5.876814    -1.276615    -0.941135     213.32
 H       5.627696    -0.278404    -0.862588      23.34
 C       3.493926    -1.982983    -1.088182      71.78
 H       2.783621    -2.796230    -0.880923      23.96
 C       3.470417    -1.728316    -2.616602     108.24
 O       3.767595    -3.061543    -3.193321     269.61
 H       4.579503    -2.898712    -3.746244      24.86
 H       4.151673    -0.956987    -2.936944      25.48
 H       2.458023    -1.492780    -2.858379      26.67
 C      -0.705813    -1.087709     0.257274      41.58
 H      -1.423013    -1.879341     0.553399      20.45
 C      -0.140312     1.306243    -0.084348      64.27
 H      -0.545422     2.237288    -0.324378      21.08
 C       1.183622     0.895512    -0.225710      -2.73
 O       2.220351     1.762084    -0.671671     146.03
 C       2.055098     3.278330    -0.276400      89.10
 H       2.957517     3.666905    -0.744988      24.68
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 H       1.181043     3.858283    -1.033267      21.78
 H       2.086883     3.319118     0.891166      24.34
 C       1.593184    -0.517605    -0.211535      16.61
 O       2.924578    -0.771219    -0.308102     136.99
 C       0.632448    -1.448449     0.059154      57.16
 H       0.845682    -2.450185     0.124217      22.94
 C      -1.107408     0.312432     0.126762      42.69
 C      -2.587938     0.614296     0.382377      91.18
 H      -2.967737    -0.109963     1.095241      24.70
 O      -2.883476     1.935310     0.947552     320.09
 H      -2.560565     1.862709     1.801430      32.61
 C      -3.431377     0.621670    -0.895289      94.58
 H      -2.887857     1.327609    -1.614288      24.65
 O      -3.318544    -0.727544    -1.410736     270.66
 H      -3.128060    -0.737578    -2.390304      25.43
 C      -4.850577     1.192514    -0.909061     115.38
 O      -4.857458     2.634442    -0.798718     271.69
 H      -5.131593     2.852726     0.142959      27.42
 H      -5.487230     0.799227    -0.293652      32.77
 H      -5.258406     0.949879    -1.965664      29.69
55
name = lig-etoh-Waterframe_231
 C       5.532562    -1.770679     1.954198      58.43
 H       5.622238    -0.729682     1.606745      26.48
 C       4.777165    -3.948010     1.432722      49.12
 H       4.498299    -4.643236     0.627496      16.09
 C       4.930146    -4.421530     2.742892      25.96
 O       4.807994    -5.808940     3.175353     282.87
 C       4.538278    -6.754540     2.193884     120.31
 H       5.231067    -6.695983     1.291370      30.73
 H       3.522652    -6.692240     1.779938      31.59
 H       4.657896    -7.710102     2.705152      25.15
 C       5.458465    -3.476868     3.653634       9.22
 O       5.768148    -3.876067     4.971335      96.45
 H       5.702278    -4.967331     4.963370      22.04
 C       5.759022    -2.130200     3.278623      73.31
 H       6.094374    -1.392142     3.977841      23.43
 C       5.041203    -2.634714     1.009440      33.71
 C       4.906522    -2.289765    -0.523021      62.90
 H       5.122541    -3.155300    -1.303767      20.14
 O       5.906234    -1.261695    -0.943428     205.28
 H       5.401866    -0.386189    -0.829643      26.39
 C       3.447632    -1.872739    -1.018016      86.14
 H       2.901256    -2.812217    -0.784618      22.93
 C       3.468704    -1.774767    -2.623131     109.68
 O       3.787517    -3.056892    -3.207104     276.75
 H       4.551253    -3.016756    -3.876571      25.15
 H       4.156602    -1.007690    -3.015432      24.30
 H       2.553366    -1.464075    -2.980096      27.07
 C      -0.726423    -1.081804     0.273180      31.17
 H      -1.469094    -1.893906     0.522664      18.91
 C      -0.219407     1.312887    -0.037058      64.44
 H      -0.488458     2.264736    -0.217934      19.53
 C       1.160038     0.883554    -0.314614       2.88
 O       2.187206     1.819292    -0.687696     177.11
 C       2.146506     3.288088    -0.315675      94.40
 H       3.124656     3.640434    -0.518488      24.49
 H       1.103481     3.852675    -0.756659      21.56
 H       1.899055     3.445822     0.807898      24.70
 C       1.573603    -0.474393    -0.262008      16.90
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 O       2.972244    -0.741183    -0.323429     185.42
 C       0.613731    -1.512968     0.026355      36.23
 H       0.929302    -2.557447    -0.063639      18.59
 C      -1.158209     0.273302     0.196220      46.85
 C      -2.614651     0.602921     0.364611      86.20
 H      -2.967099    -0.245490     0.961975      25.69
 O      -2.901837     1.888182     0.956179     328.21
 H      -2.629083     1.864910     1.843565      32.74
 C      -3.398080     0.604827    -0.931717      84.38
 H      -2.792359     1.389770    -1.695326      22.28
 O      -3.315011    -0.781020    -1.388866     269.13
 H      -3.208269    -0.644808    -2.382244      23.70
 C      -4.783229     1.184059    -0.958313     103.32
 O      -4.864120     2.636482    -0.862382     255.52
 H      -5.096733     2.964050     0.080180      26.75
 H      -5.485068     0.553833    -0.274088      28.92
 H      -5.187756     0.925425    -1.991265      29.39
55
name = lig-etoh-Waterframe_232
 C       5.524608    -1.717117     1.893823      49.08
 H       5.815207    -0.708468     1.532173      23.03
 C       4.722896    -3.999412     1.393483      39.66
 H       4.416083    -4.781574     0.734201      15.00
 C       4.941507    -4.442308     2.708407      31.97
 O       4.830380    -5.730337     3.171801     277.41
 C       4.536667    -6.720276     2.157095     120.49
 H       5.217272    -6.631581     1.248468      32.41
 H       3.424447    -6.650752     1.778229      29.60
 H       4.678902    -7.704047     2.546708      27.24
 C       5.503428    -3.499286     3.693569      -5.05
 O       5.720256    -3.877200     4.952466     -13.70
 H       5.695068    -4.968697     5.120014      21.59
 C       5.713332    -2.165157     3.259639      62.68
 H       6.149668    -1.507864     3.932221      21.76
 C       5.026679    -2.656549     0.942803      44.23
 C       4.894155    -2.241408    -0.473719      99.10
 H       5.228274    -3.179038    -0.903409      22.08
 O       5.897728    -1.266844    -0.920506     198.64
 H       5.575116    -0.304251    -0.842018      25.36
 C       3.457643    -1.868254    -0.988715      83.59
 H       2.766733    -2.683835    -0.676498      21.84
 C       3.453906    -1.772645    -2.608549      94.52
 O       3.777909    -3.091279    -3.221555     270.23
 H       4.659722    -3.013750    -3.757891      25.49
 H       4.331259    -1.114579    -2.846929      20.68
 H       2.462647    -1.484082    -2.992133      25.05
 C      -0.731888    -1.108139     0.286111      23.66
 H      -1.556386    -1.851022     0.443644      17.52
 C      -0.206010     1.256512    -0.041617      68.62
 H      -0.430258     2.304275     0.047727      18.67
 C       1.137110     0.957036    -0.386001       8.69
 O       2.151706     1.881898    -0.675344     236.09
 C       2.157306     3.231419    -0.310684     126.52
 H       3.090045     3.686870    -0.490543      25.10
 H       1.548258     3.812330    -0.954930      25.76
 H       1.962904     3.309127     0.742042      25.86
 C       1.551133    -0.452157    -0.293221      16.59
 O       3.007531    -0.668452    -0.350220     181.21
 C       0.586338    -1.489852    -0.027623      60.03
 H       0.865685    -2.619519    -0.010855      18.71
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 C      -1.156975     0.230854     0.285291      43.01
 C      -2.681817     0.581377     0.404199      71.86
 H      -3.271920    -0.211258     0.932328      22.39
 O      -2.898085     1.855553     1.000169     337.57
 H      -2.668243     1.729415     1.919227      28.80
 C      -3.279271     0.599233    -1.004905      86.77
 H      -2.563290     1.108859    -1.780791      22.89
 O      -3.346721    -0.818559    -1.390953     245.03
 H      -3.159751    -0.816497    -2.387488      24.31
 C      -4.797532     1.153761    -1.027885      80.34
 O      -4.893974     2.635785    -0.920952     235.21
 H      -4.780203     2.870249     0.079248      25.03
 H      -5.421378     0.664813    -0.011181      26.50
 H      -5.179924     0.929292    -2.018744      28.20
55
name = lig-etoh-Waterframe_233
 C       5.504125    -1.734801     1.882830      61.28
 H       5.965746    -0.776940     1.694880      21.29
 C       4.688833    -4.035545     1.335661      25.54
 H       4.247958    -4.674510     0.626567      14.91
 C       5.004199    -4.388956     2.691756      19.91
 O       4.841475    -5.667903     3.158022     269.17
 C       4.534350    -6.722987     2.099593      86.55
 H       5.247045    -6.513085     1.296221      29.66
 H       3.439589    -6.615691     1.749198      30.06
 H       4.708317    -7.641856     2.611087      24.27
 C       5.486139    -3.518231     3.627848     -18.31
 O       5.704851    -3.875529     4.976607      77.49
 H       5.728416    -4.912188     5.187605      25.44
 C       5.698693    -2.178820     3.230083      36.31
 H       6.150794    -1.583435     3.986047      21.26
 C       5.005808    -2.664701     0.983712      38.73
 C       4.888235    -2.218322    -0.492579      98.53
 H       5.118320    -3.041207    -1.070123      25.89
 O       5.883171    -1.272131    -0.880667     203.18
 H       5.697819    -0.301936    -0.781716      26.06
 C       3.474996    -1.944524    -1.014663      72.48
 H       2.753831    -2.694051    -0.666481      20.77
 C       3.482903    -1.794750    -2.548617      94.69
 O       3.739258    -3.126464    -3.207128     272.56
 H       4.622533    -2.959260    -3.689369      24.37
 H       4.204475    -0.967800    -2.854458      22.65
 H       2.455295    -1.359025    -2.928088      24.03
 C      -0.761942    -1.141150     0.284112      37.99
 H      -1.422577    -2.006399     0.453314      19.09
 C      -0.183491     1.223542    -0.031335      75.96
 H      -0.618516     2.283507     0.185906      18.43
 C       1.132428     0.967841    -0.395403      14.14
 O       2.144411     1.852937    -0.688350     223.14
 C       2.138189     3.243417    -0.284702     121.96
 H       3.228042     3.433624    -0.438030      23.35
 H       1.598045     3.835425    -0.874492      27.59
 H       1.865503     3.380037     0.709257      26.99
 C       1.573630    -0.423940    -0.327329      15.01
 O       2.974081    -0.562036    -0.389497     122.73
 C       0.599595    -1.401525    -0.077670      68.27
 H       0.888507    -2.542275     0.054168      20.08
 C      -1.150003     0.212427     0.360382      46.99
 C      -2.689780     0.548130     0.424468      70.03
 H      -3.291804    -0.232244     0.963649      22.49
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 O      -2.891295     1.846413     1.076706     340.36
 H      -2.691627     1.638705     2.031826      27.28
 C      -3.239937     0.573442    -1.074655      89.75
 H      -2.606009     1.091859    -1.703941      26.93
 O      -3.388469    -0.858989    -1.397876     258.68
 H      -3.097478    -0.927787    -2.357419      25.29
 C      -4.743951     1.176641    -1.087693      95.98
 O      -4.916394     2.601931    -0.969933     256.54
 H      -4.576173     2.878848    -0.033823      25.63
 H      -5.348936     0.636619    -0.179112      27.33
 H      -5.335158     0.800891    -1.869550      28.36
55
name = lig-etoh-Waterframe_234
 C       5.516195    -1.787726     1.959505      66.88
 H       5.785350    -0.829730     1.563599      24.28
 C       4.700866    -3.963138     1.328416       7.95
 H       4.200849    -4.603457     0.658669      11.24
 C       5.012565    -4.420680     2.593333      72.05
 O       4.821480    -5.683620     3.110802     261.48
 C       4.580943    -6.680599     2.104377     149.05
 H       5.249497    -6.664377     1.269324      35.54
 H       3.579737    -6.771635     1.596457      31.29
 H       4.721441    -7.633066     2.618493      22.90
 C       5.475412    -3.482342     3.626420      41.09
 O       5.711792    -3.852358     4.966834     165.33
 H       5.689781    -4.824149     4.998716      33.22
 C       5.723938    -2.186051     3.245334      66.63
 H       6.087519    -1.426115     3.981213      24.73
 C       4.966816    -2.665765     0.966928      53.49
 C       4.876777    -2.255137    -0.516409      86.66
 H       5.134225    -3.053412    -1.241273      21.02
 O       5.896197    -1.252840    -0.848447     208.35
 H       5.473518    -0.403994    -0.638947      28.49
 C       3.464626    -1.923887    -1.007094      77.57
 H       2.880076    -2.794428    -0.708853      21.25
 C       3.477888    -1.812739    -2.513620      99.35
 O       3.696655    -3.113902    -3.165421     266.50
 H       4.437254    -3.187550    -3.826395      25.19
 H       4.279134    -1.150791    -2.898567      22.98
 H       2.385340    -1.498843    -2.829196      23.64
 C      -0.732577    -1.149112     0.266253      36.84
 H      -1.315906    -2.003502     0.543943      20.39
 C      -0.240183     1.220628     0.043077      83.47
 H      -0.567162     2.377836    -0.076192      18.02
 C       1.126649     0.922996    -0.350956      10.54
 O       2.142544     1.810139    -0.711873     182.22
 C       2.141923     3.255809    -0.253696      94.66
 H       3.276484     3.557030    -0.213503      22.28
 H       1.398703     3.975876    -0.896538      22.21
 H       1.744954     3.375626     0.752079      25.29
 C       1.586689    -0.363184    -0.359599      26.00
 O       2.940568    -0.541706    -0.475824     135.80
 C       0.625418    -1.366593    -0.081739      51.56
 H       1.081710    -2.410058    -0.069408      18.95
 C      -1.168271     0.182767     0.374124      57.33
 C      -2.626878     0.550492     0.413623      75.96
 H      -3.076921    -0.338818     0.905352      23.38
 O      -2.888674     1.825322     1.145157     315.58
 H      -2.693172     1.629099     2.149008      27.45
 C      -3.301329     0.552448    -1.055892      88.20
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 H      -2.672352     1.052254    -1.690061      27.30
 O      -3.410199    -0.884446    -1.406269     244.58
 H      -3.179784    -0.803703    -2.388090      24.52
 C      -4.695517     1.149990    -1.102192     116.95
 O      -4.903257     2.564520    -1.023389     261.05
 H      -4.694151     2.906625    -0.065143      27.32
 H      -5.087812     0.697016    -0.321673      32.16
 H      -5.179254     0.854491    -2.037319      29.07
55
name = lig-etoh-Waterframe_235
 C       5.507126    -1.795546     1.905823      49.46
 H       5.648471    -0.740044     1.676329      22.27
 C       4.692847    -3.951187     1.321301      37.64
 H       4.302396    -4.689115     0.647933      13.87
 C       5.019029    -4.410843     2.627860      48.75
 O       4.783818    -5.711737     3.034425     317.36
 C       4.634130    -6.729529     2.087622     125.16
 H       5.413863    -6.663916     1.351317      27.56
 H       3.638457    -6.569362     1.725696      27.32
 H       4.731096    -7.706952     2.641487      19.26
 C       5.468432    -3.505903     3.640879      39.30
 O       5.721751    -3.844053     4.901998     223.13
 H       5.671042    -4.753105     5.091968      32.43
 C       5.764488    -2.149837     3.309062      36.04
 H       6.068575    -1.342866     4.087959      23.98
 C       4.979087    -2.605250     0.934755      45.73
 C       4.893291    -2.265806    -0.517685      76.67
 H       5.221369    -3.312146    -0.995303      18.99
 O       5.880411    -1.226216    -0.816351     175.79
 H       5.588366    -0.308492    -0.687921      24.47
 C       3.455154    -1.860711    -0.986973      94.11
 H       2.763013    -2.636120    -0.645443      22.49
 C       3.443654    -1.829436    -2.562276     104.30
 O       3.633082    -3.145181    -3.120331     276.10
 H       4.418507    -2.986952    -3.709812      25.12
 H       4.208477    -1.131483    -2.831795      25.51
 H       2.469285    -1.434600    -2.893851      25.95
 C      -0.649406    -1.152259     0.269689      36.54
 H      -1.329276    -1.919688     0.537962      19.38
 C      -0.228139     1.236893     0.081324      81.37
 H      -0.639726     2.302159    -0.141981      18.64
 C       1.076949     0.981768    -0.269100       8.65
 O       2.142204     1.851132    -0.714922     175.94
 C       2.104059     3.223470    -0.205905      92.86
 H       3.124154     3.791566    -0.231268      23.37
 H       1.523478     3.893263    -1.151178      21.30
 H       1.660701     3.149665     0.826347      24.25
 C       1.550925    -0.389082    -0.360770      13.47
 O       2.963817    -0.609808    -0.589650     167.54
 C       0.686727    -1.406432    -0.070080      58.28
 H       0.970114    -2.428927    -0.132310      20.42
 C      -1.147380     0.208190     0.308495      43.48
 C      -2.612048     0.549349     0.428770      79.76
 H      -3.155920    -0.235211     0.964620      21.12
 O      -2.888533     1.772785     1.172476     295.91
 H      -2.617409     1.459101     2.183546      25.05
 C      -3.291478     0.549135    -0.963335      87.71
 H      -2.605316     1.030089    -1.777663      23.09
 O      -3.417819    -0.869698    -1.418028     227.94
 H      -3.269508    -0.822938    -2.409068      24.68
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 C      -4.711427     1.090444    -1.091375     102.41
 O      -4.857575     2.559438    -1.060915     220.66
 H      -4.950027     2.772953    -0.045349      27.71
 H      -5.383740     0.633681    -0.362523      30.75
 H      -4.994801     0.825112    -2.170375      29.36
55
name = lig-etoh-Waterframe_236
 C       5.517222    -1.693426     1.950963      55.35
 H       5.702470    -0.626527     1.729611      23.52
 C       4.713109    -3.965312     1.346775      28.43
 H       4.457358    -4.679063     0.558212      18.41
 C       4.980680    -4.384967     2.644270      34.12
 O       4.775072    -5.702254     3.038534     220.92
 C       4.658430    -6.807131     2.034976      87.43
 H       5.447459    -6.732685     1.266637      25.93
 H       3.744126    -6.763237     1.457755      30.16
 H       4.669331    -7.764986     2.647157      22.81
 C       5.491836    -3.471672     3.605817      13.24
 O       5.747628    -3.880409     4.913009      86.51
 H       5.683020    -4.811652     5.029425      28.30
 C       5.738607    -2.146041     3.243809      50.93
 H       6.105001    -1.494153     4.115521      20.54
 C       4.995764    -2.625158     0.966618      20.83
 C       4.896957    -2.192477    -0.479408      66.08
 H       5.204197    -3.095405    -1.206800      20.62
 O       5.878255    -1.225258    -0.819435     185.46
 H       5.574958    -0.312684    -0.749468      26.45
 C       3.426278    -1.895349    -1.056039      87.78
 H       2.766402    -2.663473    -0.620742      22.53
 C       3.379537    -1.813907    -2.581813     110.51
 O       3.593160    -3.179835    -3.112822     267.74
 H       4.477695    -3.232527    -3.576988      26.10
 H       4.152138    -1.164045    -2.940183      25.47
 H       2.518387    -1.396426    -2.955187      28.08
 C      -0.628636    -1.104121     0.299790      35.68
 H      -1.302473    -1.938583     0.427933      17.66
 C      -0.212545     1.319614     0.061771      78.30
 H      -0.668870     2.290415     0.136028      18.12
 C       1.177546     0.994106    -0.237213       6.59
 O       2.128076     1.898993    -0.682051     223.17
 C       2.041042     3.201585    -0.217450     126.89
 H       3.088229     3.461917    -0.098002      25.00
 H       1.269969     3.891128    -0.747599      24.33
 H       1.513893     3.369372     0.795143      25.32
 C       1.595370    -0.401254    -0.341432       7.27
 O       2.968608    -0.595663    -0.664057     149.84
 C       0.708653    -1.512399    -0.047823      60.31
 H       0.927436    -2.501621    -0.113471      21.30
 C      -1.089120     0.183341     0.249955      54.54
 C      -2.656426     0.506519     0.474932      74.81
 H      -3.107797    -0.341310     1.001612      25.17
 O      -2.874903     1.712997     1.176571     318.40
 H      -2.593729     1.470298     2.220996      25.80
 C      -3.269961     0.526727    -0.901925      86.95
 H      -2.600298     1.307744    -1.624188      22.09
 O      -3.407419    -0.843646    -1.399806     247.10
 H      -3.180692    -0.723988    -2.370889      24.80
 C      -4.755360     1.074874    -1.099036      86.57
 O      -4.814594     2.541297    -1.057034     198.30
 H      -4.961246     2.838648    -0.077629      26.85
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 H      -5.732821     0.529681    -0.518765      28.00
 H      -5.025138     0.719503    -2.179410      29.12
55
name = lig-etoh-Waterframe_237
 C       5.488519    -1.615802     1.956740      58.82
 H       5.800524    -0.608493     1.602236      21.92
 C       4.770899    -3.932157     1.337968      50.67
 H       4.489223    -4.679941     0.554969      14.79
 C       4.928937    -4.407249     2.643475      24.47
 O       4.764251    -5.722168     3.052410     253.81
 C       4.663750    -6.830151     1.984693     103.29
 H       5.602292    -6.900688     1.374231      32.10
 H       3.772823    -6.877450     1.339907      33.26
 H       4.715571    -7.745272     2.631549      29.11
 C       5.503942    -3.489608     3.599522       0.20
 O       5.783336    -3.917251     4.924423      40.74
 H       5.734342    -4.899989     4.855614      24.10
 C       5.714506    -2.146938     3.226103      53.50
 H       6.182808    -1.492082     3.977270      21.47
 C       5.027179    -2.593347     1.030725      32.11
 C       4.857093    -2.145162    -0.503042      88.89
 H       5.140400    -3.002542    -1.100449      20.87
 O       5.894347    -1.204441    -0.845512     219.36
 H       5.566895    -0.296770    -0.702705      26.00
 C       3.423235    -1.929500    -1.105005      71.59
 H       2.848102    -2.822440    -0.778803      21.83
 C       3.360951    -1.836618    -2.625763     104.63
 O       3.553520    -3.219769    -3.130195     250.77
 H       4.442311    -3.296612    -3.585758      24.92
 H       4.196382    -1.230765    -3.031008      23.37
 H       2.361153    -1.577369    -2.911025      26.20
 C      -0.598806    -1.147257     0.292890      37.30
 H      -1.398701    -1.909003     0.460882      15.74
 C      -0.151588     1.319794     0.035152      50.30
 H      -0.419071     2.264816     0.234031      17.65
 C       1.209466     0.940141    -0.238428       5.59
 O       2.118660     1.895809    -0.643259     219.31
 C       1.945700     3.278698    -0.167086     123.60
 H       2.903542     3.686473    -0.169073      26.79
 H       1.488881     3.825959    -0.835803      28.15
 H       1.637569     3.179589     0.900667      25.16
 C       1.651158    -0.441963    -0.296252      20.88
 O       2.950180    -0.523887    -0.696603     134.90
 C       0.717656    -1.492090    -0.022955      61.35
 H       1.008128    -2.486022    -0.060338      23.17
 C      -1.081884     0.243459     0.259136      58.24
 C      -2.625054     0.405498     0.518594      63.52
 H      -2.944249    -0.500792     1.060945      24.25
 O      -2.864439     1.674564     1.179300     324.70
 H      -2.622299     1.490336     2.218595      25.47
 C      -3.380995     0.538655    -0.870035      86.23
 H      -2.647827     1.197947    -1.490243      22.63
 O      -3.344075    -0.815299    -1.387353     272.41
 H      -3.157398    -0.739422    -2.370761      25.08
 C      -4.788822     1.084042    -1.132323      91.48
 O      -4.807551     2.514403    -1.035501     235.78
 H      -4.678497     2.796016    -0.060491      26.61
 H      -5.477992     0.558897    -0.253959      27.62
 H      -5.002028     0.923946    -2.208499      28.82
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name = lig-etoh-Waterframe_238
 C       5.447484    -1.626696     1.933691      54.57
 H       5.781265    -0.604749     1.672594      24.47
 C       4.822047    -3.900571     1.332941      62.32
 H       4.439242    -4.568424     0.505010      14.52
 C       4.929390    -4.425875     2.649217       8.78
 O       4.730282    -5.775400     3.013249     301.77
 C       4.694065    -6.830001     2.011106      77.97
 H       5.645972    -6.734267     1.414586      30.57
 H       3.770125    -6.596995     1.411648      34.79
 H       4.574462    -7.727758     2.611554      26.20
 C       5.480127    -3.537100     3.629892     -10.51
 O       5.821901    -3.943209     4.870473      41.39
 H       5.766812    -5.005668     5.104511      18.32
 C       5.731673    -2.120868     3.288296      51.42
 H       6.207139    -1.493982     3.981946      22.51
 C       5.011890    -2.490067     0.961230      37.05
 C       4.858845    -2.181525    -0.516381      90.98
 H       5.157734    -3.076053    -0.887297      23.40
 O       5.890272    -1.180933    -0.886764     195.09
 H       5.675630    -0.207932    -0.680082      23.97
 C       3.472630    -1.865921    -1.107461      99.25
 H       2.729048    -2.599136    -0.753658      22.93
 C       3.370715    -1.921384    -2.678022      97.62
 O       3.520429    -3.276622    -3.165226     255.76
 H       4.340885    -3.156263    -3.730706      23.11
 H       4.018598    -1.090504    -3.158894      24.38
 H       2.290587    -1.555487    -2.918757      24.56
 C      -0.623564    -1.111732     0.260521      52.16
 H      -1.298730    -1.977140     0.563278      21.12
 C      -0.104585     1.228131     0.049067      71.49
 H      -0.287645     2.260796     0.011519      19.94
 C       1.174689     0.890277    -0.248546       8.17
 O       2.153955     1.897197    -0.601762     190.88
 C       1.913693     3.327210    -0.125003     105.67
 H       2.823361     3.870238    -0.156541      25.74
 H       1.211593     3.787428    -0.835806      25.40
 H       1.454938     3.374520     0.888941      25.62
 C       1.642902    -0.415736    -0.252374      23.20
 O       2.963278    -0.540401    -0.720011     134.79
 C       0.750527    -1.431123     0.003614      61.75
 H       1.090359    -2.485852     0.018421      22.31
 C      -1.071323     0.216879     0.300066      61.65
 C      -2.569434     0.388585     0.510713      76.42
 H      -2.942109    -0.449812     1.143225      24.72
 O      -2.870393     1.636135     1.190829     319.27
 H      -2.640324     1.417659     2.168714      27.14
 C      -3.400527     0.514699    -0.865536      87.26
 H      -2.826490     1.116513    -1.425333      25.93
 O      -3.271588    -0.829134    -1.394829     287.63
 H      -3.240838    -0.667765    -2.393840      24.71
 C      -4.790551     1.103953    -1.091992     117.22
 O      -4.822814     2.522887    -0.993750     288.81
 H      -4.508270     2.719154    -0.069709      28.65
 H      -5.534321     0.676074    -0.466794      30.75
 H      -5.174153     0.774047    -2.012053      30.44
55
name = lig-etoh-Waterframe_239
 C       5.457587    -1.642333     2.018275      52.42
 H       5.612395    -0.578112     1.844603      24.25
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 C       4.828287    -3.844321     1.319839      41.89
 H       4.481351    -4.555734     0.528408      13.12
 C       4.966319    -4.431927     2.600103      34.70
 O       4.704278    -5.767395     3.003412     296.84
 C       4.687488    -6.774267     2.037844     113.61
 H       5.560305    -6.849607     1.344666      28.54
 H       3.860172    -6.643412     1.254371      31.28
 H       4.526613    -7.735165     2.430567      24.60
 C       5.457698    -3.512371     3.627567      13.90
 O       5.879292    -3.967569     4.860875      80.37
 H       5.631926    -5.068062     4.909962      24.56
 C       5.718203    -2.162946     3.297359      68.93
 H       6.128021    -1.573685     4.053639      23.04
 C       4.950530    -2.508655     0.934778      42.09
 C       4.922461    -2.173638    -0.536265      78.38
 H       5.229665    -3.077088    -1.148599      20.69
 O       5.884562    -1.207295    -0.950464     210.70
 H       5.470787    -0.279138    -0.699996      22.01
 C       3.485172    -1.811652    -1.122120      96.93
 H       2.850415    -2.576644    -0.651691      22.17
 C       3.332493    -1.948288    -2.678025      88.74
 O       3.520670    -3.310942    -3.221809     251.37
 H       4.298698    -3.420411    -3.848825      23.85
 H       4.085485    -1.333035    -3.277958      23.53
 H       2.216195    -1.632307    -2.933436      24.00
 C      -0.598804    -1.124527     0.260063      55.25
 H      -1.255853    -1.991567     0.531914      21.87
 C      -0.148468     1.181927     0.081680      73.39
 H      -0.616697     2.200082    -0.199266      18.36
 C       1.241175     0.959051    -0.263909       1.79
 O       2.188968     1.924298    -0.522399     204.09
 C       1.852839     3.315573    -0.138051      94.68
 H       2.869743     3.822059    -0.144271      23.89
 H       0.876996     3.771156    -0.754335      22.52
 H       1.477415     3.453361     0.871416      26.36
 C       1.690900    -0.405042    -0.271841      18.26
 O       3.001682    -0.565427    -0.724630     178.32
 C       0.737043    -1.406446     0.040638      60.97
 H       1.061038    -2.530683     0.093367      19.87
 C      -1.082833     0.153847     0.323418      40.33
 C      -2.590559     0.457312     0.483027      83.60
 H      -3.005410    -0.446370     1.002767      22.54
 O      -2.880228     1.618162     1.208169     354.44
 H      -2.664354     1.394877     2.105858      29.56
 C      -3.291615     0.464335    -0.871387      84.21
 H      -2.766341     1.185523    -1.475748      23.83
 O      -3.225498    -0.874981    -1.429464     265.84
 H      -3.211085    -0.693495    -2.425286      24.08
 C      -4.850551     1.067950    -0.996360     103.04
 O      -4.825572     2.546536    -0.959610     296.57
 H      -4.741675     2.854686    -0.020718      26.96
 H      -5.578038     0.724524    -0.362731      30.84
 H      -5.086409     0.787564    -2.010875      30.00
55
name = lig-etoh-Waterframe_240
 C       5.430471    -1.664888     2.035625      70.50
 H       5.526563    -0.601930     1.933419      23.75
 C       4.772325    -3.894031     1.283127      36.97
 H       4.575398    -4.607012     0.485654      17.94
 C       5.016537    -4.378946     2.586493      44.73
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 O       4.697991    -5.684049     3.013327     254.78
 C       4.645765    -6.767064     1.945614     122.88
 H       5.660912    -6.815596     1.568409      21.45
 H       3.791900    -6.613963     1.254873      25.49
 H       4.530645    -7.637337     2.573542      20.27
 C       5.461237    -3.552280     3.601515      27.84
 O       5.909631    -3.988595     4.845172     168.58
 H       5.864056    -5.074373     4.940279      28.33
 C       5.686186    -2.209159     3.305424      37.00
 H       6.021902    -1.570097     4.120741      25.01
 C       4.974738    -2.503496     1.031221      18.60
 C       4.940945    -2.150099    -0.614458      56.75
 H       5.199268    -3.179055    -1.238563      19.37
 O       5.885906    -1.225680    -1.011182     198.66
 H       5.665084    -0.200256    -0.795768      19.82
 C       3.498604    -1.898643    -1.136822      79.69
 H       2.945419    -2.738734    -0.715455      23.40
 C       3.320321    -1.972143    -2.702794      98.83
 O       3.500828    -3.353689    -3.237701     259.87
 H       4.401996    -3.222280    -3.732217      21.37
 H       4.039930    -1.276135    -3.139166      24.60
 H       2.272969    -1.683259    -2.956890      25.76
 C      -0.591083    -1.218683     0.321125      43.02
 H      -1.281289    -2.046329     0.455488      21.09
 C      -0.169600     1.200676     0.055012      57.52
 H      -0.748715     2.264696    -0.007562      17.00
 C       1.241622     0.998242    -0.229293       1.64
 O       2.211395     1.976047    -0.436304     206.05
 C       1.775503     3.289272    -0.128239     107.47
 H       2.694448     3.969971    -0.418458      23.55
 H       1.117944     3.754909    -1.052868      22.80
 H       1.607573     3.242482     0.907065      26.11
 C       1.705621    -0.375490    -0.313343      14.99
 O       3.050338    -0.539216    -0.704320     139.96
 C       0.794266    -1.411301     0.044900      52.11
 H       1.114988    -2.551403     0.061009      20.26
 C      -1.093766     0.148924     0.321239      27.34
 C      -2.615259     0.436889     0.462204      80.99
 H      -3.062480    -0.449177     0.950840      22.96
 O      -2.898804     1.648872     1.225101     347.61
 H      -2.644101     1.387365     2.076914      28.79
 C      -3.265493     0.475094    -0.907040      70.92
 H      -2.631165     1.173594    -1.684002      22.15
 O      -3.192270    -0.919533    -1.468527     236.08
 H      -3.045713    -0.787647    -2.458127      24.38
 C      -4.817445     1.048657    -0.910292      86.12
 O      -4.830879     2.543439    -0.927781     267.25
 H      -5.033504     2.866293    -0.037072      28.06
 H      -5.465274     0.557332    -0.044646      27.49
 H      -5.156299     0.861398    -1.986129      27.09
55
name = lig-etoh-Waterframe_241
 C       5.384566    -1.658988     2.048401      55.46
 H       5.556601    -0.619389     1.816943      23.12
 C       4.743738    -3.925078     1.268087      40.72
 H       4.536657    -4.589257     0.469871      18.67
 C       4.995887    -4.405739     2.556069      48.16
 O       4.692006    -5.620469     2.981332     233.52
 C       4.620356    -6.734707     1.942169     104.38
 H       5.568071    -6.775035     1.427912      24.76
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 H       3.868873    -6.539607     1.189254      28.71
 H       4.361794    -7.601780     2.599087      22.86
 C       5.538166    -3.579216     3.619220      17.44
 O       5.930663    -4.017654     4.830381     111.71
 H       5.882583    -4.962498     5.025201      24.88
 C       5.649465    -2.205098     3.341830      42.96
 H       5.977347    -1.502294     4.182665      21.96
 C       5.012339    -2.540605     0.962730      22.01
 C       4.898064    -2.172526    -0.601931      80.77
 H       5.347936    -3.190373    -0.937246      18.97
 O       5.925880    -1.224331    -1.084416     182.95
 H       5.661492    -0.256321    -0.739299      22.13
 C       3.501132    -1.993589    -1.158382      75.75
 H       2.800778    -2.682206    -0.689647      21.37
 C       3.312103    -1.985933    -2.696866     105.94
 O       3.507416    -3.344843    -3.206136     260.98
 H       4.366411    -3.373307    -3.833025      21.82
 H       3.928371    -1.269581    -3.137470      25.47
 H       2.350872    -1.657265    -2.916688      26.97
 C      -0.569412    -1.215442     0.378095      45.94
 H      -1.149941    -2.080249     0.548480      21.74
 C      -0.176871     1.226687     0.023007      61.28
 H      -0.356390     2.358933     0.271269      17.61
 C       1.185019     0.976870    -0.182325       6.57
 O       2.221517     1.971928    -0.374090     196.76
 C       1.759083     3.330622    -0.178572     118.08
 H       2.682014     4.029097    -0.158436      23.36
 H       0.793776     3.506873    -0.673942      24.61
 H       1.268980     3.618360     0.777334      25.11
 C       1.680347    -0.339270    -0.332869       6.67
 O       3.078916    -0.544198    -0.676612      92.87
 C       0.843319    -1.431014     0.024840      46.94
 H       1.350857    -2.441227    -0.080640      19.68
 C      -1.064082     0.093345     0.308601      29.33
 C      -2.598817     0.385484     0.452593      75.87
 H      -3.069417    -0.406049     1.025193      24.17
 O      -2.909337     1.668872     1.217510     297.78
 H      -2.636174     1.431551     2.133967      26.54
 C      -3.319066     0.498745    -0.980372      70.87
 H      -2.601830     1.206025    -1.715148      22.01
 O      -3.178448    -0.938209    -1.480471     230.74
 H      -2.977908    -0.736483    -2.446876      24.25
 C      -4.695229     1.065686    -0.894448      98.63
 O      -4.852314     2.492773    -0.890824     290.99
 H      -4.854682     2.840628     0.068819      24.59
 H      -5.238479     0.528435     0.115326      26.37
 H      -5.447169     0.566385    -1.640383      26.80
55
name = lig-etoh-Waterframe_242
 C       5.338939    -1.693504     2.010071      49.05
 H       5.577195    -0.643754     1.808052      23.74
 C       4.766837    -3.885211     1.243398      62.29
 H       4.383285    -4.581578     0.562360      19.74
 C       4.983014    -4.374740     2.552739       9.85
 O       4.667446    -5.688083     2.937112     293.40
 C       4.586096    -6.659446     1.982731     103.32
 H       5.489853    -6.900806     1.437504      29.48
 H       3.824577    -6.441438     1.252122      33.82
 H       4.297556    -7.690452     2.399600      26.98
 C       5.595707    -3.561732     3.571170     -10.74
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 O       5.961222    -4.050725     4.855283     138.34
 H       5.756552    -4.956873     4.919435      23.49
 C       5.612548    -2.162125     3.348321      34.54
 H       5.977261    -1.461309     4.199224      17.43
 C       5.027401    -2.557668     0.902309      43.12
 C       4.954174    -2.243835    -0.532667      94.71
 H       5.228335    -3.075582    -1.114539      24.01
 O       5.909422    -1.254909    -1.125380     196.83
 H       5.670672    -0.308053    -0.851910      23.53
 C       3.472291    -1.967892    -1.145856      65.68
 H       2.839188    -2.763917    -0.689728      23.76
 C       3.310582    -1.980816    -2.673016     104.92
 O       3.515307    -3.331094    -3.159752     264.03
 H       4.310670    -3.281963    -3.823938      23.91
 H       4.040968    -1.375038    -3.177558      24.38
 H       2.291225    -1.751326    -2.840173      26.79
 C      -0.456884    -1.195611     0.385591      47.82
 H      -1.072003    -1.982749     0.753147      22.46
 C      -0.159007     1.203759     0.059199      66.40
 H      -0.582912     2.185419     0.310730      22.70
 C       1.213894     0.981287    -0.180194       2.62
 O       2.178799     1.952433    -0.287439     200.45
 C       1.679863     3.394356    -0.174596     105.36
 H       2.547333     4.039308    -0.390633      25.84
 H       1.067979     3.574284    -0.991611      26.78
 H       1.303477     3.530701     0.891588      23.99
 C       1.704072    -0.390586    -0.334031       9.52
 O       3.053396    -0.583570    -0.657639     122.94
 C       0.846400    -1.409548    -0.009472      69.46
 H       1.130563    -2.436137     0.008336      23.94
 C      -1.062169     0.111575     0.300752      22.01
 C      -2.570441     0.397938     0.434383      85.32
 H      -3.010085    -0.452417     0.941042      25.25
 O      -2.884366     1.649733     1.171024     290.53
 H      -2.696455     1.415498     2.182792      25.26
 C      -3.249862     0.471870    -0.987412      86.68
 H      -2.711893     1.209698    -1.635298      26.19
 O      -3.197528    -0.899640    -1.480350     238.42
 H      -3.080078    -0.794776    -2.468718      25.15
 C      -4.700302     1.010953    -0.836906     101.97
 O      -4.867208     2.427031    -0.876214     286.68
 H      -4.621703     2.769843     0.036174      25.70
 H      -4.889203     0.843695     0.255130      26.26
 H      -5.354478     0.568496    -1.649024      27.53
55
name = lig-etoh-Waterframe_243
 C       5.342782    -1.699303     1.972040      65.13
 H       5.466484    -0.612680     1.783002      25.26
 C       4.790480    -3.902717     1.261838      63.10
 H       4.335651    -4.528920     0.540922      18.28
 C       4.996352    -4.355162     2.565676       6.37
 O       4.662124    -5.710841     2.971506     262.41
 C       4.522303    -6.691314     1.909373      89.25
 H       5.540706    -6.792353     1.495759      28.12
 H       3.736659    -6.403879     1.191464      32.07
 H       4.225022    -7.583670     2.558710      25.68
 C       5.597519    -3.540649     3.575613     -13.85
 O       5.978669    -4.051465     4.826715     140.72
 H       5.800139    -5.078724     4.949637      24.67
 C       5.588428    -2.148106     3.278120      45.16
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 H       5.914221    -1.405083     4.062016      16.68
 C       5.047032    -2.548318     0.937997      41.55
 C       4.983324    -2.257332    -0.627616      99.13
 H       5.144696    -3.143303    -1.129363      25.19
 O       5.869101    -1.304002    -1.128736     249.70
 H       5.628410    -0.394742    -0.923299      26.77
 C       3.488330    -1.895905    -1.057248      88.97
 H       2.856325    -2.739937    -0.707730      23.59
 C       3.317311    -1.972691    -2.630648      92.15
 O       3.522919    -3.329949    -3.118087     280.98
 H       4.348371    -3.290453    -3.649852      24.76
 H       4.010459    -1.181607    -3.117018      24.21
 H       2.253164    -1.618522    -2.927185      25.43
 C      -0.474829    -1.125415     0.392081      45.71
 H      -1.007954    -1.999739     0.802284      21.70
 C      -0.150073     1.170819     0.128552      61.29
 H      -0.609798     2.066551     0.038974      25.01
 C       1.254216     0.942885    -0.191214      13.12
 O       2.142323     2.000758    -0.203807     190.81
 C       1.631946     3.383849    -0.208803     118.98
 H       2.553002     3.902454    -0.238755      27.31
 H       1.043979     3.677094    -1.063555      26.94
 H       1.185073     3.567193     0.839885      26.13
 C       1.745068    -0.386845    -0.330456      30.69
 O       3.030433    -0.642722    -0.652555     166.23
 C       0.838507    -1.451083    -0.027382      60.96
 H       1.095062    -2.425729     0.037025      23.96
 C      -1.016062     0.133649     0.312667      36.45
 C      -2.508093     0.412531     0.408070      94.48
 H      -2.963058    -0.471875     0.895895      25.30
 O      -2.838755     1.614537     1.113712     272.77
 H      -2.702155     1.323808     2.158009      24.37
 C      -3.163377     0.470308    -0.945976     101.62
 H      -2.674461     1.053070    -1.573120      29.07
 O      -3.229969    -0.857034    -1.480678     246.88
 H      -3.141683    -0.707349    -2.464788      26.47
 C      -4.717721     0.934100    -0.720075     104.55
 O      -4.858397     2.383306    -0.921852     272.04
 H      -4.900078     2.821690     0.006812      25.57
 H      -5.153571     0.560440     0.114893      30.96
 H      -5.314903     0.497764    -1.484485      30.26
55
name = lig-etoh-Waterframe_244
 C       5.379103    -1.628183     1.936509      53.80
 H       5.380350    -0.533669     1.727647      24.69
 C       4.806124    -3.924534     1.295726      48.92
 H       4.475817    -4.602607     0.506109      18.34
 C       5.006621    -4.437442     2.602569      34.85
 O       4.669317    -5.652744     3.016807     189.55
 C       4.472135    -6.732996     1.870505      93.05
 H       5.428956    -6.895278     1.292666      26.99
 H       3.724278    -6.503560     1.057315      28.58
 H       4.185599    -7.655553     2.404634      25.78
 C       5.543376    -3.536505     3.598395      20.16
 O       5.989557    -4.010079     4.771356      25.48
 H       5.902878    -5.112642     4.927167      28.63
 C       5.606222    -2.162902     3.244865      54.71
 H       5.847556    -1.426127     3.984970      20.93
 C       5.056224    -2.584919     0.891731      34.72
 C       4.903824    -2.251569    -0.664604      95.28
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 H       5.221665    -3.244131    -1.063484      21.65
 O       5.876766    -1.319786    -1.139378     250.50
 H       5.569688    -0.472296    -0.868469      28.19
 C       3.502272    -1.937144    -1.052526      93.31
 H       2.879484    -2.654708    -0.511751      22.31
 C       3.321881    -1.932470    -2.570076      87.28
 O       3.538009    -3.304325    -3.074655     270.36
 H       4.320191    -3.385408    -3.634688      26.09
 H       4.091956    -1.202734    -3.072845      23.05
 H       2.207748    -1.623383    -2.866521      24.90
 C      -0.505304    -1.178446     0.398740      41.80
 H      -1.244954    -2.007238     0.651070      20.08
 C      -0.064507     1.202291     0.127351      69.78
 H      -0.303432     2.159488    -0.132051      24.02
 C       1.236726     0.937058    -0.158267       6.63
 O       2.133059     2.043782    -0.160677     201.37
 C       1.640650     3.362040    -0.212391     129.93
 H       2.468703     3.962535    -0.045094      27.26
 H       0.803605     3.563218    -1.006584      24.92
 H       0.909062     3.687424     0.556891      27.93
 C       1.705198    -0.415944    -0.303400      16.45
 O       3.077234    -0.618055    -0.629648     136.48
 C       0.813214    -1.452898    -0.014880      67.54
 H       1.215418    -2.388735    -0.058515      24.93
 C      -0.994776     0.145326     0.355632      29.73
 C      -2.436242     0.370328     0.424773      96.27
 H      -2.927677    -0.472223     0.986403      25.29
 O      -2.785023     1.595543     1.086491     259.27
 H      -2.606887     1.458097     2.162101      24.76
 C      -3.213924     0.492128    -0.885566      90.93
 H      -2.725179     1.186512    -1.573472      27.17
 O      -3.249866    -0.854015    -1.497464     226.24
 H      -3.119368    -0.632255    -2.463913      25.67
 C      -4.700787     0.882797    -0.679616     108.56
 O      -4.865088     2.334401    -0.942526     222.53
 H      -5.263886     2.774981    -0.116148      27.35
 H      -5.242486     0.514359     0.146991      30.16
 H      -5.138936     0.409740    -1.522787      30.05
55
name = lig-etoh-Waterframe_245
 C       5.393414    -1.646539     1.872632      48.90
 H       5.474343    -0.558998     1.733747      21.21
 C       4.836839    -3.939888     1.293999      52.96
 H       4.661872    -4.746470     0.534000      18.77
 C       5.014487    -4.416086     2.592516      17.92
 O       4.653466    -5.723591     2.996322     248.24
 C       4.449611    -6.738849     1.889108     112.04
 H       5.419601    -6.913021     1.348138      24.22
 H       3.597011    -6.353139     1.283438      25.00
 H       4.221692    -7.648339     2.376310      23.11
 C       5.472055    -3.528690     3.542464      -4.10
 O       6.016370    -3.960781     4.773540     167.95
 H       5.775839    -5.039950     4.807909      24.80
 C       5.638712    -2.135232     3.223941      31.35
 H       5.895066    -1.565379     4.056511      24.83
 C       5.059475    -2.581480     0.877043      33.50
 C       4.894980    -2.296346    -0.574056      71.12
 H       5.133573    -3.222224    -1.316843      20.25
 O       5.887467    -1.306032    -1.148363     232.24
 H       5.753897    -0.405478    -0.896047      26.87
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 C       3.461834    -1.987269    -1.070237      67.55
 H       2.858841    -2.765130    -0.613208      25.41
 C       3.325243    -1.935747    -2.549816     105.27
 O       3.536424    -3.278730    -3.036823     265.69
 H       4.281441    -3.165109    -3.690824      24.88
 H       4.092621    -1.242883    -2.966832      24.58
 H       2.259748    -1.624905    -2.766047      26.24
 C      -0.540546    -1.237309     0.386004      46.43
 H      -1.317659    -2.052388     0.484220      21.48
 C      -0.067066     1.227752     0.086226      60.36
 H      -0.457561     2.274537     0.100324      21.20
 C       1.312491     0.961804    -0.099593      11.39
 O       2.166074     2.012861    -0.144717     175.62
 C       1.561243     3.394215    -0.186244     105.73
 H       2.335330     4.171221    -0.249276      26.53
 H       1.375764     3.479644    -1.338441      24.36
 H       0.948647     3.452395     0.687165      25.09
 C       1.715275    -0.407926    -0.266069      11.42
 O       3.110947    -0.541048    -0.575630      93.09
 C       0.797010    -1.464306     0.011157      54.76
 H       1.090160    -2.511081    -0.129946      24.11
 C      -0.926859     0.135152     0.380777      20.23
 C      -2.451731     0.342931     0.495293      83.72
 H      -2.829327    -0.552295     1.058441      25.68
 O      -2.726723     1.623860     1.102355     274.56
 H      -2.486004     1.508790     2.159610      25.40
 C      -3.283206     0.456316    -0.824119      74.02
 H      -2.855133     1.395817    -1.518852      25.04
 O      -3.247330    -0.854611    -1.520514     213.59
 H      -3.133280    -0.669192    -2.496671      25.13
 C      -4.708678     0.873257    -0.736308      99.97
 O      -4.905707     2.283435    -0.934539     204.09
 H      -5.200518     2.645296    -0.026313      27.50
 H      -5.052552     0.706553     0.378718      26.92
 H      -5.218458     0.344709    -1.599446      27.68
55
name = lig-etoh-Waterframe_246
 C       5.415636    -1.693021     1.892824      68.50
 H       5.636236    -0.684976     1.555592      25.09
 C       4.885559    -3.961196     1.233737      62.69
 H       4.692819    -4.690955     0.384879      17.83
 C       4.963485    -4.429976     2.546781      20.30
 O       4.660042    -5.804822     2.956588     234.45
 C       4.446288    -6.714493     1.963432     124.73
 H       5.327091    -6.783929     1.297516      28.80
 H       3.618782    -6.466520     1.236109      29.07
 H       4.208733    -7.593175     2.485248      25.23
 C       5.485614    -3.470455     3.552231      -0.06
 O       6.002090    -3.911582     4.753621     115.42
 H       5.876810    -4.920130     5.064169      24.99
 C       5.645932    -2.133217     3.179219      70.00
 H       6.036473    -1.479575     3.926456      23.65
 C       5.059725    -2.622315     0.905541      36.73
 C       4.936290    -2.268540    -0.581203      69.67
 H       5.191325    -3.323962    -1.084661      20.16
 O       5.882412    -1.320532    -1.134639     242.67
 H       5.693575    -0.429424    -0.831548      27.23
 C       3.449834    -1.937473    -0.992475      77.48
 H       2.709624    -2.662666    -0.703837      24.32
 C       3.305402    -1.919393    -2.548705     108.68
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 O       3.538718    -3.263057    -3.044066     266.47
 H       4.344243    -3.293267    -3.732852      22.36
 H       3.973098    -1.230589    -2.951946      26.68
 H       2.380322    -1.561544    -2.851601      27.87
 C      -0.527919    -1.205821     0.337892      53.95
 H      -1.174400    -2.065319     0.572251      24.47
 C      -0.104569     1.184167     0.082558      57.31
 H      -0.727761     2.167342     0.345358      18.23
 C       1.311021     0.991039    -0.039980      14.70
 O       2.274137     2.012046    -0.138025     154.83
 C       1.573116     3.379072    -0.223761      96.98
 H       2.476298     4.030723     0.112747      24.08
 H       0.890905     3.551716    -1.183700      24.67
 H       0.738190     3.555202     0.471842      24.80
 C       1.769673    -0.369285    -0.203395       7.43
 O       3.098936    -0.551982    -0.522318     131.06
 C       0.811717    -1.485184     0.019036      47.59
 H       1.065769    -2.602231    -0.207859      20.40
 C      -0.946755     0.096061     0.364812      33.32
 C      -2.476298     0.354389     0.549667      85.90
 H      -2.887176    -0.411765     1.220521      25.19
 O      -2.676015     1.667978     1.161265     293.19
 H      -2.515294     1.496981     2.204382      25.59
 C      -3.274322     0.394390    -0.817677      75.07
 H      -2.582843     1.165005    -1.482256      24.06
 O      -3.223937    -0.860038    -1.525808     213.88
 H      -3.201614    -0.540160    -2.476599      25.12
 C      -4.778533     0.867086    -0.749562      96.74
 O      -4.966825     2.278844    -0.908230     250.98
 H      -4.817965     2.684985     0.024701      25.92
 H      -5.214194     0.530055     0.360744      26.32
 H      -5.568233     0.247578    -1.324043      26.88
55
name = lig-etoh-Waterframe_247
 C       5.438057    -1.718102     1.864874      59.94
 H       5.754228    -0.730534     1.576703      26.60
 C       4.909125    -4.032561     1.177709      65.42
 H       4.601541    -4.694288     0.325735      18.97
 C       4.928241    -4.463225     2.561729      11.36
 O       4.702967    -5.730558     2.974445     249.62
 C       4.436796    -6.760105     1.941621     105.94
 H       5.314382    -6.939243     1.332961      29.59
 H       3.566335    -6.553337     1.315995      32.39
 H       4.298386    -7.723021     2.451229      26.42
 C       5.488316    -3.535765     3.530157      -7.69
 O       5.980433    -3.848636     4.771039     117.24
 H       5.892547    -4.842016     4.849151      22.39
 C       5.670899    -2.133241     3.204759      51.16
 H       6.184702    -1.360748     3.828984      20.31
 C       5.078016    -2.635548     0.897712      23.23
 C       4.940699    -2.256359    -0.588425      81.63
 H       5.191225    -3.162338    -1.120968      23.10
 O       5.875800    -1.342221    -1.101970     244.84
 H       5.590415    -0.443153    -0.846871      27.28
 C       3.470008    -1.854627    -0.969585      94.39
 H       2.888324    -2.601908    -0.384849      23.46
 C       3.308032    -1.866341    -2.554962      99.56
 O       3.529003    -3.260050    -3.069110     255.77
 H       4.426477    -3.233711    -3.671586      22.05
 H       4.042656    -1.246441    -2.982285      25.97
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 H       2.312969    -1.650822    -2.829016      27.01
 C      -0.468822    -1.221031     0.295700      45.56
 H      -1.086942    -2.005805     0.661569      22.82
 C      -0.121103     1.131730     0.150177      62.31
 H      -0.484456     2.275108     0.170405      18.68
 C       1.272115     0.983731    -0.007225      -4.68
 O       2.294471     2.045182    -0.141382     190.16
 C       1.612015     3.328014    -0.228120     106.59
 H       2.418351     4.165568    -0.007677      24.46
 H       1.168496     3.558385    -1.194469      27.89
 H       0.880194     3.396815     0.622436      25.10
 C       1.741827    -0.384262    -0.117205      15.78
 O       3.095534    -0.602222    -0.468214     163.48
 C       0.879021    -1.422091    -0.010612      66.74
 H       1.233951    -2.543625    -0.148610      21.18
 C      -1.063100     0.074082     0.326384      33.49
 C      -2.499966     0.382162     0.594312      99.53
 H      -2.956435    -0.321626     1.267167      24.47
 O      -2.640924     1.711833     1.231604     307.86
 H      -2.634604     1.499443     2.232386      27.66
 C      -3.253416     0.371457    -0.823838      81.96
 H      -2.726021     1.083089    -1.403344      26.61
 O      -3.187961    -0.892726    -1.525390     234.33
 H      -3.241256    -0.654203    -2.499370      25.03
 C      -4.861512     0.830708    -0.669951      83.85
 O      -5.024250     2.293781    -0.865577     254.47
 H      -4.608870     2.779838    -0.074040      27.33
 H      -5.259697     0.641746     0.385395      27.11
 H      -5.389019     0.397068    -1.582232      25.91
55
name = lig-etoh-Waterframe_248
 C       5.486129    -1.728501     1.862494      60.70
 H       5.697829    -0.703569     1.620062      26.33
 C       4.893951    -4.053023     1.200450      62.29
 H       4.589984    -4.829231     0.491994      16.97
 C       4.963329    -4.424615     2.522200      17.80
 O       4.731473    -5.699480     3.003280     225.60
 C       4.456519    -6.829712     1.925908      88.68
 H       5.341038    -6.896014     1.297809      31.11
 H       3.566113    -6.503134     1.425328      32.07
 H       4.299475    -7.716821     2.637858      26.05
 C       5.500572    -3.509114     3.491733      -8.78
 O       5.939717    -3.846415     4.800009     133.03
 H       5.979435    -4.774447     4.980685      23.33
 C       5.692770    -2.178928     3.173741      50.18
 H       6.166339    -1.611415     4.063603      19.75
 C       5.102573    -2.687953     0.835445      27.44
 C       4.914125    -2.271524    -0.594627      95.94
 H       4.971728    -3.053146    -1.227169      24.80
 O       5.907180    -1.318837    -1.065407     193.67
 H       5.712201    -0.342885    -0.945378      26.13
 C       3.517473    -1.863921    -0.989862      84.09
 H       2.977807    -2.773203    -0.554302      22.73
 C       3.310656    -1.878844    -2.533081      95.84
 O       3.513414    -3.228073    -3.069864     266.93
 H       4.271786    -3.194920    -3.815852      22.54
 H       4.007733    -1.115006    -3.014854      23.41
 H       2.226534    -1.544290    -2.760957      24.36
 C      -0.493745    -1.230762     0.293613      43.81
 H      -0.991059    -2.138921     0.500799      20.14
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 C      -0.114383     1.152591     0.215005      67.24
 H      -0.499751     2.200956    -0.000855      19.85
 C       1.287556     0.948969     0.003948      10.79
 O       2.219825     2.011474    -0.151246     211.02
 C       1.688412     3.322612    -0.198303     118.11
 H       2.472082     4.122884    -0.251901      25.36
 H       1.292985     3.397421    -1.138546      29.22
 H       1.021660     3.452885     0.690994      25.76
 C       1.784871    -0.341991    -0.083537      30.86
 O       3.107676    -0.574444    -0.390840     131.05
 C       0.879548    -1.409946    -0.021680      56.31
 H       1.370931    -2.457697    -0.011218      21.53
 C      -1.049490     0.051977     0.307541      31.05
 C      -2.550126     0.408285     0.602488      89.50
 H      -2.946137    -0.418567     1.197234      24.77
 O      -2.630454     1.733565     1.278863     332.81
 H      -2.627490     1.517935     2.226042      28.94
 C      -3.332459     0.426551    -0.778882      85.29
 H      -3.026441     1.172033    -1.368560      27.05
 O      -3.154476    -0.942143    -1.498143     216.97
 H      -3.141410    -0.702631    -2.476786      24.64
 C      -4.845145     0.860639    -0.620813     113.52
 O      -5.050410     2.286208    -0.825515     272.73
 H      -4.762705     2.783612     0.025599      26.91
 H      -5.337969     0.482700     0.183537      30.95
 H      -5.312702     0.419862    -1.489560      28.29
55
name = lig-etoh-Waterframe_249
 C       5.526950    -1.767390     1.816096      62.82
 H       5.577760    -0.715371     1.552230      23.35
 C       4.855021    -4.021986     1.198637      50.04
 H       4.610837    -4.770449     0.490251      19.66
 C       5.048545    -4.422243     2.551269      39.63
 O       4.745534    -5.741711     2.986543     237.01
 C       4.501806    -6.794534     2.013924     113.14
 H       5.315794    -6.944336     1.266835      25.80
 H       3.622321    -6.665991     1.370304      27.01
 H       4.316863    -7.765933     2.642272      23.29
 C       5.527409    -3.530176     3.521247      20.16
 O       5.879846    -3.862339     4.812152     123.66
 H       5.851758    -4.804491     4.960150      29.00
 C       5.732068    -2.208323     3.131209      34.74
 H       6.022491    -1.519641     4.008883      23.22
 C       5.148422    -2.705613     0.829059      32.97
 C       4.933971    -2.254555    -0.633526      86.88
 H       5.131216    -3.197605    -1.250775      21.06
 O       5.971706    -1.292595    -1.029905     164.67
 H       5.596812    -0.351543    -0.796165      22.89
 C       3.517356    -1.905628    -1.002972      68.77
 H       2.737276    -2.652584    -0.769608      23.68
 C       3.300329    -1.863943    -2.515731      93.88
 O       3.482386    -3.179934    -3.063174     281.29
 H       4.189677    -3.209019    -3.731608      25.11
 H       4.012298    -1.101282    -3.065858      23.65
 H       2.174369    -1.492075    -2.688967      25.10
 C      -0.509094    -1.258843     0.286645      43.91
 H      -1.158878    -2.104315     0.423245      21.27
 C      -0.103768     1.169623     0.218821      75.15
 H      -0.615673     2.071938     0.190747      22.34
 C       1.273397     0.984331     0.020419      17.90
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 O       2.175323     1.922435    -0.147505     204.17
 C       1.740445     3.348297    -0.201866     116.20
 H       2.702133     3.776710    -0.156651      24.66
 H       0.914776     3.450703    -0.971517      25.87
 H       1.101804     3.814288     0.566655      27.03
 C       1.807386    -0.359618    -0.100995      17.23
 O       3.173823    -0.541878    -0.326065     112.82
 C       0.859046    -1.411439     0.022748      56.01
 H       1.202053    -2.447630     0.014579      23.27
 C      -0.993696     0.092460     0.341495      22.49
 C      -2.537642     0.420823     0.557220      90.47
 H      -2.993156    -0.372040     1.212323      23.69
 O      -2.651132     1.707128     1.295499     342.02
 H      -2.509961     1.482563     2.177763      31.00
 C      -3.418735     0.483539    -0.712482      82.53
 H      -2.921242     1.232147    -1.471785      24.79
 O      -3.150548    -0.927361    -1.421651     188.65
 H      -3.018183    -0.582623    -2.354394      24.71
 C      -4.851437     0.857971    -0.637657     125.98
 O      -5.042534     2.277919    -0.752692     260.16
 H      -5.141191     2.701880     0.168966      25.79
 H      -5.364151     0.483357     0.197051      30.57
 H      -5.386360     0.396926    -1.414864      29.81
55
name = lig-etoh-Waterframe_250
 C       5.558264    -1.796119     1.776176      55.62
 H       5.649529    -0.722243     1.531765      21.68
 C       4.848134    -4.011770     1.220004      50.53
 H       4.540946    -4.644598     0.446489      21.39
 C       5.097764    -4.506577     2.550095      35.50
 O       4.765360    -5.764497     2.968463     260.13
 C       4.540310    -6.773682     2.074366     125.50
 H       5.474147    -6.967616     1.479676      23.13
 H       3.623150    -6.615176     1.473989      25.10
 H       4.478776    -7.728911     2.665125      21.60
 C       5.571520    -3.565924     3.552907      14.77
 O       5.812622    -3.886513     4.839924      93.00
 H       5.722926    -4.915978     4.922675      26.31
 C       5.772741    -2.182644     3.112510      42.35
 H       5.963592    -1.302055     3.736758      26.39
 C       5.164457    -2.686859     0.806071      40.57
 C       5.024222    -2.292641    -0.640871      79.93
 H       5.444512    -3.242355    -1.299428      20.92
 O       5.994350    -1.267747    -0.996889     171.63
 H       5.694743    -0.289235    -0.689349      21.48
 C       3.495070    -1.878348    -1.012979      71.08
 H       2.913879    -2.586771    -0.437397      24.23
 C       3.281419    -1.776567    -2.537708      94.14
 O       3.428550    -3.157045    -3.045376     278.02
 H       4.237241    -3.160577    -3.584362      26.39
 H       4.071424    -1.120684    -3.034052      24.50
 H       2.206002    -1.515637    -2.761166      26.52
 C      -0.531527    -1.195781     0.282549      54.54
 H      -1.252141    -1.990685     0.554523      24.58
 C      -0.132613     1.197308     0.214375      67.60
 H      -0.412659     2.138152     0.428231      22.23
 C       1.235800     0.916350     0.024300      11.44
 O       2.177304     1.941119    -0.134769     161.36
 C       1.762778     3.344678    -0.197316     111.48
 H       2.655790     3.848406    -0.472708      26.41
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 H       1.156028     3.706122    -1.224129      23.86
 H       1.510802     3.551198     0.842943      24.96
 C       1.747469    -0.392451    -0.113462       9.04
 O       3.229819    -0.566959    -0.301427     107.32
 C       0.863154    -1.456118     0.083578      59.60
 H       1.110311    -2.433522    -0.044539      24.32
 C      -1.012376     0.092047     0.380059      28.10
 C      -2.488900     0.438021     0.562484      90.32
 H      -2.925694    -0.402642     1.185521      25.08
 O      -2.687376     1.660423     1.286480     347.32
 H      -2.464426     1.438019     2.152568      30.83
 C      -3.353702     0.474071    -0.717792      73.23
 H      -2.776372     1.302936    -1.485034      24.51
 O      -3.187144    -0.835794    -1.319341     206.62
 H      -3.026181    -0.687691    -2.295915      26.07
 C      -4.942855     0.826012    -0.642208      95.88
 O      -5.037988     2.292864    -0.671046     214.41
 H      -5.191336     2.632973     0.260442      26.35
 H      -5.291931     0.557153     0.445754      27.22
 H      -5.402701     0.420299    -1.559916      28.25
55
name = lig-etoh-Waterframe_251
 C       5.599170    -1.778572     1.775569      55.50
 H       5.888446    -0.733768     1.507264      21.76
 C       4.878889    -4.033797     1.234092      41.99
 H       4.436444    -4.734820     0.558178      17.86
 C       5.126590    -4.496763     2.511137      53.28
 O       4.795012    -5.734832     3.033837     230.50
 C       4.597969    -6.855865     2.070760     110.81
 H       5.463488    -6.879456     1.382393      28.37
 H       3.711949    -6.613790     1.440034      28.28
 H       4.397432    -7.660964     2.713776      24.78
 C       5.613502    -3.525141     3.500219      -6.58
 O       5.738397    -3.902920     4.882785    -151.24
 H       5.916461    -4.996128     5.094259      25.65
 C       5.787958    -2.191382     3.110054      61.75
 H       6.068273    -1.517634     3.872141      21.92
 C       5.157121    -2.721081     0.799651      43.03
 C       5.106173    -2.287103    -0.656255      81.74
 H       5.263361    -3.178054    -1.420814      21.52
 O       6.016610    -1.246019    -0.979481     179.54
 H       5.706117    -0.272887    -0.653394      20.17
 C       3.566991    -1.828248    -0.970932      73.45
 H       3.053147    -2.701384    -0.577125      23.32
 C       3.248522    -1.740649    -2.536296     103.61
 O       3.374018    -3.133108    -3.020817     260.48
 H       4.217608    -3.234447    -3.668858      22.88
 H       3.957728    -1.056743    -2.939237      26.60
 H       2.348789    -1.312170    -2.825653      27.73
 C      -0.536519    -1.157663     0.316486      47.73
 H      -1.163247    -2.066231     0.533439      22.99
 C      -0.129514     1.205432     0.237564      66.63
 H      -0.354963     2.243349     0.416235      20.17
 C       1.235541     0.911861    -0.007103       5.43
 O       2.200889     1.954856    -0.152767     196.93
 C       1.851244     3.327811    -0.204188     116.10
 H       2.705599     3.931391    -0.436189      25.44
 H       0.821308     3.521438    -0.867790      23.53
 H       1.458101     3.646878     0.801647      25.57
 C       1.769189    -0.444721    -0.112315       0.24
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 O       3.183557    -0.615762    -0.303783     142.38
 C       0.819221    -1.513914     0.109600      48.60
 H       1.138430    -2.463005    -0.019917      22.14
 C      -1.055768     0.165376     0.380240      36.72
 C      -2.500053     0.410411     0.617819      88.93
 H      -2.876205    -0.480493     1.144630      25.08
 O      -2.727141     1.637061     1.282059     343.70
 H      -2.564171     1.481697     2.236705      29.11
 C      -3.285778     0.483876    -0.751383      79.06
 H      -2.932744     1.376418    -1.429156      23.76
 O      -3.230970    -0.786615    -1.259502     233.70
 H      -3.167473    -0.720314    -2.255453      25.74
 C      -4.902803     0.863748    -0.590388      81.91
 O      -5.059701     2.294329    -0.614222     240.15
 H      -4.887653     2.716043     0.281602      25.89
 H      -5.484128     0.222826     0.309639      26.80
 H      -5.534826     0.407085    -1.459492      26.93
55
name = lig-etoh-Waterframe_252
 C       5.647960    -1.783904     1.775225      55.67
 H       6.024898    -0.795495     1.442721      23.10
 C       4.901937    -4.085745     1.187838      43.57
 H       4.421267    -4.834819     0.525710      14.70
 C       5.151783    -4.437509     2.557315      16.44
 O       4.824075    -5.718665     3.072438     259.58
 C       4.638358    -6.874779     2.069207     100.43
 H       5.514975    -7.099151     1.441107      29.79
 H       3.744445    -6.738096     1.424563      31.21
 H       4.486206    -7.761529     2.593997      26.38
 C       5.622544    -3.556910     3.502259     -21.83
 O       5.685202    -3.866753     4.877253       0.87
 H       5.811221    -4.895458     4.783912      25.34
 C       5.814991    -2.206484     3.144668      51.78
 H       6.221017    -1.668549     3.950210      21.46
 C       5.203005    -2.721855     0.828595      31.28
 C       5.065401    -2.220221    -0.672286      94.91
 H       5.246634    -3.025719    -1.321658      23.67
 O       6.070517    -1.234098    -0.980521     195.35
 H       5.676897    -0.311268    -0.684265      23.32
 C       3.632449    -1.849002    -0.980593      81.27
 H       2.975751    -2.689834    -0.753003      23.43
 C       3.280588    -1.724655    -2.492523     107.53
 O       3.319502    -3.097730    -3.002364     247.97
 H       4.123504    -3.102420    -3.754519      21.04
 H       4.015881    -1.200909    -3.021273      25.82
 H       2.285807    -1.377768    -2.572988      25.98
 C      -0.542950    -1.168696     0.367800      28.22
 H      -1.303499    -1.982692     0.476454      19.96
 C      -0.064765     1.223967     0.263092      66.48
 H      -0.575973     2.282915     0.196511      20.45
 C       1.298501     0.937345    -0.049293       9.75
 O       2.256077     1.907406    -0.187688     197.05
 C       1.828721     3.315656    -0.170983     120.46
 H       2.719286     3.838563    -0.493995      26.47
 H       1.015957     3.377157    -0.824755      27.21
 H       1.474734     3.715600     0.803010      27.19
 C       1.756748    -0.470393    -0.090808      25.05
 O       3.098751    -0.649575    -0.299908     136.72
 C       0.811860    -1.483015     0.084672      65.28
 H       1.059980    -2.530277     0.111438      22.70
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 C      -1.028012     0.178729     0.375970      39.47
 C      -2.563958     0.386599     0.627289      84.53
 H      -2.999376    -0.424732     1.188322      24.69
 O      -2.785470     1.654975     1.304781     330.91
 H      -2.673706     1.447783     2.328373      26.43
 C      -3.355452     0.563761    -0.684341      99.05
 H      -2.808142     1.181544    -1.317676      26.05
 O      -3.258704    -0.835346    -1.294780     198.43
 H      -3.249902    -0.621252    -2.276556      25.57
 C      -4.801647     0.890988    -0.546084     103.64
 O      -5.094607     2.284286    -0.566127     257.53
 H      -4.700377     2.712298     0.216535      29.01
 H      -5.345331     0.478025     0.374585      28.03
 H      -5.254178     0.608257    -1.561429      26.05
55
name = lig-etoh-Waterframe_253
 C       5.722252    -1.829534     1.829476      49.89
 H       5.982873    -0.823129     1.508283      23.10
 C       4.952456    -4.073085     1.192381      36.79
 H       4.595918    -4.791076     0.382924      16.39
 C       5.114382    -4.491385     2.533660      47.43
 O       4.845972    -5.752504     3.041750     200.85
 C       4.682643    -6.857569     2.103800     112.03
 H       5.643190    -6.956094     1.578337      28.52
 H       3.817134    -6.655880     1.438269      29.53
 H       4.551469    -7.713511     2.775398      24.65
 C       5.595550    -3.514150     3.555661      10.00
 O       5.653475    -3.840455     4.825518     -54.01
 H       5.684019    -4.756897     5.151149      14.94
 C       5.878275    -2.211355     3.152528      69.24
 H       6.285950    -1.438836     3.812022      24.37
 C       5.246731    -2.725735     0.810825      45.76
 C       5.042029    -2.190309    -0.610820     100.19
 H       5.301783    -2.971150    -1.207114      24.30
 O       6.094227    -1.221044    -0.985107     191.80
 H       5.937628    -0.248290    -0.783797      24.95
 C       3.584020    -1.875103    -1.020125      79.52
 H       3.066367    -2.751604    -0.555578      21.24
 C       3.340060    -1.728521    -2.457078     100.13
 O       3.269207    -3.072537    -3.006253     247.97
 H       4.162512    -3.231359    -3.593547      22.49
 H       3.956137    -1.053618    -3.096425      23.22
 H       2.259181    -1.341457    -2.459945      24.30
 C      -0.573549    -1.162061     0.391829      29.79
 H      -1.306924    -1.963774     0.526158      19.10
 C      -0.036872     1.217077     0.241959      74.65
 H      -0.410099     2.358770     0.093937      18.59
 C       1.321105     0.921138    -0.047120       9.26
 O       2.337167     1.870354    -0.218753     208.82
 C       1.789804     3.263844    -0.171754     113.67
 H       2.641384     3.885050    -0.551905      25.28
 H       1.156985     3.492572    -0.915643      28.48
 H       1.552948     3.360081     0.891346      25.63
 C       1.703205    -0.423681    -0.084493      22.32
 O       3.082230    -0.668185    -0.288914     132.95
 C       0.770802    -1.453600     0.076309      61.24
 H       1.140859    -2.550462     0.114276      20.84
 C      -0.989609     0.129237     0.408795      48.12
 C      -2.574171     0.432325     0.626849      81.09
 H      -2.948229    -0.396157     1.230587      24.40
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 O      -2.856228     1.686846     1.345210     299.59
 H      -2.634919     1.396850     2.387782      24.07
 C      -3.332787     0.525375    -0.628639     101.25
 H      -2.848301     1.180775    -1.230178      26.54
 O      -3.297867    -0.860891    -1.362660     190.85
 H      -3.155963    -0.601597    -2.326499      23.69
 C      -4.778629     0.948866    -0.547350     118.90
 O      -5.110022     2.316369    -0.540114     278.30
 H      -4.837782     2.735602     0.300308      28.93
 H      -5.104206     0.462598     0.278500      31.49
 H      -5.195711     0.442327    -1.416745      28.50
55
name = lig-etoh-Waterframe_254
 C       5.779980    -1.866246     1.807225      55.46
 H       5.932440    -0.825420     1.633328      22.41
 C       5.015480    -4.037708     1.194610      63.36
 H       4.797069    -4.787222     0.370055      18.92
 C       5.094615    -4.495033     2.527154      23.41
 O       4.858369    -5.766100     3.018610     273.97
 C       4.749499    -6.829524     2.150308     114.51
 H       5.654932    -6.939605     1.514662      26.01
 H       3.939152    -6.722636     1.395018      28.93
 H       4.480093    -7.738818     2.808982      21.67
 C       5.517618    -3.533846     3.492651      11.38
 O       5.637338    -3.813201     4.893325     238.67
 H       5.733930    -4.794732     4.956164      22.15
 C       5.961326    -2.202621     3.158245      36.57
 H       6.249354    -1.399588     3.923321      24.23
 C       5.290928    -2.696869     0.853844      46.02
 C       5.093539    -2.179720    -0.553591      89.89
 H       5.277928    -3.072603    -1.280020      22.10
 O       6.094397    -1.216843    -0.987523     216.98
 H       5.764980    -0.340904    -0.676624      25.48
 C       3.550991    -1.868604    -0.919219      72.01
 H       2.987983    -2.821692    -0.647037      21.17
 C       3.298215    -1.740959    -2.478523      89.06
 O       3.251889    -3.080588    -3.025715     270.97
 H       4.111748    -3.203944    -3.525637      24.40
 H       4.107197    -0.978926    -2.879859      22.42
 H       2.264113    -1.228201    -2.746635      24.26
 C      -0.596373    -1.208643     0.395161      59.05
 H      -1.229666    -2.043283     0.630757      20.31
 C      -0.045740     1.177672     0.183666      66.45
 H      -0.366028     2.293820     0.245401      14.18
 C       1.320253     0.926801    -0.018078      16.95
 O       2.370617     1.850694    -0.273645     227.07
 C       1.841923     3.184222    -0.197158     113.20
 H       2.703179     3.923618    -0.129893      22.94
 H       0.825967     3.429486    -0.828238      23.80
 H       1.345433     3.413407     0.790865      26.32
 C       1.708017    -0.438845    -0.112974      24.97
 O       3.094733    -0.671353    -0.277122     169.67
 C       0.738065    -1.447927     0.091450      48.18
 H       1.184871    -2.548183    -0.050226      18.86
 C      -1.020848     0.215252     0.465661      51.17
 C      -2.482860     0.471834     0.694066      73.99
 H      -2.850044    -0.426045     1.266893      21.73
 O      -2.908005     1.697704     1.381118     293.55
 H      -2.599164     1.505156     2.432238      22.72
 C      -3.247234     0.449948    -0.723311      68.60
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 H      -2.806424     1.276292    -1.357906      23.30
 O      -3.325999    -0.823996    -1.405187     257.88
 H      -3.071995    -0.606922    -2.348579      25.18
 C      -4.823338     0.926963    -0.536493     102.74
 O      -5.105989     2.378406    -0.537588     259.57
 H      -5.039451     2.765775     0.359686      27.94
 H      -5.284238     0.515047     0.334185      30.12
 H      -5.455247     0.544998    -1.301735      29.38
55
name = lig-etoh-Waterframe_255
 C       5.853483    -1.768447     1.842524      59.45
 H       6.033682    -0.771356     1.485513      22.08
 C       5.072108    -4.051011     1.180167      57.38
 H       4.835900    -4.783749     0.385488      17.72
 C       5.103965    -4.444239     2.533979      21.14
 O       4.869162    -5.717398     3.047472     228.71
 C       4.787579    -6.867262     2.102086     114.27
 H       5.747569    -7.137059     1.625808      27.54
 H       3.946474    -6.714145     1.428075      30.11
 H       4.611239    -7.842051     2.722677      23.45
 C       5.499846    -3.502065     3.539535      23.37
 O       5.618152    -3.819971     4.922596     188.01
 H       5.816262    -4.776587     4.973205      20.86
 C       5.972791    -2.275019     3.144691      51.04
 H       6.269146    -1.674886     4.081463      23.83
 C       5.330125    -2.695151     0.866985      27.83
 C       5.113695    -2.218932    -0.571733      78.87
 H       5.289570    -3.203147    -1.308755      20.92
 O       6.045812    -1.204428    -0.968508     212.05
 H       5.769392    -0.338481    -0.647170      25.95
 C       3.544671    -1.871254    -0.861613      72.79
 H       2.914309    -2.708135    -0.474782      22.08
 C       3.260753    -1.728314    -2.460036      91.31
 O       3.273110    -3.095817    -3.044027     272.60
 H       3.999807    -3.098262    -3.650085      27.18
 H       4.231904    -1.352530    -2.895319      22.17
 H       2.271372    -1.223555    -2.726013      23.91
 C      -0.621391    -1.158115     0.410525      65.57
 H      -1.274170    -1.964297     0.665964      21.82
 C      -0.063346     1.209796     0.159641      83.30
 H      -0.467448     2.183939     0.305960      16.14
 C       1.355753     0.885235    -0.031088       6.31
 O       2.330116     1.824127    -0.319804     189.92
 C       1.864483     3.179852    -0.145275      85.48
 H       2.743708     3.892672    -0.317750      22.96
 H       1.179544     3.329828    -1.256030      22.28
 H       1.318372     3.264079     0.805865      24.22
 C       1.726949    -0.466331    -0.131983      28.72
 O       3.101640    -0.661151    -0.246605     165.00
 C       0.761189    -1.469767     0.067004      55.92
 H       0.931374    -2.610484    -0.059692      19.27
 C      -1.001424     0.186477     0.511875      33.89
 C      -2.461387     0.479310     0.715522      68.64
 H      -2.889436    -0.403878     1.278308      21.00
 O      -2.920536     1.691658     1.392371     310.06
 H      -2.672535     1.515304     2.434975      23.31
 C      -3.293303     0.475944    -0.784895      50.49
 H      -2.638234     1.198416    -1.529864      21.66
 O      -3.304305    -0.782862    -1.433197     234.94
 H      -3.171765    -0.642577    -2.406613      25.41
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 C      -4.866164     0.917225    -0.512633      87.92
 O      -5.080892     2.415938    -0.555383     221.99
 H      -4.948042     2.822665     0.349257      25.85
 H      -5.287926     0.619886     0.539412      27.35
 H      -5.406108     0.623739    -1.407641      27.92
55
name = lig-etoh-Waterframe_256
 C       5.876830    -1.728306     1.842693      57.53
 H       6.303509    -0.732114     1.621641      20.69
 C       5.120287    -4.051888     1.194558      56.55
 H       4.803097    -4.736539     0.438846      17.92
 C       5.127613    -4.430417     2.567916      19.32
 O       4.879370    -5.702341     3.055605     203.98
 C       4.818497    -6.904024     2.071634      96.71
 H       5.798013    -6.931093     1.585914      27.63
 H       4.061047    -6.728851     1.311867      30.69
 H       4.529616    -7.674934     2.827616      24.40
 C       5.512625    -3.524433     3.616137      18.24
 O       5.599666    -3.848692     4.913121      87.79
 H       5.747222    -4.758274     5.171617      19.69
 C       5.967575    -2.258670     3.175830      28.33
 H       6.504508    -1.640838     3.944134      24.76
 C       5.395909    -2.664323     0.863281      12.13
 C       5.063560    -2.266006    -0.584302      68.92
 H       5.387567    -3.106883    -1.325389      21.38
 O       5.989930    -1.189681    -0.959640     188.35
 H       5.755536    -0.314594    -0.680014      27.11
 C       3.550485    -1.904464    -0.893230      77.38
 H       3.039921    -2.692266    -0.370002      23.77
 C       3.307254    -1.788763    -2.397031     110.52
 O       3.280947    -3.113380    -3.037728     265.78
 H       4.069432    -3.122585    -3.686194      24.15
 H       3.973931    -1.069161    -2.882697      26.36
 H       2.421302    -1.224106    -2.533085      26.87
 C      -0.555046    -1.130006     0.422423      46.99
 H      -1.332125    -1.868115     0.581199      20.72
 C      -0.041747     1.227225     0.193414      70.34
 H      -0.322569     2.185503     0.124159      22.13
 C       1.284847     0.878519    -0.078761       5.46
 O       2.294235     1.783824    -0.335793     207.02
 C       1.893968     3.186739    -0.192198     117.22
 H       2.840798     3.750113    -0.202743      25.31
 H       1.217638     3.645955    -1.023811      25.88
 H       1.365813     3.415131     0.720829      27.42
 C       1.730252    -0.511436    -0.118670       7.68
 O       3.135411    -0.640600    -0.209907     107.25
 C       0.714280    -1.507112     0.036899      60.07
 H       0.978897    -2.556736    -0.037186      24.56
 C      -0.967128     0.187496     0.514242      38.73
 C      -2.559393     0.457820     0.644022      73.68
 H      -2.962356    -0.406892     1.201517      24.22
 O      -2.892728     1.678301     1.381937     310.96
 H      -2.737575     1.415811     2.366163      25.92
 C      -3.366801     0.567074    -0.729355      72.56
 H      -2.903912     1.423616    -1.428011      23.94
 O      -3.265596    -0.786045    -1.451015     209.83
 H      -3.278409    -0.522883    -2.406234      25.16
 C      -4.837183     1.019173    -0.523083      99.62
 O      -5.041106     2.412885    -0.583267     263.72
 H      -4.817979     2.836706     0.308515      26.40
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 H      -5.151308     0.394310     0.453517      27.73
 H      -5.425485     0.414723    -1.291612      27.96
55
name = lig-etoh-Waterframe_257
 C       5.882635    -1.800157     1.864174      51.68
 H       6.349406    -0.801932     1.671596      26.56
 C       5.156129    -3.984035     1.259284      60.61
 H       4.804231    -4.654351     0.532878      17.65
 C       5.162131    -4.460206     2.596587      22.04
 O       4.871669    -5.738267     3.021738     250.31
 C       4.844485    -6.829749     2.095978     112.34
 H       5.837797    -7.016577     1.649000      27.83
 H       4.099892    -6.763942     1.284645      31.90
 H       4.622002    -7.734686     2.629739      25.22
 C       5.555866    -3.529334     3.587435      -8.07
 O       5.588628    -3.878165     4.966111      30.74
 H       5.646021    -4.850853     4.920368      26.68
 C       5.981929    -2.180301     3.218399      47.93
 H       6.543405    -1.536339     3.856177      22.93
 C       5.430588    -2.660237     0.851807      38.03
 C       5.069439    -2.234060    -0.570855      90.84
 H       5.233943    -3.039176    -1.179986      25.19
 O       5.949783    -1.181199    -0.983128     229.18
 H       5.575619    -0.377501    -0.635308      28.47
 C       3.605916    -1.958493    -0.871576      82.63
 H       2.983552    -2.794960    -0.592436      24.28
 C       3.319100    -1.813131    -2.356416     111.45
 O       3.296630    -3.112830    -3.018839     246.57
 H       4.246957    -3.234829    -3.519205      21.87
 H       3.994573    -1.104269    -2.756432      26.15
 H       2.295397    -1.593466    -2.402934      27.34
 C      -0.554154    -1.144665     0.431296      31.96
 H      -1.286318    -1.979650     0.493780      20.49
 C      -0.051137     1.236825     0.237662      69.48
 H      -0.297866     2.222610     0.020504      23.10
 C       1.249049     0.824766    -0.129109      14.62
 O       2.245889     1.787196    -0.351037     186.43
 C       1.945066     3.229163    -0.242842     129.33
 H       2.886669     3.662521    -0.128579      27.82
 H       1.350547     3.569706    -0.897324      30.60
 H       1.471861     3.403800     0.716881      27.86
 C       1.700704    -0.499610    -0.089486      22.40
 O       3.157447    -0.665284    -0.205095      91.47
 C       0.769908    -1.541134     0.015457      59.21
 H       1.024371    -2.525567    -0.081559      24.33
 C      -1.034918     0.253476     0.470229      20.40
 C      -2.610180     0.445122     0.563157      91.75
 H      -3.009490    -0.438910     1.030561      25.00
 O      -2.849525     1.649729     1.363132     340.90
 H      -2.705713     1.391738     2.286382      28.62
 C      -3.378733     0.628675    -0.690415      95.43
 H      -2.947733     1.421135    -1.244467      27.08
 O      -3.239018    -0.731716    -1.434728     209.84
 H      -3.223218    -0.483168    -2.394193      25.39
 C      -4.802798     1.005384    -0.523315     108.48
 O      -5.000694     2.421118    -0.606938     243.94
 H      -4.923031     2.790970     0.339498      26.91
 H      -5.274018     0.845539     0.503495      28.41
 H      -5.508942     0.643059    -1.358180      27.79
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name = lig-etoh-Waterframe_258
 C       5.924505    -1.822816     1.893669      61.70
 H       6.139609    -0.819121     1.477453      24.52
 C       5.140270    -3.976535     1.295835      52.35
 H       4.821881    -4.661384     0.533840      17.59
 C       5.226036    -4.445004     2.601459      39.83
 O       4.850303    -5.759093     3.012107     228.83
 C       4.882131    -6.802426     2.077445     106.71
 H       5.899146    -6.966220     1.656663      27.00
 H       4.105115    -6.575732     1.293493      28.28
 H       4.633344    -7.666251     2.612309      23.68
 C       5.629567    -3.471334     3.629212      -6.34
 O       5.585592    -3.907134     4.966560     -40.26
 H       5.697462    -4.909004     5.038819      22.65
 C       5.984202    -2.189148     3.248343      78.93
 H       6.277913    -1.554639     4.027444      24.09
 C       5.428534    -2.677921     0.892941      43.74
 C       5.124469    -2.229010    -0.529204      98.08
 H       5.295040    -3.081263    -1.139664      24.61
 O       5.915572    -1.167420    -1.026145     241.78
 H       5.717107    -0.258528    -0.670931      25.01
 C       3.612707    -1.980071    -0.809459      80.53
 H       3.044070    -2.859835    -0.429680      21.87
 C       3.273288    -1.832729    -2.339020      94.12
 O       3.354742    -3.135225    -2.986390     243.75
 H       4.265259    -3.171143    -3.624598      21.99
 H       3.920241    -1.172525    -2.904709      22.55
 H       2.193653    -1.497589    -2.433834      23.94
 C      -0.592771    -1.135793     0.382300      26.25
 H      -1.287658    -1.999764     0.548861      18.73
 C      -0.107946     1.228320     0.223260      68.58
 H      -0.453855     2.320949     0.183855      19.39
 C       1.254702     0.864355    -0.123704       7.05
 O       2.215681     1.804191    -0.389348     206.92
 C       2.000564     3.221292    -0.223519     107.37
 H       2.917103     3.728813    -0.415965      25.01
 H       1.428640     3.590075    -1.167979      24.97
 H       1.481628     3.374321     0.747915      25.32
 C       1.762959    -0.507262    -0.096314      15.74
 O       3.128540    -0.734701    -0.217303     145.92
 C       0.781796    -1.524919     0.044925      60.36
 H       1.002603    -2.504574    -0.088091      22.14
 C      -1.099835     0.170465     0.391221      42.83
 C      -2.556173     0.452668     0.592293      89.27
 H      -2.983994    -0.444403     1.045628      24.56
 O      -2.817438     1.614949     1.356169     367.49
 H      -2.614444     1.394677     2.229709      30.80
 C      -3.324460     0.609786    -0.766556      96.97
 H      -2.860483     1.308120    -1.330402      27.71
 O      -3.229001    -0.622712    -1.405395     274.58
 H      -3.072719    -0.475463    -2.366985      25.54
 C      -4.886753     1.008609    -0.487754      94.60
 O      -4.954111     2.498532    -0.621192     235.82
 H      -5.028730     2.844355     0.336963      27.42
 H      -5.237561     0.598433     0.437475      30.16
 H      -5.382026     0.529641    -1.365732      28.76
55
name = lig-etoh-Waterframe_259
 C       5.949206    -1.770703     1.886417      54.16
 H       6.090470    -0.698636     1.711316      22.05
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 C       5.098281    -4.053507     1.282105      45.44
 H       4.778771    -4.774899     0.494732      16.57
 C       5.286709    -4.423089     2.641340      11.94
 O       4.855238    -5.684892     3.056097     263.22
 C       4.906160    -6.813655     2.009010      91.46
 H       5.911133    -6.829869     1.549006      25.78
 H       4.208038    -6.626598     1.140969      26.81
 H       4.555536    -7.632448     2.594326      22.39
 C       5.664611    -3.554134     3.678260       8.18
 O       5.595183    -3.896004     4.956010      26.15
 H       5.922491    -4.879923     5.141962      21.53
 C       5.997739    -2.195397     3.301321      26.57
 H       6.043691    -1.454962     4.085779      24.35
 C       5.435482    -2.675382     0.972707      37.74
 C       5.143209    -2.236307    -0.488876      84.90
 H       5.524072    -3.103953    -1.229079      22.15
 O       5.927298    -1.154793    -1.071048     227.54
 H       5.721820    -0.237375    -0.630987      24.02
 C       3.571785    -1.999381    -0.796489      76.74
 H       3.125999    -2.838686    -0.197373      19.62
 C       3.229772    -1.884359    -2.331452      87.34
 O       3.420744    -3.181047    -2.962351     260.73
 H       4.213093    -3.031798    -3.631036      23.27
 H       3.893030    -1.069946    -2.787499      22.17
 H       2.185262    -1.352199    -2.463591      23.36
 C      -0.604200    -1.195482     0.284006      37.31
 H      -1.319781    -1.981809     0.576380      21.13
 C      -0.148630     1.155223     0.152841      68.52
 H      -0.523153     2.275445     0.401522      16.55
 C       1.228377     0.928770    -0.063388       7.18
 O       2.246365     1.814919    -0.437211     210.93
 C       2.023898     3.200367    -0.256181     105.90
 H       3.033274     3.673083    -0.317958      22.57
 H       1.116683     3.694254    -1.126412      22.60
 H       1.582444     3.612898     0.708572      25.48
 C       1.745241    -0.509823    -0.112999       8.30
 O       3.113560    -0.775159    -0.212357     156.38
 C       0.737434    -1.453803     0.091318      61.67
 H       0.988307    -2.501922     0.037503      20.35
 C      -1.045405     0.109829     0.320729      33.72
 C      -2.519647     0.435130     0.610555      77.18
 H      -2.985566    -0.439180     1.158049      21.37
 O      -2.785791     1.608118     1.386678     367.12
 H      -2.559156     1.432192     2.243383      32.02
 C      -3.311269     0.641933    -0.768917      80.84
 H      -2.879635     1.470525    -1.403697      24.87
 O      -3.224768    -0.599074    -1.430629     267.42
 H      -3.034310    -0.419942    -2.383586      25.40
 C      -4.867679     1.041394    -0.519260     101.20
 O      -4.938009     2.548442    -0.596039     211.08
 H      -4.948143     2.863674     0.374492      28.00
 H      -5.207989     0.587010     0.345473      30.99
 H      -5.508233     0.630230    -1.277610      29.76
55
name = lig-etoh-Waterframe_260
 C       5.930557    -1.743984     2.013498      55.71
 H       6.120057    -0.701305     1.783148      24.78
 C       5.124329    -4.029113     1.306898      22.27
 H       4.695375    -4.755414     0.539736      12.73
 C       5.283548    -4.474897     2.616734      52.60
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 O       4.872689    -5.664770     3.070689     208.78
 C       4.908008    -6.755041     1.976921     103.66
 H       5.953325    -6.927910     1.677871      28.28
 H       4.177158    -6.619936     1.165045      29.39
 H       4.703510    -7.753701     2.465955      23.98
 C       5.717718    -3.539644     3.635305       0.03
 O       5.625163    -3.882433     5.024839    -160.99
 H       5.890600    -4.920641     5.109061      20.51
 C       5.985512    -2.213288     3.306579      60.82
 H       6.115614    -1.424911     4.102774      23.35
 C       5.432461    -2.686591     0.957622      53.00
 C       5.141647    -2.218669    -0.506677      80.66
 H       5.372754    -3.250211    -1.152377      21.57
 O       5.954038    -1.158409    -1.067717     217.17
 H       5.597476    -0.265081    -0.614339      23.62
 C       3.548399    -2.054842    -0.794719      65.56
 H       2.943147    -2.919219    -0.418256      20.12
 C       3.224975    -1.922186    -2.286901      92.07
 O       3.466032    -3.210580    -2.959955     255.84
 H       4.286672    -3.228606    -3.480546      25.95
 H       4.031244    -1.185689    -2.604398      21.93
 H       2.112047    -1.827538    -2.481015      24.04
 C      -0.649216    -1.267052     0.208801      45.99
 H      -1.278502    -2.131316     0.404150      23.92
 C      -0.109725     1.142732     0.097576      60.91
 H      -0.572732     2.229922     0.253264      16.70
 C       1.280091     0.877771    -0.054353      17.97
 O       2.262645     1.809368    -0.453896     181.93
 C       2.002030     3.250288    -0.298899      98.41
 H       2.994734     3.777804    -0.457748      23.84
 H       1.186712     3.651971    -1.125770      24.03
 H       1.658676     3.265643     0.768580      24.99
 C       1.641271    -0.416609    -0.106088      17.93
 O       3.100605    -0.746717    -0.182310     110.46
 C       0.749354    -1.477843     0.101515      48.05
 H       1.155262    -2.554460     0.233416      18.51
 C      -1.045828     0.094351     0.289320      25.77
 C      -2.530269     0.421716     0.581311      80.50
 H      -2.977130    -0.512887     1.055120      22.20
 O      -2.735589     1.625443     1.434446     343.02
 H      -2.567804     1.376815     2.314291      30.12
 C      -3.352857     0.692955    -0.695376      69.89
 H      -2.771179     1.628949    -1.256173      23.29
 O      -3.221860    -0.636075    -1.503765     200.93
 H      -3.143734    -0.409475    -2.476593      23.78
 C      -4.780578     1.108009    -0.576838     114.54
 O      -4.943832     2.560071    -0.531195     198.44
 H      -4.695491     2.779613     0.434521      27.58
 H      -5.186052     0.918946     0.436909      28.57
 H      -5.433782     0.869874    -1.378592      29.33
55
name = lig-etoh-Waterframe_261
 C       5.841302    -1.785201     1.999240      66.06
 H       6.132018    -0.774833     1.751983      26.31
 C       5.175688    -3.944657     1.309819      50.23
 H       4.696467    -4.598898     0.513830      16.17
 C       5.286799    -4.445190     2.631231      19.33
 O       4.876556    -5.761379     3.034794     280.38
 C       4.923631    -6.714366     2.018481      80.73
 H       5.923990    -6.710402     1.547628      27.38
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 H       4.236463    -6.438391     1.226645      31.02
 H       4.583871    -7.678404     2.575096      23.93
 C       5.727906    -3.556312     3.656616     -30.99
 O       5.679339    -3.851260     5.043047     -92.86
 H       5.745654    -4.849429     5.191537      21.14
 C       5.979604    -2.205611     3.349401      47.18
 H       6.407027    -1.618670     4.242627      19.75
 C       5.458868    -2.609140     0.967905      39.87
 C       5.084917    -2.251318    -0.510928      79.44
 H       5.343609    -3.105882    -1.196282      21.78
 O       5.947564    -1.199318    -1.018854     227.46
 H       5.677024    -0.204735    -0.752468      23.38
 C       3.526820    -2.057195    -0.768679      68.39
 H       3.021305    -2.946279    -0.354372      22.16
 C       3.272407    -1.999460    -2.263750     109.61
 O       3.501049    -3.268995    -2.959892     270.21
 H       4.337526    -3.203430    -3.381443      26.62
 H       3.654350    -1.128851    -2.843640      25.30
 H       2.235136    -1.719498    -2.392942      26.03
 C      -0.642722    -1.298103     0.171259      53.92
 H      -1.353489    -2.098601     0.256016      23.99
 C      -0.088765     1.151712     0.083698      65.82
 H      -0.398705     2.194961    -0.077363      21.44
 C       1.296480     0.933053    -0.124750      -1.93
 O       2.282993     1.800801    -0.473027     213.07
 C       1.944405     3.230192    -0.310812     122.28
 H       2.907213     3.805609    -0.509253      25.73
 H       1.285205     3.566871    -0.903430      30.92
 H       1.564226     3.482215     0.694854      27.53
 C       1.688868    -0.497521    -0.080007       6.07
 O       3.050379    -0.713243    -0.150783     104.36
 C       0.739353    -1.536209     0.090938      57.74
 H       1.291877    -2.575651     0.273118      21.84
 C      -1.082530     0.078900     0.260364      25.49
 C      -2.554468     0.427595     0.571942      86.38
 H      -2.981883    -0.456137     1.076743      24.88
 O      -2.674406     1.614124     1.464464     302.37
 H      -2.587855     1.250288     2.386409      27.54
 C      -3.312439     0.667086    -0.714467      78.58
 H      -2.679049     1.481478    -1.315229      24.68
 O      -3.238830    -0.618730    -1.541600     208.08
 H      -3.212512    -0.342967    -2.512046      23.70
 C      -4.767975     1.205453    -0.570089      99.51
 O      -4.921299     2.610781    -0.455817     241.63
 H      -4.523635     2.894236     0.441177      27.27
 H      -5.291077     0.527929     0.318916      27.02
 H      -5.209227     0.733392    -1.483316      27.95
55
name = lig-etoh-Waterframe_262
 C       5.806137    -1.718819     2.003683      50.96
 H       6.069222    -0.687611     1.774115      23.74
 C       5.203574    -3.919791     1.326489      33.69
 H       4.864162    -4.588822     0.520471      13.77
 C       5.272456    -4.433707     2.665780      65.17
 O       4.900726    -5.753816     3.030001     279.09
 C       4.920588    -6.716569     1.996495     105.67
 H       5.892467    -6.837538     1.496069      29.06
 H       4.165257    -6.516229     1.234758      29.94
 H       4.625368    -7.746975     2.412686      23.43
 C       5.684511    -3.570688     3.736808      18.41
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 O       5.740399    -3.811082     5.029433    -131.22
 H       5.909039    -4.780551     5.137013      16.71
 C       5.994563    -2.234794     3.361885      42.15
 H       6.518857    -1.544983     4.099473      24.51
 C       5.423394    -2.596332     0.944799      44.57
 C       5.055396    -2.236522    -0.466746     108.45
 H       5.281577    -3.036184    -1.011622      23.90
 O       5.936528    -1.246679    -0.983638     248.60
 H       5.614379    -0.310489    -0.634207      23.34
 C       3.572830    -1.998210    -0.724671      81.94
 H       3.082099    -2.779109    -0.155451      20.87
 C       3.234862    -2.028051    -2.305206     102.09
 O       3.532864    -3.315199    -2.945344     271.88
 H       4.303010    -3.198071    -3.527667      26.06
 H       3.812110    -1.248514    -2.808529      23.08
 H       2.190581    -1.896592    -2.296283      24.64
 C      -0.632352    -1.243088     0.172579      39.16
 H      -1.376088    -2.013660     0.311423      20.48
 C      -0.100133     1.153022     0.049795      73.80
 H      -0.467010     2.084169    -0.082092      20.06
 C       1.253639     0.841295    -0.200796      -1.84
 O       2.295419     1.832123    -0.482498     193.61
 C       1.894295     3.193238    -0.300868     108.51
 H       2.894305     3.705910    -0.430918      24.32
 H       1.118009     3.471605    -1.065029      25.57
 H       1.509120     3.447543     0.667340      27.37
 C       1.708076    -0.548081    -0.049435      22.59
 O       3.058860    -0.749147    -0.145891     163.85
 C       0.769107    -1.567429     0.065496      63.89
 H       0.947584    -2.724067     0.102208      18.96
 C      -1.041972     0.070676     0.234692      34.84
 C      -2.527722     0.423687     0.593723      82.34
 H      -3.010164    -0.376240     1.114086      24.12
 O      -2.621905     1.575868     1.457235     296.53
 H      -2.495016     1.233830     2.460687      25.13
 C      -3.248291     0.648142    -0.803893      92.60
 H      -2.717124     1.349431    -1.379017      25.87
 O      -3.285649    -0.562290    -1.519385     265.17
 H      -3.132465    -0.363076    -2.503872      24.07
 C      -4.751274     1.185990    -0.572596      85.99
 O      -4.882558     2.665709    -0.383230     232.45
 H      -4.649152     2.943027     0.577559      26.21
 H      -5.427175     0.571812     0.195280      27.07
 H      -5.279819     1.146145    -1.624030      26.88
55
name = lig-etoh-Waterframe_263
 C       5.805722    -1.659550     2.050340      54.74
 H       5.971440    -0.588975     1.890842      22.06
 C       5.208543    -3.978372     1.366508      41.19
 H       5.047869    -4.718675     0.632693      15.55
 C       5.246299    -4.432492     2.686896      41.94
 O       4.938308    -5.692982     3.039902     204.19
 C       4.892933    -6.778714     1.908853     113.83
 H       5.908790    -6.873274     1.514893      28.45
 H       4.100021    -6.561495     1.168055      28.21
 H       4.728707    -7.688129     2.481922      23.36
 C       5.631594    -3.489270     3.693507      40.89
 O       5.814406    -3.822980     5.085365     197.56
 H       6.025585    -4.791409     5.182398      24.11
 C       6.017472    -2.213112     3.272366      55.52
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 H       6.355828    -1.535253     4.055364      22.64
 C       5.363181    -2.591305     1.024366      34.42
 C       5.075302    -2.224430    -0.419188     104.97
 H       5.169793    -3.171377    -0.965261      21.10
 O       5.938759    -1.251815    -0.972139     261.86
 H       5.742590    -0.326405    -0.575779      22.42
 C       3.582835    -1.975339    -0.714521      87.10
 H       3.051328    -2.819144    -0.268672      19.93
 C       3.199702    -2.052803    -2.296243      95.53
 O       3.555072    -3.343191    -2.927333     257.21
 H       4.328851    -3.273771    -3.575481      25.65
 H       3.821286    -1.275375    -2.708472      22.33
 H       2.120278    -1.967398    -2.517601      23.47
 C      -0.586545    -1.215920     0.200120      41.05
 H      -1.282605    -2.027860     0.430615      20.26
 C      -0.114662     1.126543    -0.017845      67.91
 H      -0.468602     2.075588     0.090188      17.92
 C       1.256450     0.758468    -0.245943       8.54
 O       2.253405     1.773933    -0.466409     190.71
 C       1.849384     3.173790    -0.297926      80.22
 H       2.689980     3.862352    -0.447908      23.77
 H       1.051650     3.526253    -1.322226      22.29
 H       1.390379     3.193581     0.655797      25.34
 C       1.698088    -0.560415    -0.069943      18.29
 O       3.135744    -0.767545    -0.152436     176.58
 C       0.718223    -1.606628     0.024651      73.86
 H       0.973468    -2.664354    -0.103948      17.53
 C      -1.018254     0.120648     0.252653      34.48
 C      -2.457382     0.406962     0.563577      77.83
 H      -2.907321    -0.487418     0.966219      23.45
 O      -2.586350     1.558434     1.423889     284.39
 H      -2.292014     1.204188     2.450771      22.47
 C      -3.262014     0.709858    -0.802726      92.10
 H      -2.748334     1.427810    -1.286591      27.11
 O      -3.338933    -0.559097    -1.490652     271.04
 H      -3.118958    -0.443224    -2.472513      24.70
 C      -4.727263     1.230653    -0.646446     101.84
 O      -4.825392     2.694412    -0.295550     243.21
 H      -4.920500     2.809185     0.711918      25.97
 H      -5.277213     0.765810     0.119069      29.28
 H      -5.301434     1.184677    -1.629945      28.28
55
name = lig-etoh-Waterframe_264
 C       5.768608    -1.649352     1.986972      61.17
 H       5.887359    -0.571671     1.808130      20.72
 C       5.209186    -3.985093     1.380135      56.09
 H       5.088176    -4.653026     0.586125      15.71
 C       5.232830    -4.398496     2.709547      11.65
 O       4.961476    -5.724015     3.014419     254.74
 C       4.890319    -6.790596     1.913317      99.48
 H       5.837345    -6.756855     1.365783      28.45
 H       4.102747    -6.575763     1.131228      29.82
 H       4.626540    -7.591694     2.521380      23.55
 C       5.628391    -3.453428     3.702398      22.17
 O       5.884099    -3.816843     5.090763     231.40
 H       5.923750    -4.852409     5.115233      23.03
 C       6.032269    -2.142855     3.317923      47.05
 H       6.280943    -1.557795     4.148923      22.42
 C       5.318106    -2.590580     1.123142      33.06
 C       5.075230    -2.255571    -0.385718      85.30
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 H       5.427929    -3.215624    -1.095876      19.61
 O       5.973060    -1.238243    -0.978007     222.52
 H       5.762129    -0.321801    -0.649078      22.94
 C       3.534862    -2.050000    -0.760704      75.76
 H       3.048160    -2.924373    -0.271059      18.53
 C       3.234730    -2.063969    -2.274507      92.86
 O       3.558882    -3.369443    -2.906358     244.70
 H       4.516915    -3.199020    -3.307988      22.97
 H       3.651430    -1.223701    -2.846092      22.40
 H       2.129829    -1.766177    -2.480863      22.74
 C      -0.600660    -1.244693     0.259088      37.78
 H      -1.351929    -2.037409     0.457101      17.18
 C      -0.073610     1.116041    -0.083897      66.27
 H      -0.269813     2.190655     0.074331      15.25
 C       1.271283     0.792206    -0.248309      15.74
 O       2.214977     1.688803    -0.460545     217.75
 C       1.778933     3.121706    -0.325645     101.92
 H       2.644340     3.716532    -0.262392      24.24
 H       0.851201     3.532687    -1.095690      23.24
 H       1.247056     3.375729     0.604678      26.54
 C       1.737420    -0.606258    -0.155169      17.42
 O       3.147997    -0.738460    -0.151149     158.98
 C       0.753658    -1.610291    -0.037979      65.64
 H       1.044122    -2.584263    -0.077009      21.04
 C      -1.007478     0.110991     0.266257      50.43
 C      -2.447347     0.419732     0.487237      75.53
 H      -2.837389    -0.533973     0.946452      23.18
 O      -2.563344     1.554041     1.386557     272.43
 H      -2.295958     1.181022     2.397804      21.38
 C      -3.289813     0.779707    -0.747526      85.05
 H      -2.629966     1.481095    -1.335768      25.22
 O      -3.383115    -0.579016    -1.464611     214.74
 H      -3.252070    -0.371364    -2.443635      24.04
 C      -4.715446     1.345458    -0.672762     120.59
 O      -4.761012     2.705373    -0.229302     265.74
 H      -4.972180     2.732483     0.759995      25.72
 H      -5.164206     0.703416    -0.030051      30.77
 H      -5.123952     1.022836    -1.596145      30.12
55
name = lig-etoh-Waterframe_265
 C       5.740700    -1.640930     2.042243      44.11
 H       5.862080    -0.655458     1.568556      20.97
 C       5.192644    -3.934405     1.394758      62.05
 H       4.951446    -4.589374     0.569384      14.08
 C       5.232083    -4.416183     2.710731      22.09
 O       4.984242    -5.777895     2.991456     279.35
 C       4.886295    -6.718829     1.959221     107.75
 H       5.830811    -6.936580     1.410483      30.35
 H       4.006023    -6.497169     1.296060      32.73
 H       4.709678    -7.694527     2.341327      26.07
 C       5.696111    -3.442222     3.781222      11.55
 O       5.928766    -3.799456     5.022136      57.08
 H       5.982540    -4.841150     5.154085      18.48
 C       5.982237    -2.076795     3.403560      60.33
 H       6.386671    -1.395132     4.103404      24.48
 C       5.280847    -2.600807     1.033089      43.25
 C       5.084657    -2.273065    -0.412455      81.36
 H       5.554898    -3.294551    -0.908528      20.78
 O       5.987113    -1.237011    -0.969172     204.13
 H       5.645309    -0.371450    -0.731412      27.05
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 C       3.582169    -2.118342    -0.785361      69.24
 H       2.936329    -2.846619    -0.241165      19.86
 C       3.254785    -2.041549    -2.289707      89.26
 O       3.553999    -3.349210    -2.875235     231.13
 H       4.543493    -3.397410    -3.271772      24.08
 H       3.931098    -1.296702    -2.791152      21.62
 H       2.112401    -2.044164    -2.269656      22.62
 C      -0.597707    -1.273933     0.294125      33.14
 H      -1.352458    -2.071637     0.454560      15.68
 C      -0.040868     1.097951    -0.093543      69.51
 H      -0.445029     2.214653    -0.203155      17.65
 C       1.271300     0.719069    -0.229099      16.16
 O       2.220797     1.725659    -0.463093     207.85
 C       1.707611     3.074338    -0.320271     117.57
 H       2.640285     3.543884    -0.452056      25.81
 H       1.199014     3.261819    -1.155626      28.21
 H       1.267577     3.204244     0.715126      25.05
 C       1.741824    -0.570715    -0.247385      23.06
 O       3.108343    -0.768990    -0.185619     136.02
 C       0.802956    -1.608080    -0.066113      73.17
 H       1.015420    -2.593054     0.045766      23.89
 C      -0.979710     0.052684     0.217576      47.15
 C      -2.484140     0.449397     0.480631      78.94
 H      -3.075166    -0.406551     0.972177      24.15
 O      -2.557231     1.572146     1.360436     284.64
 H      -2.390462     1.187406     2.290078      25.13
 C      -3.250383     0.770892    -0.770340      87.94
 H      -2.561552     1.432643    -1.529777      23.24
 O      -3.428362    -0.546829    -1.432895     237.11
 H      -3.386360    -0.375339    -2.418446      25.90
 C      -4.677058     1.379336    -0.629490     103.79
 O      -4.719909     2.734002    -0.201763     281.04
 H      -4.776981     2.836749     0.803806      27.28
 H      -5.375201     0.719118    -0.001513      28.02
 H      -5.091208     1.517617    -1.616144      28.24
55
name = lig-etoh-Waterframe_266
 C       5.679396    -1.687204     2.066388      58.72
 H       6.017936    -0.642765     1.901293      24.26
 C       5.128564    -3.925196     1.400834      50.60
 H       4.784568    -4.720818     0.686482      15.39
 C       5.281519    -4.397132     2.730042      -0.93
 O       5.033413    -5.765497     3.043434     279.65
 C       4.873112    -6.708290     1.953214      85.24
 H       5.818735    -6.693544     1.346343      28.09
 H       4.091506    -6.414808     1.226823      30.72
 H       4.661780    -7.669538     2.490189      24.13
 C       5.740947    -3.450485     3.699352     -25.44
 O       5.981848    -3.812694     5.036622      72.68
 H       6.192474    -4.844379     5.095345      22.50
 C       5.892263    -2.041499     3.404098      56.51
 H       6.419101    -1.350926     4.084150      22.91
 C       5.319329    -2.533380     1.043113      43.80
 C       5.126561    -2.288465    -0.469561      98.58
 H       5.282596    -3.184668    -1.036813      23.00
 O       5.949256    -1.249163    -0.953959     292.38
 H       5.647507    -0.382095    -0.732324      28.62
 C       3.636981    -2.096763    -0.779988      76.19
 H       3.125475    -3.000935    -0.359336      21.03
 C       3.302043    -2.082634    -2.277409      93.99
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 O       3.542856    -3.342998    -2.864818     246.05
 H       4.424768    -3.323509    -3.497347      22.87
 H       3.791214    -1.159364    -2.740470      23.13
 H       2.259372    -1.794316    -2.543989      24.28
 C      -0.514875    -1.316587     0.259425      48.60
 H      -1.182907    -2.133247     0.555011      19.12
 C      -0.108059     1.009542    -0.073247      66.07
 H      -0.544218     2.085623    -0.407200      18.78
 C       1.299602     0.765552    -0.255816       8.57
 O       2.249834     1.738144    -0.451607     237.62
 C       1.743261     3.035202    -0.339530     123.14
 H       2.513669     3.841741    -0.456494      25.72
 H       1.041904     3.287962    -1.052611      28.19
 H       1.119457     3.226645     0.630788      25.41
 C       1.724472    -0.623886    -0.283461      12.86
 O       3.104254    -0.837496    -0.260304     152.41
 C       0.755943    -1.618022    -0.029399      63.35
 H       1.147922    -2.643939     0.074363      23.02
 C      -1.031917     0.031816     0.175597      43.17
 C      -2.482032     0.458104     0.505914      75.93
 H      -3.044488    -0.402670     0.931463      23.99
 O      -2.559325     1.624714     1.358353     299.10
 H      -2.356743     1.307774     2.219813      29.35
 C      -3.234711     0.727873    -0.857524      89.43
 H      -2.651553     1.502258    -1.549197      23.20
 O      -3.471436    -0.507630    -1.420598     269.02
 H      -3.425965    -0.435393    -2.414673      25.75
 C      -4.634540     1.408802    -0.608238      86.48
 O      -4.681583     2.819297    -0.156520     271.51
 H      -4.499708     2.929953     0.826967      27.79
 H      -5.476775     0.748683    -0.012184      26.11
 H      -5.084273     1.534848    -1.642686      26.66
55
name = lig-etoh-Waterframe_267
 C       5.661934    -1.621608     2.074257      64.19
 H       5.939626    -0.568113     1.895673      22.89
 C       5.059298    -3.906482     1.428836      43.45
 H       4.700489    -4.580531     0.575822      17.02
 C       5.332403    -4.384908     2.701412      43.95
 O       5.092583    -5.685475     3.122285     267.07
 C       4.879806    -6.679184     1.930465      83.31
 H       5.840420    -6.711382     1.367681      26.76
 H       4.023761    -6.458694     1.306145      29.80
 H       4.646975    -7.672208     2.472430      23.75
 C       5.775852    -3.455297     3.694822      12.58
 O       6.049203    -3.838662     5.041612      -0.50
 H       6.184879    -4.867247     5.091731      29.36
 C       5.812598    -2.129983     3.371756      56.97
 H       6.182521    -1.437868     4.209618      21.51
 C       5.344834    -2.603190     1.050664      39.53
 C       5.129649    -2.271355    -0.476561     107.46
 H       5.410468    -3.050622    -1.042512      23.01
 O       5.925364    -1.234072    -0.971958     295.75
 H       5.631709    -0.391530    -0.594781      25.00
 C       3.616600    -2.085516    -0.805387      83.96
 H       3.236229    -2.981174    -0.315908      17.53
 C       3.334135    -2.044817    -2.297814      92.21
 O       3.551609    -3.365552    -2.912465     245.81
 H       4.305228    -3.184775    -3.642724      23.14
 H       4.050482    -1.356004    -2.821267      20.25
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 H       2.325014    -1.735725    -2.397740      23.99
 C      -0.591910    -1.336385     0.241841      49.28
 H      -1.142449    -2.170969     0.657446      25.25
 C      -0.107367     0.978137    -0.121429      58.72
 H      -0.513155     2.053481    -0.178563      16.12
 C       1.274395     0.742668    -0.297756       6.75
 O       2.297947     1.724562    -0.440088     185.24
 C       1.739329     3.107683    -0.365351      94.15
 H       2.608846     3.884619    -0.311304      22.11
 H       0.728956     3.309114    -1.044865      22.32
 H       1.328894     3.168369     0.695515      24.45
 C       1.715489    -0.620619    -0.268178      14.08
 O       3.112250    -0.888777    -0.322248     174.46
 C       0.822693    -1.654198     0.000093      48.75
 H       1.166124    -2.792262     0.063805      14.24
 C      -1.079050    -0.049546     0.190738      40.60
 C      -2.470767     0.447895     0.468167      83.04
 H      -2.909046    -0.368771     1.010076      22.71
 O      -2.555243     1.676163     1.360346     299.81
 H      -2.317539     1.371500     2.185287      29.61
 C      -3.266144     0.792604    -0.829551      93.59
 H      -2.629120     1.338273    -1.483838      24.03
 O      -3.504706    -0.527582    -1.469516     244.26
 H      -3.390976    -0.404677    -2.455053      24.29
 C      -4.630487     1.497385    -0.623068      89.13
 O      -4.629428     2.893252    -0.132037     282.04
 H      -4.386923     2.776518     0.837648      27.06
 H      -5.114911     0.756215     0.143738      26.14
 H      -5.128282     1.280490    -1.630757      25.87
55
name = lig-etoh-Waterframe_268
 C       5.655050    -1.612025     2.030280      55.91
 H       5.700862    -0.583947     1.688901      22.34
 C       5.020360    -3.902905     1.417019      48.93
 H       4.654136    -4.608272     0.609366      19.43
 C       5.361774    -4.394860     2.710374      42.72
 O       5.134825    -5.652758     3.123513     286.91
 C       4.898027    -6.622429     1.999664      97.77
 H       5.790994    -6.754664     1.373089      26.54
 H       4.047726    -6.313766     1.437998      30.02
 H       4.790746    -7.669578     2.449173      21.09
 C       5.787747    -3.534686     3.753983      15.24
 O       6.117713    -3.868995     5.003995     189.73
 H       6.063643    -4.851420     5.150935      31.66
 C       5.789539    -2.142799     3.372985      50.78
 H       5.821871    -1.440371     4.289553      22.13
 C       5.349414    -2.575643     1.035819      41.10
 C       5.116942    -2.268521    -0.430925      88.62
 H       5.566406    -3.177810    -0.955029      20.19
 O       5.923911    -1.161713    -0.999552     223.63
 H       5.640775    -0.255870    -0.609777      21.77
 C       3.614787    -2.161431    -0.847983      70.41
 H       2.954599    -2.886025    -0.404575      18.52
 C       3.388292    -2.029915    -2.366788      93.95
 O       3.541921    -3.376010    -2.988780     258.28
 H       4.402861    -3.422142    -3.586185      25.05
 H       4.152671    -1.366840    -2.744904      20.95
 H       2.364386    -1.750991    -2.494808      24.65
 C      -0.622963    -1.430506     0.255915      40.97
 H      -1.355822    -2.172279     0.578830      23.58
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 C      -0.097848     0.975425    -0.170873      61.75
 H      -0.396550     1.950033     0.057576      16.67
 C       1.270769     0.702605    -0.333455       2.67
 O       2.285284     1.717297    -0.450606     152.55
 C       1.721981     3.166569    -0.293758      87.90
 H       2.662419     3.684996    -0.682131      22.29
 H       1.094981     3.334113    -1.362600      22.34
 H       1.444235     3.268505     0.731969      24.27
 C       1.753100    -0.650299    -0.230287      20.86
 O       3.096474    -0.836245    -0.333195     165.74
 C       0.799351    -1.662555     0.027628      57.20
 H       1.153497    -2.813902     0.096718      16.25
 C      -1.028950    -0.042570     0.183229      29.06
 C      -2.501548     0.447615     0.470587      80.45
 H      -3.108201    -0.263060     0.987103      22.24
 O      -2.527849     1.694178     1.336956     286.75
 H      -2.336486     1.325543     2.197592      26.10
 C      -3.258888     0.836919    -0.803624      92.59
 H      -2.618289     1.350105    -1.390999      25.56
 O      -3.526781    -0.519573    -1.521154     224.63
 H      -3.377461    -0.340391    -2.490079      24.66
 C      -4.618704     1.533613    -0.597526     109.14
 O      -4.570498     2.913035    -0.155654     292.87
 H      -4.445149     2.852087     0.835512      27.68
 H      -5.105425     1.092364     0.213058      27.98
 H      -5.351859     1.618685    -1.437022      26.49
55
name = lig-etoh-Waterframe_269
 C       5.640249    -1.680744     2.036275      55.61
 H       5.626996    -0.616184     1.897847      21.99
 C       5.056106    -3.901785     1.413976      44.68
 H       4.685407    -4.656714     0.719885      16.28
 C       5.354435    -4.381795     2.699654      41.60
 O       5.168238    -5.712375     3.091185     281.86
 C       4.948347    -6.594416     2.096674     106.64
 H       5.759926    -6.523328     1.395387      30.02
 H       4.119189    -6.341049     1.396511      30.79
 H       4.691707    -7.534278     2.616474      23.65
 C       5.783570    -3.486429     3.704561       7.20
 O       6.182622    -3.917461     5.001461     231.60
 H       6.162421    -4.880684     5.138161      29.83
 C       5.781680    -2.101661     3.393036      53.31
 H       5.766584    -1.319546     4.180904      23.31
 C       5.302247    -2.542040     1.030084      54.08
 C       5.125952    -2.247619    -0.426462      75.64
 H       5.510194    -3.252678    -1.063841      20.29
 O       5.910880    -1.120718    -1.013269     174.29
 H       5.533749    -0.151145    -0.730651      19.46
 C       3.600279    -2.175564    -0.885987      59.76
 H       2.990194    -3.033281    -0.529204      19.85
 C       3.465274    -2.073066    -2.442164     103.57
 O       3.529156    -3.379040    -3.072312     277.06
 H       4.493311    -3.437680    -3.364477      25.10
 H       4.072205    -1.275673    -2.806516      24.05
 H       2.497012    -1.627598    -2.821897      24.94
 C      -0.605470    -1.419410     0.263976      57.96
 H      -1.325441    -2.235153     0.401520      18.39
 C      -0.083861     0.968317    -0.161224      60.86
 H      -0.362423     1.920774    -0.058768      22.29
 C       1.311445     0.695339    -0.345021       6.95
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 O       2.201252     1.711983    -0.456660     205.35
 C       1.823505     3.129201    -0.322462     115.00
 H       2.715359     3.748949    -0.464772      25.10
 H       0.822131     3.421735    -0.880525      24.46
 H       1.379274     3.561349     0.500827      28.11
 C       1.719222    -0.678504    -0.198960      11.59
 O       3.120003    -0.788967    -0.333365     129.60
 C       0.718993    -1.696909     0.060839      61.07
 H       1.133729    -2.756627     0.153860      23.61
 C      -1.018606    -0.053141     0.173831      24.76
 C      -2.515888     0.473853     0.498109      76.77
 H      -3.121653    -0.336130     0.941742      26.01
 O      -2.476278     1.673314     1.306011     274.05
 H      -2.328934     1.356636     2.257074      26.62
 C      -3.258165     0.804650    -0.861675      85.59
 H      -2.669265     1.568052    -1.452801      25.81
 O      -3.527225    -0.432233    -1.534799     255.57
 H      -3.421173    -0.325136    -2.518560      25.39
 C      -4.650214     1.563644    -0.508134     102.15
 O      -4.491338     2.959148    -0.190060     275.70
 H      -4.588373     3.175869     0.782072      26.93
 H      -5.237253     0.990618     0.144362      29.58
 H      -5.186229     1.467353    -1.482842      28.80
55
name = lig-etoh-Waterframe_270
 C       5.605019    -1.667602     2.106213      52.68
 H       5.730401    -0.604069     1.938976      24.90
 C       5.123754    -3.923225     1.394035      69.25
 H       4.794927    -4.556181     0.621512      17.86
 C       5.337946    -4.371301     2.701602      10.75
 O       5.214010    -5.677892     3.135056     256.49
 C       4.975888    -6.660231     2.062425     108.01
 H       5.895602    -6.840125     1.514811      28.69
 H       4.019420    -6.444956     1.497391      30.38
 H       4.866780    -7.620660     2.510407      24.98
 C       5.801933    -3.433460     3.724826      -6.68
 O       6.225607    -3.924609     4.963312     157.03
 H       6.359916    -4.888183     4.966977      25.97
 C       5.779309    -2.070018     3.416327      64.71
 H       6.069441    -1.345448     4.136315      21.56
 C       5.239781    -2.591812     1.021281      26.36
 C       5.097041    -2.197196    -0.515044      72.26
 H       5.585431    -3.108046    -1.104586      21.79
 O       5.886229    -1.139818    -1.017252     222.53
 H       5.484065    -0.231445    -0.612747      21.56
 C       3.613358    -2.079679    -0.939445      71.49
 H       3.158019    -2.987222    -0.440906      21.90
 C       3.491806    -2.059907    -2.512144      97.61
 O       3.556794    -3.377165    -3.137896     262.78
 H       4.453237    -3.494144    -3.506546      26.48
 H       4.389459    -1.574321    -2.931685      23.37
 H       2.408053    -1.656871    -2.674682      25.24
 C      -0.641220    -1.345192     0.257023      52.34
 H      -1.300651    -2.202748     0.488032      20.51
 C      -0.076476     0.944635    -0.111968      65.77
 H      -0.439074     1.921358    -0.315252      24.04
 C       1.236506     0.678376    -0.295812      21.16
 O       2.167593     1.731604    -0.461326     207.63
 C       1.852354     3.110859    -0.345895     120.49
 H       2.735027     3.649437    -0.577033      27.12
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 H       1.155052     3.369376    -1.046217      27.60
 H       1.631823     3.201678     0.815432      24.84
 C       1.680327    -0.665262    -0.192972      -3.10
 O       3.124668    -0.847575    -0.341335     121.38
 C       0.778710    -1.720812     0.069899      51.79
 H       0.983634    -2.739915     0.184241      23.94
 C      -1.073986    -0.033860     0.178437      30.05
 C      -2.456309     0.467485     0.442872      93.14
 H      -2.953397    -0.380102     1.022612      26.26
 O      -2.421269     1.644313     1.286290     253.48
 H      -2.202224     1.321593     2.271728      26.56
 C      -3.297262     0.835585    -0.828121      84.69
 H      -2.676206     1.601859    -1.567564      25.14
 O      -3.525227    -0.338464    -1.542272     262.17
 H      -3.413636    -0.249095    -2.526259      25.52
 C      -4.649960     1.543752    -0.481197      98.49
 O      -4.432450     3.018551    -0.225057     250.66
 H      -4.847160     3.203833     0.662782      27.39
 H      -5.240269     0.943878     0.311119      28.26
 H      -5.116054     1.483840    -1.444829      30.04
55
name = lig-etoh-Waterframe_271
 C       5.527263    -1.627763     2.065391      52.95
 H       5.789863    -0.613486     1.734938      23.54
 C       5.164668    -3.967564     1.341638      58.78
 H       4.974572    -4.699705     0.608959      15.31
 C       5.358329    -4.338597     2.742800       0.83
 O       5.253798    -5.652176     3.164027     260.66
 C       5.012829    -6.779878     2.051840      79.19
 H       5.879143    -6.834255     1.348829      28.30
 H       4.132593    -6.448767     1.416737      30.71
 H       4.841514    -7.616390     2.656643      25.06
 C       5.799557    -3.467575     3.743448      -8.16
 O       6.266507    -3.886240     4.911959     161.44
 H       6.362152    -4.887631     4.955527      23.23
 C       5.822755    -2.052597     3.467625      49.60
 H       6.347036    -1.459686     4.148423      23.31
 C       5.235579    -2.534762     1.049519      23.04
 C       5.080122    -2.207361    -0.552967      95.84
 H       5.356968    -3.057769    -1.052213      24.76
 O       5.882276    -1.141432    -1.011719     260.07
 H       5.703615    -0.212828    -0.602640      23.40
 C       3.655388    -2.025063    -0.993058      87.00
 H       3.038549    -2.885862    -0.615964      20.94
 C       3.507477    -2.043244    -2.545219      85.57
 O       3.571609    -3.405767    -3.165107     289.14
 H       4.336652    -3.344631    -3.719787      26.58
 H       4.315095    -1.330555    -2.973563      22.51
 H       2.554910    -1.490774    -2.887382      24.86
 C      -0.614898    -1.347046     0.257656      57.38
 H      -1.379487    -2.032082     0.655391      24.29
 C      -0.164208     0.980080    -0.083874      60.27
 H      -0.485040     2.057346    -0.370188      20.98
 C       1.219414     0.703707    -0.224117     -18.40
 O       2.196785     1.655132    -0.503330     180.18
 C       1.869709     3.093419    -0.336882     110.96
 H       2.808957     3.490168    -0.630060      25.20
 H       1.166217     3.493225    -0.964113      26.83
 H       1.575652     3.274954     0.866049      23.99
 C       1.741595    -0.694299    -0.207609       1.08
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 O       3.068911    -0.896892    -0.349127     158.67
 C       0.757410    -1.682454     0.069581      68.69
 H       1.068304    -2.633909     0.140742      22.62
 C      -1.064711    -0.006831     0.155045      35.18
 C      -2.438563     0.453183     0.404330      87.16
 H      -3.052657    -0.357999     0.900993      24.78
 O      -2.358670     1.629853     1.283873     210.57
 H      -2.110931     1.186267     2.255397      24.53
 C      -3.303458     0.918736    -0.751234      92.39
 H      -2.646131     1.686035    -1.370657      25.61
 O      -3.544673    -0.307471    -1.554187     248.48
 H      -3.408183    -0.125792    -2.527646      25.63
 C      -4.619674     1.562107    -0.506982     106.24
 O      -4.427384     3.020832    -0.241761     249.03
 H      -4.915902     3.272127     0.578013      27.37
 H      -5.122813     1.235403     0.525102      26.85
 H      -5.391139     1.486349    -1.249892      29.85
55
name = lig-etoh-Waterframe_272
 C       5.497358    -1.596074     2.079503      46.23
 H       5.679809    -0.542354     1.790385      23.11
 C       5.206557    -3.931355     1.380860      41.71
 H       5.124989    -4.718043     0.643158      14.61
 C       5.366383    -4.374589     2.663993      26.27
 O       5.283355    -5.701686     3.125308     260.33
 C       5.047113    -6.789349     2.113517     106.00
 H       5.982792    -6.830602     1.458770      27.49
 H       4.156927    -6.581334     1.486400      31.37
 H       4.809697    -7.646991     2.697534      22.29
 C       5.780102    -3.398183     3.698189       8.53
 O       6.332148    -3.861220     4.924581     137.28
 H       6.223238    -4.875996     5.087026      25.56
 C       5.875983    -2.063273     3.392312      54.24
 H       6.361054    -1.406205     4.101013      22.80
 C       5.227995    -2.554115     1.010183      32.35
 C       5.076633    -2.233760    -0.474064     104.92
 H       5.396043    -3.063644    -0.989870      23.54
 O       5.943152    -1.131305    -1.023692     228.64
 H       5.568091    -0.309137    -0.594740      23.27
 C       3.596774    -2.081155    -1.051397      69.01
 H       3.083479    -3.016259    -0.831303      20.16
 C       3.520768    -1.969000    -2.606406      86.91
 O       3.583319    -3.387654    -3.148638     292.13
 H       4.354000    -3.377146    -3.703965      26.62
 H       4.327100    -1.292296    -3.042439      20.64
 H       2.552544    -1.622111    -2.919437      24.85
 C      -0.606992    -1.342976     0.288244      45.43
 H      -1.255604    -2.173089     0.597290      19.06
 C      -0.120433     1.071793    -0.123133      78.84
 H      -0.557848     2.204726    -0.061986      17.15
 C       1.249152     0.681029    -0.183358       8.75
 O       2.219052     1.587558    -0.548806     180.76
 C       1.926061     3.044718    -0.315383     115.70
 H       2.862481     3.612551    -0.454629      24.85
 H       0.950681     3.419161    -0.874891      24.27
 H       1.553457     3.481735     0.669096      26.37
 C       1.672680    -0.654737    -0.209345      18.27
 O       3.049784    -0.875116    -0.358035     159.25
 C       0.739388    -1.657338     0.057914      60.69
 H       1.091741    -2.656436     0.154044      20.52
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 C      -1.043913    -0.039383     0.113800      29.29
 C      -2.509858     0.465338     0.448532      81.37
 H      -3.088032    -0.376638     0.845765      25.64
 O      -2.301967     1.602834     1.314664     232.58
 H      -2.162908     1.230231     2.350955      23.87
 C      -3.266883     0.950200    -0.804603      96.74
 H      -2.714987     1.673313    -1.293321      27.93
 O      -3.559800    -0.269321    -1.539713     266.12
 H      -3.494202    -0.164600    -2.537975      25.14
 C      -4.652250     1.657240    -0.422346      97.83
 O      -4.449097     3.026317    -0.270763     279.73
 H      -4.748310     3.311841     0.621649      27.64
 H      -4.949165     1.092870     0.538627      27.47
 H      -5.339288     1.253843    -1.230921      28.45
55
name = lig-etoh-Waterframe_273
 C       5.499835    -1.611179     2.038768      59.07
 H       5.445873    -0.514608     1.948211      22.88
 C       5.229638    -3.900705     1.364814      45.17
 H       5.085567    -4.584718     0.485014      16.61
 C       5.403042    -4.412419     2.694015      13.85
 O       5.303987    -5.737044     3.063021     290.69
 C       5.073447    -6.749245     2.184018     127.31
 H       6.013491    -7.070685     1.639817      24.42
 H       4.234619    -6.593279     1.537003      33.26
 H       4.967926    -7.693741     2.733405      21.86
 C       5.795682    -3.446556     3.668497      -6.42
 O       6.371214    -3.809187     4.921868     223.60
 H       6.248481    -4.847395     4.998470      23.05
 C       5.916145    -2.041566     3.268086      40.20
 H       6.169120    -1.271901     4.062760      24.37
 C       5.229294    -2.537396     1.035870      32.23
 C       5.079333    -2.243955    -0.470461      84.91
 H       5.626173    -3.155196    -0.984627      21.91
 O       5.973817    -1.146952    -0.993862     227.18
 H       5.609708    -0.271169    -0.764796      24.05
 C       3.557329    -2.115597    -1.072501      60.59
 H       2.982190    -2.958761    -0.736808      20.95
 C       3.509186    -1.936067    -2.654626      99.63
 O       3.606571    -3.319102    -3.114833     301.87
 H       4.476827    -3.509922    -3.486792      28.63
 H       4.353291    -1.403059    -3.068792      21.96
 H       2.550279    -1.574974    -2.832930      26.45
 C      -0.621355    -1.349913     0.299619      52.50
 H      -1.296065    -2.189502     0.471505      16.65
 C      -0.077416     1.027681    -0.124485      73.90
 H      -0.376013     2.148419     0.091359      17.70
 C       1.235318     0.736968    -0.222773      10.32
 O       2.271440     1.612661    -0.547488     207.42
 C       1.947208     3.004612    -0.286683     106.11
 H       2.846034     3.614402    -0.650586      23.88
 H       1.227485     3.206257    -1.260283      22.44
 H       1.730981     2.952332     0.699604      27.31
 C       1.618175    -0.645057    -0.206285      14.09
 O       3.041091    -0.860155    -0.383752     131.69
 C       0.750107    -1.679138     0.054697      60.74
 H       1.048676    -2.781719     0.186209      20.33
 C      -1.068895     0.026015     0.102352      38.75
 C      -2.482013     0.467764     0.464722      82.59
 H      -3.029679    -0.311636     0.948884      25.80
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 O      -2.288992     1.585890     1.384056     243.25
 H      -2.220432     1.155051     2.398620      23.52
 C      -3.277165     0.971032    -0.851896     100.06
 H      -2.701040     1.571544    -1.461377      27.02
 O      -3.569962    -0.236219    -1.521888     268.17
 H      -3.527384    -0.160870    -2.519522      26.31
 C      -4.620535     1.607214    -0.340803      97.94
 O      -4.503289     3.091843    -0.281547     283.60
 H      -4.549854     3.304801     0.673951      29.52
 H      -5.054916     1.222474     0.567842      28.68
 H      -5.381045     1.533675    -1.221086      27.16
55
name = lig-etoh-Waterframe_274
 C       5.508612    -1.574710     1.982836      53.26
 H       5.286637    -0.524695     1.736489      20.53
 C       5.232714    -3.917126     1.342828      60.73
 H       4.966294    -4.668192     0.517265      14.69
 C       5.449482    -4.401231     2.682225      28.73
 O       5.342607    -5.695199     3.091005     275.84
 C       5.107646    -6.826824     2.169814      86.28
 H       5.966403    -6.970096     1.516473      27.42
 H       4.317639    -6.590473     1.467364      34.09
 H       4.731022    -7.564992     2.936665      24.27
 C       5.898047    -3.460033     3.654217      17.69
 O       6.368885    -3.756976     4.879612     148.58
 H       6.500199    -4.779105     5.097085      19.67
 C       5.918035    -2.102055     3.257075      51.39
 H       6.065420    -1.308535     4.086716      24.55
 C       5.216635    -2.534042     1.006496      31.75
 C       5.086204    -2.219458    -0.535395      82.95
 H       5.492435    -3.272925    -1.086712      21.85
 O       5.970614    -1.182186    -0.945326     227.59
 H       5.648215    -0.311408    -0.712820      26.99
 C       3.590814    -2.052708    -1.036451      80.42
 H       2.943179    -2.873278    -0.738668      21.85
 C       3.499826    -1.957123    -2.602224     107.81
 O       3.611903    -3.281126    -3.096285     292.72
 H       4.572330    -3.297920    -3.399883      25.23
 H       4.222619    -1.263240    -2.952900      24.92
 H       2.612976    -1.417574    -3.018034      25.41
 C      -0.653270    -1.309973     0.246341      41.64
 H      -1.463833    -1.991650     0.478639      19.10
 C      -0.110892     1.011585    -0.075861      77.18
 H      -0.427553     2.057315    -0.135029      19.94
 C       1.298537     0.724517    -0.327369       5.81
 O       2.346573     1.612420    -0.532672     219.14
 C       1.986717     2.946112    -0.344258     117.01
 H       2.984228     3.523744    -0.396184      23.54
 H       0.999993     3.478122    -0.771235      23.62
 H       1.619670     3.138268     0.661779      26.62
 C       1.703821    -0.665635    -0.230616      10.04
 O       3.016567    -0.858993    -0.422708     170.62
 C       0.691435    -1.701447     0.072945      55.41
 H       1.135735    -2.810559     0.128824      18.59
 C      -1.049170     0.000642     0.142225      38.45
 C      -2.399329     0.519490     0.434116      86.56
 H      -2.973527    -0.325668     0.816879      24.66
 O      -2.318014     1.583326     1.471047     243.55
 H      -2.177788     1.041840     2.391691      24.64
 C      -3.297759     0.965457    -0.768031      92.36
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 H      -2.737488     1.726839    -1.453806      24.10
 O      -3.593380    -0.259187    -1.531504     238.50
 H      -3.494388    -0.054289    -2.505968      25.19
 C      -4.594913     1.623008    -0.358456     103.21
 O      -4.561119     3.158567    -0.241845     271.76
 H      -4.406828     3.347383     0.703979      30.21
 H      -4.963511     1.285649     0.535523      29.95
 H      -5.427223     1.422118    -1.102742      27.68
55
name = lig-etoh-Waterframe_275
 C       5.511048    -1.600243     1.963305      44.95
 H       5.497469    -0.520987     1.781096      20.89
 C       5.210987    -3.949361     1.337440      59.51
 H       4.900581    -4.783159     0.647922      16.91
 C       5.514570    -4.367026     2.604117      17.86
 O       5.387527    -5.667157     3.136882     245.35
 C       5.097990    -6.843056     2.144089      94.73
 H       6.027738    -7.167173     1.712548      27.27
 H       4.252629    -6.573763     1.476935      29.79
 H       4.788255    -7.790174     2.749211      24.51
 C       6.010045    -3.432913     3.569221      -9.59
 O       6.384330    -3.725277     4.889026     122.23
 H       6.445011    -4.766663     5.004636      23.83
 C       5.869636    -2.080158     3.262885      46.17
 H       6.191407    -1.448213     4.150114      19.84
 C       5.212483    -2.585672     0.910664      29.26
 C       5.046101    -2.224683    -0.551645      90.37
 H       5.310219    -3.114428    -1.248765      23.05
 O       5.975316    -1.203095    -0.921087     219.62
 H       5.659163    -0.426161    -0.478202      28.08
 C       3.603768    -1.981677    -1.008173      91.10
 H       3.165031    -2.977038    -0.681790      22.84
 C       3.492259    -1.895847    -2.508037      93.93
 O       3.640257    -3.271881    -3.099052     241.31
 H       4.527845    -3.349374    -3.653845      24.96
 H       4.350870    -1.322840    -2.861313      22.87
 H       2.397729    -1.601422    -2.865055      23.80
 C      -0.682460    -1.338732     0.193753      43.63
 H      -1.417490    -2.089214     0.503330      20.77
 C      -0.013692     1.050952    -0.087795      64.74
 H      -0.468520     1.923569    -0.263010      19.60
 C       1.292750     0.627379    -0.388303       7.96
 O       2.372260     1.576754    -0.540289     149.80
 C       2.007078     3.013464    -0.291373     104.31
 H       2.942566     3.603015    -0.497892      25.04
 H       1.307161     3.299518    -1.058393      25.25
 H       1.740305     3.233504     0.840284      23.80
 C       1.669343    -0.714284    -0.259010      29.68
 O       3.059521    -0.845693    -0.448818     187.78
 C       0.710521    -1.651403     0.049147      64.39
 H       0.877822    -2.807518     0.156744      19.15
 C      -0.983191     0.044280     0.168936      34.81
 C      -2.405615     0.551962     0.461628      82.65
 H      -2.977453    -0.348727     0.828831      22.37
 O      -2.364485     1.566163     1.533690     281.05
 H      -2.166533     1.095765     2.393549      26.36
 C      -3.273681     0.976171    -0.710666      73.12
 H      -2.702209     1.829352    -1.393816      23.32
 O      -3.606453    -0.267522    -1.533410     210.07
 H      -3.473425    -0.088512    -2.513504      24.06
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 C      -4.639734     1.716513    -0.346359     102.56
 O      -4.602107     3.173228    -0.197448     290.42
 H      -4.416770     3.283741     0.752772      29.87
 H      -4.859236     1.264544     0.599406      28.80
 H      -5.258227     1.339036    -1.126205      28.59
55
name = lig-etoh-Waterframe_276
 C       5.512777    -1.694986     1.926561      59.02
 H       5.713671    -0.653317     1.762461      21.11
 C       5.164261    -3.982508     1.266419      60.73
 H       4.855161    -4.719690     0.527178      19.09
 C       5.605634    -4.393471     2.613664       9.60
 O       5.414400    -5.697137     3.118768     285.74
 C       5.100840    -6.805352     2.182098      83.06
 H       5.999975    -7.081861     1.650437      25.20
 H       4.353723    -6.531417     1.367489      30.92
 H       4.744656    -7.658773     2.847440      23.75
 C       6.071755    -3.402359     3.517825     -15.00
 O       6.407957    -3.723917     4.872264     157.47
 H       6.273742    -4.729744     5.001031      25.35
 C       5.848502    -2.019668     3.243811      52.14
 H       6.174539    -1.250419     3.934763      20.97
 C       5.238487    -2.624798     0.918225      36.63
 C       5.031802    -2.254852    -0.564737     107.75
 H       5.328437    -3.042334    -1.111271      25.23
 O       5.986800    -1.192047    -0.912206     222.94
 H       5.834790    -0.365525    -0.460271      26.01
 C       3.616241    -2.025551    -0.980599      82.46
 H       2.979358    -2.887152    -0.557506      19.99
 C       3.504156    -1.898386    -2.494800      84.11
 O       3.659494    -3.266377    -3.093040     248.04
 H       4.524321    -3.231384    -3.740061      23.69
 H       4.185058    -1.116113    -2.974117      21.43
 H       2.411669    -1.465273    -2.609206      23.25
 C      -0.648385    -1.309495     0.175433      56.61
 H      -1.305868    -2.163310     0.412430      21.38
 C       0.033941     1.054027    -0.145507      58.67
 H      -0.106325     2.078354    -0.190832      19.59
 C       1.321171     0.656892    -0.390169       9.54
 O       2.351312     1.547450    -0.539795     183.10
 C       2.065434     3.061496    -0.274547      98.08
 H       2.968763     3.526794    -0.552327      24.83
 H       1.397905     3.257625    -0.985292      27.13
 H       1.652199     3.046154     0.824339      23.46
 C       1.670610    -0.731337    -0.315105      18.73
 O       3.078155    -0.803221    -0.416000     166.58
 C       0.679226    -1.700302     0.009614      50.66
 H       1.028049    -2.738357     0.125491      18.01
 C      -0.975662     0.098388     0.179265      44.13
 C      -2.429119     0.516798     0.555326      69.72
 H      -2.955252    -0.386114     0.989580      22.78
 O      -2.416457     1.558165     1.558445     305.46
 H      -2.232337     1.120941     2.345440      27.60
 C      -3.265345     1.042585    -0.739343      72.41
 H      -2.539987     1.590295    -1.446160      23.00
 O      -3.594738    -0.215419    -1.491941     229.43
 H      -3.460254    -0.100153    -2.478085      25.26
 C      -4.640104     1.736825    -0.307689      99.39
 O      -4.624316     3.157907    -0.159118     307.95
 H      -4.590451     3.355900     0.792309      29.05
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 H      -5.187415     1.293169     0.648800      25.79
 H      -5.346589     1.649963    -1.107511      27.53
55
name = lig-etoh-Waterframe_277
 C       5.548791    -1.709212     1.881408      56.25
 H       5.591265    -0.744679     1.437898      21.20
 C       5.167189    -4.047786     1.276523      53.04
 H       4.868504    -4.690870     0.501682      20.21
 C       5.628796    -4.437428     2.555289      19.79
 O       5.443054    -5.706471     3.079118     270.90
 C       5.121143    -6.745155     2.215333      91.93
 H       5.990624    -7.052887     1.627147      24.80
 H       4.292830    -6.433721     1.511506      29.50
 H       4.684817    -7.466788     2.880285      22.45
 C       6.062182    -3.381005     3.572159      11.38
 O       6.431612    -3.736096     4.813584     180.60
 H       6.325887    -4.701345     5.027477      30.16
 C       5.888773    -2.025742     3.206081      67.00
 H       6.047953    -1.186547     3.795576      22.08
 C       5.247161    -2.682545     0.931731      39.73
 C       5.110082    -2.271458    -0.515852     106.04
 H       5.461582    -3.093755    -1.061489      23.27
 O       6.005149    -1.188937    -0.928999     219.16
 H       5.645064    -0.338924    -0.554157      24.42
 C       3.606305    -2.060366    -0.955766      68.09
 H       2.925994    -2.892477    -0.680902      20.24
 C       3.468191    -1.932864    -2.511326      91.89
 O       3.661858    -3.223570    -3.091348     259.85
 H       4.633986    -3.173537    -3.578022      22.92
 H       4.152065    -1.117513    -2.936469      20.40
 H       2.471543    -1.646201    -2.808530      24.42
 C      -0.607919    -1.231922     0.184341      35.41
 H      -1.475207    -1.895809     0.396534      19.54
 C      -0.017814     1.072277    -0.185563      87.43
 H      -0.141768     2.156199     0.080124      18.16
 C       1.351700     0.671871    -0.363985       9.30
 O       2.365078     1.586842    -0.541085     216.87
 C       2.110697     2.976974    -0.306760     127.32
 H       3.028035     3.452236    -0.287170      24.87
 H       1.254907     3.548103    -0.784055      26.21
 H       1.744446     3.283173     0.730008      27.08
 C       1.712259    -0.687332    -0.362287      15.45
 O       3.077670    -0.801688    -0.361364     169.36
 C       0.737171    -1.744022    -0.068163      45.53
 H       0.988639    -2.726268     0.054540      18.02
 C      -1.016465     0.097804     0.177407      43.07
 C      -2.433690     0.502752     0.587117      69.01
 H      -2.964274    -0.421386     0.899565      23.11
 O      -2.466137     1.567478     1.570308     314.19
 H      -2.242844     1.169975     2.376738      27.69
 C      -3.268787     1.028860    -0.715190      87.20
 H      -2.712358     1.732480    -1.229950      26.42
 O      -3.579605    -0.143594    -1.430511     259.46
 H      -3.518126     0.001943    -2.416082      25.41
 C      -4.648080     1.728769    -0.327007      84.46
 O      -4.612276     3.183754    -0.101005     292.02
 H      -4.820592     3.432046     0.816832      27.89
 H      -5.108780     1.061395     0.582022      25.62
 H      -5.324113     1.568307    -1.211715      27.02
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name = lig-etoh-Waterframe_278
 C       5.590732    -1.705042     1.813005      55.35
 H       5.501659    -0.657151     1.592444      19.49
 C       5.212965    -4.099584     1.292877      51.89
 H       4.938106    -4.883331     0.655934      20.17
 C       5.612727    -4.404741     2.569848      15.85
 O       5.508875    -5.654287     3.088820     316.26
 C       5.080423    -6.733433     2.200688     114.29
 H       5.925098    -7.217633     1.650918      23.56
 H       4.241286    -6.417467     1.593259      29.11
 H       4.819511    -7.565215     2.766892      23.36
 C       5.966997    -3.423774     3.520897       4.75
 O       6.473488    -3.759872     4.802220     339.27
 H       6.429043    -4.723929     4.881267      34.09
 C       5.952652    -2.040392     3.168260      53.73
 H       6.080710    -1.385148     3.994046      25.47
 C       5.262782    -2.728280     0.936171      39.07
 C       5.164199    -2.304027    -0.505129     107.35
 H       5.517317    -3.204059    -1.220138      22.29
 O       6.001955    -1.185103    -0.939101     263.51
 H       5.490801    -0.324367    -0.734985      22.34
 C       3.606007    -2.054681    -0.975549      76.31
 H       3.185945    -2.955558    -0.599005      20.98
 C       3.410062    -1.935660    -2.511975      99.64
 O       3.685257    -3.210428    -3.112766     264.95
 H       4.660037    -3.346999    -3.485299      26.85
 H       4.221453    -1.280503    -2.849283      20.70
 H       2.455478    -1.697596    -2.783390      26.60
 C      -0.573052    -1.228009     0.185258      44.25
 H      -1.323206    -1.992865     0.470990      16.76
 C      -0.044609     1.097446    -0.150665      63.70
 H      -0.547045     2.145365     0.036002      14.93
 C       1.256813     0.712107    -0.344110       8.30
 O       2.386269     1.635972    -0.552366     188.01
 C       2.131428     2.971016    -0.252785     110.14
 H       3.119133     3.460839    -0.455320      22.75
 H       1.480022     3.534852    -1.206751      22.13
 H       1.891775     2.991935     0.770280      26.20
 C       1.718219    -0.677688    -0.353843      15.78
 O       3.111904    -0.870914    -0.321656     168.69
 C       0.767572    -1.652191    -0.150678      62.08
 H       0.894387    -2.651738    -0.087862      20.67
 C      -0.995058     0.129837     0.149480      62.03
 C      -2.453065     0.534110     0.538144      76.45
 H      -2.957220    -0.352690     0.906179      23.73
 O      -2.508881     1.578295     1.569634     296.68
 H      -2.177876     1.126444     2.419225      25.45
 C      -3.280282     1.058060    -0.593131     104.15
 H      -2.752480     1.778008    -1.121928      27.62
 O      -3.566491    -0.113728    -1.410401     240.50
 H      -3.597023     0.088851    -2.386272      25.70
 C      -4.647502     1.705384    -0.354883      92.79
 O      -4.588348     3.195625    -0.042417     267.66
 H      -5.020206     3.211766     0.824151      27.50
 H      -5.085475     1.207472     0.560519      27.61
 H      -5.234606     1.438489    -1.289823      27.71
55
name = lig-etoh-Waterframe_279
 C       5.636816    -1.705233     1.866022      49.79
 H       5.579681    -0.639118     1.616495      19.12
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 C       5.270905    -4.086351     1.270759      52.34
 H       5.045799    -4.883960     0.574830      14.84
 C       5.551426    -4.395419     2.627845      25.78
 O       5.573180    -5.678306     3.115620     237.85
 C       5.041428    -6.763885     2.202365     121.42
 H       5.846258    -6.931251     1.420652      27.37
 H       4.204946    -6.498392     1.579937      31.27
 H       4.766595    -7.510656     2.926382      23.54
 C       5.936906    -3.408730     3.517512      13.66
 O       6.497889    -3.791738     4.765688     271.83
 H       6.422435    -4.727765     4.961739      29.02
 C       5.981740    -2.101206     3.130456      63.56
 H       6.268157    -1.407081     3.960845      25.01
 C       5.305907    -2.731890     0.872787      23.39
 C       5.131164    -2.308797    -0.611734     123.74
 H       5.544103    -3.285713    -1.272619      24.35
 O       5.986335    -1.193663    -0.944007     256.99
 H       5.562663    -0.284618    -0.635121      20.82
 C       3.660813    -2.105016    -0.977159      89.26
 H       3.117358    -2.943736    -0.567294      20.85
 C       3.432109    -1.942087    -2.497089      97.36
 O       3.681345    -3.269067    -3.138618     276.75
 H       4.616520    -3.097320    -3.508087      26.28
 H       3.993153    -1.112625    -2.904213      23.08
 H       2.423430    -1.528543    -2.674750      25.19
 C      -0.571012    -1.237660     0.166025      35.39
 H      -1.084445    -2.127246     0.482745      18.02
 C      -0.099983     1.165349    -0.080655      80.67
 H      -0.269652     2.300422    -0.363263      16.44
 C       1.304211     0.778859    -0.352315      11.26
 O       2.359572     1.581150    -0.573754     186.43
 C       2.198620     3.047516    -0.224378      96.74
 H       3.223535     3.546126    -0.404407      22.92
 H       1.227255     3.352062    -0.945687      21.10
 H       1.705627     3.208275     0.695986      25.21
 C       1.731569    -0.595000    -0.318036       9.33
 O       3.119808    -0.937681    -0.291031     189.50
 C       0.709512    -1.565666    -0.192957      56.50
 H       1.063342    -2.602667    -0.266741      18.25
 C      -1.012065     0.093700     0.141621      40.10
 C      -2.451270     0.556914     0.555521      79.59
 H      -2.922409    -0.347229     0.944406      23.78
 O      -2.521496     1.587236     1.564923     259.46
 H      -2.187781     1.036608     2.442633      23.46
 C      -3.295789     1.113885    -0.576919      92.78
 H      -2.582880     1.753650    -1.221660      23.86
 O      -3.549835    -0.119456    -1.414574     235.93
 H      -3.573938     0.158143    -2.370425      26.63
 C      -4.657053     1.721664    -0.306835     112.86
 O      -4.578985     3.148062    -0.001472     296.67
 H      -4.982293     3.288942     0.867641      28.97
 H      -5.247027     1.293160     0.393517      30.33
 H      -5.283543     1.677237    -1.231685      28.62
55
name = lig-etoh-Waterframe_280
 C       5.644940    -1.746510     1.831200      49.20
 H       5.797368    -0.677059     1.546212      22.84
 C       5.322185    -4.030795     1.256907      59.64
 H       5.150502    -4.755229     0.417044      15.45
 C       5.469900    -4.440364     2.615332      20.09
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 O       5.586608    -5.758455     3.110989     265.37
 C       5.027572    -6.743250     2.221925     125.79
 H       5.793060    -7.058613     1.439376      29.86
 H       4.060072    -6.404186     1.861247      31.74
 H       4.890230    -7.699903     2.858021      23.20
 C       5.973853    -3.461044     3.600018      -4.88
 O       6.514704    -3.808919     4.736995     161.57
 H       6.234421    -4.700428     4.991749      26.53
 C       6.006880    -2.102816     3.170372      50.76
 H       6.494250    -1.222377     3.743522      22.28
 C       5.375034    -2.668481     0.829415      25.90
 C       5.122619    -2.312552    -0.660290     113.09
 H       5.478667    -3.123454    -1.372791      24.04
 O       5.971634    -1.196963    -0.971116     255.34
 H       5.585741    -0.407510    -0.393971      21.65
 C       3.650045    -2.159712    -0.995271      78.66
 H       3.051405    -3.087074    -0.767055      19.70
 C       3.442525    -1.955067    -2.484839      89.85
 O       3.663113    -3.275600    -3.156074     259.00
 H       4.502348    -3.301559    -3.661079      28.55
 H       4.073820    -1.203681    -2.951963      20.77
 H       2.255628    -1.837032    -2.617650      21.87
 C      -0.624223    -1.247624     0.143984      22.58
 H      -1.386460    -1.959467     0.421247      16.23
 C      -0.008287     1.167666    -0.092939      75.54
 H      -0.420925     2.211376    -0.309208      18.22
 C       1.305788     0.788496    -0.315513      17.83
 O       2.380580     1.638424    -0.572504     202.49
 C       2.164410     3.061843    -0.242015     117.45
 H       3.130001     3.683494    -0.378608      23.89
 H       1.536749     3.626536    -0.848614      25.73
 H       1.898840     3.300900     0.833512      24.29
 C       1.728038    -0.550303    -0.288512      15.32
 O       3.102074    -0.944149    -0.255368     175.86
 C       0.753904    -1.511125    -0.223782      76.86
 H       1.062157    -2.658845    -0.279732      17.85
 C      -1.064808     0.144713     0.179561      56.60
 C      -2.461821     0.542308     0.606992      67.67
 H      -3.040831    -0.363365     0.912340      22.61
 O      -2.489983     1.589325     1.582437     257.88
 H      -2.275828     1.186746     2.594391      23.41
 C      -3.290301     1.065613    -0.667991      76.05
 H      -2.705718     1.977795    -1.247897      23.02
 O      -3.535985    -0.114134    -1.420065     258.93
 H      -3.486576     0.024441    -2.410308      25.37
 C      -4.704804     1.775492    -0.264205     103.57
 O      -4.573638     3.133905     0.048669     298.36
 H      -4.711042     3.350586     0.974724      29.42
 H      -5.199312     1.090698     0.385498      30.14
 H      -5.186367     1.716193    -1.248072      29.88
55
name = lig-etoh-Waterframe_281
 C       5.696289    -1.736793     1.813551      45.25
 H       5.922508    -0.676110     1.565899      22.64
 C       5.339471    -4.003767     1.246316      74.73
 H       5.160034    -4.844790     0.493314      15.08
 C       5.480201    -4.448903     2.614645      18.12
 O       5.567553    -5.794195     3.079670     305.63
 C       5.016179    -6.783652     2.251554     120.42
 H       5.569158    -6.961866     1.309557      31.28
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 H       4.013811    -6.465584     1.865542      31.44
 H       4.950414    -7.797897     2.827140      23.09
 C       5.959798    -3.475343     3.532329     -21.83
 O       6.547186    -3.860680     4.803991     222.00
 H       6.276151    -4.789948     5.070755      27.68
 C       6.021701    -2.100300     3.165872      44.20
 H       6.550594    -1.361505     3.882608      21.90
 C       5.415802    -2.680838     0.812407      36.89
 C       5.166326    -2.326327    -0.631340     112.19
 H       5.455077    -3.071014    -1.211801      27.30
 O       5.947804    -1.178676    -1.016403     244.55
 H       5.651083    -0.290284    -0.532842      20.68
 C       3.581453    -2.145253    -1.013364      68.51
 H       3.139810    -3.131445    -0.605770      19.21
 C       3.412680    -2.024423    -2.523663      94.07
 O       3.620191    -3.288482    -3.163587     287.41
 H       4.496587    -3.289045    -3.554280      28.41
 H       4.062806    -1.217689    -2.918133      21.16
 H       2.266991    -1.706592    -2.775158      23.01
 C      -0.672495    -1.145391     0.101128      50.36
 H      -1.422921    -1.931173     0.215884      18.65
 C      -0.031669     1.113141    -0.114510      74.37
 H      -0.297615     2.140019     0.004354      17.95
 C       1.350174     0.807443    -0.270965      13.62
 O       2.405552     1.781915    -0.562406     206.77
 C       2.147716     3.118355    -0.242370     120.23
 H       3.174354     3.474829    -0.479701      22.09
 H       1.482237     3.541937    -0.824362      28.65
 H       1.975005     3.015294     0.897206      24.59
 C       1.745180    -0.604073    -0.273839      22.46
 O       3.084363    -0.934795    -0.237037     180.72
 C       0.695027    -1.543184    -0.193575      71.37
 H       1.006515    -2.714743    -0.183302      17.33
 C      -0.987982     0.173858     0.226491      26.46
 C      -2.494348     0.559038     0.580675      58.32
 H      -3.030638    -0.352695     0.983063      20.13
 O      -2.452303     1.624081     1.609432     271.86
 H      -2.200868     1.004618     2.515624      19.17
 C      -3.311161     1.048468    -0.672384      77.40
 H      -2.682733     1.795901    -1.354243      21.58
 O      -3.535235    -0.129791    -1.455116     268.85
 H      -3.323798    -0.087666    -2.430553      24.42
 C      -4.685448     1.734622    -0.301400      84.48
 O      -4.566011     3.177807     0.121664     295.25
 H      -4.495757     3.064350     1.069559      28.63
 H      -5.217428     1.135436     0.612192      25.84
 H      -5.342714     1.672229    -1.185600      27.80
55
name = lig-etoh-Waterframe_282
 C       5.801646    -1.682993     1.851307      51.35
 H       5.853267    -0.641360     1.522578      20.41
 C       5.319621    -4.084171     1.266069      47.42
 H       5.039118    -4.868685     0.500480      15.47
 C       5.564356    -4.452943     2.588731      20.26
 O       5.537998    -5.755458     3.049343     244.83
 C       4.968819    -6.864028     2.197386     119.22
 H       5.566616    -6.887094     1.332954      30.81
 H       3.882152    -6.719520     1.920712      29.60
 H       5.006702    -7.719821     2.927541      23.22
 C       5.981178    -3.493646     3.541734      -6.58
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 O       6.542770    -3.889158     4.828186     286.66
 H       6.409435    -4.894353     5.077983      25.79
 C       6.036892    -2.149964     3.128479      61.46
 H       6.333261    -1.520802     3.984615      25.70
 C       5.431228    -2.707616     0.858906       7.60
 C       5.155186    -2.290545    -0.607023      96.76
 H       5.524979    -3.143847    -1.175811      25.01
 O       5.945128    -1.154254    -1.086024     207.04
 H       5.463463    -0.287003    -0.773415      23.03
 C       3.582613    -2.119887    -0.953198      76.27
 H       2.986010    -2.945831    -0.463387      20.85
 C       3.332217    -2.037221    -2.560784     100.56
 O       3.577914    -3.335793    -3.162138     289.99
 H       4.460040    -3.242279    -3.493654      27.85
 H       4.092534    -1.293076    -2.920418      22.34
 H       2.398360    -1.571269    -2.846999      25.30
 C      -0.646143    -1.143773     0.036762      49.92
 H      -1.419600    -1.929012     0.182490      21.74
 C       0.007457     1.167638    -0.080904      74.16
 H      -0.178643     2.135107     0.125604      19.33
 C       1.430464     0.802937    -0.267482       0.90
 O       2.376052     1.777098    -0.569338     206.59
 C       2.174333     3.184126    -0.192492     112.27
 H       3.018801     3.825114    -0.412499      24.87
 H       1.170378     3.516003    -0.698716      24.64
 H       1.822490     3.488251     0.870330      26.13
 C       1.712130    -0.624580    -0.260768      15.45
 O       3.088846    -0.951829    -0.260605     193.41
 C       0.612692    -1.578302    -0.121605      54.43
 H       0.792470    -2.713586    -0.130862      17.46
 C      -1.015709     0.206673     0.246976      27.43
 C      -2.456354     0.625107     0.539072      78.87
 H      -2.923786    -0.284505     0.970413      20.86
 O      -2.418274     1.639624     1.614732     286.51
 H      -2.065012     1.108050     2.456596      23.10
 C      -3.319061     1.054913    -0.666049      90.51
 H      -2.672353     1.701582    -1.194972      25.18
 O      -3.557658    -0.192392    -1.490524     248.63
 H      -3.242330     0.022570    -2.406890      25.19
 C      -4.643770     1.709863    -0.319738      93.52
 O      -4.542700     3.164534     0.174871     290.82
 H      -4.414216     3.112886     1.123477      28.85
 H      -5.191559     1.208177     0.653851      25.03
 H      -5.421463     1.634551    -1.091439      27.98
55
name = lig-etoh-Waterframe_283
 C       5.855805    -1.732293     1.816132      55.85
 H       5.865256    -0.667086     1.643665      19.39
 C       5.288282    -4.091138     1.252226      57.37
 H       4.885187    -4.807262     0.533375      18.46
 C       5.654299    -4.494892     2.563118      19.18
 O       5.472800    -5.756232     3.019154     255.95
 C       4.945553    -6.889981     2.174228     121.17
 H       5.566338    -7.165276     1.332295      27.98
 H       3.861845    -6.795975     1.955981      28.53
 H       5.169746    -7.744666     2.768831      24.35
 C       6.053718    -3.555011     3.595224      10.53
 O       6.511635    -3.876086     4.794264     220.98
 H       6.207777    -4.866789     5.035533      28.50
 C       6.082265    -2.184184     3.203979      48.09
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 H       6.189073    -1.408953     3.899983      25.79
 C       5.443970    -2.681612     0.935257      27.05
 C       5.108787    -2.265785    -0.590708      85.04
 H       5.455933    -3.186927    -1.350660      23.31
 O       5.922219    -1.146374    -1.150719     181.97
 H       5.474575    -0.292636    -0.834757      24.46
 C       3.576982    -2.122779    -0.919602      80.51
 H       3.091742    -3.046985    -0.633477      22.50
 C       3.309866    -2.008295    -2.516063      97.52
 O       3.525775    -3.384382    -3.145202     243.87
 H       4.372563    -3.415767    -3.638052      28.04
 H       4.106913    -1.412788    -2.975023      23.17
 H       2.345814    -1.796015    -2.719363      27.11
 C      -0.725966    -1.152379     0.031442      40.43
 H      -1.538942    -1.877747     0.285744      22.19
 C       0.098412     1.223139     0.023293      52.33
 H      -0.175876     2.229589     0.052328      18.94
 C       1.362101     0.776426    -0.266845       9.82
 O       2.381555     1.746500    -0.545945     147.84
 C       2.092794     3.259691    -0.133978      87.21
 H       2.914023     3.832347    -0.487885      25.55
 H       1.186346     3.676593    -0.938389      21.38
 H       2.001520     3.302977     0.973521      24.36
 C       1.689838    -0.625495    -0.250035      19.23
 O       3.079471    -0.934844    -0.291123     180.58
 C       0.682205    -1.583753    -0.080049      52.95
 H       0.805448    -2.621181    -0.107302      19.45
 C      -0.994662     0.266443     0.159348      39.57
 C      -2.398633     0.654185     0.574615      76.82
 H      -2.934082    -0.235838     0.910800      22.13
 O      -2.391190     1.664353     1.593284     324.24
 H      -2.137710     1.214358     2.407042      27.96
 C      -3.284509     1.042218    -0.695181      84.68
 H      -2.806967     1.711780    -1.234687      28.42
 O      -3.574978    -0.212114    -1.475602     251.86
 H      -3.417936    -0.104893    -2.459550      24.50
 C      -4.647781     1.749231    -0.225509     104.02
 O      -4.494726     3.095308     0.158965     322.89
 H      -4.548127     3.230712     1.110622      28.56
 H      -5.024133     0.969919     0.468372      28.09
 H      -5.202297     1.684489    -1.184188      28.63
55
name = lig-etoh-Waterframe_284
 C       5.886062    -1.816469     1.917327      41.86
 H       5.970081    -0.781888     1.632225      19.99
 C       5.280737    -4.014592     1.268005      53.97
 H       4.828988    -4.695120     0.600695      20.14
 C       5.686138    -4.515630     2.514883      -2.56
 O       5.402160    -5.841472     2.997759     279.91
 C       4.977466    -6.908179     2.187487     105.00
 H       5.476996    -6.957791     1.152170      28.49
 H       3.929249    -6.773805     1.886786      30.58
 H       4.991414    -7.739488     2.815647      24.21
 C       6.122527    -3.545974     3.514655     -10.49
 O       6.480078    -3.896276     4.818814     189.37
 H       6.146852    -4.808348     5.239463      23.30
 C       6.119341    -2.177359     3.231365      65.69
 H       6.300700    -1.461568     3.972173      23.76
 C       5.419173    -2.687381     0.843910      26.27
 C       5.081837    -2.252810    -0.586309     101.41
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 H       5.376001    -3.253913    -1.259610      23.19
 O       5.866768    -1.162222    -1.181686     244.63
 H       5.672613    -0.322176    -0.717028      25.85
 C       3.578056    -2.141691    -0.964241      82.26
 H       3.131851    -3.023306    -0.567767      21.05
 C       3.357246    -2.062489    -2.451697      99.06
 O       3.450307    -3.422218    -3.102096     248.15
 H       4.367860    -3.329452    -3.570759      25.38
 H       3.827583    -1.206707    -2.967263      23.17
 H       2.294255    -1.815926    -2.552765      25.52
 C      -0.713192    -1.091072     0.071212      45.20
 H      -1.506756    -1.813260     0.287843      19.63
 C       0.057116     1.227552     0.123099      78.79
 H      -0.133866     2.332073     0.027519      18.00
 C       1.347488     0.804512    -0.259175      -1.32
 O       2.381356     1.750391    -0.494630     154.56
 C       2.040435     3.214560    -0.141102      95.42
 H       2.997360     3.510076    -0.398460      24.50
 H       0.981034     3.660950    -0.610694      20.85
 H       1.846219     3.141688     0.887693      25.60
 C       1.709323    -0.624191    -0.244433      10.62
 O       3.044661    -0.895255    -0.308395     172.64
 C       0.660005    -1.571589    -0.065200      51.29
 H       1.040687    -2.499151    -0.020119      21.21
 C      -0.928450     0.252269     0.079257      47.19
 C      -2.372768     0.648018     0.558327      75.82
 H      -2.817778    -0.248210     1.009533      23.22
 O      -2.372410     1.704552     1.570197     343.85
 H      -2.260290     1.256503     2.350340      29.12
 C      -3.259369     1.029270    -0.681443      89.94
 H      -2.557613     1.592878    -1.237949      24.82
 O      -3.589374    -0.195576    -1.409294     270.36
 H      -3.576589    -0.126831    -2.394090      25.88
 C      -4.608782     1.682906    -0.197234     110.85
 O      -4.448090     3.051889     0.139875     335.65
 H      -4.747829     3.208648     1.044499      28.90
 H      -5.176610     1.172839     0.491570      29.84
 H      -5.247211     1.718630    -1.120549      27.93
55
name = lig-etoh-Waterframe_285
 C       5.863340    -1.814767     1.896126      50.04
 H       6.077175    -0.771818     1.691608      21.18
 C       5.257554    -4.007623     1.238621      52.74
 H       4.818613    -4.705968     0.588327      19.83
 C       5.661035    -4.532078     2.522428       0.73
 O       5.386740    -5.848270     3.011005     303.06
 C       4.945333    -6.920006     2.134560     108.22
 H       5.715795    -6.968351     1.244850      29.12
 H       3.921600    -6.769044     1.818255      29.93
 H       5.008331    -7.850001     2.671577      24.65
 C       6.163818    -3.619955     3.490462     -29.44
 O       6.452175    -3.908508     4.854416     147.29
 H       6.224721    -4.902493     5.018155      25.01
 C       6.170828    -2.207433     3.233331      53.20
 H       6.549732    -1.601586     4.055423      22.26
 C       5.432066    -2.649172     0.848985      39.67
 C       5.078025    -2.262670    -0.617966     121.89
 H       5.447769    -3.099220    -1.168357      24.01
 O       5.819731    -1.191672    -1.176250     314.31
 H       5.616541    -0.425636    -0.646827      27.22
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 C       3.597453    -2.137212    -0.936392      79.31
 H       2.999037    -2.908510    -0.450668      20.36
 C       3.291350    -2.126886    -2.429168      85.58
 O       3.413037    -3.405243    -3.045330     239.59
 H       4.396245    -3.512332    -3.462294      25.19
 H       3.940210    -1.373697    -2.948704      20.66
 H       2.141793    -1.796139    -2.468142      23.02
 C      -0.599246    -1.118771     0.103703      42.92
 H      -1.424512    -1.787388     0.242636      18.76
 C       0.056947     1.221081     0.109354      84.26
 H      -0.362549     2.325715     0.349604      15.62
 C       1.378230     0.834855    -0.216887      14.73
 O       2.338346     1.753857    -0.443168     251.23
 C       2.020888     3.056342    -0.112855     120.37
 H       2.817240     3.795168    -0.286275      24.74
 H       1.249319     3.474686    -0.748749      25.06
 H       1.792503     3.271696     0.892368      26.36
 C       1.666402    -0.554771    -0.245176      19.21
 O       3.045168    -0.881142    -0.338326     186.15
 C       0.665389    -1.531036    -0.065475      65.34
 H       0.860171    -2.581678     0.113714      21.64
 C      -0.991092     0.268654     0.128131      56.93
 C      -2.351949     0.613430     0.535336      91.74
 H      -2.757532    -0.279835     1.057022      23.52
 O      -2.348475     1.733309     1.532255     328.92
 H      -2.269068     1.333721     2.334320      29.17
 C      -3.246819     0.992648    -0.606480      98.32
 H      -2.632981     1.706958    -1.254794      24.30
 O      -3.604636    -0.200000    -1.330719     263.30
 H      -3.549691     0.074061    -2.265539      25.87
 C      -4.584750     1.626585    -0.258610     102.10
 O      -4.406014     3.059092     0.129576     300.26
 H      -4.689267     3.215139     1.053430      28.09
 H      -5.021764     1.166515     0.626267      28.74
 H      -5.313017     1.432655    -1.087909      28.32
55
name = lig-etoh-Waterframe_286
 C       5.869603    -1.711512     1.870534      51.10
 H       6.006061    -0.643328     1.669455      23.19
 C       5.246522    -4.063329     1.228577      57.21
 H       4.837663    -4.717693     0.468369      17.92
 C       5.583623    -4.550239     2.527765       1.63
 O       5.393923    -5.818166     3.031298     242.90
 C       4.937482    -6.909030     2.053409     117.89
 H       5.692874    -7.092246     1.237655      30.86
 H       3.959147    -6.764102     1.587439      29.91
 H       5.022381    -7.839739     2.678128      25.52
 C       6.168106    -3.651568     3.557831       5.37
 O       6.428180    -3.942354     4.831725      55.28
 H       6.309780    -4.892754     5.112207      17.11
 C       6.235649    -2.327463     3.167989      49.83
 H       6.665926    -1.568389     3.900168      21.55
 C       5.432365    -2.652755     0.912397      18.24
 C       5.105222    -2.314468    -0.620538     109.70
 H       5.360499    -3.084710    -1.193217      25.79
 O       5.801688    -1.177900    -1.146394     302.87
 H       5.431823    -0.364401    -0.819066      27.07
 C       3.522959    -2.125878    -0.854696      73.34
 H       3.055887    -3.070187    -0.397814      18.73
 C       3.203866    -2.130046    -2.413838      89.83
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 O       3.386174    -3.436918    -2.986956     228.55
 H       4.385471    -3.451633    -3.431755      23.95
 H       3.950644    -1.497895    -2.909043      20.27
 H       2.080703    -1.824156    -2.703429      22.56
 C      -0.637273    -1.105285     0.132372      50.48
 H      -1.276924    -1.948049     0.281782      19.79
 C       0.003605     1.211581     0.062803      74.91
 H      -0.172725     2.299561     0.517121      13.49
 C       1.317394     0.838474    -0.149270      21.29
 O       2.373174     1.718406    -0.395422     223.97
 C       1.986858     3.054248    -0.084830     112.41
 H       2.930792     3.712626    -0.303254      22.93
 H       1.305808     3.235347    -0.773146      29.95
 H       1.571062     3.113873     0.989981      27.39
 C       1.714764    -0.532767    -0.264384      22.77
 O       3.070139    -0.841490    -0.367152     194.14
 C       0.754714    -1.517241    -0.060708      63.36
 H       0.869770    -2.676073     0.018621      15.88
 C      -0.949540     0.220173     0.222990      37.55
 C      -2.373134     0.602847     0.622231      74.50
 H      -2.919709    -0.289893     1.029904      21.11
 O      -2.323236     1.741053     1.487763     354.37
 H      -2.155393     1.394880     2.332228      28.76
 C      -3.261131     0.993528    -0.581429      85.67
 H      -2.864494     1.749655    -1.290926      23.55
 O      -3.601448    -0.233430    -1.290721     264.03
 H      -3.528198    -0.113340    -2.258395      25.96
 C      -4.588018     1.638626    -0.210732      89.58
 O      -4.389166     3.058620     0.068101     295.70
 H      -4.463723     3.111792     1.053103      27.98
 H      -4.833002     0.923133     0.690915      27.18
 H      -5.237171     1.463241    -1.080990      28.01
55
name = lig-etoh-Waterframe_287
 C       5.888665    -1.736625     1.895129      56.06
 H       5.923475    -0.662784     1.670357      24.30
 C       5.267125    -4.068317     1.267404      59.49
 H       4.924835    -4.758801     0.454389      18.35
 C       5.519544    -4.539412     2.565063      19.17
 O       5.374419    -5.850410     2.985642     257.15
 C       4.985988    -6.878707     2.013816     111.96
 H       5.691140    -6.963248     1.237363      29.70
 H       4.003988    -6.591530     1.559359      29.43
 H       4.719703    -7.728699     2.732647      23.88
 C       6.081179    -3.663182     3.496040     -11.17
 O       6.442368    -3.985564     4.844238     271.66
 H       6.092339    -4.885796     5.142399      21.82
 C       6.312227    -2.311086     3.054531      41.79
 H       6.665661    -1.640628     3.936469      23.37
 C       5.404558    -2.687066     0.900570      10.16
 C       5.069774    -2.319910    -0.557453      85.30
 H       5.331120    -3.219988    -1.229583      21.72
 O       5.803863    -1.146522    -1.112663     276.50
 H       5.292789    -0.366872    -0.877469      26.14
 C       3.448235    -2.142228    -0.846501      74.07
 H       2.927324    -2.948721    -0.203877      18.92
 C       3.154823    -2.122074    -2.381352      93.51
 O       3.371709    -3.509986    -2.933303     241.63
 H       4.292219    -3.363017    -3.493012      22.82
 H       3.747698    -1.322256    -2.806046      22.80
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 H       2.147019    -1.757400    -2.631251      24.52
 C      -0.590493    -1.191324     0.153207      40.88
 H      -1.390538    -1.908245     0.390573      21.77
 C      -0.016130     1.216327     0.072364      76.57
 H      -0.311102     2.304042     0.212876      16.62
 C       1.331288     0.798409    -0.141512       6.88
 O       2.414705     1.654323    -0.318009     159.58
 C       1.959837     3.117540    -0.086414      87.42
 H       3.012340     3.641134    -0.111586      22.74
 H       1.096719     3.495495    -0.775070      23.56
 H       1.488002     3.130410     1.008279      24.64
 C       1.759976    -0.572488    -0.254139      16.89
 O       3.114137    -0.789273    -0.379744     189.30
 C       0.745419    -1.514123    -0.056449      59.39
 H       1.268962    -2.551213    -0.245272      16.32
 C      -0.982406     0.162629     0.333915      27.66
 C      -2.406101     0.600836     0.669327      81.90
 H      -2.948248    -0.194054     1.220529      21.09
 O      -2.308827     1.756208     1.495721     330.73
 H      -2.051968     1.457674     2.378178      28.54
 C      -3.279440     0.995371    -0.623011      80.37
 H      -2.501306     1.563140    -1.175586      23.28
 O      -3.587690    -0.300281    -1.278043     265.05
 H      -3.438601    -0.232814    -2.239983      27.51
 C      -4.572392     1.632446    -0.121980     107.13
 O      -4.406612     3.043868     0.015734     288.82
 H      -4.244009     3.244805     0.973684      28.44
 H      -5.283658     1.251217     0.764913      26.11
 H      -5.295849     1.616680    -0.932267      27.28
55
name = lig-etoh-Waterframe_288
 C       5.870233    -1.843038     1.818998      51.17
 H       5.981430    -0.757798     1.658343      23.16
 C       5.276535    -4.033904     1.269611      70.22
 H       4.994920    -4.850641     0.532191      18.88
 C       5.479542    -4.562466     2.579757       9.32
 O       5.357062    -5.892067     2.940034     282.01
 C       4.972867    -6.814140     1.999552     133.46
 H       5.765617    -7.128121     1.374530      27.34
 H       4.091902    -6.441199     1.412661      28.31
 H       4.781654    -7.851497     2.449568      22.74
 C       6.030423    -3.614334     3.489780     -12.29
 O       6.451562    -3.982745     4.796317     233.84
 H       6.073365    -4.902944     5.024710      19.84
 C       6.357995    -2.295642     3.098117      42.92
 H       6.753984    -1.623133     3.925066      23.78
 C       5.375340    -2.704009     0.886429      41.09
 C       4.974426    -2.283917    -0.529639      91.92
 H       5.453187    -3.230429    -1.214135      21.50
 O       5.781176    -1.158286    -1.064478     229.49
 H       5.437919    -0.309565    -0.647965      24.00
 C       3.478288    -2.130224    -0.845446      87.98
 H       2.820607    -2.802501    -0.270367      21.91
 C       3.109857    -2.155313    -2.325433      98.14
 O       3.365364    -3.503410    -2.898948     235.96
 H       4.252667    -3.552158    -3.454585      26.15
 H       3.813388    -1.486656    -2.821917      22.52
 H       2.114510    -2.001160    -2.392658      26.41
 C      -0.575260    -1.256618     0.228362      45.97
 H      -1.326968    -2.094940     0.346107      17.54
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 C      -0.013637     1.135566     0.109600      72.17
 H      -0.395367     2.056089    -0.111579      18.95
 C       1.362118     0.772874    -0.161459      19.39
 O       2.387321     1.701267    -0.235092     190.21
 C       1.983915     3.101161    -0.057612     109.79
 H       2.832898     3.828278    -0.075917      24.83
 H       1.354395     3.659507    -0.994213      22.54
 H       1.562269     3.324308     0.978499      23.89
 C       1.721514    -0.547686    -0.193288      24.48
 O       3.138947    -0.772750    -0.389180     173.39
 C       0.787447    -1.572700    -0.098458      72.21
 H       0.863173    -2.727217    -0.233962      19.31
 C      -0.988418     0.128590     0.384643      48.01
 C      -2.427171     0.565012     0.690358      87.71
 H      -2.938703    -0.198748     1.276522      23.34
 O      -2.308295     1.810026     1.543105     285.00
 H      -2.085070     1.418572     2.454614      26.56
 C      -3.247587     0.882126    -0.560189      82.12
 H      -2.778480     1.632393    -1.279563      22.89
 O      -3.562648    -0.359617    -1.282647     271.87
 H      -3.383286    -0.141887    -2.212811      26.77
 C      -4.635893     1.678672    -0.128777      90.57
 O      -4.420427     3.089371    -0.020096     290.91
 H      -4.157400     3.277575     0.919227      28.83
 H      -4.939788     1.237564     0.879523      28.27
 H      -5.308267     1.409925    -0.955956      27.97
55
name = lig-etoh-Waterframe_289
 C       5.913037    -1.864646     1.830776      55.13
 H       6.066012    -0.831862     1.462757      24.11
 C       5.241247    -4.114799     1.255889      51.58
 H       4.933205    -4.776974     0.396567      14.51
 C       5.480772    -4.531578     2.539034      20.54
 O       5.360337    -5.877069     2.965489     228.93
 C       4.940327    -6.843742     1.899294     112.11
 H       5.844769    -7.062689     1.279303      27.85
 H       4.160389    -6.516899     1.179954      31.14
 H       4.571159    -7.687323     2.519974      24.02
 C       6.040785    -3.589253     3.562417      22.62
 O       6.447630    -3.960202     4.725871     151.76
 H       6.315679    -4.921251     5.027248      19.39
 C       6.302448    -2.298712     3.132376      76.41
 H       6.809419    -1.571666     3.732642      25.98
 C       5.322138    -2.721333     0.865230      22.97
 C       4.969117    -2.267882    -0.542920     115.02
 H       5.226060    -3.176021    -1.298612      23.93
 O       5.737498    -1.178151    -1.002105     229.91
 H       5.664943    -0.356383    -0.421666      26.85
 C       3.506104    -2.085182    -0.808520      95.80
 H       3.054258    -2.920801    -0.329476      22.26
 C       3.122826    -2.235524    -2.298184      95.85
 O       3.340263    -3.496424    -2.877562     253.03
 H       4.273047    -3.357600    -3.247630      25.57
 H       3.582127    -1.433269    -2.964311      22.59
 H       2.065307    -2.055617    -2.392293      25.09
 C      -0.567067    -1.266833     0.317243      34.34
 H      -1.214288    -2.170311     0.362561      17.84
 C      -0.006565     1.029303     0.112353      72.39
 H      -0.292434     1.976362    -0.071276      21.43
 C       1.311003     0.820374    -0.127256      11.68
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 O       2.351003     1.800210    -0.165880     202.31
 C       2.040473     3.149119    -0.030089     119.15
 H       3.002799     3.516832    -0.082310      24.36
 H       1.336176     3.227753    -0.979861      22.81
 H       1.359049     3.282544     0.746350      26.02
 C       1.783140    -0.603609    -0.160577       0.61
 O       3.099539    -0.764579    -0.388864     174.24
 C       0.717360    -1.647868    -0.109840      70.71
 H       0.955297    -2.725197    -0.211142      21.46
 C      -0.954378     0.034208     0.389839      52.71
 C      -2.384539     0.554195     0.736557      83.15
 H      -2.926272    -0.257917     1.234925      23.85
 O      -2.323125     1.828183     1.580996     281.90
 H      -2.237689     1.419914     2.560426      24.74
 C      -3.302045     0.828911    -0.494643      89.26
 H      -2.833361     1.554859    -1.206690      23.74
 O      -3.521790    -0.401625    -1.288604     262.94
 H      -3.476271    -0.177954    -2.238217      26.76
 C      -4.623406     1.645298    -0.144974      99.94
 O      -4.438711     3.146745    -0.076467     267.23
 H      -4.300553     3.192547     0.921779      27.17
 H      -4.854298     1.274947     0.795022      30.02
 H      -5.439530     1.377812    -0.855855      28.63
55
name = lig-etoh-Waterframe_290
 C       5.929591    -1.864852     1.809422      59.14
 H       6.231141    -0.831397     1.579349      23.29
 C       5.170499    -4.128145     1.177437      62.33
 H       4.815797    -4.907104     0.482636      13.79
 C       5.521491    -4.522087     2.553501       1.84
 O       5.343757    -5.835344     2.948578     271.62
 C       4.925297    -6.874297     1.837627      69.94
 H       5.870885    -7.215620     1.254049      25.58
 H       4.151893    -6.423429     1.224662      29.91
 H       4.485685    -7.649324     2.419935      24.04
 C       6.007975    -3.614550     3.468817     -16.81
 O       6.490149    -3.975557     4.788708     224.22
 H       6.167335    -4.958102     4.860471      33.17
 C       6.215980    -2.244041     3.110251      61.04
 H       6.742274    -1.653269     3.780968      22.45
 C       5.318677    -2.770183     0.907995      41.45
 C       5.013056    -2.298505    -0.554105     121.39
 H       5.237761    -3.057256    -1.179454      28.12
 O       5.755404    -1.169046    -0.964928     215.76
 H       5.438318    -0.385927    -0.370980      24.96
 C       3.503658    -2.086097    -0.798547      88.42
 H       3.045358    -2.825560    -0.163687      21.46
 C       3.076879    -2.217590    -2.293561      83.62
 O       3.352951    -3.525698    -2.870809     265.84
 H       4.173427    -3.536752    -3.387142      27.99
 H       3.539059    -1.368341    -2.899540      22.29
 H       1.904884    -2.033409    -2.319516      23.15
 C      -0.570153    -1.371460     0.365102      33.98
 H      -1.399678    -2.019854     0.650587      17.02
 C      -0.031011     1.037735     0.091755      53.90
 H      -0.402530     2.059226     0.313756      17.77
 C       1.374269     0.749091    -0.056908       7.71
 O       2.323432     1.753354    -0.092663     219.52
 C       2.007763     3.198248    -0.069264     123.58
 H       2.891536     3.770663     0.016423      25.94
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 H       1.579239     3.672170    -0.906067      27.79
 H       1.480090     3.522690     0.800276      26.96
 C       1.702989    -0.626990    -0.152110      24.74
 O       3.065977    -0.787250    -0.376760     215.02
 C       0.763481    -1.630927    -0.080927      73.00
 H       1.127063    -2.588677    -0.185541      22.78
 C      -0.987023     0.016123     0.402626      44.12
 C      -2.353303     0.535940     0.788624      79.77
 H      -2.822897    -0.224222     1.447963      21.46
 O      -2.343469     1.772933     1.592725     274.15
 H      -2.327914     1.461155     2.631358      24.45
 C      -3.325529     0.868348    -0.523887      84.37
 H      -2.594925     1.443868    -1.035962      26.24
 O      -3.486894    -0.434864    -1.268446     241.82
 H      -3.604123    -0.180191    -2.209106      26.51
 C      -4.603159     1.590431    -0.120950     110.22
 O      -4.458179     3.125547    -0.131566     237.30
 H      -4.561013     3.464149     0.828658      26.06
 H      -5.088701     1.418073     0.783939      30.11
 H      -5.428644     1.435673    -0.864079      29.00
55
name = lig-etoh-Waterframe_291
 C       5.912497    -1.838711     1.777559      65.81
 H       6.120683    -0.826707     1.426806      25.16
 C       5.129149    -4.112639     1.229388      62.71
 H       4.713833    -4.768707     0.484642      19.57
 C       5.511617    -4.575139     2.453753       6.25
 O       5.315082    -5.855957     2.876354     251.44
 C       4.917358    -6.843378     1.877786      98.47
 H       5.809150    -7.297265     1.283792      24.72
 H       4.191412    -6.436320     1.188367      31.08
 H       4.540258    -7.693679     2.356044      23.57
 C       6.037017    -3.596869     3.465101     -24.79
 O       6.496255    -4.012817     4.796324     241.68
 H       6.124824    -4.936885     5.104951      29.55
 C       6.147583    -2.256904     3.115355      61.97
 H       6.533263    -1.638038     3.884140      20.27
 C       5.354226    -2.768129     0.862688      42.53
 C       5.040386    -2.343594    -0.541706     100.85
 H       5.419341    -3.076889    -1.157612      25.69
 O       5.805536    -1.130324    -0.931212     178.58
 H       5.299908    -0.249933    -0.671201      24.02
 C       3.481213    -2.143732    -0.803381      80.69
 H       2.892989    -2.864126    -0.190991      20.41
 C       3.026144    -2.185762    -2.283563      84.32
 O       3.342182    -3.557978    -2.871881     253.54
 H       4.106690    -3.422356    -3.452866      26.59
 H       3.629094    -1.442843    -2.820254      22.21
 H       1.836430    -2.140383    -2.364090      22.41
 C      -0.617875    -1.376241     0.388795      43.27
 H      -1.180309    -2.235184     0.748000      23.06
 C      -0.034308     1.050648     0.123857      64.71
 H      -0.332241     2.139508     0.503649      18.19
 C       1.291931     0.751736     0.023975      19.30
 O       2.327604     1.707215    -0.035111     145.29
 C       1.970904     3.262692    -0.086144      96.47
 H       3.025252     3.683083     0.080874      24.51
 H       1.563741     3.635169    -0.964260      27.03
 H       1.390257     3.494807     0.881980      24.39
 C       1.677339    -0.579344    -0.173307      15.32
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 O       3.055034    -0.815259    -0.355058     174.14
 C       0.759658    -1.665835     0.012557      52.69
 H       1.076944    -2.621549    -0.090644      21.09
 C      -0.963667     0.013405     0.398814      28.30
 C      -2.409225     0.491623     0.834139      79.65
 H      -2.913377    -0.333017     1.418483      23.43
 O      -2.356822     1.706909     1.590092     292.17
 H      -2.230976     1.324645     2.628323      23.73
 C      -3.223969     0.845404    -0.481586      70.83
 H      -2.764507     1.593491    -1.155439      25.96
 O      -3.471396    -0.419177    -1.226377     227.50
 H      -3.630774    -0.235083    -2.178955      26.56
 C      -4.639875     1.633857    -0.119726      90.19
 O      -4.477448     3.059328    -0.200322     248.79
 H      -4.678715     3.443459     0.725935      25.67
 H      -5.018850     1.191445     0.914145      27.64
 H      -5.217398     1.266722    -0.998931      28.73
55
name = lig-etoh-Waterframe_292
 C       5.864362    -1.824726     1.759570      60.64
 H       5.944937    -0.802022     1.428622      22.47
 C       5.096480    -4.056651     1.223852      61.73
 H       4.648337    -4.659299     0.492105      23.10
 C       5.524959    -4.591816     2.470162      26.24
 O       5.297246    -5.908158     2.816649     337.11
 C       4.908053    -6.848193     1.905301     111.64
 H       5.820062    -7.049347     1.320843      23.43
 H       4.145590    -6.561240     1.171754      28.69
 H       4.476363    -7.624748     2.533430      24.25
 C       6.060226    -3.687321     3.503580      12.59
 O       6.469292    -4.028024     4.741397     159.28
 H       6.118431    -4.985833     4.947597      29.21
 C       6.113757    -2.284141     3.131331      28.49
 H       6.305525    -1.463588     3.869128      21.22
 C       5.407569    -2.720975     0.837461      40.42
 C       5.042953    -2.309506    -0.573272      78.89
 H       5.431450    -3.150570    -1.374074      20.64
 O       5.834382    -1.114406    -0.919297     190.34
 H       5.341592    -0.212116    -0.707971      22.94
 C       3.441541    -2.201088    -0.813790      67.33
 H       3.013797    -3.137796    -0.306579      18.61
 C       3.028838    -2.254885    -2.288451     102.51
 O       3.284217    -3.533851    -2.879850     246.71
 H       4.228739    -3.446053    -3.315791      23.21
 H       3.471996    -1.468749    -2.840618      24.67
 H       1.962767    -1.918222    -2.439622      24.27
 C      -0.585732    -1.327069     0.391524      56.60
 H      -1.229731    -2.161616     0.651664      25.19
 C      -0.095887     1.055556     0.249760      64.00
 H      -0.426351     2.220422     0.258109      17.96
 C       1.271207     0.816060     0.043163       0.79
 O       2.312008     1.727152     0.007697     182.04
 C       1.983466     3.226650    -0.045212      92.25
 H       3.107608     3.570084    -0.016310      21.92
 H       1.449840     3.232672    -1.007144      24.84
 H       1.122330     3.456800     0.730286      21.92
 C       1.694694    -0.630854    -0.168473      -2.43
 O       3.055627    -0.830978    -0.327542     142.19
 C       0.714365    -1.658583     0.121497      59.96
 H       0.950707    -2.705732     0.093797      21.08
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 C      -1.016571    -0.012016     0.438457      32.51
 C      -2.430271     0.435477     0.781430      85.79
 H      -3.050628    -0.403940     1.176603      23.28
 O      -2.371993     1.632916     1.619075     270.79
 H      -2.015258     1.275052     2.619977      24.93
 C      -3.194615     0.833811    -0.420582      81.17
 H      -2.642692     1.562357    -1.110797      24.34
 O      -3.465413    -0.383881    -1.166546     237.84
 H      -3.438221    -0.153473    -2.127390      26.29
 C      -4.603178     1.582982    -0.175471      88.55
 O      -4.519666     2.994739    -0.260843     268.06
 H      -4.461454     3.327703     0.715364      24.91
 H      -5.041349     1.198331     0.926742      26.90
 H      -5.343687     1.221645    -0.912262      28.57
55
name = lig-etoh-Waterframe_293
 C       5.830356    -1.813301     1.849305      54.00
 H       5.922836    -0.745880     1.767167      22.21
 C       5.113685    -4.014925     1.204065      72.75
 H       4.666102    -4.716913     0.580381      25.46
 C       5.519168    -4.568735     2.502190      25.16
 O       5.303259    -5.878567     2.852595     275.96
 C       4.882985    -6.918026     1.848090      97.90
 H       5.677222    -7.303545     1.272360      25.94
 H       4.001887    -6.560350     1.280537      28.58
 H       4.615652    -7.831359     2.488628      23.31
 C       6.046526    -3.694466     3.433815      21.82
 O       6.432837    -4.083617     4.713724     152.59
 H       6.243987    -5.066890     4.842497      31.49
 C       6.077956    -2.315048     3.096449      34.99
 H       6.279363    -1.579829     3.975115      19.01
 C       5.400623    -2.727509     0.798448      16.35
 C       5.030788    -2.225192    -0.635678      90.93
 H       5.363368    -3.151749    -1.440282      22.32
 O       5.828125    -1.112464    -0.949839     218.68
 H       5.430396    -0.312170    -0.388371      23.42
 C       3.479726    -2.211972    -0.835681      73.40
 H       3.016477    -3.001325    -0.165582      19.33
 C       3.031131    -2.253331    -2.313418     101.84
 O       3.208003    -3.522210    -2.901971     239.03
 H       4.136653    -3.637792    -3.344889      26.52
 H       3.647424    -1.542053    -2.834305      23.20
 H       2.006598    -2.119878    -2.318364      26.69
 C      -0.618261    -1.298483     0.421222      31.22
 H      -1.459547    -1.976195     0.525774      17.95
 C      -0.121929     1.075499     0.357354      52.80
 H      -0.659431     2.061726     0.194662      16.22
 C       1.292693     0.746386     0.027842       6.48
 O       2.291625     1.754834     0.064921     202.05
 C       1.963201     3.064177    -0.050350     131.73
 H       2.731150     3.904934     0.004144      24.87
 H       1.564462     3.409090    -1.128056      24.66
 H       1.406640     3.602442     0.782314      25.40
 C       1.665565    -0.616563    -0.077667      20.71
 O       3.044948    -0.899360    -0.301797     177.21
 C       0.769220    -1.622691     0.182192      61.97
 H       1.040446    -2.735947     0.257856      19.98
 C      -1.066652     0.020049     0.493438      36.73
 C      -2.450944     0.395112     0.762898      92.55
 H      -2.967475    -0.417831     1.273999      24.00
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 O      -2.391974     1.544802     1.670304     273.17
 H      -2.026860     1.099741     2.611871      26.22
 C      -3.258454     0.877319    -0.466380      97.09
 H      -2.440327     1.469987    -0.928047      23.57
 O      -3.458296    -0.368920    -1.138783     264.47
 H      -3.233031    -0.213486    -2.093772      25.53
 C      -4.561634     1.460722    -0.205153     110.69
 O      -4.568532     2.959740    -0.297357     258.56
 H      -4.154887     3.292208     0.579015      27.12
 H      -4.987203     1.322937     0.819060      28.58
 H      -5.287031     1.162783    -0.937865      27.94
55
name = lig-etoh-Waterframe_294
 C       5.778903    -1.802355     1.869451      52.20
 H       5.875793    -0.720943     1.780463      21.63
 C       5.169242    -4.065729     1.204817      40.19
 H       4.755683    -4.726989     0.463258      16.02
 C       5.463793    -4.551389     2.421150      26.44
 O       5.310418    -5.881947     2.881165     263.02
 C       4.864605    -6.975623     1.836720      75.39
 H       5.581872    -7.196834     1.070189      31.27
 H       3.930328    -6.643338     1.301782      33.04
 H       4.612355    -7.883287     2.513416      25.96
 C       6.028118    -3.683634     3.408643       0.14
 O       6.402108    -4.147695     4.690146     146.87
 H       6.188337    -5.099971     4.849821      27.25
 C       6.069847    -2.348739     3.149460      55.00
 H       6.459091    -1.729222     4.038850      17.05
 C       5.363270    -2.669540     0.796853      36.36
 C       5.037991    -2.240940    -0.637086     121.62
 H       5.452971    -2.988828    -1.359624      24.33
 O       5.784976    -1.064683    -1.000512     239.66
 H       5.629821    -0.287870    -0.342815      24.69
 C       3.515173    -2.151070    -0.833817      85.57
 H       3.111098    -3.017347    -0.288831      17.73
 C       3.033693    -2.213959    -2.305578      86.55
 O       3.131084    -3.590575    -2.939836     259.28
 H       3.970174    -3.385610    -3.525360      24.02
 H       3.598383    -1.438048    -2.917324      20.99
 H       2.007744    -1.989553    -2.342845      25.41
 C      -0.650660    -1.304471     0.452116      38.98
 H      -1.298188    -2.189464     0.527692      19.66
 C      -0.064467     1.059455     0.378069      75.88
 H      -0.271144     2.074943     0.474553      19.94
 C       1.215735     0.751081     0.071688      21.25
 O       2.305804     1.688220     0.114928     188.43
 C       1.908446     3.106243    -0.077735     107.00
 H       2.959189     3.388869     0.004739      20.99
 H       1.271210     3.316218    -1.073127      23.42
 H       1.195229     3.203889     0.707962      23.70
 C       1.725767    -0.605446     0.022316       9.75
 O       3.018065    -0.932855    -0.268259     200.66
 C       0.707300    -1.617778     0.251687      51.86
 H       1.242942    -2.677234     0.246997      17.20
 C      -1.010857     0.050965     0.512323      42.95
 C      -2.520032     0.407642     0.833714      81.63
 H      -2.999440    -0.478307     1.247655      24.98
 O      -2.428045     1.467552     1.744532     326.41
 H      -2.269702     1.020891     2.649335      26.83
 C      -3.205570     0.843867    -0.488268      83.71
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 H      -2.779504     1.641914    -1.144667      24.20
 O      -3.443399    -0.399685    -1.190903     255.14
 H      -3.238260    -0.390773    -2.169856      24.81
 C      -4.627007     1.479029    -0.202204     105.66
 O      -4.601450     2.918026    -0.341947     252.87
 H      -4.137212     3.252775     0.506060      26.15
 H      -4.874196     1.039227     0.677650      30.99
 H      -5.197146     1.038053    -1.008782      28.67
55
name = lig-etoh-Waterframe_295
 C       5.725716    -1.794289     1.861551      55.20
 H       5.821326    -0.730555     1.578449      23.21
 C       5.207755    -4.058444     1.072918      87.03
 H       4.893110    -4.768048     0.253324      12.59
 C       5.442198    -4.622357     2.420184      35.77
 O       5.295438    -5.925066     2.826746     280.44
 C       4.843945    -6.949442     1.881533     103.37
 H       5.654722    -6.949095     1.125504      32.10
 H       3.855867    -6.690236     1.435545      33.69
 H       4.777596    -7.893820     2.519529      23.51
 C       5.983353    -3.751687     3.454577     -18.20
 O       6.373110    -4.205803     4.653573     156.48
 H       6.006318    -5.093483     4.751394      27.23
 C       6.095576    -2.323187     3.210951      41.44
 H       6.567890    -1.638165     3.927350      19.61
 C       5.328065    -2.658821     0.886459      46.46
 C       5.086989    -2.236524    -0.594272     102.85
 H       5.383024    -2.956332    -1.180874      25.39
 O       5.744841    -0.997639    -1.062720     268.17
 H       5.445532    -0.185765    -0.525783      24.43
 C       3.498414    -2.145046    -0.855301      77.13
 H       3.127156    -3.056978    -0.465919      18.69
 C       3.005295    -2.194893    -2.318697      83.51
 O       3.086437    -3.576474    -2.969963     237.30
 H       3.909029    -3.661147    -3.603490      25.01
 H       3.593355    -1.508315    -3.052509      20.75
 H       1.955584    -1.756688    -2.342436      23.31
 C      -0.625339    -1.336442     0.475373      55.49
 H      -1.349999    -2.152713     0.728606      22.61
 C      -0.040645     1.079458     0.386253      62.66
 H      -0.203449     1.992108     0.770813      21.03
 C       1.332309     0.716828     0.149206      12.27
 O       2.285733     1.599884     0.113141     183.14
 C       1.864100     3.096493    -0.066958     104.39
 H       2.785565     3.689770    -0.049877      24.98
 H       1.397781     3.154712    -1.044431      25.51
 H       1.272683     3.480217     0.748384      24.94
 C       1.663807    -0.671420     0.097770      31.87
 O       3.030011    -0.885405    -0.210234     189.82
 C       0.733516    -1.601631     0.294125      59.89
 H       0.858980    -2.757504     0.264888      17.58
 C      -1.055010     0.008753     0.542467      35.61
 C      -2.460415     0.420255     0.829966      83.21
 H      -3.114774    -0.438333     1.062770      22.75
 O      -2.513152     1.453021     1.849604     334.32
 H      -2.298455     1.039577     2.652656      28.58
 C      -3.220747     0.810760    -0.506466      71.70
 H      -2.648618     1.506777    -1.170579      24.22
 O      -3.418819    -0.468298    -1.265980     219.49
 H      -3.310589    -0.176260    -2.233627      23.94
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 C      -4.666957     1.451606    -0.232563     100.63
 O      -4.634208     2.877148    -0.364405     243.08
 H      -4.427863     3.283769     0.556736      25.31
 H      -5.146227     1.131422     0.709305      29.33
 H      -5.402924     1.151813    -1.048604      28.05
55
name = lig-etoh-Waterframe_296
 C       5.719251    -1.798815     1.968879      57.85
 H       5.853485    -0.729457     1.698431      21.41
 C       5.252897    -4.099608     1.067725      24.23
 H       5.059903    -4.725281     0.113087       8.56
 C       5.444236    -4.630980     2.363320      47.44
 O       5.269348    -5.948905     2.786008     264.92
 C       4.846992    -6.901404     1.918066     160.10
 H       5.559200    -7.080690     1.008546      30.11
 H       3.833131    -6.768741     1.542979      31.91
 H       4.967282    -7.862515     2.374861      21.20
 C       5.907422    -3.720176     3.420161      -1.37
 O       6.345366    -4.291520     4.658295     285.59
 H       6.069466    -5.207362     4.853310      31.67
 C       6.099450    -2.315951     3.163000      69.55
 H       6.517166    -1.712904     3.902308      25.09
 C       5.297612    -2.694039     0.881634      38.96
 C       5.063309    -2.159289    -0.560906      90.06
 H       5.481239    -2.981407    -1.181291      22.71
 O       5.705419    -0.961228    -1.106978     285.19
 H       5.201514    -0.193699    -0.757570      24.82
 C       3.495374    -2.167385    -0.874743      63.96
 H       2.975396    -2.918535    -0.298283      18.18
 C       3.013790    -2.170576    -2.405291      86.50
 O       3.031136    -3.517859    -2.967216     236.36
 H       4.007204    -3.547998    -3.307571      23.21
 H       3.732983    -1.507496    -2.979098      22.11
 H       1.855823    -1.982353    -2.409135      22.78
 C      -0.647213    -1.314235     0.531577      52.00
 H      -1.408898    -2.093716     0.789135      23.36
 C      -0.040240     1.008113     0.432402      69.25
 H      -0.447055     1.963237     0.736445      19.58
 C       1.297548     0.639357     0.265860      12.33
 O       2.343035     1.660850     0.095154     165.95
 C       1.872951     3.030380    -0.047609     130.61
 H       2.667326     3.738722    -0.199422      26.78
 H       1.352287     3.107416    -0.923270      27.99
 H       1.277347     3.517690     0.743778      26.32
 C       1.708202    -0.697871     0.103110       9.39
 O       3.054337    -0.864040    -0.154862     147.81
 C       0.691337    -1.732323     0.328329      46.91
 H       1.021388    -2.791860     0.248207      17.26
 C      -1.019451     0.008331     0.561867      36.95
 C      -2.454557     0.417003     0.785546      78.83
 H      -2.944331    -0.492527     1.245544      23.33
 O      -2.586760     1.482816     1.881776     299.78
 H      -2.216977     1.011529     2.645985      26.90
 C      -3.295847     0.772986    -0.517481      83.14
 H      -2.570660     1.393093    -1.027367      25.11
 O      -3.381149    -0.499052    -1.313390     211.66
 H      -3.422480    -0.268888    -2.316783      23.84
 C      -4.693319     1.385849    -0.290720      99.32
 O      -4.664385     2.882792    -0.364658     210.66
 H      -4.698815     3.208193     0.604348      24.89
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 H      -5.195500     1.246889     0.759093      27.83
 H      -5.385621     1.037183    -1.139548      28.43
55
name = lig-etoh-Waterframe_297
 C       5.687125    -1.822339     1.925011      60.93
 H       5.817347    -0.726001     1.927901      20.07
 C       5.286915    -4.106420     1.077183      39.12
 H       5.141990    -4.862959     0.227058      13.27
 C       5.463056    -4.599455     2.352122      22.58
 O       5.279444    -5.885796     2.798913     301.38
 C       4.842312    -6.971540     1.840902     117.44
 H       5.357396    -6.898320     0.825697      27.85
 H       3.782964    -6.812715     1.650181      31.61
 H       4.903470    -7.809598     2.436989      20.69
 C       5.860316    -3.756036     3.402445      11.71
 O       6.310090    -4.320516     4.642117     298.46
 H       6.059156    -5.285264     4.712624      27.92
 C       6.097758    -2.401968     3.201627      49.59
 H       6.437043    -1.833954     4.010771      24.01
 C       5.324604    -2.646417     0.886534      16.52
 C       4.987345    -2.145016    -0.587014      78.96
 H       5.586978    -2.968682    -1.327989      19.92
 O       5.647019    -0.954892    -1.117691     302.74
 H       5.305904    -0.112675    -0.773568      24.49
 C       3.482547    -2.128660    -0.859475      72.04
 H       3.030848    -3.025344    -0.312086      16.92
 C       3.020283    -2.150208    -2.405811      97.59
 O       3.039668    -3.463711    -2.953209     260.03
 H       3.963638    -3.655385    -3.345286      24.83
 H       3.572547    -1.450625    -2.971365      23.38
 H       1.965323    -1.688624    -2.542730      23.32
 C      -0.652433    -1.374766     0.602150      36.59
 H      -1.456700    -2.127200     0.690062      15.90
 C      -0.040629     0.971836     0.519049      71.57
 H      -0.335792     2.093245     0.314998      16.43
 C       1.300161     0.663630     0.343998      -3.58
 O       2.380664     1.700655     0.104559     168.39
 C       1.869718     3.005603    -0.067195     110.04
 H       2.862964     3.450051    -0.208882      23.24
 H       1.104074     3.090593    -0.853010      24.96
 H       1.253141     3.124082     0.886344      23.39
 C       1.717682    -0.753844     0.121855      -2.41
 O       3.080922    -0.890405    -0.141374     157.02
 C       0.702634    -1.803421     0.327939      43.93
 H       0.994361    -2.792757     0.290699      19.28
 C      -1.012657     0.017853     0.571271      42.75
 C      -2.529817     0.393237     0.825852      70.46
 H      -2.885067    -0.560592     1.304996      23.71
 O      -2.606031     1.516368     1.789637     292.72
 H      -2.264053     1.071850     2.715012      25.48
 C      -3.302250     0.710559    -0.520457      87.81
 H      -2.901471     1.559343    -1.088602      23.64
 O      -3.354684    -0.509010    -1.313696     253.98
 H      -3.336410    -0.339898    -2.320749      23.13
 C      -4.728940     1.385636    -0.337547      94.69
 O      -4.699492     2.871071    -0.367124     255.84
 H      -4.647176     3.165732     0.610031      24.92
 H      -5.030834     0.796413     0.635441      28.33
 H      -5.316442     0.917152    -1.138999      29.66
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name = lig-etoh-Waterframe_298
 C       5.704655    -1.832178     1.949007      56.91
 H       5.623984    -0.750358     1.751602      22.12
 C       5.309660    -4.035428     1.059088      35.03
 H       5.063978    -4.751688     0.263362       7.48
 C       5.464745    -4.600168     2.362251      51.73
 O       5.290833    -5.879377     2.772594     276.92
 C       4.797632    -6.977074     1.790891     146.84
 H       5.409702    -6.932393     0.878605      35.01
 H       3.717615    -6.833937     1.683764      31.13
 H       5.067382    -7.881994     2.267128      25.44
 C       5.905659    -3.812310     3.476232      24.35
 O       6.260236    -4.315750     4.601686     130.60
 H       5.963938    -5.291132     4.678542      26.55
 C       6.044438    -2.462465     3.217590      66.47
 H       6.371889    -1.840860     4.062110      23.62
 C       5.352108    -2.638352     0.804461      27.74
 C       4.982606    -2.160283    -0.634812      92.25
 H       5.254778    -3.117257    -1.371200      21.80
 O       5.595488    -0.953536    -1.114694     347.59
 H       5.453143    -0.244258    -0.488381      27.68
 C       3.451173    -2.093507    -0.851830      80.20
 H       3.066317    -3.121772    -0.492330      16.46
 C       3.033921    -2.053811    -2.345685      93.84
 O       3.075599    -3.451212    -2.937817     244.02
 H       3.891073    -3.452410    -3.530338      26.36
 H       3.764629    -1.592737    -2.925355      20.45
 H       2.018150    -1.689314    -2.404766      23.78
 C      -0.623329    -1.422034     0.629588      23.04
 H      -1.365613    -2.199887     0.687485      16.02
 C       0.014473     1.034400     0.551551      54.48
 H      -0.337917     2.152453     0.235384      14.75
 C       1.416394     0.647316     0.344291       3.06
 O       2.349989     1.588805     0.118135     176.38
 C       1.850457     2.983402    -0.039739     102.34
 H       2.635735     3.814322    -0.202197      23.46
 H       1.146174     3.169980    -0.990193      22.09
 H       1.528009     3.499688     0.942231      23.42
 C       1.674091    -0.739533     0.194051      13.84
 O       3.058148    -0.946305    -0.149214     190.80
 C       0.736592    -1.756750     0.321939      62.69
 H       0.881927    -2.747957     0.220349      19.52
 C      -1.094662    -0.084512     0.630612      43.92
 C      -2.543380     0.363744     0.854433      80.70
 H      -3.218204    -0.431902     1.206080      23.28
 O      -2.613150     1.533702     1.646799     266.53
 H      -2.428442     1.226161     2.697858      25.25
 C      -3.298702     0.724815    -0.535476      80.00
 H      -2.626833     1.455788    -1.115098      21.67
 O      -3.334172    -0.528944    -1.286066     257.26
 H      -3.211237    -0.194436    -2.220842      24.03
 C      -4.735288     1.312966    -0.350873     105.56
 O      -4.744496     2.793856    -0.352799     275.36
 H      -4.561685     3.167563     0.547224      26.78
 H      -5.369633     1.065332     0.552326      28.09
 H      -5.360079     1.198219    -1.203394      28.02
55
name = lig-etoh-Waterframe_299
 C       5.716742    -1.860995     1.935814      56.99
 H       5.687506    -0.765860     1.927705      23.10
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 C       5.306075    -4.014588     1.055074      52.29
 H       4.981756    -4.576631     0.243333      11.97
 C       5.468294    -4.586976     2.332317      35.32
 O       5.277664    -5.974339     2.696963     304.43
 C       4.803481    -6.913453     1.794430     139.75
 H       5.252987    -6.819191     0.827439      37.58
 H       3.696761    -6.928800     1.544671      34.68
 H       5.093339    -7.924953     2.186246      26.72
 C       5.934931    -3.806270     3.389585     -16.10
 O       6.235719    -4.353460     4.681011     126.84
 H       5.964844    -5.355529     4.855889      22.40
 C       5.972292    -2.394577     3.193272      49.29
 H       6.291688    -1.719103     4.064066      18.72
 C       5.402898    -2.643046     0.767200      30.17
 C       4.975833    -2.210243    -0.670050      96.67
 H       5.320373    -2.918204    -1.368690      24.97
 O       5.573631    -0.974078    -1.106183     338.58
 H       5.481136    -0.334979    -0.415146      29.25
 C       3.436805    -2.139530    -0.858701      85.75
 H       2.901244    -2.980343    -0.381039      18.56
 C       3.081890    -2.000018    -2.312317      89.61
 O       3.109096    -3.420419    -2.916980     271.21
 H       3.893551    -3.325910    -3.491654      26.20
 H       3.790994    -1.287608    -2.814434      20.81
 H       2.108054    -1.665297    -2.452966      25.88
 C      -0.627722    -1.422641     0.623331      30.88
 H      -1.209254    -2.287371     0.790787      20.40
 C      -0.001899     0.933928     0.531084      81.82
 H      -0.362939     2.034443     0.683425      16.86
 C       1.303003     0.641529     0.344962      19.17
 O       2.359312     1.547455     0.116057     183.23
 C       1.877423     3.027423     0.004962      91.25
 H       2.859299     3.447920    -0.413300      21.50
 H       1.013991     2.932485    -0.848451      22.21
 H       1.232055     3.370029     0.862954      23.22
 C       1.739568    -0.726792     0.240245      18.51
 O       2.975997    -0.973435    -0.123589     201.95
 C       0.719326    -1.691944     0.338892      54.76
 H       1.091858    -2.677844     0.083741      17.48
 C      -1.026825    -0.084153     0.718515      69.85
 C      -2.572037     0.334934     0.790326      79.76
 H      -3.158454    -0.424827     1.309903      24.06
 O      -2.633984     1.580994     1.532478     258.79
 H      -2.368366     1.277986     2.583068      23.78
 C      -3.264533     0.722663    -0.506448      82.00
 H      -2.542860     1.425814    -1.034428      22.71
 O      -3.314616    -0.539650    -1.261630     237.54
 H      -3.297941    -0.415177    -2.252714      24.48
 C      -4.766008     1.313160    -0.373544     101.47
 O      -4.771904     2.729730    -0.348799     303.34
 H      -4.679509     3.031533     0.577939      26.60
 H      -5.329815     0.894968     0.436360      29.36
 H      -5.221518     0.977440    -1.322479      28.18
55
name = lig-etoh-Waterframe_300
 C       5.714615    -1.812103     1.867907      64.92
 H       5.846050    -0.743237     1.844125      22.19
 C       5.269570    -4.061041     1.016574      61.02
 H       4.948739    -4.705701     0.280600      15.43
 C       5.478913    -4.669581     2.291284      37.61
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 O       5.282899    -5.977786     2.650352     265.08
 C       4.801382    -6.910260     1.695123     117.50
 H       5.206764    -6.727898     0.725232      36.54
 H       3.665747    -6.807385     1.710402      31.48
 H       5.029720    -7.944616     2.189363      24.73
 C       5.949075    -3.796536     3.387837     -25.98
 O       6.214510    -4.344359     4.738961     108.33
 H       5.994076    -5.363785     4.716167      26.65
 C       5.929924    -2.378433     3.186974      32.61
 H       6.135674    -1.624739     4.047665      16.85
 C       5.448016    -2.654467     0.791992      35.74
 C       4.996730    -2.241617    -0.653893      90.24
 H       5.395643    -2.893615    -1.289358      25.26
 O       5.574087    -1.003090    -1.093610     310.37
 H       5.349890    -0.193196    -0.622029      27.31
 C       3.399943    -2.199784    -0.805842      77.62
 H       2.969762    -3.107069    -0.435558      20.28
 C       3.092593    -2.014727    -2.327942      92.75
 O       3.165223    -3.330823    -2.907954     289.06
 H       3.986093    -3.522269    -3.381691      27.81
 H       3.823698    -1.226418    -2.788925      20.53
 H       2.090226    -1.621244    -2.468154      25.57
 C      -0.626841    -1.424095     0.624826      52.78
 H      -1.370487    -2.176621     0.811993      21.85
 C      -0.118035     0.875147     0.560410      76.14
 H      -0.397303     1.838057     0.895608      18.74
 C       1.278228     0.617041     0.326139      14.09
 O       2.328671     1.586846     0.138564     187.09
 C       1.889045     2.939176    -0.016033     117.06
 H       2.829106     3.509237    -0.224403      24.59
 H       1.152383     3.038199    -0.839964      25.36
 H       1.587398     3.309390     0.949867      25.74
 C       1.676980    -0.705593     0.253553      26.76
 O       3.002394    -0.959810    -0.096162     187.25
 C       0.740833    -1.684683     0.350652      67.41
 H       1.028245    -2.806938     0.163681      17.77
 C      -1.026760    -0.087072     0.762338      45.91
 C      -2.523794     0.339247     0.781167      80.18
 H      -2.917703    -0.540252     1.293689      22.25
 O      -2.663902     1.637906     1.470787     276.13
 H      -2.239398     1.397947     2.478775      22.39
 C      -3.238710     0.670673    -0.522715      85.99
 H      -2.792228     1.530476    -1.006937      24.62
 O      -3.305026    -0.575876    -1.250505     230.12
 H      -3.407860    -0.312460    -2.205784      25.21
 C      -4.730142     1.263350    -0.426159      96.20
 O      -4.810618     2.700001    -0.353341     296.80
 H      -4.900992     3.005006     0.566797      26.48
 H      -5.118944     0.663595     0.341194      29.52
 H      -5.174423     0.839676    -1.377721      28.70
55
name = lig-etoh-Waterframe_301
 C       5.741082    -1.774705     1.862861      67.38
 H       5.840005    -0.775289     1.489063      23.05
 C       5.250624    -4.134701     1.023367      39.09
 H       4.953594    -4.739409     0.199548      18.92
 C       5.529052    -4.666809     2.288798      28.50
 O       5.321604    -5.950906     2.639924     230.73
 C       4.752651    -6.939309     1.593539     105.19
 H       5.220255    -6.855234     0.599523      30.27
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 H       3.651329    -6.815823     1.572550      28.87
 H       5.118043    -7.987494     1.922974      23.62
 C       5.922148    -3.801958     3.452031       7.82
 O       6.182438    -4.280359     4.691665     139.63
 H       6.049576    -5.305761     4.742426      28.03
 C       5.912542    -2.408270     3.154922      56.48
 H       6.054149    -1.771885     4.071072      21.30
 C       5.428425    -2.710385     0.785872      11.87
 C       5.011455    -2.227386    -0.575960      78.44
 H       5.332259    -3.112854    -1.315875      20.62
 O       5.601046    -1.016579    -1.096531     295.43
 H       5.080116    -0.278063    -0.725325      25.61
 C       3.417793    -2.201949    -0.773889      74.41
 H       2.997693    -3.112306    -0.417043      19.96
 C       3.086346    -2.033526    -2.306747      91.09
 O       3.199996    -3.292166    -2.919751     268.78
 H       4.124925    -3.245259    -3.423626      22.71
 H       3.936768    -1.429338    -2.785649      18.13
 H       2.009725    -1.664628    -2.448846      22.54
 C      -0.638849    -1.441278     0.644159       8.91
 H      -1.391833    -2.252695     0.682609      16.68
 C      -0.085312     0.975923     0.626333      69.09
 H      -0.437217     1.917625     0.647212      18.98
 C       1.266220     0.661479     0.319330      16.91
 O       2.262442     1.573718     0.167281     240.39
 C       1.921510     2.909586    -0.022097     141.31
 H       2.737961     3.528286    -0.240487      26.99
 H       1.252681     3.172872    -0.709389      28.47
 H       1.566602     3.338879     0.879452      27.04
 C       1.668070    -0.721573     0.194371      13.77
 O       3.059769    -0.951172    -0.058641     167.10
 C       0.680592    -1.778162     0.377625      60.54
 H       0.976221    -2.946795     0.347554      18.39
 C      -1.111393    -0.134943     0.723721      71.28
 C      -2.468500     0.373743     0.838453      95.41
 H      -3.179425    -0.362670     1.272901      24.51
 O      -2.679602     1.658648     1.457483     260.69
 H      -2.297941     1.631865     2.486828      30.38
 C      -3.234942     0.642725    -0.567831      93.82
 H      -2.578334     1.281472    -1.143447      25.16
 O      -3.300606    -0.619069    -1.278640     236.69
 H      -3.328455    -0.344896    -2.231288      26.06
 C      -4.654507     1.140904    -0.453446     101.73
 O      -4.867281     2.656532    -0.372244     238.46
 H      -4.961509     2.993031     0.532225      28.12
 H      -5.299214     0.794579     0.426639      28.04
 H      -5.254233     1.088835    -1.396607      27.51
55
name = lig-etoh-Waterframe_302
 C       5.755029    -1.890998     1.824215      64.80
 H       5.814526    -0.794499     1.732569      23.90
 C       5.281263    -4.118381     1.052885      34.13
 H       4.998746    -4.808607     0.225143      17.65
 C       5.568498    -4.619832     2.329844       4.80
 O       5.345619    -6.024338     2.600972     296.89
 C       4.760743    -6.937507     1.539678      89.95
 H       5.192957    -6.679199     0.527950      25.72
 H       3.700116    -6.920145     1.385642      32.10
 H       5.012844    -7.924827     1.946965      20.11
 C       5.847604    -3.783726     3.367431      16.64
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 O       6.157744    -4.218372     4.651721     261.96
 H       5.997103    -5.204344     4.830862      33.93
 C       5.926985    -2.393130     3.153569      49.49
 H       6.123494    -1.799210     4.006631      21.16
 C       5.389088    -2.754397     0.832968      55.91
 C       4.985937    -2.259295    -0.562289      81.12
 H       5.351127    -3.130969    -1.426629      23.22
 O       5.629873    -1.042603    -1.087590     221.30
 H       5.147833    -0.254948    -0.727032      26.06
 C       3.491608    -2.138981    -0.761105      83.83
 H       2.953794    -2.944518    -0.238666      18.00
 C       3.100483    -2.028993    -2.232368      90.51
 O       3.206471    -3.329343    -2.941868     257.36
 H       4.016730    -3.300602    -3.699321      22.63
 H       3.668768    -1.205942    -2.651301      21.08
 H       2.048870    -1.562176    -2.399820      22.63
 C      -0.712039    -1.471715     0.649516      37.17
 H      -1.399137    -2.364984     0.723890      16.71
 C      -0.087610     1.000247     0.666964      76.04
 H      -0.399108     1.979152     0.425748      18.52
 C       1.207825     0.634899     0.331938       5.25
 O       2.253785     1.542411     0.171498     164.46
 C       1.929288     3.008592     0.005631     114.39
 H       2.910658     3.273103    -0.310273      24.31
 H       1.151034     3.010318    -0.824346      24.37
 H       1.328629     3.358807     0.857199      24.50
 C       1.662443    -0.803235     0.141454      12.34
 O       3.047828    -0.954394    -0.013229     190.51
 C       0.696263    -1.800364     0.397409      43.86
 H       1.023034    -2.921003     0.373681      17.77
 C      -1.032243    -0.044613     0.675450      59.78
 C      -2.584605     0.410078     0.838475      79.36
 H      -3.165935    -0.380522     1.399648      23.97
 O      -2.669737     1.695938     1.470800     282.06
 H      -2.403587     1.543886     2.512937      28.95
 C      -3.168573     0.601275    -0.593571      87.49
 H      -2.511882     1.251008    -1.212206      23.15
 O      -3.300045    -0.686947    -1.320956     239.81
 H      -3.123349    -0.558235    -2.281065      24.73
 C      -4.677496     1.169680    -0.465053      79.96
 O      -4.905285     2.596833    -0.407339     264.00
 H      -4.807547     2.868437     0.521311      29.05
 H      -5.247924     0.513650     0.408663      26.55
 H      -5.088007     0.683593    -1.408852      26.71
55
name = lig-etoh-Waterframe_303
 C       5.765987    -1.946780     1.879859      61.19
 H       5.777378    -0.822108     1.755674      24.57
 C       5.329721    -4.120420     1.081365      37.50
 H       5.022076    -4.856825     0.243738      10.54
 C       5.511207    -4.734630     2.295853      44.06
 O       5.361939    -6.085605     2.552258     303.84
 C       4.807461    -6.896750     1.523481     152.76
 H       5.368119    -6.767167     0.534403      32.21
 H       3.757104    -6.731683     1.482688      30.97
 H       5.027340    -7.878055     1.806197      24.40
 C       5.819066    -3.752851     3.372281      30.54
 O       6.132519    -4.166724     4.639000     177.56
 H       5.867580    -5.124887     4.703991      31.43
 C       5.959178    -2.380954     3.142563      72.91
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 H       6.249792    -1.706813     3.864116      23.56
 C       5.347070    -2.756236     0.783615      78.73
 C       4.998320    -2.278504    -0.603559     100.69
 H       5.348279    -3.115846    -1.341700      24.93
 O       5.668274    -1.084319    -1.058654     235.53
 H       5.488753    -0.226363    -0.562025      26.00
 C       3.495371    -2.104966    -0.714689      80.12
 H       3.069415    -3.106652    -0.302791      16.90
 C       3.093307    -2.004428    -2.208071      88.22
 O       3.161303    -3.351889    -2.943630     229.92
 H       4.119814    -3.372367    -3.357045      24.76
 H       3.742729    -1.334385    -2.704070      21.11
 H       1.994654    -1.882097    -2.143611      23.03
 C      -0.682257    -1.404604     0.622591      47.64
 H      -1.551985    -2.065152     0.914984      20.07
 C      -0.091013     0.968298     0.616942      56.95
 H      -0.426577     2.088884     0.650520      16.24
 C       1.252117     0.530868     0.324864      10.66
 O       2.259256     1.539181     0.180331     140.39
 C       1.891573     2.997301    -0.003155      95.60
 H       2.886231     3.604749    -0.129610      23.89
 H       1.312726     3.112199    -1.101082      21.96
 H       1.537936     3.615499     0.927910      23.27
 C       1.611375    -0.778349     0.163783      27.75
 O       3.010803    -0.943801     0.017817     188.14
 C       0.672882    -1.792841     0.405418      43.39
 H       0.980650    -2.807446     0.267198      15.19
 C      -1.073902    -0.040054     0.695220      46.50
 C      -2.585983     0.410977     0.768039      80.37
 H      -2.949718    -0.507361     1.295714      23.19
 O      -2.665731     1.734040     1.495127     292.28
 H      -2.476477     1.338490     2.454155      26.93
 C      -3.174171     0.569230    -0.612549      81.84
 H      -2.596958     1.383203    -1.137771      23.45
 O      -3.279947    -0.761289    -1.311067     247.84
 H      -3.080523    -0.474198    -2.233567      24.29
 C      -4.684776     1.134299    -0.522048      91.54
 O      -4.929007     2.514467    -0.448195     280.62
 H      -4.782372     2.867418     0.448553      29.07
 H      -5.046009     0.592537     0.425220      27.15
 H      -5.189440     0.768882    -1.436047      27.19
55
name = lig-etoh-Waterframe_304
 C       5.721316    -1.872211     1.816957      58.18
 H       5.852190    -0.782471     1.557984      23.60
 C       5.328154    -4.189506     1.014521      66.95
 H       5.080683    -4.803225     0.065581       7.97
 C       5.459844    -4.746765     2.323671      53.86
 O       5.410947    -6.107555     2.553938     299.78
 C       4.870434    -6.901704     1.494782     170.12
 H       5.376490    -6.750843     0.506116      37.67
 H       3.803337    -6.639275     1.308572      32.78
 H       4.934061    -7.918222     1.781982      24.94
 C       5.819570    -3.816851     3.395935      20.10
 O       6.095297    -4.165160     4.666375     162.78
 H       5.930920    -5.124288     4.827159      23.08
 C       6.001690    -2.417477     3.152565      55.93
 H       6.356719    -1.778868     3.942609      23.22
 C       5.382838    -2.747554     0.798324      52.58
 C       5.028728    -2.254304    -0.605759     125.91
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 H       5.213197    -2.965746    -1.249653      27.34
 O       5.749859    -1.106785    -1.038469     235.82
 H       5.598955    -0.439314    -0.299122      27.56
 C       3.459050    -2.144313    -0.716229      73.16
 H       3.015836    -3.133838    -0.326926      16.21
 C       3.035287    -2.058028    -2.208739     100.04
 O       3.118120    -3.351424    -2.886255     267.64
 H       4.027474    -3.391885    -3.263447      26.45
 H       3.545446    -1.331265    -2.820840      22.41
 H       2.005931    -1.743561    -2.304180      24.58
 C      -0.683799    -1.317930     0.627440      49.04
 H      -1.374229    -2.164211     0.842879      23.15
 C      -0.063125     0.903318     0.523244      82.15
 H      -0.267174     2.004098     0.971500      17.16
 C       1.250215     0.633955     0.325513      19.48
 O       2.275051     1.575063     0.194280     220.58
 C       1.916421     2.954103    -0.032421     106.28
 H       2.938960     3.513766    -0.078143      23.41
 H       1.198901     3.322652    -0.948669      22.94
 H       1.130719     3.298332     0.792147      22.47
 C       1.633256    -0.776068     0.217032      13.06
 O       2.981759    -0.955034     0.034579     184.66
 C       0.609845    -1.777120     0.379984      34.51
 H       0.786490    -2.757621     0.269976      16.67
 C      -1.108956    -0.014853     0.697330      73.09
 C      -2.474995     0.389940     0.722281      90.49
 H      -3.186035    -0.293697     1.163165      23.56
 O      -2.670889     1.690159     1.504523     293.43
 H      -2.479762     1.473120     2.464336      26.65
 C      -3.263435     0.572545    -0.647615      84.31
 H      -2.593943     1.167625    -1.317260      22.93
 O      -3.223767    -0.776550    -1.252616     226.38
 H      -3.323057    -0.638165    -2.244350      24.20
 C      -4.682046     1.009770    -0.555141     117.63
 O      -4.931793     2.475707    -0.498235     281.20
 H      -4.902450     2.840521     0.414586      28.70
 H      -5.198638     0.665245     0.249531      29.91
 H      -5.296047     0.805807    -1.380772      28.41
55
name = lig-etoh-Waterframe_305
 C       5.707547    -1.830081     1.822644      61.17
 H       5.902547    -0.767710     1.658274      22.53
 C       5.307820    -4.181696     0.974031      69.35
 H       5.182587    -4.868926     0.101198      19.37
 C       5.449136    -4.695808     2.300150      10.07
 O       5.467953    -6.104746     2.588943     273.40
 C       4.906877    -6.932396     1.439803     142.74
 H       5.573250    -6.806935     0.594071      31.29
 H       3.836960    -6.625382     1.152740      27.82
 H       4.890581    -7.959108     1.871568      23.42
 C       5.828414    -3.842723     3.364269      -1.68
 O       6.060768    -4.225345     4.751646     233.97
 H       6.043797    -5.187507     4.907508      22.76
 C       6.008346    -2.452569     3.073655      38.24
 H       6.364388    -1.947520     4.032981      20.72
 C       5.433824    -2.806806     0.804366       8.32
 C       5.018449    -2.268672    -0.580636      93.57
 H       5.287960    -3.011215    -1.316847      22.77
 O       5.829048    -1.102837    -1.001750     211.31
 H       5.638367    -0.288873    -0.403671      25.15
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 C       3.423475    -2.170612    -0.753568      75.47
 H       2.979513    -2.999437    -0.221022      21.03
 C       2.930082    -2.085333    -2.238484     100.92
 O       3.095278    -3.373360    -2.821553     297.50
 H       3.821945    -3.371984    -3.421298      29.45
 H       3.630286    -1.306104    -2.687798      22.54
 H       1.931678    -1.718333    -2.316942      25.97
 C      -0.747930    -1.367264     0.647750      40.66
 H      -1.458149    -2.174759     0.666292      14.13
 C      -0.061635     0.974376     0.505402      59.60
 H      -0.405524     2.092832     0.675578      19.14
 C       1.293041     0.659879     0.305485      12.76
 O       2.298274     1.604554     0.186420     214.38
 C       1.877606     2.949897    -0.030964     120.77
 H       2.827081     3.511969     0.057673      25.03
 H       1.487331     2.901382    -0.985603      27.41
 H       1.258537     3.199943     0.832181      24.88
 C       1.646403    -0.750093     0.263251      19.65
 O       2.986556    -1.004772     0.030290     199.59
 C       0.624007    -1.698089     0.336349      79.28
 H       0.748021    -2.721066     0.283742      24.78
 C      -1.045703     0.000067     0.647369      56.17
 C      -2.541279     0.453649     0.732449      77.76
 H      -3.033885    -0.453849     1.160871      25.99
 O      -2.672539     1.625066     1.482201     326.54
 H      -2.402695     1.380642     2.376036      30.23
 C      -3.235710     0.554256    -0.708224      92.27
 H      -2.851225     1.264984    -1.476504      25.46
 O      -3.188667    -0.802554    -1.177626     221.18
 H      -3.357962    -0.687310    -2.165856      25.49
 C      -4.784201     0.967757    -0.557948      96.92
 O      -4.905955     2.447506    -0.551842     247.77
 H      -4.993701     2.731879     0.393391      27.07
 H      -5.256322     0.396757     0.221257      29.98
 H      -5.132852     0.482173    -1.491641      29.30
55
name = lig-etoh-Waterframe_306
 C       5.740902    -1.915479     1.862899      70.12
 H       5.795021    -0.862575     1.746047      24.26
 C       5.309817    -4.165515     1.015265      47.01
 H       5.142099    -4.818996     0.193907      20.65
 C       5.495447    -4.743128     2.278526      32.21
 O       5.474588    -6.072468     2.569686     229.80
 C       4.977278    -6.945167     1.450562     151.75
 H       5.700233    -7.058040     0.681184      30.35
 H       3.967836    -6.555524     1.090949      25.92
 H       4.931698    -8.029895     1.869693      23.11
 C       5.846243    -3.849897     3.383398       0.34
 O       6.028567    -4.280287     4.763504     161.15
 H       5.971899    -5.240409     4.724433      26.14
 C       5.999177    -2.496105     3.068997      56.22
 H       6.313285    -1.734366     3.901401      22.82
 C       5.424935    -2.764397     0.748924      17.79
 C       5.009079    -2.290141    -0.591022      67.72
 H       5.439939    -3.112385    -1.428425      19.59
 O       5.865876    -1.092325    -0.952254     208.15
 H       5.457055    -0.168684    -0.701960      25.68
 C       3.389843    -2.175686    -0.744771      82.17
 H       3.077669    -3.112756    -0.375208      23.36
 C       2.886875    -2.061810    -2.218067      95.09
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 O       3.076704    -3.430275    -2.812511     260.48
 H       3.779006    -3.287502    -3.412629      29.31
 H       3.630862    -1.379193    -2.773612      22.48
 H       1.813016    -1.868168    -2.246727      25.22
 C      -0.740052    -1.402229     0.608742      31.88
 H      -1.588271    -2.007047     0.675048      15.94
 C      -0.050510     1.094088     0.504139      64.56
 H      -0.457400     2.028041     0.184157      19.74
 C       1.319256     0.648881     0.301923       8.53
 O       2.358994     1.574955     0.189705     181.44
 C       1.862381     2.960130    -0.010303     131.01
 H       2.645567     3.653883    -0.002231      27.75
 H       1.484164     3.059382    -0.943175      29.97
 H       1.185850     3.431568     0.616470      28.49
 C       1.657632    -0.693203     0.256937      21.86
 O       3.018062    -1.032118     0.022894     198.72
 C       0.606740    -1.669978     0.337386      56.34
 H       1.078722    -2.705339     0.203274      22.55
 C      -1.061640     0.009103     0.589417      34.12
 C      -2.574952     0.442670     0.679356      86.03
 H      -2.994643    -0.409219     1.247846      25.04
 O      -2.693381     1.605713     1.487559     324.07
 H      -2.331473     1.280074     2.263827      31.81
 C      -3.252036     0.556805    -0.665874      95.87
 H      -2.783807     1.305018    -1.315623      25.77
 O      -3.185893    -0.849505    -1.127922     248.34
 H      -3.078297    -0.750725    -2.135948      25.09
 C      -4.819576     0.935463    -0.597753      87.80
 O      -4.888769     2.368433    -0.581831     244.18
 H      -5.016720     2.776629     0.318209      27.68
 H      -5.277930     0.426098     0.376436      27.65
 H      -5.327750     0.647091    -1.622657      26.97
55
name = lig-etoh-Waterframe_307
 C       5.766251    -1.997402     1.810201      55.41
 H       5.749197    -0.943086     1.741240      26.59
 C       5.326729    -4.152733     1.032079      55.77
 H       5.032709    -4.759566     0.254759      16.58
 C       5.586800    -4.728969     2.313884      27.75
 O       5.453151    -6.089436     2.521670     271.94
 C       5.075194    -6.969047     1.505008     108.85
 H       5.776794    -7.024477     0.672053      26.48
 H       4.164788    -6.628545     0.985416      30.16
 H       4.784062    -7.931051     2.065847      22.21
 C       5.863400    -3.896966     3.440214      15.73
 O       5.997141    -4.329564     4.679970      98.94
 H       5.870033    -5.277199     4.851118      22.91
 C       5.998832    -2.516629     3.177725      39.85
 H       6.237179    -1.731724     3.971807      22.35
 C       5.377411    -2.756280     0.761385      16.58
 C       5.027295    -2.242694    -0.650828      64.29
 H       5.255741    -3.159987    -1.480287      21.30
 O       5.838762    -1.087676    -0.923603     241.47
 H       5.205564    -0.294582    -0.729793      26.61
 C       3.426349    -2.187804    -0.754583      80.81
 H       3.026963    -3.149516    -0.385462      21.41
 C       2.907189    -2.102007    -2.187700      95.43
 O       3.068299    -3.462722    -2.840543     232.04
 H       3.916253    -3.442665    -3.301940      27.74
 H       3.220883    -1.304710    -2.879467      24.94
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 H       1.805989    -1.814321    -2.235019      24.79
 C      -0.710275    -1.302974     0.538966      51.75
 H      -1.378762    -2.123769     0.730509      23.13
 C      -0.078462     1.050469     0.439837      74.49
 H      -0.278276     1.972707     0.128609      20.89
 C       1.301125     0.727584     0.327091       4.93
 O       2.394316     1.596011     0.200922     190.81
 C       1.888148     3.014393    -0.029498     105.74
 H       2.814330     3.534936     0.013436      25.01
 H       1.310075     3.189753    -1.029041      25.78
 H       1.089168     3.168314     0.725770      24.74
 C       1.646386    -0.708341     0.213800      11.32
 O       3.025163    -1.019625     0.043577     169.63
 C       0.664900    -1.695214     0.355254      46.49
 H       0.978382    -2.875081     0.265646      18.71
 C      -1.066546     0.066064     0.530284      45.10
 C      -2.535872     0.369183     0.675091      89.71
 H      -3.165116    -0.367159     1.164186      25.82
 O      -2.719382     1.621316     1.518468     305.09
 H      -2.359451     1.399556     2.300255      32.59
 C      -3.347225     0.515771    -0.616542     101.59
 H      -2.701635     1.099414    -1.241153      25.13
 O      -3.185253    -0.883299    -1.122218     239.15
 H      -2.902099    -0.815952    -2.091726      26.14
 C      -4.769308     0.913602    -0.627252     106.69
 O      -4.884900     2.331611    -0.585110     256.54
 H      -4.879481     2.725596     0.334660      27.76
 H      -5.424081     0.523053     0.305714      27.43
 H      -5.452089     0.565786    -1.481787      27.10
55
name = lig-etoh-Waterframe_308
 C       5.800328    -1.985428     1.898843      51.80
 H       5.901121    -0.920960     1.678141      24.84
 C       5.337131    -4.184625     1.032553      48.83
 H       4.995961    -4.879837     0.319759      15.98
 C       5.640666    -4.706298     2.275520      26.63
 O       5.459997    -6.084468     2.551564     276.10
 C       5.105919    -7.006652     1.501810     108.76
 H       6.010225    -7.224217     0.852824      24.58
 H       4.241620    -6.716544     0.979355      30.94
 H       4.945272    -7.966990     2.024814      22.15
 C       5.882064    -3.903806     3.410360      -5.56
 O       5.981597    -4.399567     4.684939     172.56
 H       5.870195    -5.383458     4.828745      25.67
 C       5.977281    -2.501853     3.190391      66.69
 H       6.157615    -1.976749     4.108094      21.90
 C       5.343950    -2.840352     0.760273      15.39
 C       5.012125    -2.248824    -0.653689      92.14
 H       5.363587    -2.936699    -1.402119      25.51
 O       5.742658    -1.076697    -0.930227     271.75
 H       5.322394    -0.197842    -0.565100      25.16
 C       3.500783    -2.157386    -0.779122      72.55
 H       3.086137    -3.038348    -0.167619      20.77
 C       2.888416    -2.173047    -2.220499      97.64
 O       3.077887    -3.462371    -2.874582     236.53
 H       4.003006    -3.445718    -3.231348      27.96
 H       3.481996    -1.419317    -2.754005      22.98
 H       1.773275    -2.148887    -2.022270      23.55
 C      -0.614359    -1.243869     0.481269      49.15
 H      -1.358167    -2.043691     0.757224      23.45
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 C      -0.059556     1.039097     0.321885      65.47
 H      -0.395727     2.040647     0.449273      19.67
 C       1.319522     0.678034     0.326510      12.06
 O       2.354514     1.654667     0.184635     164.59
 C       1.931441     3.037628    -0.024240      97.18
 H       2.825390     3.708220     0.095432      25.08
 H       1.432496     3.032745    -1.154026      22.84
 H       1.411588     3.288898     0.988817      23.33
 C       1.674144    -0.701428     0.182370      25.22
 O       3.016838    -0.988099     0.061169     182.85
 C       0.693056    -1.687758     0.365527      54.94
 H       0.752763    -2.865973     0.450620      17.64
 C      -1.095496     0.049944     0.487151      28.75
 C      -2.573499     0.382700     0.775418      73.28
 H      -2.832566    -0.575683     1.305174      22.84
 O      -2.740582     1.619678     1.525169     347.66
 H      -2.457081     1.402292     2.342877      32.10
 C      -3.318259     0.408548    -0.642403      84.85
 H      -2.958374     1.152077    -1.399106      23.88
 O      -3.198745    -0.931337    -1.134109     248.61
 H      -3.018381    -0.712795    -2.116246      23.98
 C      -4.815198     0.894000    -0.584211     100.45
 O      -4.870395     2.356033    -0.575581     251.06
 H      -4.685997     2.595274     0.378434      27.04
 H      -5.253370     0.365386     0.274441      29.71
 H      -5.061346     0.443988    -1.523107      29.72
55
name = lig-etoh-Waterframe_309
 C       5.781472    -1.966598     1.906414      64.20
 H       6.059924    -0.881148     1.766782      23.70
 C       5.325097    -4.263645     0.981134      39.99
 H       5.029725    -4.984814     0.189081      17.26
 C       5.645400    -4.779553     2.261148      25.79
 O       5.481707    -6.065561     2.614107     254.59
 C       5.152089    -7.076695     1.509994     110.44
 H       6.071438    -7.230052     0.827814      26.02
 H       4.320251    -6.809857     0.888436      28.98
 H       4.956466    -7.970265     2.022437      22.19
 C       5.899017    -3.911989     3.364474       1.11
 O       5.981449    -4.439049     4.714432     163.62
 H       5.952689    -5.436928     4.629497      34.47
 C       5.958626    -2.522013     3.207051      63.71
 H       6.152743    -1.899796     4.009651      24.69
 C       5.403211    -2.810517     0.834427      35.29
 C       5.020023    -2.275178    -0.578336     100.64
 H       5.371231    -2.893586    -1.256317      26.39
 O       5.651029    -1.015351    -0.962130     239.23
 H       5.468753    -0.280334    -0.244272      25.87
 C       3.482212    -2.146983    -0.744348      77.19
 H       3.137032    -3.135508    -0.238475      18.14
 C       2.896494    -2.243298    -2.206182     102.35
 O       3.122750    -3.474187    -2.913144     249.96
 H       4.026698    -3.350198    -3.417345      24.45
 H       3.245599    -1.399898    -2.814887      23.95
 H       1.792553    -2.035602    -2.242873      23.98
 C      -0.627523    -1.278598     0.474900      39.56
 H      -1.462200    -2.026252     0.691059      21.59
 C      -0.061831     1.056568     0.255893      76.58
 H      -0.347921     2.098109     0.707996      19.67
 C       1.320843     0.666395     0.245493      10.24
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 O       2.320298     1.669084     0.170175     180.31
 C       2.001069     3.041581     0.049536     129.08
 H       2.938762     3.624187    -0.219291      25.23
 H       1.281076     3.336967    -0.878379      23.88
 H       1.230642     3.667777     0.630459      23.86
 C       1.738864    -0.703922     0.173256      22.72
 O       3.071955    -0.950056     0.037317     191.14
 C       0.709442    -1.656667     0.361354      51.98
 H       1.103062    -2.674960     0.440852      19.39
 C      -1.038934     0.088073     0.444717      31.75
 C      -2.559241     0.382687     0.796284      82.66
 H      -2.943249    -0.420076     1.509317      22.73
 O      -2.770170     1.596805     1.525163     337.27
 H      -2.539480     1.352636     2.377817      30.75
 C      -3.293068     0.363037    -0.586005      78.80
 H      -2.725152     1.113923    -1.259839      22.91
 O      -3.216564    -0.985849    -1.182661     221.77
 H      -3.244562    -0.861530    -2.197815      25.30
 C      -4.799909     0.825549    -0.543270     105.04
 O      -4.843343     2.335242    -0.538015     245.66
 H      -4.658734     2.773434     0.350043      26.99
 H      -5.425518     0.449401     0.190865      30.10
 H      -5.303498     0.697852    -1.484252      28.44
55
name = lig-etoh-Waterframe_310
 C       5.764396    -1.974462     1.907494      60.21
 H       5.899379    -0.850902     1.781343      22.70
 C       5.346242    -4.251590     0.978791      39.15
 H       5.096733    -4.791804    -0.009009      18.11
 C       5.599252    -4.819064     2.236359      39.34
 O       5.490540    -6.151921     2.635452     297.60
 C       5.219867    -7.121092     1.573447     120.91
 H       6.086975    -7.196486     0.858090      30.48
 H       4.323663    -6.753420     0.975664      29.65
 H       4.959243    -7.986437     2.103291      25.46
 C       5.908071    -3.943178     3.421904      -7.20
 O       5.996664    -4.413381     4.651729     114.06
 H       5.909473    -5.428975     4.870845      17.97
 C       5.959399    -2.540137     3.204923      61.73
 H       6.196587    -1.862918     3.979646      24.20
 C       5.468835    -2.809312     0.852090      61.92
 C       5.048104    -2.245998    -0.502341      90.68
 H       5.344413    -3.085847    -1.267203      22.91
 O       5.580899    -0.955721    -0.974598     260.75
 H       5.480285    -0.338076    -0.145232      23.44
 C       3.436063    -2.216837    -0.688964      73.60
 H       2.916273    -3.055880    -0.203631      18.70
 C       2.895271    -2.211205    -2.207763      91.09
 O       3.196189    -3.497226    -2.951713     230.93
 H       4.090677    -3.331229    -3.540799      23.52
 H       3.260849    -1.399530    -2.829856      22.47
 H       1.808785    -2.166967    -2.164215      23.35
 C      -0.687472    -1.304654     0.483323      51.75
 H      -1.374058    -2.178468     0.633874      18.21
 C      -0.030892     1.081708     0.291657      62.41
 H      -0.206306     2.279299     0.389970      18.32
 C       1.300731     0.729111     0.115466      15.85
 O       2.303846     1.659552     0.178614     191.68
 C       1.984852     3.135047     0.015170     113.14
 H       3.062533     3.411062    -0.101217      23.44
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 H       1.475823     3.130443    -0.847322      26.28
 H       1.635495     3.460008     1.058742      22.76
 C       1.741421    -0.638397     0.169267       7.10
 O       3.155230    -0.941317    -0.020581     159.30
 C       0.773019    -1.646545     0.346916      45.59
 H       1.092943    -2.601584     0.375415      19.32
 C      -1.016097     0.059061     0.449687      58.36
 C      -2.494709     0.325256     0.767861      89.21
 H      -2.985476    -0.497456     1.326358      26.17
 O      -2.795161     1.594732     1.520965     310.20
 H      -2.541135     1.349500     2.411935      28.72
 C      -3.321946     0.340155    -0.526125      82.44
 H      -2.658857     0.990455    -1.150922      23.32
 O      -3.235143    -1.034465    -1.212771     220.10
 H      -3.259909    -0.668784    -2.184256      22.87
 C      -4.774679     0.848058    -0.523856     108.27
 O      -4.803939     2.296879    -0.494752     267.17
 H      -4.796945     2.699758     0.436195      26.71
 H      -5.382120     0.440772     0.289357      29.21
 H      -5.375829     0.574485    -1.424811      28.30
55
name = lig-etoh-Waterframe_311
 C       5.765818    -1.993309     1.952392      53.06
 H       5.630266    -0.907553     1.794276      18.63
 C       5.405867    -4.179316     1.009206      65.29
 H       5.167277    -4.854535     0.091670      20.46
 C       5.550840    -4.825161     2.288265      42.89
 O       5.508445    -6.227668     2.634532     364.64
 C       5.242064    -7.142424     1.640338     156.83
 H       6.078225    -7.359734     0.978460      33.90
 H       4.279687    -6.831008     1.058042      26.50
 H       5.104040    -8.155002     2.072897      24.19
 C       5.863811    -3.970147     3.345357       3.19
 O       6.037187    -4.385654     4.664692     199.13
 H       5.776179    -5.398310     4.744178      23.61
 C       5.984377    -2.557873     3.196856      60.56
 H       6.211162    -2.007518     4.143385      22.95
 C       5.496658    -2.817289     0.808778      65.68
 C       5.021960    -2.246511    -0.517279     105.09
 H       5.536923    -2.978775    -1.454720      23.31
 O       5.530803    -0.955326    -0.948719     305.33
 H       5.368898    -0.091736    -0.377572      21.87
 C       3.442132    -2.256813    -0.667131      71.52
 H       2.983175    -2.983412    -0.072075      18.18
 C       2.913158    -2.220960    -2.208177      87.90
 O       3.255407    -3.493695    -2.961948     224.97
 H       4.245966    -3.328676    -3.348475      23.98
 H       3.433335    -1.359010    -2.630253      19.52
 H       1.865890    -2.280362    -2.118798      22.52
 C      -0.564821    -1.331595     0.480577      18.20
 H      -1.337199    -2.065339     0.692442      16.02
 C      -0.031428     1.089258     0.332997      75.61
 H      -0.500133     2.122198     0.074483      16.79
 C       1.316807     0.774332     0.040575      21.70
 O       2.335779     1.681381     0.169843     196.97
 C       2.042295     3.115844     0.012246     121.11
 H       2.966098     3.718750    -0.108231      24.78
 H       1.387061     3.410768    -0.742168      27.39
 H       1.632592     3.460383     0.988963      25.11
 C       1.753885    -0.603814     0.127902      10.44
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 O       3.133998    -0.917041    -0.074164     177.23
 C       0.752086    -1.614056     0.330782      58.61
 H       0.909728    -2.624898     0.339345      18.47
 C      -1.040058     0.012928     0.511807      45.26
 C      -2.504195     0.274742     0.758429      83.87
 H      -2.680490    -0.619161     1.332580      24.18
 O      -2.794560     1.558833     1.498653     305.12
 H      -2.460684     1.321713     2.424729      28.03
 C      -3.309212     0.312632    -0.562339      91.26
 H      -2.994029     1.024108    -1.294969      23.82
 O      -3.267177    -1.026990    -1.191635     260.98
 H      -3.102742    -0.796634    -2.179478      21.30
 C      -4.779747     0.871217    -0.472716      95.22
 O      -4.774635     2.287353    -0.457882     280.95
 H      -4.933949     2.469154     0.520653      27.16
 H      -5.142750     0.389173     0.510031      28.31
 H      -5.077771     0.355578    -1.422463      28.39
55
name = lig-etoh-Waterframe_312
 C       5.743583    -1.978309     1.940142      59.12
 H       5.655812    -0.910084     1.939821      23.67
 C       5.462266    -4.228731     1.039734      65.83
 H       5.231732    -4.945427     0.208282      19.15
 C       5.525601    -4.852558     2.304096      27.56
 O       5.538724    -6.196504     2.664151     297.62
 C       5.226440    -7.237641     1.628871     143.93
 H       6.011557    -7.233314     0.926130      34.75
 H       4.294165    -7.064152     1.003228      29.96
 H       5.086397    -8.184353     2.271326      23.96
 C       5.832876    -3.957063     3.357752      14.05
 O       6.073155    -4.377033     4.679542     240.98
 H       5.883416    -5.399221     4.751742      22.96
 C       6.004361    -2.607765     3.190990      51.61
 H       6.173756    -2.016206     4.177490      20.47
 C       5.501826    -2.776006     0.815387      39.07
 C       5.001605    -2.228706    -0.588116     115.58
 H       5.454943    -2.950038    -1.424483      24.00
 O       5.526264    -0.960419    -0.930758     332.52
 H       4.989923    -0.228759    -0.432040      21.11
 C       3.470399    -2.239693    -0.681226      83.83
 H       3.147803    -3.057593    -0.087392      19.12
 C       2.974416    -2.311078    -2.144485     105.29
 O       3.293759    -3.460710    -2.916158     263.18
 H       4.160695    -3.323281    -3.409432      26.44
 H       3.310298    -1.357414    -2.630902      21.67
 H       1.926137    -2.072860    -2.324906      23.88
 C      -0.543163    -1.276253     0.527154      49.90
 H      -1.136127    -2.128837     0.740996      20.82
 C      -0.123982     1.038094     0.309472      69.10
 H      -0.524508     2.022557     0.212660      17.79
 C       1.330514     0.764424     0.077965      26.54
 O       2.414303     1.750427     0.101408     232.25
 C       2.078682     3.114943     0.060908     123.49
 H       2.997772     3.650971    -0.156081      23.62
 H       1.229203     3.463248    -0.724426      24.75
 H       1.503190     3.452734     0.850808      27.15
 C       1.751950    -0.613269     0.051289      29.61
 O       3.048580    -0.886128    -0.122523     197.72
 C       0.814824    -1.611017     0.286057      39.12
 H       1.153169    -2.675507     0.300788      14.36
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 C      -0.962861     0.030638     0.555320      32.75
 C      -2.510325     0.255136     0.747916      71.43
 H      -2.997364    -0.520483     1.367890      22.79
 O      -2.772879     1.469689     1.465290     275.01
 H      -2.353959     1.302800     2.416243      25.68
 C      -3.295133     0.317875    -0.619536      90.35
 H      -2.748084     1.023057    -1.257403      23.94
 O      -3.297844    -1.020073    -1.120183     266.30
 H      -3.147535    -0.926661    -2.085901      25.69
 C      -4.718568     0.772676    -0.400062     100.11
 O      -4.775721     2.283303    -0.418155     232.17
 H      -4.941978     2.752011     0.472272      25.84
 H      -5.435690     0.463528     0.485480      26.72
 H      -5.480731     0.588714    -1.242725      27.08
55
name = lig-etoh-Waterframe_313
 C       5.724664    -1.952403     1.936136      59.87
 H       5.841590    -0.898775     1.867367      25.47
 C       5.481609    -4.282568     1.019950      51.40
 H       5.328469    -4.836957     0.136657      18.19
 C       5.551188    -4.843533     2.303202      17.94
 O       5.534603    -6.171260     2.659990     254.00
 C       5.206396    -7.291461     1.626535     115.89
 H       6.003624    -7.361239     0.913705      31.38
 H       4.241006    -7.086258     1.222639      31.24
 H       5.235970    -8.236071     2.295167      24.25
 C       5.839218    -3.972975     3.473002      11.67
 O       6.101850    -4.395886     4.691061     238.37
 H       6.064115    -5.384480     4.929849      21.54
 C       5.987140    -2.595255     3.166199      54.25
 H       6.229538    -1.881658     4.051859      21.39
 C       5.468101    -2.806430     0.818157      29.28
 C       5.041013    -2.240503    -0.605644     109.74
 H       5.242819    -2.947992    -1.249312      24.67
 O       5.544038    -0.947648    -0.923055     352.86
 H       4.885103    -0.333937    -0.443008      20.41
 C       3.475780    -2.209588    -0.695870      86.08
 H       3.074960    -3.066995    -0.085355      20.14
 C       2.996954    -2.285134    -2.126631     100.26
 O       3.316295    -3.475485    -2.862616     246.74
 H       4.091768    -3.235194    -3.352842      28.02
 H       3.592832    -1.505227    -2.686299      20.66
 H       1.838343    -2.240964    -2.085236      22.57
 C      -0.491174    -1.333722     0.598079      35.60
 H      -1.195879    -2.100776     0.835165      21.18
 C      -0.035718     1.094921     0.248154      88.10
 H      -0.321867     2.036591     0.455874      22.45
 C       1.314509     0.787966     0.165805      12.05
 O       2.441251     1.735167     0.010131     149.39
 C       2.021122     3.189483     0.084552     108.76
 H       2.995540     3.646737     0.063969      25.42
 H       1.548435     3.115298    -0.983923      22.03
 H       1.720939     3.384044     1.107706      24.49
 C       1.701394    -0.572016    -0.014468      23.11
 O       3.044938    -0.893659    -0.190938     191.49
 C       0.839475    -1.622493     0.243705      39.35
 H       1.303349    -2.710364     0.276187      15.59
 C      -1.032396    -0.013609     0.593447      46.75
 C      -2.502538     0.238709     0.736006      78.77
 H      -3.017637    -0.698615     1.150969      23.46
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 O      -2.738770     1.421223     1.448137     262.49
 H      -2.285980     1.222046     2.423311      22.90
 C      -3.266018     0.331195    -0.583637      84.14
 H      -2.676011     0.960094    -1.314430      25.05
 O      -3.320557    -1.061737    -1.056552     226.10
 H      -3.317569    -0.842336    -1.992661      26.74
 C      -4.776283     0.804140    -0.346960      92.78
 O      -4.787002     2.283034    -0.395645     229.40
 H      -4.813870     2.757597     0.513393      24.93
 H      -5.031658     0.258552     0.641745      27.99
 H      -5.402782     0.478090    -1.237805      27.61
55
name = lig-etoh-Waterframe_314
 C       5.719761    -1.999398     1.899346      52.82
 H       5.911246    -0.964675     1.660243      23.85
 C       5.466664    -4.236192     0.974725      53.47
 H       5.384714    -4.897426     0.186474      17.89
 C       5.617102    -4.808578     2.337481      15.44
 O       5.515408    -6.210638     2.620892     349.28
 C       5.198462    -7.260868     1.696131     120.29
 H       5.851879    -7.361819     0.773861      29.66
 H       4.216116    -7.146594     1.348146      32.07
 H       5.266677    -8.224164     2.262962      22.05
 C       5.845221    -3.966247     3.427020     -11.34
 O       6.149396    -4.431527     4.789386     318.31
 H       5.981489    -5.422844     4.769926      30.69
 C       5.951002    -2.544083     3.197250      54.56
 H       6.337300    -1.898711     4.003795      24.44
 C       5.435280    -2.863834     0.819154      46.53
 C       5.058676    -2.284778    -0.531559     119.31
 H       5.418530    -2.936772    -1.324140      23.59
 O       5.578665    -0.956287    -0.924791     313.40
 H       5.181439    -0.138586    -0.473386      21.29
 C       3.488357    -2.189188    -0.684402      80.97
 H       2.956193    -3.002794    -0.042720      19.50
 C       3.003986    -2.222042    -2.157568      87.38
 O       3.332702    -3.534331    -2.821604     245.25
 H       4.193790    -3.417360    -3.272434      27.27
 H       3.352838    -1.278294    -2.663163      22.09
 H       1.844525    -2.135925    -2.109160      23.05
 C      -0.499018    -1.387789     0.664996      20.56
 H      -1.165491    -2.200954     0.955668      18.96
 C      -0.020550     1.114989     0.287835      68.11
 H      -0.268598     2.124941     0.479864      20.31
 C       1.385629     0.828156     0.181363      16.89
 O       2.406136     1.682939    -0.045288     171.33
 C       2.052960     3.156223     0.069413     114.01
 H       2.933292     3.771267     0.127440      25.82
 H       1.334270     3.770858    -0.652766      24.06
 H       1.259981     3.392133     0.958339      22.94
 C       1.709931    -0.577239    -0.040629      19.90
 O       3.078587    -0.876018    -0.261591     190.58
 C       0.804620    -1.619292     0.230624      54.91
 H       1.131023    -2.774179     0.219865      16.40
 C      -0.964265    -0.043766     0.557826      33.89
 C      -2.481252     0.187356     0.717304      80.44
 H      -2.753111    -0.733619     1.308222      23.46
 O      -2.706274     1.420717     1.486173     248.36
 H      -2.332112     1.178713     2.517088      23.31
 C      -3.276440     0.331309    -0.540169      87.27
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 H      -2.910012     0.970704    -1.384640      25.34
 O      -3.349674    -1.098183    -1.038146     195.15
 H      -3.356224    -1.029005    -1.995723      27.07
 C      -4.743251     0.867639    -0.314043     112.61
 O      -4.826617     2.272752    -0.377239     257.59
 H      -4.704096     2.558554     0.593175      25.61
 H      -5.012055     0.506529     0.646224      30.10
 H      -5.269199     0.323491    -1.056121      29.94
55
name = lig-etoh-Waterframe_315
 C       5.737526    -2.062353     1.897576      53.37
 H       5.818360    -0.977312     1.678014      18.96
 C       5.445207    -4.280603     1.032495      26.06
 H       5.282198    -4.959306     0.216722      16.30
 C       5.653377    -4.828884     2.275774      25.39
 O       5.530000    -6.198520     2.619047     303.53
 C       5.151631    -7.222912     1.725170     125.23
 H       5.778989    -7.104237     0.763208      30.78
 H       4.083411    -7.194474     1.422584      31.49
 H       5.328381    -8.116894     2.284612      23.40
 C       5.899322    -3.922724     3.460212     -23.29
 O       6.174045    -4.448278     4.797478     316.26
 H       5.864811    -5.389785     4.902151      31.12
 C       5.926577    -2.524846     3.215831      71.73
 H       6.263223    -1.953144     4.014084      28.67
 C       5.425327    -2.866931     0.813909      58.83
 C       5.032079    -2.258754    -0.497168     111.87
 H       5.623953    -2.940984    -1.380561      21.66
 O       5.655670    -0.994091    -0.926695     249.01
 H       5.462060    -0.261490    -0.264908      23.71
 C       3.494176    -2.174501    -0.717592      78.77
 H       2.984918    -2.983878    -0.087375      18.60
 C       3.000743    -2.223971    -2.192964      96.61
 O       3.340246    -3.547652    -2.789463     261.40
 H       4.214474    -3.458875    -3.292458      26.95
 H       3.380251    -1.395689    -2.777777      21.98
 H       1.907256    -2.191633    -2.328531      23.51
 C      -0.524633    -1.352705     0.682540      14.27
 H      -1.123061    -2.228119     0.992505      15.07
 C      -0.013715     1.040613     0.398800      81.34
 H      -0.559770     2.055887     0.244641      16.75
 C       1.368780     0.745649     0.120210       6.07
 O       2.371682     1.752696    -0.107596     193.52
 C       2.020639     3.136816     0.078973     103.49
 H       3.009370     3.542950     0.370857      24.01
 H       1.548299     3.548141    -0.809639      25.10
 H       1.371707     3.074028     1.118148      21.65
 C       1.772873    -0.622343    -0.010286      15.27
 O       3.099857    -0.806077    -0.304461     208.86
 C       0.785431    -1.633057     0.249249      69.85
 H       1.104268    -2.719378     0.086857      15.78
 C      -0.860325    -0.014998     0.512502      64.71
 C      -2.367743     0.188491     0.767946      79.00
 H      -2.877088    -0.584642     1.348295      23.09
 O      -2.673117     1.424056     1.543553     225.53
 H      -2.389309     1.125714     2.597020      23.62
 C      -3.327324     0.273105    -0.548180      85.85
 H      -2.760546     0.949557    -1.216707      23.64
 O      -3.398090    -1.118193    -1.038175     238.91
 H      -3.180170    -0.947061    -1.990984      24.99
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 C      -4.684296     0.840048    -0.250863     120.56
 O      -4.875605     2.275893    -0.370250     244.76
 H      -4.624981     2.808024     0.473084      25.23
 H      -5.214564     0.663638     0.616381      29.96
 H      -5.417214     0.517255    -0.955498      29.02
55
name = lig-etoh-Waterframe_316
 C       5.751858    -2.050384     1.923193      49.28
 H       5.692265    -0.922888     1.903193      16.83
 C       5.404136    -4.335149     1.040215      21.92
 H       5.037645    -4.962504     0.176990       9.31
 C       5.672019    -4.846290     2.343240      27.94
 O       5.566653    -6.126292     2.675485     272.38
 C       5.091311    -7.182025     1.700529     120.81
 H       5.683447    -7.140677     0.734238      34.15
 H       3.945459    -7.091618     1.570039      30.56
 H       5.412205    -8.087537     2.105511      25.32
 C       5.954412    -3.967809     3.495860      11.67
 O       6.178582    -4.427014     4.726529     285.89
 H       5.834095    -5.297973     4.961621      25.66
 C       5.944522    -2.579677     3.254802      64.15
 H       6.034931    -1.850317     3.992248      28.10
 C       5.435349    -2.878288     0.843592      49.20
 C       5.051201    -2.216375    -0.570847     117.65
 H       5.223349    -3.213210    -1.324714      25.94
 O       5.755818    -1.040178    -0.895431     258.68
 H       5.587500    -0.370313    -0.186310      26.52
 C       3.487676    -2.121857    -0.792830      82.84
 H       3.042426    -2.892002    -0.170629      21.02
 C       3.016197    -2.292792    -2.255951     110.41
 O       3.354945    -3.542835    -2.784533     259.65
 H       4.166001    -3.335151    -3.407512      25.75
 H       3.632392    -1.636511    -2.794692      20.96
 H       1.968979    -2.174418    -2.238500      24.61
 C      -0.451914    -1.338893     0.630733      16.72
 H      -1.300470    -2.012134     0.892422      16.05
 C       0.056367     0.993975     0.433419      80.02
 H      -0.431152     2.065659     0.155914      18.26
 C       1.333283     0.712259     0.045688       5.80
 O       2.334307     1.746228    -0.185191     204.55
 C       1.993251     3.080879     0.147143     116.12
 H       2.964011     3.617175     0.393141      24.21
 H       1.712427     3.455416    -0.753000      26.80
 H       1.329821     3.333605     1.016903      24.49
 C       1.785272    -0.640434     0.053419       9.07
 O       3.124158    -0.764641    -0.328166     211.91
 C       0.847603    -1.673759     0.271610      81.08
 H       1.070032    -2.692589     0.144930      19.51
 C      -0.944241    -0.033660     0.586168      61.63
 C      -2.355812     0.254307     0.824329      88.26
 H      -2.635683    -0.694284     1.314604      23.85
 O      -2.624026     1.425018     1.596701     252.13
 H      -2.347411     1.144622     2.643162      23.83
 C      -3.268218     0.220053    -0.461042      82.76
 H      -2.826536     0.814451    -1.272848      23.69
 O      -3.443590    -1.115539    -1.066281     221.86
 H      -3.129106    -0.905688    -2.007995      24.35
 C      -4.756978     0.834377    -0.185207      85.24
 O      -4.895544     2.309266    -0.389398     209.99
 H      -4.567429     2.963138     0.338041      24.19
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 H      -5.013754     0.314911     0.870502      26.38
 H      -5.366853     0.468301    -1.071686      26.31
55
name = lig-etoh-Waterframe_317
 C       5.744170    -2.044875     1.997914      44.44
 H       5.642704    -0.936795     1.875799      21.44
 C       5.362738    -4.274182     1.060686      20.64
 H       4.940539    -5.044549     0.310206      11.63
 C       5.661275    -4.796539     2.380571      27.64
 O       5.594652    -6.169045     2.736624     318.51
 C       5.074142    -7.102015     1.702078     138.87
 H       5.384160    -6.934093     0.683544      36.87
 H       3.912105    -6.978084     1.643573      30.29
 H       5.273034    -8.072496     2.109677      25.51
 C       5.979267    -3.990552     3.428862      20.59
 O       6.193863    -4.425242     4.727373     313.03
 H       5.858572    -5.326503     4.756908      28.72
 C       5.973307    -2.608124     3.249209      58.02
 H       5.909938    -1.975103     4.157047      22.93
 C       5.435656    -2.897347     0.839421      25.15
 C       5.035159    -2.301138    -0.598061      82.25
 H       5.407566    -2.894510    -1.423896      24.19
 O       5.877552    -1.098822    -0.871315     208.98
 H       5.576591    -0.336530    -0.339224      27.85
 C       3.527442    -2.055426    -0.814365      90.91
 H       3.079969    -2.784334    -0.221677      21.31
 C       3.063081    -2.272917    -2.291091     102.42
 O       3.379188    -3.587896    -2.837871     244.49
 H       4.229690    -3.545895    -3.482644      24.31
 H       3.437495    -1.411656    -2.905299      23.65
 H       2.025143    -2.013791    -2.399997      25.35
 C      -0.455043    -1.340816     0.572905      59.72
 H      -1.070465    -2.270040     0.687040      20.61
 C       0.013860     1.001952     0.375856      65.71
 H      -0.067964     2.141688     0.501660      17.78
 C       1.367090     0.722141     0.027315      22.43
 O       2.288238     1.645163    -0.235131     230.43
 C       1.985060     3.099188     0.177920     108.61
 H       2.982635     3.550334     0.387154      23.03
 H       1.480902     3.784144    -0.594626      24.83
 H       1.224718     3.204163     0.809951      27.59
 C       1.816338    -0.632508     0.066008      22.42
 O       3.125582    -0.769771    -0.346050     208.23
 C       0.933138    -1.719846     0.301689      55.47
 H       1.167212    -2.688397     0.292955      18.37
 C      -0.900763    -0.012004     0.681463      52.02
 C      -2.428755     0.222904     0.880647      90.39
 H      -2.766873    -0.615046     1.528960      25.02
 O      -2.582228     1.443537     1.655440     255.56
 H      -2.196505     1.155823     2.623054      23.54
 C      -3.259271     0.269202    -0.396010      77.34
 H      -2.854574     0.922049    -1.167167      25.01
 O      -3.456747    -1.110126    -1.072966     184.49
 H      -3.298508    -0.904300    -2.074900      24.67
 C      -4.762381     0.845607    -0.158348      80.30
 O      -4.898964     2.291345    -0.401140     203.16
 H      -4.618131     2.785799     0.457663      24.42
 H      -5.173906     0.533668     0.997708      25.85
 H      -5.396913     0.210530    -0.907215      26.42
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name = lig-etoh-Waterframe_318
 C       5.697577    -2.048557     1.968104      49.72
 H       5.725994    -0.961163     1.847615      22.26
 C       5.324356    -4.241502     1.137765      35.71
 H       4.998008    -4.913881     0.261532      14.98
 C       5.626473    -4.837262     2.334144      23.39
 O       5.618037    -6.216876     2.742248     332.39
 C       5.013077    -7.008095     1.741511     153.53
 H       5.452847    -6.787652     0.801742      35.21
 H       3.920255    -6.857272     1.769369      28.67
 H       5.251967    -8.092290     1.980744      23.07
 C       6.010074    -3.957997     3.429491     -17.31
 O       6.203383    -4.459266     4.737801     258.66
 H       6.009380    -5.399160     4.790812      29.72
 C       5.983039    -2.579249     3.246796      52.60
 H       6.125352    -2.063910     4.278672      20.33
 C       5.418475    -2.860076     0.840681      39.51
 C       5.116080    -2.329850    -0.574220      93.12
 H       5.431115    -2.980443    -1.244535      23.98
 O       5.975284    -1.159432    -0.848541     225.32
 H       5.580711    -0.343407    -0.533738      26.26
 C       3.569265    -2.074478    -0.830933      85.64
 H       3.056837    -2.847864    -0.301867      20.37
 C       3.106682    -2.179159    -2.346236      82.32
 O       3.387073    -3.621588    -2.912565     200.32
 H       4.360081    -3.457860    -3.340874      22.89
 H       3.629272    -1.426934    -3.073855      21.77
 H       1.986226    -2.303640    -2.394448      23.20
 C      -0.400619    -1.406971     0.526634      55.31
 H      -1.090542    -2.265388     0.673067      23.82
 C       0.011352     1.053484     0.333965      67.16
 H      -0.459890     1.955321     0.681219      19.78
 C       1.318891     0.671933     0.075878      12.15
 O       2.281015     1.666924    -0.283669     161.56
 C       1.970219     3.089826     0.157116      98.18
 H       2.932271     3.398512     0.584287      24.92
 H       1.520153     3.652310    -0.832161      23.03
 H       1.494614     2.910496     1.077188      25.75
 C       1.838823    -0.652280     0.027457      18.44
 O       3.160142    -0.768632    -0.360235     203.32
 C       0.938694    -1.667934     0.344323      58.52
 H       1.265389    -2.621195     0.278595      19.52
 C      -0.878490    -0.046253     0.713475      25.81
 C      -2.434433     0.155194     0.972984      75.40
 H      -3.005287    -0.602532     1.543447      23.65
 O      -2.554316     1.478041     1.710212     275.28
 H      -2.170450     1.204543     2.605290      25.75
 C      -3.349828     0.334679    -0.384583      74.26
 H      -2.748520     1.043235    -0.951124      25.34
 O      -3.433810    -1.060986    -1.045588     189.71
 H      -3.359459    -0.717042    -2.025216      24.63
 C      -4.735259     0.839844    -0.117838     113.04
 O      -4.882843     2.222980    -0.401861     230.99
 H      -4.811890     2.746735     0.481651      25.30
 H      -5.178899     0.848216     0.884938      27.53
 H      -5.517194     0.355327    -0.766844      27.39
55
name = lig-etoh-Waterframe_319
 C       5.670948    -1.984085     1.938840      51.51
 H       5.806690    -0.934966     1.801521      23.43
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 C       5.275569    -4.264043     1.118502      75.57
 H       5.053898    -4.854565     0.213224      20.17
 C       5.636549    -4.870902     2.414061      10.12
 O       5.646377    -6.185771     2.726001     356.95
 C       4.936103    -6.985829     1.751686     120.89
 H       5.372507    -6.764101     0.773013      30.70
 H       3.906479    -6.780526     1.708132      31.44
 H       5.189667    -8.103985     1.934503      23.40
 C       5.999543    -3.991233     3.470864      -1.35
 O       6.223368    -4.484103     4.722233     187.04
 H       6.032912    -5.428187     4.805229      23.46
 C       5.991421    -2.569804     3.260691      51.38
 H       6.396180    -1.733384     3.961857      22.23
 C       5.382241    -2.832504     0.903726      30.49
 C       5.203607    -2.305415    -0.525264      92.06
 H       5.387893    -3.277270    -1.117427      19.77
 O       6.040317    -1.215217    -0.839649     256.13
 H       5.622040    -0.408443    -0.555696      28.17
 C       3.631523    -2.130740    -0.901015      69.70
 H       3.101522    -2.980852    -0.373215      16.79
 C       3.154683    -2.221328    -2.399950      83.45
 O       3.397701    -3.578065    -2.959585     236.88
 H       4.321105    -3.510614    -3.445175      25.40
 H       3.687068    -1.434612    -3.071635      21.01
 H       1.998789    -1.977417    -2.354404      22.79
 C      -0.421875    -1.414897     0.556703      57.33
 H      -1.125381    -2.203533     0.794830      23.42
 C      -0.091264     0.987351     0.407244      51.69
 H      -0.455957     1.963060     0.369371      20.77
 C       1.334398     0.735919     0.081646      -3.22
 O       2.281343     1.709185    -0.322988     205.07
 C       2.011852     2.969422     0.158806     117.44
 H       2.924078     3.560983     0.226622      25.32
 H       1.405423     3.716561    -0.627436      23.45
 H       1.305718     3.121023     1.128885      22.80
 C       1.833273    -0.616909    -0.012895      10.31
 O       3.210853    -0.774004    -0.362552     172.61
 C       0.972626    -1.656453     0.336463      60.51
 H       1.232611    -2.702248     0.145776      17.39
 C      -0.920427    -0.156031     0.659162      23.48
 C      -2.423550     0.175649     1.014579      80.95
 H      -2.699381    -0.742980     1.592472      23.92
 O      -2.529811     1.473061     1.752080     295.78
 H      -2.296353     1.281463     2.631212      29.80
 C      -3.341809     0.316818    -0.304495      78.51
 H      -2.899525     1.041733    -1.040306      24.83
 O      -3.390333    -0.934297    -1.014322     229.24
 H      -3.279112    -0.775719    -2.032354      24.66
 C      -4.802650     0.841896    -0.047048     113.41
 O      -4.851321     2.227872    -0.416561     231.68
 H      -4.936663     2.902962     0.360391      24.99
 H      -4.893905     0.516210     0.901113      29.97
 H      -5.424948     0.289495    -0.711021      29.65
55
name = lig-etoh-Waterframe_320
 C       5.697372    -1.951437     2.028431      44.29
 H       5.822829    -0.925837     1.801458      22.53
 C       5.277641    -4.274069     1.145186      13.77
 H       5.066466    -4.940336     0.368070      17.30
 C       5.620860    -4.782579     2.406740      28.25
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 O       5.653904    -6.177209     2.705565     293.22
 C       4.890460    -7.004121     1.715233     124.42
 H       5.186886    -6.871859     0.628965      29.33
 H       3.850255    -6.743607     1.782285      29.68
 H       4.965103    -8.050011     2.168042      23.11
 C       5.951916    -3.950574     3.506379      -4.12
 O       6.269263    -4.504793     4.739942     343.82
 H       5.896287    -5.417365     4.795828      34.66
 C       6.014105    -2.531718     3.202450      74.58
 H       6.490835    -1.909247     4.011692      23.86
 C       5.316730    -2.872314     0.949633      41.65
 C       5.179808    -2.349531    -0.491808     100.29
 H       5.764720    -3.160427    -1.326890      20.06
 O       6.080483    -1.240004    -0.846616     219.84
 H       5.709280    -0.451252    -0.470656      26.35
 C       3.710958    -2.150096    -0.955553      67.74
 H       3.198532    -2.987889    -0.334997      15.16
 C       3.224267    -2.254109    -2.419954      98.62
 O       3.368881    -3.516750    -2.986428     297.43
 H       4.132126    -3.345697    -3.572302      25.71
 H       3.751400    -1.499115    -2.997061      20.99
 H       2.176762    -1.869652    -2.536192      23.74
 C      -0.428250    -1.472682     0.633678      29.87
 H      -0.952883    -2.367096     0.864190      17.80
 C      -0.064181     0.899767     0.444106      77.25
 H      -0.417824     1.848467     0.163952      20.41
 C       1.306844     0.767082     0.061331      10.63
 O       2.257169     1.697772    -0.335496     208.28
 C       2.027157     3.029319     0.140380     113.70
 H       2.983540     3.539712     0.124152      24.75
 H       1.322725     3.409144    -0.500976      25.32
 H       1.374705     3.027823     1.236378      21.45
 C       1.860804    -0.559141    -0.036326      -0.69
 O       3.224958    -0.811087    -0.369276     172.04
 C       0.951633    -1.680421     0.270134      44.66
 H       1.322272    -2.800896     0.190731      16.36
 C      -1.007069    -0.126209     0.594335      43.30
 C      -2.387771     0.207214     0.999077     106.23
 H      -2.729129    -0.598178     1.674331      24.33
 O      -2.515594     1.425966     1.773922     316.20
 H      -2.340842     1.146455     2.602481      30.55
 C      -3.294674     0.328987    -0.236650      79.92
 H      -2.880051     1.182331    -0.865004      23.08
 O      -3.337697    -0.865422    -0.990107     265.18
 H      -3.161770    -0.527233    -1.951995      23.44
 C      -4.814811     0.810103     0.027576      88.91
 O      -4.841543     2.272452    -0.418178     219.88
 H      -4.890157     2.897301     0.403310      24.71
 H      -5.163253     0.629465     1.126691      27.92
 H      -5.456139     0.261899    -0.619776      28.46
55
name = lig-etoh-Waterframe_321
 C       5.695312    -1.996041     1.985182      64.46
 H       5.809415    -0.918180     1.888896      21.47
 C       5.293782    -4.241742     1.183364      43.66
 H       5.053517    -4.902990     0.427094      16.07
 C       5.591472    -4.760218     2.428904       2.94
 O       5.635083    -6.159966     2.634005     292.49
 C       4.826473    -7.015853     1.741897     130.46
 H       5.270668    -7.146138     0.694153      26.11
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 H       3.763581    -6.654349     1.816078      27.76
 H       4.935083    -8.025647     2.146439      22.77
 C       5.906197    -3.889934     3.505596       3.46
 O       6.315135    -4.492987     4.749455     292.82
 H       5.824037    -5.357617     4.942915      26.46
 C       6.091307    -2.539455     3.307241      46.53
 H       6.382301    -2.025021     4.184633      21.10
 C       5.283024    -2.851112     0.971418      32.79
 C       5.198591    -2.373716    -0.533095      95.71
 H       5.599511    -3.326154    -1.200497      21.55
 O       6.068687    -1.217880    -0.828160     232.38
 H       5.783469    -0.435177    -0.386801      25.79
 C       3.705817    -2.157863    -0.924668      80.59
 H       3.119205    -2.998770    -0.438758      18.47
 C       3.298085    -2.145663    -2.418852      97.81
 O       3.315249    -3.507723    -3.031574     257.85
 H       4.172232    -3.541662    -3.581466      26.45
 H       3.976426    -1.590866    -2.941714      22.77
 H       2.263707    -1.974752    -2.410029      25.54
 C      -0.396568    -1.499417     0.674080      37.88
 H      -0.977773    -2.356927     0.948427      17.96
 C       0.001192     0.913906     0.370425      62.52
 H      -0.513158     1.898366     0.426968      18.47
 C       1.336397     0.657180     0.022789      13.06
 O       2.232451     1.688700    -0.321245     174.13
 C       1.975328     3.115351     0.118405     117.04
 H       2.949062     3.602546     0.166251      25.32
 H       1.308375     3.593091    -0.494587      25.69
 H       1.936097     2.984080     1.219977      23.73
 C       1.847382    -0.656104    -0.041740      18.30
 O       3.222184    -0.839425    -0.385016     195.27
 C       0.916195    -1.633883     0.196290      67.76
 H       1.422840    -2.710473     0.281379      18.58
 C      -0.943642    -0.175941     0.593176      28.14
 C      -2.413212     0.200007     0.999145      96.79
 H      -2.852888    -0.700778     1.467082      23.58
 O      -2.500408     1.391172     1.795792     331.69
 H      -2.229761     1.066234     2.632601      28.63
 C      -3.325171     0.418857    -0.163769      79.28
 H      -2.848039     1.266449    -0.682835      23.44
 O      -3.263145    -0.837999    -0.999639     226.62
 H      -3.198664    -0.542484    -1.979630      23.64
 C      -4.766986     0.836898     0.098450     102.47
 O      -4.855551     2.277738    -0.396052     208.72
 H      -4.707894     2.899670     0.407999      25.20
 H      -5.373944     1.108895     1.076255      25.58
 H      -5.465305     0.319585    -0.574429      27.05
55
name = lig-etoh-Waterframe_322
 C       5.734543    -2.024811     2.044519      46.44
 H       5.764673    -0.918913     1.821244      21.92
 C       5.277803    -4.207304     1.190786      25.52
 H       5.064856    -4.836501     0.341456      15.35
 C       5.546409    -4.805050     2.448322      27.31
 O       5.609619    -6.136908     2.573389     313.44
 C       4.787284    -7.032105     1.802605     141.22
 H       5.217827    -7.053178     0.776658      27.43
 H       3.707945    -6.685588     1.553981      27.81
 H       4.809987    -7.948254     2.304662      23.62
 C       5.922487    -3.954000     3.576965      13.94
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 O       6.343774    -4.441281     4.739431     314.76
 H       5.875912    -5.316467     5.023144      26.04
 C       6.104282    -2.526478     3.362063      50.78
 H       6.288516    -1.835591     4.104218      21.36
 C       5.316210    -2.800499     0.926152      38.31
 C       5.191933    -2.356766    -0.523321     103.18
 H       5.457365    -3.124615    -1.083050      25.30
 O       6.026893    -1.204254    -0.811767     250.80
 H       5.652073    -0.497275    -0.321855      28.68
 C       3.652444    -2.159222    -0.886171      84.99
 H       3.113201    -3.000266    -0.494715      21.25
 C       3.363195    -2.082490    -2.414289      86.90
 O       3.264281    -3.515463    -3.063286     241.24
 H       4.233411    -3.640007    -3.407727      24.43
 H       3.962295    -1.372218    -2.982981      24.08
 H       2.402268    -1.593528    -2.511866      26.19
 C      -0.389377    -1.468500     0.655546      41.26
 H      -1.038638    -2.285455     0.998396      19.41
 C      -0.018031     0.887534     0.282647      66.29
 H      -0.160764     1.972658     0.652750      17.90
 C       1.382511     0.640399    -0.025006       3.86
 O       2.233466     1.712773    -0.312913     194.73
 C       1.979925     3.104884     0.140693     120.62
 H       2.883571     3.535587    -0.268029      24.76
 H       1.102541     3.831335    -0.232746      24.09
 H       1.710856     3.240743     1.104975      27.81
 C       1.870660    -0.728027    -0.090240      20.80
 O       3.205436    -0.871901    -0.387691     198.39
 C       0.917073    -1.718663     0.192542      61.44
 H       1.257223    -2.820147     0.185546      20.15
 C      -0.838877    -0.186734     0.656038      39.95
 C      -2.411616     0.119901     1.020177      78.14
 H      -2.744509    -0.785152     1.546463      23.45
 O      -2.482019     1.358561     1.833591     297.21
 H      -2.102288     1.108106     2.767128      25.02
 C      -3.332552     0.471623    -0.169394      69.99
 H      -3.000405     1.249667    -0.829287      25.02
 O      -3.198967    -0.786844    -1.009330     212.03
 H      -3.260713    -0.532193    -1.977734      24.91
 C      -4.788537     1.000468     0.127802     102.07
 O      -4.876562     2.281243    -0.387331     270.05
 H      -4.536920     2.999949     0.253169      25.13
 H      -4.884622     0.652602     1.269175      27.19
 H      -5.401072     0.248855    -0.476927      27.20
55
name = lig-etoh-Waterframe_323
 C       5.777635    -2.000327     2.098355      50.05
 H       5.887945    -0.873262     2.022121      21.42
 C       5.242762    -4.169072     1.175442      19.84
 H       5.078625    -4.899051     0.327862      18.09
 C       5.505582    -4.751209     2.430798      71.22
 O       5.579859    -6.159412     2.587258     322.05
 C       4.752905    -7.033224     1.798455     156.38
 H       5.220667    -7.283307     0.859514      31.77
 H       3.693910    -6.611487     1.730636      25.13
 H       4.664913    -7.908512     2.385559      24.03
 C       5.957267    -3.964680     3.555633      15.22
 O       6.377779    -4.423880     4.809587     344.12
 H       5.987083    -5.389824     4.959134      31.41
 C       6.027395    -2.558096     3.316627      57.06
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 H       6.330977    -1.869138     4.090004      23.61
 C       5.410199    -2.817065     0.969476      45.84
 C       5.129424    -2.306919    -0.474815      98.82
 H       5.544287    -3.015693    -1.177527      21.99
 O       5.960377    -1.191247    -0.803494     254.95
 H       5.659074    -0.393535    -0.395024      27.66
 C       3.640720    -2.156659    -0.912096      86.06
 H       3.130542    -2.949950    -0.450532      21.03
 C       3.372443    -2.083906    -2.443152      82.45
 O       3.236952    -3.457174    -3.040951     241.88
 H       4.167662    -3.515642    -3.529871      23.60
 H       4.317740    -1.547783    -2.952173      21.29
 H       2.398219    -1.580307    -2.682919      24.50
 C      -0.364031    -1.480664     0.612516      34.51
 H      -1.057563    -2.319472     0.928632      23.62
 C       0.064712     0.863554     0.253459      64.82
 H      -0.324492     1.965606     0.413771      17.99
 C       1.357961     0.650635    -0.065310      20.94
 O       2.244284     1.732088    -0.300330     209.74
 C       1.953322     3.097981     0.148118     103.75
 H       2.858841     3.664453    -0.208918      24.20
 H       0.918079     3.258276    -0.530720      20.70
 H       1.935583     3.223821     1.221264      26.04
 C       1.847480    -0.705140    -0.145255       4.07
 O       3.201556    -0.907032    -0.369297     162.40
 C       0.950553    -1.875935     0.220153      47.75
 H       1.119266    -2.913519     0.061923      17.55
 C      -0.888875    -0.101187     0.719906      32.76
 C      -2.319857     0.114450     1.047093      86.43
 H      -2.747623    -0.714312     1.631576      22.34
 O      -2.464816     1.324543     1.858176     253.32
 H      -2.162964     0.896748     2.886651      20.39
 C      -3.265518     0.451492    -0.256585      68.08
 H      -2.720909     1.270063    -0.756320      24.13
 O      -3.182076    -0.733189    -1.021556     249.85
 H      -3.203859    -0.420309    -1.956992      24.94
 C      -4.731448     0.994740     0.158353      93.17
 O      -4.928166     2.347324    -0.379405     258.38
 H      -4.566827     3.062290     0.230829      26.37
 H      -4.862136     1.010914     1.292225      26.83
 H      -5.633715     0.472674    -0.339874      25.67
55
name = lig-etoh-Waterframe_324
 C       5.793883    -1.947897     2.052240      57.16
 H       5.988110    -0.860260     2.023750      19.81
 C       5.229446    -4.184144     1.186126      53.09
 H       4.944045    -4.849467     0.279867      17.46
 C       5.509609    -4.762696     2.439350      25.91
 O       5.557641    -6.152259     2.640784     295.84
 C       4.700275    -7.039788     1.809466     115.33
 H       5.100911    -7.377579     0.867403      29.75
 H       3.742450    -6.541898     1.646899      29.99
 H       4.576290    -7.960491     2.434924      24.91
 C       5.978006    -3.955641     3.507545     -13.08
 O       6.396248    -4.428496     4.856917     192.10
 H       6.008344    -5.397373     4.958106      29.13
 C       5.971574    -2.605261     3.334864      60.33
 H       6.406925    -2.104164     4.271832      20.89
 C       5.459797    -2.781278     0.999949      31.87
 C       5.111118    -2.273704    -0.437997      71.93
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 H       5.576543    -3.251999    -1.199055      21.07
 O       5.901894    -1.132391    -0.807460     257.06
 H       5.634388    -0.291012    -0.448161      26.60
 C       3.630262    -2.161324    -0.926873      79.50
 H       3.078102    -3.015885    -0.529192      20.13
 C       3.399708    -2.128811    -2.476376      89.77
 O       3.247851    -3.384472    -3.016544     261.10
 H       4.036148    -3.588213    -3.654684      25.65
 H       4.397683    -1.632321    -2.897016      21.17
 H       2.439188    -1.517569    -2.654402      24.09
 C      -0.370920    -1.479982     0.596387      51.72
 H      -1.082488    -2.324472     0.823671      22.18
 C       0.003065     0.906400     0.315239      56.76
 H      -0.423151     1.900043    -0.002163      18.04
 C       1.394992     0.634636    -0.099456      -3.70
 O       2.312835     1.690729    -0.286572     189.42
 C       1.894484     3.036084     0.102981     101.35
 H       2.600781     3.852806    -0.196625      24.97
 H       0.860941     3.483396    -0.332308      22.52
 H       1.868405     3.013140     1.266076      23.58
 C       1.792765    -0.774422    -0.155195      11.00
 O       3.187078    -0.892604    -0.339000     172.85
 C       0.959163    -1.840247     0.207971      56.20
 H       1.250313    -2.788549     0.054311      18.78
 C      -0.822082    -0.161162     0.693095      26.14
 C      -2.301849     0.195170     1.042198      89.29
 H      -2.709601    -0.773619     1.441567      22.99
 O      -2.447469     1.300138     1.893744     246.75
 H      -2.244200     0.924761     2.954169      20.84
 C      -3.152247     0.442776    -0.237553      74.37
 H      -2.619157     1.319901    -0.708494      23.18
 O      -3.199027    -0.710215    -1.086316     276.97
 H      -3.111673    -0.518959    -2.032036      25.73
 C      -4.651295     1.001593     0.168040      93.79
 O      -4.969903     2.425144    -0.383505     243.81
 H      -4.788824     3.078192     0.337988      26.27
 H      -4.796401     1.249462     1.110640      28.63
 H      -5.488702     0.351039    -0.162267      27.18
55
name = lig-etoh-Waterframe_325
 C       5.821773    -1.931025     2.086099      43.33
 H       5.960420    -0.905858     1.810592      20.90
 C       5.247267    -4.174439     1.222896      28.31
 H       4.810031    -4.770872     0.351837      14.12
 C       5.551136    -4.850020     2.428044      39.46
 O       5.517999    -6.162462     2.685914     294.20
 C       4.648325    -7.026005     1.852468     116.59
 H       5.198905    -7.171055     0.887275      30.49
 H       3.736713    -6.591481     1.539638      32.09
 H       4.429987    -7.951416     2.520373      25.28
 C       5.986112    -4.011324     3.565985      -4.34
 O       6.384192    -4.424548     4.795066     290.76
 H       5.910114    -5.293953     5.053178      26.22
 C       5.989346    -2.564870     3.350420      60.92
 H       6.283984    -1.930133     4.301171      22.70
 C       5.404365    -2.754456     0.962064      39.80
 C       5.148722    -2.270651    -0.437581      80.29
 H       5.564973    -3.203796    -1.174701      21.39
 O       5.866157    -1.061386    -0.832762     280.48
 H       5.398908    -0.370471    -0.352594      26.22
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 C       3.637591    -2.158402    -0.895392      71.74
 H       3.047859    -3.071337    -0.546320      18.47
 C       3.472765    -2.070219    -2.438117      88.94
 O       3.253704    -3.413883    -3.036810     271.90
 H       4.177693    -3.460167    -3.531555      23.48
 H       4.178505    -1.446452    -2.988487      22.15
 H       2.585549    -1.426060    -2.644750      24.54
 C      -0.381237    -1.530377     0.598654      47.24
 H      -1.095169    -2.324083     0.857110      16.82
 C       0.033945     0.931606     0.305552      76.90
 H      -0.457939     1.858434     0.125710      18.79
 C       1.335365     0.617997    -0.065143       4.51
 O       2.381406     1.626962    -0.305989     156.86
 C       1.809161     2.985741     0.100236     107.08
 H       2.656650     3.599429    -0.278048      23.77
 H       0.925224     3.303574    -0.214958      26.44
 H       1.528252     2.981130     1.256904      22.86
 C       1.828895    -0.729554    -0.130481      18.43
 O       3.147921    -0.895298    -0.325425     184.82
 C       0.909873    -1.744526     0.168436      66.39
 H       1.313707    -2.708897     0.220592      21.76
 C      -0.787189    -0.191707     0.636374      38.64
 C      -2.288412     0.164622     0.998775      90.86
 H      -2.746394    -0.732420     1.499402      22.51
 O      -2.440309     1.317364     1.937146     246.24
 H      -2.104106     0.879906     2.819973      23.73
 C      -3.109069     0.541417    -0.213202      75.75
 H      -2.718048     1.306508    -0.924302      22.63
 O      -3.215998    -0.720159    -1.134452     239.96
 H      -3.132215    -0.366526    -2.027244      25.54
 C      -4.560253     1.091180     0.158230      93.49
 O      -4.982301     2.422117    -0.415208     287.11
 H      -4.971503     3.121435     0.258932      27.66
 H      -4.512862     1.006829     1.238135      27.41
 H      -5.120320     0.270537    -0.199768      27.39
55
name = lig-etoh-Waterframe_326
 C       5.815648    -1.980889     2.070598      52.92
 H       5.956887    -0.923280     2.029711      20.43
 C       5.253744    -4.154522     1.231829      52.43
 H       4.859614    -4.816234     0.468440      17.05
 C       5.622309    -4.805266     2.462497      30.58
 O       5.446701    -6.230089     2.735185     440.51
 C       4.623802    -6.983558     1.875947     127.08
 H       5.265620    -7.331017     0.990333      26.18
 H       3.690481    -6.497221     1.659192      27.71
 H       4.415865    -8.005337     2.405995      23.07
 C       5.959595    -3.959918     3.537684      21.46
 O       6.365995    -4.442114     4.747213     374.84
 H       5.888685    -5.270703     5.000614      31.55
 C       6.047600    -2.547068     3.356391      45.28
 H       6.160985    -1.783172     4.187437      18.78
 C       5.357684    -2.774189     1.025379      46.48
 C       5.178062    -2.274236    -0.497486     114.35
 H       5.616204    -2.883607    -1.139558      26.15
 O       5.819713    -1.010855    -0.837099     306.06
 H       5.422575    -0.244817    -0.382677      24.89
 C       3.687177    -2.142708    -0.877424      77.22
 H       3.089283    -3.029799    -0.455863      18.78
 C       3.475254    -1.978559    -2.399932      91.09
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 O       3.314646    -3.427875    -3.059151     241.63
 H       4.204225    -3.568837    -3.533533      26.16
 H       4.302562    -1.586819    -2.837497      23.04
 H       2.472715    -1.660396    -2.502667      25.11
 C      -0.421763    -1.522457     0.597655      38.29
 H      -0.974104    -2.367089     0.955721      17.90
 C       0.035133     0.884893     0.275335      65.52
 H      -0.283701     1.826755     0.529724      19.52
 C       1.392039     0.656189    -0.040608      19.34
 O       2.332840     1.583978    -0.303782     223.90
 C       1.784860     2.899122     0.090922     113.39
 H       2.585179     3.641343    -0.051420      24.61
 H       1.010913     2.995804    -0.637012      24.18
 H       1.747959     2.989493     1.219525      23.67
 C       1.804956    -0.648370    -0.078048      22.49
 O       3.156222    -0.909997    -0.317952     190.43
 C       0.922157    -1.738161     0.139539      62.88
 H       1.295420    -2.797908     0.313400      21.49
 C      -0.874315    -0.156306     0.608006      41.87
 C      -2.250025     0.143251     0.968527      95.86
 H      -2.772894    -0.697332     1.433591      24.09
 O      -2.400723     1.318959     1.946960     274.11
 H      -2.157105     1.004259     2.760017      28.45
 C      -3.123667     0.638120    -0.318533      71.73
 H      -2.446413     1.335039    -0.849532      23.76
 O      -3.234220    -0.683993    -1.113738     226.21
 H      -3.241956    -0.426847    -2.055880      25.26
 C      -4.462210     1.155464     0.138152      99.23
 O      -4.969367     2.345525    -0.442963     283.49
 H      -4.837321     3.109312     0.122558      28.29
 H      -4.627687     1.115950     1.378159      24.43
 H      -5.196917     0.504844    -0.336001      25.30
55
name = lig-etoh-Waterframe_327
 C       5.801443    -1.995211     2.090052      63.42
 H       5.877980    -0.909220     2.007612      21.54
 C       5.251973    -4.222545     1.249944      41.86
 H       5.000164    -4.804662     0.425465      20.26
 C       5.615753    -4.770619     2.457666      14.51
 O       5.413363    -6.205114     2.810785     289.64
 C       4.610450    -6.996946     1.864677     108.43
 H       4.996034    -7.249669     0.835877      24.73
 H       3.672139    -6.443792     1.582704      27.72
 H       4.328571    -7.879930     2.465177      23.14
 C       5.973803    -3.887405     3.533360      14.72
 O       6.356973    -4.451004     4.738195     374.70
 H       5.891337    -5.335215     4.928003      32.00
 C       6.085208    -2.532730     3.320650      56.83
 H       6.315076    -2.005386     4.223254      22.92
 C       5.354521    -2.791479     0.999207      53.56
 C       5.188409    -2.216783    -0.486237     111.76
 H       5.665800    -2.924060    -1.117387      24.51
 O       5.800048    -0.967770    -0.823762     335.33
 H       5.451204    -0.166488    -0.356616      24.60
 C       3.696326    -2.140637    -0.878857      83.89
 H       3.196722    -3.055494    -0.486522      20.13
 C       3.430996    -2.051130    -2.386987      96.78
 O       3.400494    -3.399491    -3.043687     273.49
 H       4.247766    -3.431243    -3.559970      26.36
 H       4.200203    -1.394099    -2.780254      23.34
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 H       2.515863    -1.512321    -2.627485      25.72
 C      -0.413799    -1.463180     0.562408      39.89
 H      -1.001487    -2.253986     0.947170      20.69
 C       0.007013     0.863693     0.293679      71.39
 H      -0.223847     1.797865     0.684030      17.75
 C       1.386902     0.636925    -0.010774      14.86
 O       2.313030     1.615426    -0.275846     247.93
 C       1.860406     2.859213     0.052832     117.70
 H       2.553726     3.640768    -0.165267      25.18
 H       0.834816     3.232938    -0.699963      22.81
 H       1.312087     2.845959     0.981181      26.57
 C       1.819498    -0.750090    -0.060034      26.21
 O       3.200164    -0.882438    -0.286313     185.47
 C       0.899813    -1.745110     0.188000      51.99
 H       1.372113    -2.841444     0.087046      17.28
 C      -0.898547    -0.186581     0.586164      47.25
 C      -2.329933     0.229651     0.959820      89.02
 H      -2.774928    -0.717035     1.267707      23.10
 O      -2.345075     1.311266     1.896718     298.85
 H      -2.193253     0.915294     2.767079      26.14
 C      -3.051295     0.625319    -0.370165      88.70
 H      -2.457764     1.401031    -0.875872      23.80
 O      -3.263104    -0.591763    -1.075750     257.35
 H      -3.264060    -0.515173    -2.045737      25.61
 C      -4.478033     1.139151     0.083952      81.88
 O      -4.942370     2.348966    -0.494800     289.75
 H      -4.607102     3.090444     0.008957      29.07
 H      -4.564593     1.409144     1.300897      22.75
 H      -5.226450     0.287253    -0.120566      24.56
55
name = lig-etoh-Waterframe_328
 C       5.759807    -1.947919     2.043224      53.09
 H       5.820149    -0.871288     1.769235      21.68
 C       5.256671    -4.236214     1.179402      58.68
 H       5.067058    -4.905845     0.389208      21.11
 C       5.540692    -4.810249     2.485928      49.87
 O       5.403366    -6.109039     2.833585     337.91
 C       4.565006    -6.982150     1.859732     134.80
 H       5.190895    -7.154949     0.995952      29.41
 H       3.603385    -6.424158     1.614528      24.33
 H       4.335797    -7.848109     2.395249      25.15
 C       6.015259    -3.951410     3.546228       4.84
 O       6.368898    -4.417288     4.742380     286.14
 H       5.822148    -5.306334     5.031110      24.19
 C       6.125969    -2.524697     3.348344      55.97
 H       6.550318    -1.964168     4.108658      23.30
 C       5.399456    -2.803078     0.967476      51.28
 C       5.178956    -2.169043    -0.426651     106.88
 H       5.702263    -3.085087    -1.194155      20.90
 O       5.825856    -0.926615    -0.797684     303.16
 H       5.364390    -0.235125    -0.229153      22.80
 C       3.669449    -2.152263    -0.875456      76.52
 H       3.187157    -2.982768    -0.419313      19.75
 C       3.395469    -2.114247    -2.405522      97.59
 O       3.492724    -3.350292    -3.018676     277.13
 H       4.353559    -3.357765    -3.437352      26.89
 H       4.161293    -1.389262    -2.908401      21.48
 H       2.372107    -1.646574    -2.585778      23.83
 C      -0.430836    -1.488061     0.540743      32.00
 H      -1.153406    -2.264378     0.751550      19.54
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 C       0.032519     0.884771     0.352023      77.69
 H      -0.436856     1.902560     0.377884      16.72
 C       1.315194     0.509532     0.021551       5.21
 O       2.343789     1.607724    -0.256812     149.97
 C       1.826572     2.968235    -0.005386     100.49
 H       2.745743     3.540873     0.022236      23.76
 H       0.946819     3.354725    -0.806120      21.96
 H       1.403282     3.015059     0.990912      25.07
 C       1.873371    -0.776888    -0.064874      22.85
 O       3.228010    -0.878149    -0.251232     182.70
 C       0.928722    -1.797293     0.234019      62.01
 H       1.095612    -2.965753     0.061166      16.53
 C      -0.891991    -0.154412     0.582045      43.24
 C      -2.357339     0.257689     0.910881      94.23
 H      -2.992760    -0.537195     1.378365      22.44
 O      -2.300820     1.315736     1.851371     255.38
 H      -2.081060     0.828876     2.773802      24.44
 C      -3.062529     0.643911    -0.328894      96.23
 H      -2.604251     1.365764    -0.994371      23.26
 O      -3.277974    -0.553387    -1.081926     266.20
 H      -3.187084    -0.215982    -2.007094      25.08
 C      -4.512409     1.130282     0.075285      87.57
 O      -4.921460     2.393628    -0.607959     282.54
 H      -4.673881     3.094569     0.027745      28.38
 H      -4.283276     1.259707     1.102838      26.26
 H      -5.189673     0.227316    -0.027684      26.14
55
name = lig-etoh-Waterframe_329
 C       5.747071    -1.958494     2.029502      46.79
 H       5.901130    -0.862281     1.895981      22.58
 C       5.295281    -4.212395     1.149389      69.69
 H       5.029388    -4.886256     0.319308      15.79
 C       5.460839    -4.749519     2.460848      55.27
 O       5.344418    -6.088776     2.808287     287.07
 C       4.585560    -6.917559     1.908561     156.97
 H       5.252958    -7.153238     1.103864      35.14
 H       3.632662    -6.451850     1.491068      28.16
 H       4.437787    -7.834583     2.363694      26.86
 C       6.031532    -3.939047     3.501268     -11.06
 O       6.405845    -4.395754     4.801578     259.75
 H       5.859721    -5.255595     5.092625      22.69
 C       6.144414    -2.531833     3.288229      57.98
 H       6.614625    -1.885494     3.981015      23.51
 C       5.442618    -2.807987     0.964697      43.18
 C       5.170325    -2.211768    -0.437599      91.01
 H       5.772760    -2.896248    -1.335907      20.80
 O       5.851027    -0.919928    -0.734394     284.11
 H       5.456852    -0.071976    -0.305157      21.25
 C       3.677737    -2.137478    -0.834618      85.32
 H       3.122307    -2.935184    -0.398287      20.54
 C       3.361185    -2.054903    -2.382140      85.80
 O       3.576205    -3.389856    -3.015157     259.03
 H       4.465864    -3.499136    -3.357698      27.98
 H       4.133874    -1.333686    -2.902470      19.89
 H       2.250654    -1.970592    -2.467642      22.78
 C      -0.445037    -1.508036     0.525616      28.63
 H      -1.117824    -2.370765     0.623965      16.97
 C       0.013771     0.885267     0.395559      86.13
 H      -0.238719     1.957843     0.004948      15.07
 C       1.385597     0.565219     0.026198       6.71
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 O       2.305350     1.555990    -0.226106     170.75
 C       1.817482     3.064446    -0.035216     103.01
 H       2.780087     3.636350    -0.060627      24.36
 H       1.361303     3.387035    -0.867629      26.61
 H       1.505108     3.252064     0.990178      24.63
 C       1.854755    -0.808223    -0.021998      16.95
 O       3.227827    -0.905100    -0.238843     194.49
 C       0.925475    -1.870984     0.250116      52.61
 H       1.163933    -2.956982     0.221201      17.16
 C      -0.900818    -0.161703     0.605548      47.73
 C      -2.292868     0.218856     0.894913     102.76
 H      -2.865440    -0.627636     1.361161      23.91
 O      -2.268673     1.359418     1.843480     224.76
 H      -1.946099     1.037938     2.855769      24.89
 C      -3.193234     0.699000    -0.330471      86.44
 H      -2.577036     1.467467    -0.824980      23.02
 O      -3.265864    -0.557674    -1.146534     268.19
 H      -3.248809    -0.352563    -2.149719      24.06
 C      -4.505311     1.184332     0.096140     115.97
 O      -4.899383     2.402599    -0.701858     235.48
 H      -4.962927     3.121595    -0.028951      28.75
 H      -4.618018     1.443366     1.059183      30.16
 H      -5.339056     0.560403    -0.234985      26.64
55
name = lig-etoh-Waterframe_330
 C       5.793078    -1.986493     2.036735      54.44
 H       5.903362    -0.892660     1.949422      24.11
 C       5.329089    -4.174817     1.157295      51.23
 H       4.976981    -4.789594     0.265012      12.50
 C       5.448361    -4.684850     2.448243      50.04
 O       5.264290    -6.056867     2.793935     282.46
 C       4.645824    -6.901686     1.906500     121.91
 H       5.163946    -7.135778     0.946707      30.93
 H       3.697931    -6.472876     1.520302      31.25
 H       4.363140    -7.769584     2.525920      25.40
 C       6.026162    -3.883209     3.519564      -6.20
 O       6.434693    -4.363618     4.811266     359.63
 H       5.937961    -5.208473     4.964067      29.07
 C       6.160433    -2.553783     3.205126      63.78
 H       6.517147    -1.946176     4.075338      22.54
 C       5.450402    -2.791903     0.914721      44.41
 C       5.216740    -2.216441    -0.499384     106.23
 H       5.633968    -2.903939    -1.160477      24.98
 O       5.886484    -0.943737    -0.668653     317.65
 H       5.385872    -0.126566    -0.274711      21.38
 C       3.693763    -2.123833    -0.817523      88.20
 H       3.212448    -3.065015    -0.455056      20.01
 C       3.368444    -2.080116    -2.329475      91.59
 O       3.629447    -3.459851    -2.987189     258.21
 H       4.522227    -3.335213    -3.436300      25.64
 H       3.773170    -1.166148    -2.809825      22.93
 H       2.317766    -1.803983    -2.529625      24.01
 C      -0.421626    -1.528187     0.519028      28.97
 H      -1.125009    -2.335603     0.891924      19.73
 C       0.095245     0.852659     0.329811      73.69
 H      -0.388195     1.940991     0.285850      16.22
 C       1.380827     0.609919     0.079737      20.56
 O       2.274422     1.607546    -0.190491     232.96
 C       1.928078     3.072652    -0.062690     110.51
 H       2.921622     3.568248    -0.239011      23.00
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 H       1.277497     3.347926    -0.835566      26.29
 H       1.127512     3.283227     0.726075      23.24
 C       1.808643    -0.807527     0.055678      24.34
 O       3.191839    -0.927055    -0.219420     202.76
 C       0.902595    -1.863962     0.253504      44.22
 H       1.308939    -2.786716     0.315013      17.42
 C      -0.855182    -0.205980     0.598011      68.25
 C      -2.301856     0.208703     0.944954      85.91
 H      -2.655079    -0.751954     1.365416      23.58
 O      -2.250094     1.415438     1.834632     241.49
 H      -2.002338     0.905521     2.818317      22.98
 C      -3.188688     0.662908    -0.329056      69.91
 H      -2.723222     1.569038    -0.805583      23.20
 O      -3.261322    -0.535051    -1.211306     247.29
 H      -3.340800    -0.316521    -2.225380      23.23
 C      -4.635347     1.304569     0.071614     101.60
 O      -4.877960     2.429491    -0.781801     234.52
 H      -4.973912     3.221234    -0.198403      27.96
 H      -4.867027     1.542234     1.166662      27.92
 H      -5.299807     0.459850    -0.189681      27.54
55
name = lig-etoh-Waterframe_331
 C       5.851483    -1.957011     1.939442      55.40
 H       5.878179    -0.875989     1.823189      23.06
 C       5.319421    -4.130434     1.146762      57.98
 H       5.014124    -4.921223     0.375400      17.29
 C       5.506547    -4.695983     2.491987      28.70
 O       5.233993    -5.954369     2.816224     295.89
 C       4.616777    -6.936248     1.832572     115.91
 H       5.373829    -7.223223     1.015327      28.40
 H       3.693308    -6.516596     1.520053      28.13
 H       4.415827    -7.897533     2.473342      23.52
 C       5.999541    -3.909400     3.548037      12.47
 O       6.434517    -4.323098     4.748779     371.67
 H       6.005385    -5.148305     5.018767      27.91
 C       6.203235    -2.544946     3.262192      41.72
 H       6.454561    -1.811885     4.138547      19.83
 C       5.461315    -2.750996     0.882741      32.79
 C       5.254518    -2.193726    -0.511116     116.91
 H       5.612620    -2.862188    -1.172280      25.20
 O       5.939074    -0.972572    -0.633416     292.46
 H       5.284834    -0.316310    -0.173173      22.74
 C       3.706009    -2.155514    -0.844696      72.89
 H       3.328178    -3.104618    -0.320407      19.55
 C       3.352298    -2.151584    -2.321082     106.93
 O       3.675627    -3.447987    -2.932021     250.67
 H       4.449852    -3.340585    -3.607402      26.05
 H       4.075442    -1.557603    -2.818417      22.33
 H       2.275822    -2.025784    -2.384829      23.50
 C      -0.445089    -1.560167     0.575405      36.68
 H      -1.130997    -2.339919     1.026753      20.55
 C       0.018478     0.832176     0.279408      68.05
 H      -0.344757     1.839160     0.641142      16.74
 C       1.408522     0.589176     0.128943      13.23
 O       2.320960     1.693845    -0.152256     192.87
 C       1.969137     3.016536    -0.152854     102.22
 H       2.906475     3.625687     0.060074      23.22
 H       1.262681     3.270941    -1.157217      22.31
 H       1.519503     3.322453     0.926924      23.58
 C       1.822084    -0.730786     0.099745      23.15
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 O       3.139155    -0.940663    -0.175340     209.11
 C       0.939187    -1.815280     0.261596      65.63
 H       1.268893    -2.763023     0.316467      20.16
 C      -0.809793    -0.200255     0.556014      44.25
 C      -2.301273     0.229645     0.957405      92.03
 H      -2.890088    -0.477225     1.564078      21.60
 O      -2.250029     1.402450     1.826244     250.71
 H      -2.109188     1.083072     2.881514      23.08
 C      -3.160347     0.621777    -0.271122      62.57
 H      -2.621129     1.382271    -0.888172      22.31
 O      -3.280545    -0.472728    -1.240296     257.06
 H      -3.248000     0.011435    -2.148460      23.94
 C      -4.759578     1.318823     0.016249      80.50
 O      -4.885176     2.486597    -0.865063     229.19
 H      -4.675931     3.281948    -0.273461      26.15
 H      -4.603529     1.632333     1.200052      24.67
 H      -5.480629     0.512820    -0.175021      27.42
55
name = lig-etoh-Waterframe_332
 C       5.941446    -1.923269     1.969071      58.21
 H       6.035752    -0.869659     1.779034      23.27
 C       5.299390    -4.150006     1.203511      37.07
 H       5.055692    -4.833463     0.354071      21.28
 C       5.552811    -4.658069     2.422810      32.92
 O       5.193289    -5.971375     2.837337     245.07
 C       4.612070    -6.935632     1.812507     120.41
 H       5.423388    -7.072932     1.023004      26.75
 H       3.747847    -6.649660     1.250237      28.69
 H       4.490991    -7.930700     2.424246      22.38
 C       6.005984    -3.833918     3.516663      -0.85
 O       6.431934    -4.326087     4.739721     327.27
 H       5.970181    -5.148042     5.062478      30.17
 C       6.181713    -2.455270     3.234871      51.10
 H       6.543037    -1.777583     4.106210      21.36
 C       5.490510    -2.775733     0.884626      21.64
 C       5.247228    -2.203688    -0.499199      83.52
 H       5.794981    -2.912524    -1.409060      21.30
 O       5.979255    -0.964378    -0.633251     222.66
 H       5.549542    -0.103457    -0.215894      23.02
 C       3.717985    -2.188815    -0.806108      76.55
 H       3.236729    -3.085170    -0.309236      20.54
 C       3.381492    -2.230400    -2.343445     109.85
 O       3.700215    -3.468552    -2.889712     255.81
 H       4.546431    -3.371774    -3.505357      25.05
 H       3.909137    -1.394592    -2.815237      24.85
 H       2.322951    -1.996096    -2.541911      24.97
 C      -0.410829    -1.557022     0.643088      21.67
 H      -1.070159    -2.415662     0.845810      17.65
 C       0.003022     0.880981     0.292143      65.50
 H      -0.307691     1.867689     0.459426      18.89
 C       1.404731     0.699602     0.131431      10.85
 O       2.416768     1.629227    -0.105675     203.42
 C       1.967682     3.037825    -0.157281     109.75
 H       2.911396     3.591440    -0.315316      24.00
 H       1.436331     3.511577    -1.205933      23.22
 H       1.378700     3.328246     0.759482      25.11
 C       1.861991    -0.712634     0.087627      12.26
 O       3.184055    -0.960427    -0.149505     177.94
 C       0.915837    -1.771674     0.319632      53.27
 H       1.303617    -2.802718     0.222530      20.85
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 C      -0.947882    -0.244778     0.561405      43.96
 C      -2.309470     0.240299     0.987691      94.36
 H      -2.810331    -0.600905     1.530540      23.60
 O      -2.261407     1.416753     1.822774     252.08
 H      -2.074417     1.005495     2.796107      24.26
 C      -3.216289     0.645729    -0.265816      81.60
 H      -2.571543     1.486785    -0.594408      23.66
 O      -3.310544    -0.404137    -1.224467     265.87
 H      -3.110217    -0.135135    -2.214433      23.71
 C      -4.688672     1.287383    -0.036656      96.42
 O      -4.907552     2.527807    -0.913893     213.13
 H      -4.495838     3.271250    -0.362623      27.11
 H      -4.827641     1.800000     1.049895      25.47
 H      -5.645360     0.828500    -0.225982      26.45
55
name = lig-etoh-Waterframe_333
 C       5.982843    -1.906073     1.942726      65.27
 H       6.254639    -0.876301     1.784407      24.59
 C       5.281955    -4.140052     1.147851      68.66
 H       4.921861    -4.765610     0.345988      20.39
 C       5.555939    -4.684683     2.468614       5.87
 O       5.141732    -6.020608     2.826021     253.34
 C       4.689440    -6.901067     1.806119     112.78
 H       5.427104    -7.056921     1.026277      28.10
 H       3.724466    -6.563727     1.341471      25.94
 H       4.430015    -7.851090     2.345647      24.03
 C       6.038003    -3.760436     3.472320     -12.81
 O       6.422668    -4.318960     4.741641     183.79
 H       5.892665    -5.172999     4.929371      30.76
 C       6.163518    -2.387528     3.239473      52.24
 H       6.618374    -1.772286     4.035281      20.06
 C       5.562475    -2.784109     0.958285      36.59
 C       5.254815    -2.198930    -0.464567      56.88
 H       5.816078    -3.012280    -1.332860      21.13
 O       6.020761    -0.940114    -0.676864     189.68
 H       5.585554    -0.080025    -0.249040      23.17
 C       3.694642    -2.193560    -0.771805      85.91
 H       3.257046    -3.098007    -0.357900      22.88
 C       3.395200    -2.190375    -2.325503      96.30
 O       3.744059    -3.549862    -2.897271     219.33
 H       4.717506    -3.475031    -3.289739      24.56
 H       3.848402    -1.293272    -2.808190      25.64
 H       2.293404    -2.106530    -2.522769      25.83
 C      -0.438789    -1.504027     0.682565      43.79
 H      -0.995548    -2.407293     0.770209      18.45
 C       0.005659     0.910418     0.335826      74.27
 H      -0.427516     1.796755     0.103400      20.85
 C       1.390542     0.679812     0.105639       7.03
 O       2.464302     1.585422    -0.067347     161.10
 C       2.009713     3.103035    -0.183393     108.30
 H       2.958204     3.576797    -0.252295      24.70
 H       1.284153     3.021193    -0.993435      25.87
 H       1.380510     3.396900     0.550214      28.15
 C       1.833660    -0.705709     0.071617      12.59
 O       3.283691    -0.965881    -0.145350     165.03
 C       0.963431    -1.715315     0.369775      52.44
 H       1.314172    -2.854415     0.227041      20.69
 C      -0.972165    -0.199457     0.583222      30.66
 C      -2.414084     0.197820     1.001068      89.17
 H      -2.751074    -0.726508     1.509861      25.39
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 O      -2.278422     1.422124     1.843822     253.40
 H      -1.994989     1.095999     2.733732      28.42
 C      -3.290165     0.741289    -0.268863      87.19
 H      -2.768854     1.631233    -0.644566      24.52
 O      -3.333527    -0.373783    -1.198612     263.70
 H      -3.131688    -0.175826    -2.198537      24.39
 C      -4.621748     1.362549    -0.070091     106.41
 O      -4.892488     2.533448    -0.939151     237.45
 H      -4.675989     3.386041    -0.392516      27.12
 H      -4.781241     1.548805     0.967859      28.88
 H      -5.333005     0.532923    -0.350915      26.85
55
name = lig-etoh-Waterframe_334
 C       6.014874    -1.871871     1.942831      59.66
 H       6.217424    -0.844891     1.603356      25.18
 C       5.296416    -4.158341     1.173275      72.53
 H       4.816476    -4.687887     0.405401      20.21
 C       5.490490    -4.702572     2.464542      11.15
 O       5.150635    -6.002342     2.848114     236.24
 C       4.733558    -6.884908     1.775578     117.37
 H       5.464374    -7.073427     1.037919      30.72
 H       3.783150    -6.393028     1.378866      26.45
 H       4.524891    -7.805541     2.223356      26.77
 C       6.057078    -3.826172     3.505774      -9.26
 O       6.401230    -4.259297     4.699685     165.88
 H       6.011045    -5.173259     5.067277      22.00
 C       6.194123    -2.374770     3.273827      51.84
 H       6.571959    -1.766155     4.033682      22.26
 C       5.594967    -2.748367     0.919512      26.81
 C       5.313319    -2.189867    -0.419222      83.21
 H       5.677533    -2.924180    -1.128286      24.34
 O       6.034073    -0.948421    -0.743856     249.49
 H       5.429862    -0.232229    -0.289414      25.65
 C       3.728225    -2.167715    -0.779796      81.90
 H       3.308454    -3.021874    -0.309966      24.25
 C       3.385989    -2.181797    -2.281515      89.19
 O       3.792413    -3.581004    -2.909887     192.31
 H       4.787285    -3.567780    -3.242972      25.29
 H       4.071210    -1.555464    -2.886502      24.43
 H       2.284442    -2.228073    -2.379468      25.65
 C      -0.427799    -1.439089     0.670930      48.74
 H      -1.103496    -2.208207     0.963666      24.17
 C      -0.013758     0.903992     0.338906      70.26
 H      -0.398494     1.865775     0.032483      20.08
 C       1.412507     0.608750     0.088426       7.45
 O       2.437697     1.616133    -0.017800     184.42
 C       2.033318     3.034989    -0.217887     124.01
 H       2.855708     3.729155    -0.315097      25.89
 H       1.496575     3.050406    -1.060743      28.86
 H       1.645754     3.401757     0.710945      27.39
 C       1.899737    -0.698368     0.062171      21.10
 O       3.290421    -0.930415    -0.132999     181.64
 C       0.946677    -1.703512     0.408841      47.39
 H       1.335846    -2.854121     0.485656      19.74
 C      -0.902414    -0.108974     0.618749      24.08
 C      -2.480608     0.236751     0.958187      89.18
 H      -3.079207    -0.492460     1.496762      24.35
 O      -2.323060     1.391097     1.883561     276.23
 H      -2.031755     1.091011     2.695029      32.01
 C      -3.228111     0.822506    -0.279600      85.80
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 H      -2.540731     1.456429    -0.845095      23.95
 O      -3.353676    -0.364630    -1.172811     249.97
 H      -3.347216     0.020156    -2.117310      25.23
 C      -4.665972     1.402375    -0.067019     103.46
 O      -4.858855     2.537063    -0.927716     257.26
 H      -5.018443     3.325952    -0.256939      25.75
 H      -4.793451     1.580891     0.902737      30.38
 H      -5.227302     0.534945    -0.505472      27.07
55
name = lig-etoh-Waterframe_335
 C       6.036412    -1.884025     1.975200      58.14
 H       6.134037    -0.787906     1.793172      25.29
 C       5.314995    -4.109931     1.208949      73.39
 H       4.893488    -4.719079     0.458322      21.91
 C       5.448889    -4.657811     2.474467      28.62
 O       5.204664    -5.972899     2.879007     234.52
 C       4.741746    -6.869613     1.754217     126.14
 H       5.568679    -6.879477     1.036214      30.19
 H       3.857775    -6.538793     1.108971      27.51
 H       4.540787    -7.783472     2.195388      27.10
 C       6.016694    -3.829544     3.462907      14.38
 O       6.411030    -4.214781     4.741470     157.00
 H       6.024405    -5.145508     5.099703      19.48
 C       6.237112    -2.451840     3.252344      60.33
 H       6.490466    -1.899431     4.082803      23.76
 C       5.605848    -2.751626     0.936129      13.37
 C       5.349559    -2.199022    -0.488057      80.80
 H       5.705340    -2.856465    -1.133806      27.03
 O       5.997783    -0.984257    -0.799429     273.21
 H       5.581840    -0.094471    -0.473224      25.67
 C       3.828175    -2.126536    -0.754586      77.15
 H       3.335742    -2.954548    -0.248561      23.70
 C       3.451252    -2.291486    -2.280067     109.35
 O       3.803627    -3.566803    -2.893740     239.83
 H       4.748990    -3.404918    -3.311733      24.59
 H       3.833617    -1.382160    -2.852563      26.08
 H       2.415350    -2.006944    -2.497678      26.06
 C      -0.399439    -1.379766     0.670658      61.63
 H      -1.062873    -2.109434     1.127158      29.57
 C       0.063270     0.928122     0.272047      58.33
 H      -0.189645     2.074122     0.380236      19.97
 C       1.421203     0.643737     0.091073      10.34
 O       2.395654     1.640787     0.019663     209.31
 C       2.051525     2.957979    -0.225797     116.01
 H       3.052982     3.385213    -0.533893      24.72
 H       1.360850     3.353183    -1.021589      25.78
 H       1.459836     3.413959     0.757837      24.09
 C       1.932790    -0.740775     0.082789      13.60
 O       3.255707    -0.879520    -0.128315     169.82
 C       0.937837    -1.725562     0.438356      57.98
 H       1.273825    -2.771710     0.726341      21.83
 C      -0.937903    -0.077243     0.659786      24.80
 C      -2.417234     0.381703     0.931595      93.07
 H      -3.004075    -0.506274     1.204131      24.20
 O      -2.401679     1.370431     1.930384     303.51
 H      -2.150673     0.890000     2.660481      28.60
 C      -3.121444     0.827949    -0.328566      75.35
 H      -2.458883     1.609171    -0.799708      23.63
 O      -3.372664    -0.344816    -1.145185     244.07
 H      -3.512502    -0.162973    -2.131486      25.25
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 C      -4.666861     1.384473    -0.080005      93.65
 O      -4.849298     2.581194    -0.890335     254.88
 H      -5.058386     3.385420    -0.257829      25.01
 H      -4.991669     1.707381     0.956173      25.89
 H      -5.542470     0.736339    -0.335064      26.91
55
name = lig-etoh-Waterframe_336
 C       6.036721    -1.915851     2.003875      69.08
 H       6.162062    -0.822750     2.003526      20.34
 C       5.306285    -4.064044     1.195108      56.83
 H       5.060531    -4.712551     0.355478      22.86
 C       5.453771    -4.630873     2.525042      22.42
 O       5.221685    -5.964505     2.852544     251.02
 C       4.789957    -6.833938     1.744365     122.86
 H       5.716166    -6.967350     1.074104      25.64
 H       3.853376    -6.470673     1.275789      25.07
 H       4.618022    -7.817238     2.204849      23.62
 C       5.995578    -3.807798     3.512497      16.74
 O       6.419043    -4.189743     4.796986     205.76
 H       5.972029    -5.079482     5.044814      21.73
 C       6.271575    -2.509673     3.212392      48.32
 H       6.541399    -1.968668     4.099045      25.51
 C       5.624898    -2.715584     0.952478      11.64
 C       5.343649    -2.196571    -0.523536      63.80
 H       5.830643    -3.034205    -1.346032      21.74
 O       6.000692    -0.990948    -0.877393     261.25
 H       5.579698    -0.164799    -0.409378      24.80
 C       3.844686    -2.132686    -0.734874      72.96
 H       3.430632    -3.014817    -0.160321      24.89
 C       3.493155    -2.280657    -2.298069     103.69
 O       3.816770    -3.522508    -2.878403     227.36
 H       4.684987    -3.512671    -3.454580      25.68
 H       4.087150    -1.473839    -2.792095      26.77
 H       2.387486    -2.311721    -2.316758      26.37
 C      -0.442806    -1.336514     0.731656      34.79
 H      -0.987627    -2.243079     1.090388      27.00
 C       0.102420     0.963811     0.258959      65.55
 H      -0.138213     2.086236     0.599656      19.22
 C       1.429617     0.632395     0.100776      23.11
 O       2.367202     1.588845     0.025777     172.49
 C       2.049782     3.005741    -0.230708      94.10
 H       3.109700     3.420053    -0.386493      24.89
 H       1.152077     2.942414    -1.095254      22.66
 H       1.731888     3.635069     0.796962      24.48
 C       1.844077    -0.736146     0.118544      16.04
 O       3.284355    -0.855164    -0.158766     143.33
 C       0.987933    -1.733368     0.469208      61.22
 H       1.229550    -2.703050     0.664637      25.31
 C      -0.889936     0.006861     0.613222      30.30
 C      -2.302315     0.420918     0.891516      90.53
 H      -2.727666    -0.566372     1.171870      24.04
 O      -2.498705     1.377118     2.000177     250.61
 H      -2.199718     0.909329     2.882879      23.17
 C      -3.160528     0.859765    -0.394924      73.76
 H      -2.762718     1.740037    -0.953842      23.33
 O      -3.360642    -0.349806    -1.121639     251.81
 H      -3.349305    -0.205329    -2.120038      25.04
 C      -4.638424     1.430433    -0.065354      79.91
 O      -4.856034     2.637997    -0.867342     276.65
 H      -4.760020     3.477010    -0.239022      24.52
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 H      -4.659066     1.646975     1.170097      23.62
 H      -5.281096     0.571433    -0.356009      26.76
55
name = lig-etoh-Waterframe_337
 C       6.039753    -1.883237     2.001906      53.51
 H       6.262441    -0.832966     1.808483      21.02
 C       5.319694    -4.064101     1.224075      46.38
 H       5.109020    -4.704764     0.324093      20.65
 C       5.468444    -4.631563     2.496000      32.99
 O       5.228945    -5.958549     2.814207     244.95
 C       4.862990    -6.814951     1.768270     114.70
 H       5.593781    -6.995291     0.878717      26.35
 H       3.984724    -6.398977     1.317531      28.62
 H       4.625554    -7.827336     2.284150      23.56
 C       6.006866    -3.836786     3.626971      16.12
 O       6.403720    -4.183493     4.839139     217.05
 H       6.103953    -5.055573     5.209235      19.94
 C       6.307563    -2.486312     3.268401      37.36
 H       6.800246    -1.788118     4.027280      23.85
 C       5.623323    -2.675561     0.887157      15.22
 C       5.363119    -2.190861    -0.482716      75.72
 H       5.702630    -3.172882    -1.300909      20.46
 O       6.029894    -0.972767    -0.959404     241.77
 H       5.593970    -0.297838    -0.322908      25.73
 C       3.789580    -2.167148    -0.751645      71.42
 H       3.323621    -3.058755    -0.210667      23.95
 C       3.500673    -2.201325    -2.247098      99.26
 O       3.850289    -3.539540    -2.890783     217.08
 H       4.728522    -3.474836    -3.445533      25.37
 H       3.977136    -1.442372    -2.850011      26.06
 H       2.395214    -2.122197    -2.392435      26.44
 C      -0.401316    -1.334057     0.777718      53.51
 H      -1.287289    -2.012374     1.014423      18.46
 C       0.099313     1.029020     0.325618      67.54
 H      -0.236212     2.132041     0.313558      21.00
 C       1.409994     0.619365     0.117175      14.97
 O       2.427853     1.570062     0.027374     165.04
 C       2.062028     3.027194    -0.202524     110.36
 H       2.821952     3.619034    -0.742930      25.82
 H       1.290283     3.088506    -1.140858      24.31
 H       1.663142     3.496028     0.688532      26.42
 C       1.900603    -0.709858     0.106051       4.64
 O       3.294480    -0.868382    -0.203201     137.46
 C       0.902007    -1.721320     0.526790      59.33
 H       1.258477    -2.657034     0.466931      25.28
 C      -0.794381     0.040986     0.548582      33.06
 C      -2.273574     0.409220     0.864404      78.70
 H      -2.796341    -0.493155     1.261864      24.87
 O      -2.586496     1.388913     2.038564     171.30
 H      -2.110828     0.937954     2.965306      23.46
 C      -3.239762     0.921720    -0.392655      86.28
 H      -2.655546     1.500763    -1.126030      24.55
 O      -3.328147    -0.374451    -1.135626     251.21
 H      -3.047710    -0.219512    -2.071198      26.62
 C      -4.534345     1.481215    -0.028453     106.14
 O      -4.865508     2.668544    -0.822815     269.29
 H      -4.698337     3.468125    -0.213352      25.51
 H      -4.572210     1.683001     1.171228      24.76
 H      -5.249493     0.725315    -0.361474      27.49
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name = lig-etoh-Waterframe_338
 C       6.060453    -1.870741     1.966517      58.59
 H       6.383920    -0.866966     1.765461      24.06
 C       5.366552    -4.036650     1.218272      55.54
 H       4.970212    -4.802020     0.475319      17.02
 C       5.527607    -4.601815     2.524569      38.26
 O       5.278594    -5.938262     2.806310     295.32
 C       4.861371    -6.836209     1.736997     123.74
 H       5.701957    -6.887912     1.014113      29.71
 H       3.962174    -6.557803     1.237063      29.04
 H       4.637094    -7.860622     2.254928      23.53
 C       6.015579    -3.783219     3.593274       3.32
 O       6.404770    -4.197032     4.930532     172.75
 H       6.059590    -5.148387     5.180488      19.72
 C       6.319333    -2.426186     3.311979      33.20
 H       6.966904    -1.822079     4.081318      23.43
 C       5.626690    -2.686858     0.949461      43.68
 C       5.330996    -2.206419    -0.499705      87.85
 H       5.776959    -2.971799    -1.158940      23.17
 O       6.033226    -0.989326    -0.991068     217.31
 H       5.847813    -0.098574    -0.559429      25.76
 C       3.768084    -2.165552    -0.767639      85.10
 H       3.217619    -3.016586    -0.320769      22.71
 C       3.468179    -2.177521    -2.272084     100.29
 O       3.875398    -3.529523    -2.894699     247.45
 H       4.731329    -3.240093    -3.351185      25.48
 H       4.068656    -1.376544    -2.692251      24.49
 H       2.444979    -1.887779    -2.531679      25.76
 C      -0.418878    -1.273442     0.777002      41.00
 H      -1.238240    -2.007732     1.056030      17.86
 C       0.123170     1.107762     0.367367      72.75
 H      -0.211026     2.053015     0.021392      19.57
 C       1.489030     0.688358     0.138244      -1.45
 O       2.530665     1.644247     0.001193     188.61
 C       2.040503     2.994647    -0.238141     129.53
 H       2.970728     3.445938    -0.543298      25.07
 H       1.168833     3.117092    -0.795115      27.01
 H       1.679175     3.366026     0.592069      29.20
 C       1.917323    -0.724653     0.111240      10.89
 O       3.252761    -0.908156    -0.237154     179.07
 C       0.936761    -1.690367     0.519555      58.16
 H       1.104995    -2.801324     0.459330      20.07
 C      -0.851176     0.026361     0.585287      41.13
 C      -2.362912     0.437684     0.883516      76.98
 H      -2.833184    -0.564194     1.093597      24.43
 O      -2.614538     1.388393     2.020632     183.52
 H      -2.159892     0.753988     2.853337      22.43
 C      -3.107022     0.862113    -0.380313      82.23
 H      -2.513566     1.633628    -0.921468      24.13
 O      -3.309482    -0.386263    -1.153237     276.18
 H      -3.051640    -0.309779    -2.091249      26.66
 C      -4.522611     1.538677     0.000993     109.96
 O      -4.863846     2.697335    -0.771968     296.94
 H      -4.890399     3.495591    -0.202814      27.50
 H      -4.595965     1.809482     1.021632      28.19
 H      -5.370492     0.886404    -0.090332      28.22
55
name = lig-etoh-Waterframe_339
 C       6.140819    -1.861116     2.030512      66.98
 H       6.374257    -0.835830     1.800779      24.89
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 C       5.398579    -4.068122     1.262141      24.44
 H       4.895532    -4.633054     0.429913      11.97
 C       5.594426    -4.561844     2.544737      26.04
 O       5.324080    -5.920757     2.823831     214.44
 C       4.861912    -6.856717     1.697890     114.76
 H       5.685748    -6.965570     1.055953      31.53
 H       3.928824    -6.553375     1.196212      28.87
 H       4.806058    -7.844191     2.218604      24.71
 C       6.075372    -3.710054     3.623344      -4.74
 O       6.399410    -4.159219     4.928910     247.99
 H       5.961398    -5.096313     5.206285      26.13
 C       6.319792    -2.369494     3.269511      67.19
 H       6.809906    -1.848433     4.163438      22.17
 C       5.606631    -2.691233     0.975531      62.94
 C       5.299970    -2.190823    -0.504411     115.03
 H       5.675520    -2.849602    -1.081181      27.57
 O       6.037693    -1.031723    -1.002228     253.47
 H       5.678327    -0.204481    -0.586019      26.30
 C       3.732597    -2.167013    -0.793450      84.42
 H       3.366336    -3.029124    -0.270290      20.73
 C       3.478786    -2.168986    -2.353852     105.49
 O       3.882887    -3.436892    -2.889988     260.57
 H       4.665558    -3.358466    -3.502517      27.53
 H       4.225442    -1.491719    -2.697819      23.34
 H       2.407121    -2.060215    -2.556882      24.56
 C      -0.437031    -1.228870     0.754617      50.69
 H      -0.919500    -2.114589     1.125380      24.83
 C       0.164875     1.063536     0.350662      69.55
 H      -0.163844     1.997202     0.155800      20.78
 C       1.568235     0.752050     0.187781       5.79
 O       2.576331     1.687674    -0.056922     202.40
 C       2.049641     2.986917    -0.233719     121.37
 H       2.886501     3.634663    -0.477271      26.12
 H       1.332926     2.968036    -0.964913      26.81
 H       1.851122     3.444588     0.841802      24.76
 C       1.888004    -0.692750     0.139486      14.39
 O       3.203476    -0.934720    -0.252784     182.30
 C       0.969348    -1.650463     0.464393      49.97
 H       1.118108    -2.826281     0.628941      17.65
 C      -0.918093     0.135345     0.690610      33.48
 C      -2.429758     0.403981     0.928099      85.77
 H      -2.897234    -0.553756     1.206807      23.01
 O      -2.592139     1.334739     1.964601     247.00
 H      -2.292075     0.920640     2.917948      22.90
 C      -3.029350     0.832724    -0.382030      75.90
 H      -2.487169     1.645832    -0.860985      23.12
 O      -3.285898    -0.363393    -1.156724     276.03
 H      -3.265541    -0.198665    -2.100626      25.95
 C      -4.538467     1.571170     0.052229      91.09
 O      -4.864550     2.734272    -0.770076     301.47
 H      -4.831917     3.470285    -0.106490      27.19
 H      -4.359259     1.878415     0.966213      27.26
 H      -5.233114     0.715215    -0.052497      27.17
55
name = lig-etoh-Waterframe_340
 C       6.177990    -1.828636     1.977924      54.05
 H       6.313358    -0.748574     1.859751      28.64
 C       5.397892    -4.028251     1.280860      44.35
 H       5.040824    -4.733762     0.522906      15.04
 C       5.649942    -4.582172     2.580780      23.75
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 O       5.352457    -5.922566     2.839071     237.02
 C       4.922945    -6.844820     1.713644     109.25
 H       5.560486    -6.921620     0.868996      31.10
 H       3.937282    -6.442090     1.273109      27.63
 H       4.700659    -7.742287     2.233195      24.64
 C       6.121466    -3.720221     3.638272      50.46
 O       6.389063    -4.068294     4.877483     149.68
 H       6.111797    -4.998884     5.216584      21.24
 C       6.359763    -2.360224     3.343121      44.01
 H       6.585355    -1.578673     4.059677      21.91
 C       5.612735    -2.643733     0.983411      49.94
 C       5.279050    -2.196460    -0.469101      87.51
 H       5.559025    -3.167024    -1.158257      20.49
 O       6.015739    -1.058943    -0.975695     229.17
 H       5.528165    -0.320461    -0.577116      27.48
 C       3.721775    -2.168049    -0.820871      82.49
 H       3.302680    -3.059742    -0.384016      20.89
 C       3.530351    -2.156899    -2.379918     110.45
 O       3.888664    -3.409850    -2.919476     278.60
 H       4.598192    -3.262452    -3.567815      26.98
 H       3.957935    -1.314943    -2.906559      25.12
 H       2.457805    -1.956698    -2.644181      24.52
 C      -0.389168    -1.217234     0.749553      59.23
 H      -1.117455    -1.892204     1.122863      25.11
 C       0.165796     1.042880     0.349044      69.90
 H      -0.037191     2.071131     0.461909      22.21
 C       1.546778     0.717308     0.235847      16.47
 O       2.589439     1.669526    -0.114596     145.70
 C       2.124426     3.072413    -0.201473     106.83
 H       2.828278     3.755170    -0.664034      26.38
 H       1.339923     3.103393    -1.038960      25.67
 H       1.380365     3.457033     0.816766      23.00
 C       1.922287    -0.605888     0.136905      16.10
 O       3.185123    -0.926207    -0.254243     168.97
 C       0.860128    -1.581083     0.441588      57.98
 H       1.441687    -2.601953     0.541781      19.92
 C      -0.842897     0.112355     0.774867      31.15
 C      -2.376962     0.312789     0.968094      77.53
 H      -2.855698    -0.604964     1.286875      23.38
 O      -2.583274     1.337514     1.952065     268.25
 H      -2.194134     0.854875     2.757770      24.61
 C      -3.139558     0.897101    -0.375126      76.64
 H      -2.402332     1.450898    -0.955140      23.14
 O      -3.258022    -0.319444    -1.152859     264.04
 H      -3.340093    -0.119438    -2.081503      27.11
 C      -4.450954     1.560865     0.052085      93.82
 O      -4.868448     2.723515    -0.784690     279.65
 H      -4.827762     3.584392    -0.209094      26.11
 H      -4.358475     1.867741     1.136732      23.98
 H      -5.298877     0.761809    -0.053160      25.86
55
name = lig-etoh-Waterframe_341
 C       6.166493    -1.808522     1.992155      62.28
 H       6.268316    -0.724939     1.789692      25.79
 C       5.408226    -3.982068     1.329855      44.10
 H       5.188047    -4.667064     0.554868      22.10
 C       5.675341    -4.590111     2.550300      26.98
 O       5.399168    -5.944819     2.849453     263.26
 C       4.933150    -6.771111     1.764246     133.30
 H       5.698461    -6.876634     0.944822      30.00
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 H       3.920223    -6.346510     1.419152      26.10
 H       4.744037    -7.726752     2.157106      24.19
 C       6.150728    -3.704596     3.572197      13.26
 O       6.398417    -4.014505     4.925830     189.08
 H       6.179819    -4.982830     5.048664      24.38
 C       6.378523    -2.313124     3.292918      50.70
 H       6.526914    -1.708110     4.145997      25.99
 C       5.629964    -2.621753     0.971886      36.15
 C       5.244515    -2.259810    -0.445783      70.95
 H       5.734903    -3.258050    -1.208612      20.09
 O       5.960365    -1.081323    -0.922765     192.82
 H       5.670958    -0.226562    -0.613645      28.20
 C       3.742606    -2.139751    -0.843751      83.91
 H       3.113155    -3.006319    -0.547941      23.09
 C       3.507121    -2.096735    -2.376162      92.27
 O       3.900601    -3.437129    -2.986030     246.78
 H       4.736307    -3.294789    -3.448494      27.45
 H       4.250426    -1.335702    -2.845868      22.14
 H       2.404167    -1.962397    -2.493589      25.23
 C      -0.432902    -1.256378     0.806547      37.62
 H      -1.219626    -1.989125     0.980095      20.49
 C       0.148240     1.094932     0.441683      67.71
 H      -0.137541     2.203503     0.551423      20.29
 C       1.519778     0.759031     0.212872       2.86
 O       2.554481     1.680260    -0.141412     147.80
 C       2.109272     3.127047    -0.239575     100.58
 H       3.101272     3.645593    -0.200562      25.41
 H       1.230569     3.229177    -1.040564      23.69
 H       1.683535     3.524991     0.842437      25.16
 C       1.886314    -0.629385     0.118903      25.79
 O       3.217303    -0.892926    -0.249841     176.07
 C       0.955450    -1.529009     0.400872      69.16
 H       1.061572    -2.661433     0.389934      22.66
 C      -0.756350     0.069053     0.765464      37.24
 C      -2.293380     0.330424     0.940420      74.78
 H      -2.689382    -0.666457     1.185244      24.50
 O      -2.555700     1.338275     1.998757     271.47
 H      -2.177465     1.040244     2.792047      28.56
 C      -3.150563     0.886743    -0.326791      85.07
 H      -2.533040     1.736247    -0.767740      23.71
 O      -3.271320    -0.291587    -1.144912     269.19
 H      -3.224509    -0.183053    -2.112236      26.16
 C      -4.419507     1.583229     0.023964     101.63
 O      -4.856180     2.681920    -0.813317     263.07
 H      -4.930097     3.521984    -0.188273      25.46
 H      -4.513848     1.905923     1.209599      23.78
 H      -5.296383     0.853683    -0.060137      26.35
55
name = lig-etoh-Waterframe_342
 C       6.109719    -1.744009     1.985942      72.31
 H       6.290279    -0.676604     1.761308      23.46
 C       5.426302    -3.989464     1.304249      52.02
 H       5.082923    -4.532146     0.471106      20.82
 C       5.699107    -4.573136     2.568046      50.24
 O       5.474595    -5.928502     2.880109     271.48
 C       4.899059    -6.707279     1.806679     143.38
 H       5.735012    -6.760174     0.985307      29.82
 H       3.993628    -6.321911     1.282292      27.05
 H       4.814959    -7.716435     2.188239      24.84
 C       6.190072    -3.659305     3.563143      18.81
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 O       6.401103    -4.000084     4.947702      86.91
 H       6.171097    -4.939119     5.165543      26.73
 C       6.370593    -2.320973     3.228204      57.22
 H       6.715373    -1.828298     4.078059      23.35
 C       5.629579    -2.654268     1.004682      21.51
 C       5.234996    -2.273969    -0.449168      72.50
 H       5.707673    -3.060537    -1.159008      23.82
 O       5.929544    -1.096268    -0.887771     199.35
 H       5.580671    -0.370942    -0.385968      30.26
 C       3.717772    -2.129446    -0.846317      82.44
 H       3.154638    -2.993093    -0.350709      21.65
 C       3.533692    -2.090690    -2.378174      92.05
 O       3.861913    -3.439697    -3.019065     258.76
 H       4.760389    -3.421036    -3.396925      27.00
 H       4.219739    -1.226515    -2.806344      22.42
 H       2.492813    -1.850718    -2.671908      25.73
 C      -0.371719    -1.300492     0.809148      36.95
 H      -0.974268    -2.236506     0.882935      19.09
 C       0.202188     1.159816     0.572699      66.30
 H      -0.379823     2.196678     0.422112      19.65
 C       1.488285     0.837949     0.144408      12.31
 O       2.458619     1.731366    -0.153479     210.10
 C       2.125429     3.122161    -0.193272     127.12
 H       3.135105     3.644252    -0.354621      25.09
 H       1.614994     3.540101    -1.139196      24.91
 H       1.772509     3.377613     0.648291      29.34
 C       1.920261    -0.610778     0.067255      -2.82
 O       3.269972    -0.840060    -0.243586     158.65
 C       0.914271    -1.665204     0.417492      51.15
 H       1.170960    -2.669767     0.129871      21.78
 C      -0.809156     0.089641     0.731498      43.55
 C      -2.239729     0.428557     0.939348      99.05
 H      -2.731989    -0.555090     1.212674      24.68
 O      -2.508270     1.328888     2.049481     268.17
 H      -2.145300     0.948352     2.788086      31.10
 C      -3.019454     0.881145    -0.269137      78.31
 H      -2.541801     1.738697    -0.808707      24.01
 O      -3.302478    -0.278705    -1.134369     275.31
 H      -3.047493    -0.101282    -2.076985      26.11
 C      -4.548443     1.564978     0.048939      86.04
 O      -4.829373     2.662107    -0.857164     249.82
 H      -4.859755     3.506232    -0.248043      25.90
 H      -4.307850     2.040648     1.132710      23.66
 H      -5.191196     0.727770    -0.060583      28.10
55
name = lig-etoh-Waterframe_343
 C       6.040592    -1.717910     1.942340      56.23
 H       6.254052    -0.652927     1.787472      24.53
 C       5.442940    -4.054284     1.269871      41.43
 H       4.935776    -4.694628     0.559493      11.43
 C       5.719838    -4.548489     2.593978      36.42
 O       5.530464    -5.864380     2.912415     268.21
 C       4.909092    -6.675294     1.805072     113.09
 H       5.611454    -6.775387     0.897058      31.33
 H       3.982131    -6.240884     1.506444      32.59
 H       4.621322    -7.656032     2.290311      26.23
 C       6.198558    -3.690201     3.619326       0.35
 O       6.404296    -3.989514     4.918761      64.98
 H       6.078911    -4.909375     5.070097      24.50
 C       6.392134    -2.304126     3.247478      26.69
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 H       6.939127    -1.621106     3.860745      22.99
 C       5.586916    -2.640304     0.998756      16.37
 C       5.244804    -2.263148    -0.466943      86.19
 H       5.477868    -3.002650    -1.006668      30.48
 O       5.912911    -1.074392    -0.849520     250.23
 H       5.586442    -0.359367    -0.328407      30.75
 C       3.697431    -2.129469    -0.799803      74.58
 H       3.156450    -2.976994    -0.280339      22.36
 C       3.570533    -2.127952    -2.407143      95.22
 O       3.769100    -3.415948    -2.994039     269.99
 H       4.626086    -3.308873    -3.573959      25.07
 H       4.281903    -1.347076    -2.807613      22.18
 H       2.582994    -1.825360    -2.734374      25.71
 C      -0.322629    -1.293059     0.744526      32.05
 H      -1.158452    -2.016168     1.025594      17.67
 C       0.144766     1.129401     0.641725      64.13
 H      -0.081729     2.264828     0.437943      19.03
 C       1.460688     0.778391     0.108011       7.93
 O       2.402225     1.784976    -0.194529     203.24
 C       2.202261     3.174185    -0.176018     118.50
 H       3.220701     3.630577    -0.264997      23.69
 H       1.507162     3.425711    -0.976580      25.40
 H       1.547270     3.529179     0.679361      24.36
 C       1.888470    -0.582430     0.045269       3.18
 O       3.296140    -0.790640    -0.250996     170.70
 C       0.994169    -1.705851     0.366843      47.13
 H       1.291411    -2.679221     0.226109      20.73
 C      -0.761318     0.080181     0.742697      39.31
 C      -2.265660     0.455683     1.000028      81.34
 H      -2.817126    -0.500588     1.259503      23.12
 O      -2.435961     1.343949     2.108543     269.16
 H      -2.133442     0.790562     2.806073      28.23
 C      -3.018201     0.954992    -0.288727      74.48
 H      -2.351037     1.505965    -0.949782      22.90
 O      -3.305405    -0.262295    -1.101344     269.32
 H      -3.054149    -0.088341    -2.052693      25.88
 C      -4.525500     1.524413     0.091235      93.35
 O      -4.817683     2.640749    -0.897320     244.41
 H      -4.715466     3.535306    -0.396128      26.65
 H      -4.688188     1.913803     1.125706      27.29
 H      -5.287607     0.809551     0.036503      28.81
55
name = lig-etoh-Waterframe_344
 C       6.009049    -1.799877     1.985481      56.43
 H       6.119716    -0.764163     1.707097      23.46
 C       5.457937    -4.047719     1.306962      19.66
 H       5.039201    -4.784800     0.581320       9.96
 C       5.731620    -4.505576     2.565803      37.36
 O       5.559853    -5.848753     2.904920     271.68
 C       4.899443    -6.637772     1.854413     129.66
 H       5.505951    -6.865319     0.981173      31.10
 H       4.024499    -6.134387     1.617909      33.03
 H       4.676300    -7.653901     2.359381      24.39
 C       6.194161    -3.595329     3.603330       3.90
 O       6.411076    -4.028603     4.917992     177.92
 H       6.086373    -4.967653     5.048533      30.79
 C       6.418002    -2.251738     3.224098      64.37
 H       6.955409    -1.590287     3.962209      23.20
 C       5.505653    -2.672931     0.938881      23.96
 C       5.190238    -2.234556    -0.439125      79.97
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 H       5.591582    -3.123805    -1.172541      23.23
 O       5.919366    -1.030824    -0.830916     241.82
 H       5.625664    -0.208308    -0.451657      29.68
 C       3.715360    -2.089433    -0.778462      82.40
 H       3.096973    -2.895152    -0.406408      23.27
 C       3.553725    -2.109602    -2.379450      98.47
 O       3.685659    -3.424934    -2.976006     249.00
 H       4.518358    -3.339549    -3.623017      25.43
 H       4.360416    -1.573280    -2.733317      22.83
 H       2.567793    -1.700771    -2.543429      25.57
 C      -0.318363    -1.264396     0.660614      52.43
 H      -1.089713    -2.000452     1.028254      21.59
 C       0.185102     1.085852     0.568697      69.04
 H      -0.146816     2.105087     0.825463      20.24
 C       1.413078     0.757207     0.139490      13.39
 O       2.408286     1.753005    -0.230652     159.56
 C       2.183940     3.253624    -0.179815      97.95
 H       3.155812     3.693389    -0.060965      24.02
 H       1.598637     3.507736    -1.005501      25.05
 H       1.666200     3.757585     1.001417      21.28
 C       1.916410    -0.607063     0.017939      17.67
 O       3.258517    -0.768513    -0.274397     175.09
 C       1.061034    -1.617286     0.302567      73.02
 H       1.310326    -2.599276     0.497024      20.79
 C      -0.757856     0.048753     0.808538      75.13
 C      -2.298214     0.406957     1.045037      72.07
 H      -2.807527    -0.538386     1.266045      22.41
 O      -2.350323     1.375113     2.165551     266.39
 H      -2.101274     0.899834     3.073865      24.55
 C      -3.100518     0.974755    -0.292429      80.71
 H      -2.528788     1.784573    -0.769208      23.10
 O      -3.286569    -0.253208    -1.054725     263.61
 H      -3.241258    -0.134507    -2.060514      24.53
 C      -4.442633     1.560184     0.083155     103.88
 O      -4.819335     2.602366    -0.907753     265.11
 H      -4.620929     3.433414    -0.354486      27.94
 H      -4.589710     1.854110     1.024235      29.50
 H      -5.162359     0.762805    -0.214789      26.65
55
name = lig-etoh-Waterframe_345
 C       5.972405    -1.854779     1.933624      57.08
 H       6.059816    -0.808258     1.712173      20.35
 C       5.430036    -4.019932     1.284239      53.78
 H       5.304152    -4.754943     0.428216      20.30
 C       5.757258    -4.466626     2.598174      -3.63
 O       5.596243    -5.836294     2.874746     285.40
 C       4.876147    -6.627481     1.942868     128.71
 H       5.505941    -6.778804     1.123045      25.76
 H       3.971127    -6.227917     1.476280      29.66
 H       4.682422    -7.616647     2.469652      23.11
 C       6.178779    -3.558409     3.581453      11.57
 O       6.423707    -4.062808     4.902820     272.11
 H       6.099382    -5.030224     4.979319      23.06
 C       6.438253    -2.231609     3.244702      47.61
 H       6.757317    -1.526363     4.099882      24.07
 C       5.471892    -2.700405     1.001262      39.72
 C       5.147653    -2.181623    -0.423452      74.85
 H       5.740189    -2.974116    -1.311203      20.69
 O       5.938444    -0.987706    -0.830068     190.33
 H       5.493297    -0.229913    -0.416754      26.09
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 C       3.696660    -2.051909    -0.823077      98.40
 H       3.169547    -2.842287    -0.358863      22.49
 C       3.530492    -2.044991    -2.302213      94.82
 O       3.589261    -3.457483    -2.965669     219.89
 H       4.572095    -3.400720    -3.383859      23.94
 H       4.232631    -1.416057    -2.758126      24.97
 H       2.576723    -1.560386    -2.619335      25.30
 C      -0.323573    -1.273176     0.606400      58.69
 H      -0.756095    -2.249112     0.747007      23.06
 C       0.140746     1.069899     0.530829      55.41
 H      -0.121651     1.999058     0.872724      20.56
 C       1.517918     0.802449     0.125680       8.21
 O       2.432173     1.742918    -0.241390     147.22
 C       2.151381     3.270020    -0.140316     104.95
 H       3.133679     3.653004    -0.248917      26.52
 H       1.696873     3.801108    -0.958824      26.04
 H       1.538540     3.423908     0.949483      23.02
 C       1.956087    -0.564726    -0.016529      17.96
 O       3.244577    -0.766154    -0.318973     188.59
 C       0.984251    -1.557642     0.304810      59.17
 H       1.411540    -2.562137     0.509497      20.73
 C      -0.828482     0.026373     0.824260      45.87
 C      -2.273452     0.373817     1.094846      85.44
 H      -2.806707    -0.499872     1.427785      22.38
 O      -2.290503     1.412374     2.180397     251.80
 H      -1.861905     0.804988     3.048170      21.30
 C      -3.084150     0.949589    -0.195128      78.71
 H      -2.539903     1.775200    -0.704892      23.25
 O      -3.252945    -0.248011    -1.029798     239.83
 H      -3.339881     0.019285    -2.011082      24.72
 C      -4.446568     1.567038     0.012184      96.34
 O      -4.813235     2.593929    -0.881246     293.30
 H      -4.779335     3.499711    -0.439692      28.41
 H      -4.361705     1.916949     1.023455      26.74
 H      -5.153639     0.612473    -0.113038      25.71
55
name = lig-etoh-Waterframe_346
 C       5.994547    -1.763550     1.974027      54.87
 H       6.055636    -0.712681     1.692631      21.16
 C       5.413485    -4.079883     1.274724      20.17
 H       5.311258    -4.802724     0.414780      16.73
 C       5.734534    -4.483283     2.544925      24.60
 O       5.636596    -5.783273     2.886908     250.00
 C       4.870473    -6.665148     1.977139     124.99
 H       5.525325    -6.952249     1.151423      25.97
 H       3.862157    -6.185909     1.658750      26.06
 H       4.624760    -7.548651     2.569925      24.32
 C       6.188701    -3.619308     3.646480      17.65
 O       6.439956    -4.067573     4.854756     232.01
 H       6.086911    -5.040501     4.958261      27.51
 C       6.381484    -2.245553     3.241544      50.40
 H       6.651174    -1.412281     3.990661      23.52
 C       5.445982    -2.648921     0.981404      38.61
 C       5.221797    -2.128125    -0.449430     105.32
 H       5.459526    -3.100345    -1.063262      21.18
 O       5.923482    -0.945209    -0.806138     254.22
 H       5.568582    -0.135232    -0.329667      24.06
 C       3.667452    -2.047475    -0.824317      92.11
 H       3.168037    -2.884565    -0.351266      20.41
 C       3.470055    -2.012678    -2.352812      84.37
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 O       3.515170    -3.421362    -2.928328     230.35
 H       4.498941    -3.512832    -3.307835      25.13
 H       4.273399    -1.359531    -2.815064      22.10
 H       2.393314    -1.725954    -2.602275      24.23
 C      -0.378164    -1.344595     0.596054      33.97
 H      -1.100375    -2.130927     0.674948      18.30
 C       0.114502     1.050516     0.537955      62.88
 H      -0.151057     2.044719     0.539985      18.81
 C       1.522173     0.833882     0.104611       4.29
 O       2.477080     1.830558    -0.266811     207.77
 C       2.147090     3.194737    -0.097495     123.72
 H       3.133063     3.663963    -0.004248      24.62
 H       1.339251     3.508593    -0.883023      23.74
 H       1.696253     3.393409     0.733472      28.42
 C       1.890996    -0.487719    -0.012617      21.94
 O       3.284332    -0.751783    -0.368153     177.57
 C       1.012362    -1.502652     0.303266      58.84
 H       1.281695    -2.645644     0.145911      16.65
 C      -0.830480     0.010871     0.741244      24.80
 C      -2.279561     0.404440     1.159531      87.64
 H      -2.785862    -0.478446     1.566902      22.00
 O      -2.233337     1.417268     2.163560     242.82
 H      -1.782502     0.921242     3.091179      23.40
 C      -2.991523     0.899683    -0.121632      78.21
 H      -2.200318     1.462226    -0.642872      20.90
 O      -3.198498    -0.250187    -1.019367     271.33
 H      -3.252465     0.107890    -1.977043      25.30
 C      -4.472558     1.527410     0.057873      93.62
 O      -4.817468     2.617261    -0.893270     277.82
 H      -4.934419     3.383721    -0.258574      26.76
 H      -4.550771     2.071135     1.144938      24.08
 H      -5.410999     0.852121     0.179498      25.07
55
name = lig-etoh-Waterframe_347
 C       5.980037    -1.712316     1.985657      50.14
 H       6.157667    -0.624247     1.864163      19.01
 C       5.411805    -3.999141     1.220109      32.75
 H       5.057299    -4.778725     0.536572      11.12
 C       5.720446    -4.483800     2.528988      53.45
 O       5.654091    -5.811647     2.901880     273.96
 C       4.886371    -6.717076     2.040537     124.27
 H       5.381656    -7.147428     1.079662      30.80
 H       3.950587    -6.103113     1.654927      25.81
 H       4.638264    -7.515188     2.675712      26.11
 C       6.172295    -3.610999     3.543463      -6.16
 O       6.470988    -4.091592     4.868837     201.36
 H       6.145152    -5.053126     5.039576      30.22
 C       6.284599    -2.270764     3.264553      62.18
 H       6.747609    -1.634685     4.066532      23.61
 C       5.487382    -2.592433     0.973265      68.59
 C       5.216984    -2.151258    -0.461129     170.08
 H       5.672093    -2.746368    -1.085282      30.72
 O       5.922007    -0.917409    -0.799583     198.15
 H       5.574184    -0.106043    -0.240148      21.03
 C       3.701434    -2.027675    -0.830085      80.07
 H       3.100952    -2.871262    -0.385493      21.01
 C       3.379280    -2.061951    -2.426055      92.88
 O       3.477634    -3.362859    -2.898406     249.00
 H       4.387047    -3.466996    -3.385542      26.30
 H       4.152607    -1.345482    -2.966109      22.19
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 H       2.338222    -1.635388    -2.545454      23.97
 C      -0.413168    -1.332097     0.595589      14.32
 H      -1.174319    -2.069074     0.797440      15.96
 C       0.162872     1.087527     0.499404      85.42
 H      -0.367132     2.040550     0.322174      14.58
 C       1.430161     0.901615     0.097424       8.55
 O       2.511697     1.839098    -0.272936     210.42
 C       2.113137     3.161954    -0.048629     106.79
 H       2.916838     3.969446    -0.147926      22.46
 H       1.347494     3.432600    -0.927653      22.39
 H       1.685901     3.357355     0.980551      24.47
 C       1.935601    -0.480081    -0.013529       6.08
 O       3.245682    -0.691633    -0.377101     187.43
 C       0.970449    -1.553274     0.268177      61.86
 H       1.376708    -2.581291    -0.156649      15.31
 C      -0.793170    -0.017262     0.673963      52.12
 C      -2.258287     0.387119     1.203520      81.76
 H      -2.760896    -0.546994     1.596856      21.45
 O      -2.179066     1.444294     2.152801     278.12
 H      -1.902607     0.980572     3.101603      24.33
 C      -2.994903     0.852657    -0.100210      82.99
 H      -2.409340     1.730270    -0.491003      20.67
 O      -3.131998    -0.275848    -1.000012     278.65
 H      -3.068864     0.010953    -1.987448      23.02
 C      -4.467287     1.563109     0.182321      83.02
 O      -4.815436     2.619698    -0.885738     245.85
 H      -4.930866     3.436746    -0.330276      27.95
 H      -4.470945     2.123463     1.266262      24.78
 H      -5.138354     0.731011     0.018062      26.15
55
name = lig-etoh-Waterframe_348
 C       5.954106    -1.712814     2.011459      57.23
 H       6.156235    -0.630654     1.842759      20.61
 C       5.402322    -3.907442     1.232469      32.70
 H       4.878264    -4.406897     0.448987      12.89
 C       5.706055    -4.496876     2.479128      29.73
 O       5.668096    -5.871013     2.870972     347.23
 C       4.877764    -6.755876     2.103886     121.52
 H       5.557716    -7.127512     1.230000      30.47
 H       3.922245    -6.310968     1.687058      30.66
 H       4.550314    -7.554648     2.709936      25.76
 C       6.148387    -3.654237     3.518580     -28.75
 O       6.504602    -4.085106     4.844818     269.01
 H       6.170228    -5.032432     4.907786      31.64
 C       6.219626    -2.242659     3.288977      69.42
 H       6.695041    -1.782184     4.117013      25.08
 C       5.553639    -2.548247     0.961762      51.66
 C       5.210915    -2.115320    -0.490274     140.54
 H       5.706915    -2.784365    -1.211990      24.08
 O       5.928514    -0.886764    -0.801802     222.41
 H       5.520826    -0.073508    -0.250599      19.16
 C       3.712478    -1.976844    -0.904435      76.46
 H       3.152805    -2.784460    -0.315989      16.29
 C       3.326148    -2.029313    -2.384796      93.47
 O       3.456495    -3.381573    -2.928464     243.91
 H       4.397737    -3.362183    -3.324513      25.90
 H       3.961262    -1.347048    -3.055883      21.10
 H       2.308839    -1.701034    -2.538694      23.70
 C      -0.360502    -1.308079     0.586061      41.04
 H      -0.892094    -2.218180     0.890895      16.49
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 C       0.084669     1.139137     0.413535      83.69
 H      -0.349410     2.252949     0.495234      13.62
 C       1.519225     0.869471     0.053048       7.40
 O       2.504701     1.779165    -0.240581     207.55
 C       2.037660     3.247059    -0.037673      66.73
 H       2.988398     3.822512    -0.338773      20.81
 H       1.134349     3.582918    -0.643284      22.51
 H       1.564278     3.243666     1.213105      19.82
 C       1.871561    -0.527763     0.017152      19.04
 O       3.203063    -0.639595    -0.375132     193.22
 C       0.970954    -1.580932     0.155303      75.24
 H       1.230620    -2.685129     0.060424      17.16
 C      -0.779031     0.044244     0.704602      45.43
 C      -2.175562     0.341896     1.152261      93.58
 H      -2.684468    -0.540575     1.648010      21.23
 O      -2.143798     1.472664     2.156406     280.15
 H      -1.911970     1.001153     2.996043      25.88
 C      -3.081264     0.913262    -0.056856      77.68
 H      -2.557847     1.744512    -0.600372      21.13
 O      -3.069517    -0.292693    -0.970897     262.41
 H      -2.922795    -0.052990    -1.964177      23.13
 C      -4.414352     1.570923     0.227140     110.19
 O      -4.796909     2.588944    -0.816253     291.53
 H      -4.676630     3.480960    -0.449586      29.01
 H      -4.434752     1.937800     1.284111      27.00
 H      -5.105288     0.807915     0.119603      27.64
55
name = lig-etoh-Waterframe_349
 C       5.957947    -1.673269     2.042622      47.76
 H       6.062156    -0.599075     1.819302      22.89
 C       5.351098    -3.890931     1.237128      39.84
 H       4.946533    -4.479357     0.438810      24.51
 C       5.699358    -4.548365     2.459040      54.17
 O       5.676621    -5.866320     2.823821     416.01
 C       4.851727    -6.829983     2.106105     125.10
 H       5.493144    -7.266638     1.320939      26.72
 H       3.999120    -6.403895     1.677456      30.70
 H       4.628818    -7.667912     2.798803      25.02
 C       6.133861    -3.654218     3.565812      33.12
 O       6.522643    -4.078162     4.755952     257.08
 H       6.243866    -5.010455     4.964991      25.77
 C       6.193090    -2.268250     3.322793      53.45
 H       6.448280    -1.565458     4.038763      21.72
 C       5.574718    -2.504153     0.941436      32.86
 C       5.245680    -2.010817    -0.534000      77.65
 H       5.441459    -3.081385    -1.162515      17.70
 O       5.948557    -0.849762    -0.824739     257.85
 H       5.540028    -0.024428    -0.297046      19.90
 C       3.683530    -1.895566    -0.893645      77.42
 H       3.201561    -2.786636    -0.408495      15.51
 C       3.284837    -1.984269    -2.361793      86.24
 O       3.459803    -3.417331    -2.980018     238.81
 H       4.405752    -3.473214    -3.261986      27.07
 H       3.924304    -1.316339    -2.917176      21.77
 H       2.250201    -1.868311    -2.408935      24.61
 C      -0.268896    -1.270894     0.580756      44.83
 H      -0.978075    -2.076355     0.913348      18.56
 C       0.116083     1.150922     0.307288      66.08
 H      -0.177356     2.263320     0.648715      16.23
 C       1.446255     0.800982     0.057049      10.67
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 O       2.445501     1.790754    -0.204146     161.94
 C       1.973266     3.242091    -0.023514      99.40
 H       2.912275     3.788191    -0.197872      23.36
 H       1.122266     3.439880    -0.554102      25.02
 H       1.913269     3.578138     1.235625      22.03
 C       1.855637    -0.538637    -0.019823      17.68
 O       3.205599    -0.644524    -0.385025     183.12
 C       0.949803    -1.616938     0.079994      77.60
 H       1.268031    -2.601988     0.218763      22.48
 C      -0.745303     0.091304     0.732307      36.23
 C      -2.166264     0.419699     1.117058      89.69
 H      -2.591417    -0.528649     1.510164      21.87
 O      -2.117366     1.461313     2.153429     307.44
 H      -1.788370     1.090146     2.908630      28.53
 C      -3.046230     0.937183    -0.061860      77.14
 H      -2.359254     1.587824    -0.590115      23.21
 O      -3.047714    -0.285713    -0.928478     264.81
 H      -2.964106     0.039978    -1.904244      24.51
 C      -4.439541     1.533164     0.246240     118.60
 O      -4.749638     2.547682    -0.714030     342.36
 H      -4.486912     3.307929    -0.205735      28.98
 H      -4.377812     1.972902     1.158374      27.82
 H      -5.330387     0.922559     0.320669      26.06
55
name = lig-etoh-Waterframe_350
 C       5.950449    -1.668027     2.019181      54.64
 H       6.036595    -0.594520     2.059793      21.11
 C       5.313720    -3.928695     1.221400      68.84
 H       5.129941    -4.696316     0.475165      30.31
 C       5.696287    -4.485031     2.476016       7.74
 O       5.671016    -5.864232     2.773436     342.33
 C       4.860281    -6.916488     2.070508     100.55
 H       5.323004    -7.402544     1.265007      23.78
 H       3.988727    -6.489248     1.698354      29.11
 H       4.630717    -7.618080     2.963188      23.09
 C       6.091497    -3.636402     3.500020      13.07
 O       6.558815    -4.109900     4.741018     362.54
 H       6.183816    -5.033561     4.896565      28.29
 C       6.173113    -2.241737     3.308010      48.38
 H       6.270085    -1.645957     4.174131      23.37
 C       5.534127    -2.487393     0.954301      37.78
 C       5.194083    -1.985822    -0.497378      86.26
 H       5.808798    -2.635529    -1.359199      19.17
 O       6.002770    -0.803200    -0.892884     213.76
 H       5.649399    -0.015940    -0.303061      22.29
 C       3.696710    -1.891723    -0.823626      81.21
 H       3.237115    -2.714210    -0.310959      18.35
 C       3.276224    -2.031208    -2.397574      83.01
 O       3.468988    -3.401850    -2.994617     269.86
 H       4.341524    -3.332894    -3.417922      26.66
 H       3.725995    -1.308535    -2.984297      23.78
 H       2.220946    -1.811049    -2.468258      24.30
 C      -0.324813    -1.193651     0.613173      58.68
 H      -1.104804    -1.954437     0.895129      19.02
 C       0.131325     1.122935     0.308645      73.85
 H      -0.146502     2.222701     0.394699      20.55
 C       1.405413     0.809181     0.036634      17.01
 O       2.352081     1.842251    -0.153165     221.24
 C       2.006809     3.180933     0.028003     144.83
 H       2.656714     3.816738    -0.509351      27.10
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 H       1.189964     3.419856    -0.557074      27.46
 H       1.751419     3.400703     0.990775      28.48
 C       1.901568    -0.547463    -0.134755       6.83
 O       3.211735    -0.647526    -0.383118     168.61
 C       0.995251    -1.633022     0.079111      62.06
 H       1.351681    -2.578047     0.051068      25.58
 C      -0.693269     0.100931     0.678530      36.08
 C      -2.171251     0.492654     1.151579      92.50
 H      -2.677938    -0.407452     1.475980      24.97
 O      -2.103821     1.455516     2.154260     323.41
 H      -1.721922     1.021114     2.844577      30.12
 C      -2.943227     0.876004    -0.099305      79.58
 H      -2.539867     1.796733    -0.527883      25.07
 O      -3.059694    -0.260271    -0.895539     260.96
 H      -3.179185    -0.025732    -1.895060      24.48
 C      -4.451018     1.493039     0.311063      89.59
 O      -4.699713     2.540893    -0.632976     282.47
 H      -4.761312     3.411730    -0.178598      27.26
 H      -4.283913     1.960008     1.244319      26.65
 H      -5.243984     0.600384     0.312573      25.59
55
name = lig-etoh-Waterframe_351
 C       5.918645    -1.668121     2.021652      46.90
 H       5.972217    -0.610501     1.829427      17.85
 C       5.339473    -3.925514     1.196754      26.99
 H       5.132623    -4.562778     0.307815      16.92
 C       5.640037    -4.473256     2.426489      37.63
 O       5.674088    -5.869656     2.715136     291.38
 C       4.865484    -6.927822     2.059309     112.30
 H       5.441421    -7.429461     1.300595      28.24
 H       3.858790    -6.574939     1.727904      28.89
 H       4.621513    -7.699694     2.915520      24.95
 C       6.101456    -3.610865     3.508886       1.98
 O       6.573975    -4.146412     4.722545     316.47
 H       6.158573    -5.064823     4.885730      30.81
 C       6.135459    -2.228741     3.274163      64.77
 H       6.363724    -1.736630     4.234639      23.20
 C       5.449178    -2.543997     0.944321      41.11
 C       5.254813    -1.956848    -0.491661      97.00
 H       5.523859    -2.803563    -1.149758      24.65
 O       6.026772    -0.750409    -0.929624     253.20
 H       5.879611     0.077839    -0.384212      23.70
 C       3.725899    -1.971754    -0.843837      73.93
 H       3.267419    -2.680608    -0.208319      20.38
 C       3.279770    -2.108952    -2.403215      86.67
 O       3.480063    -3.349452    -2.987499     273.12
 H       4.272455    -3.247407    -3.560506      26.18
 H       3.839029    -1.417070    -3.005330      20.88
 H       2.153432    -1.873282    -2.427395      22.52
 C      -0.323714    -1.253798     0.597504      52.65
 H      -1.022032    -2.051909     0.918197      21.52
 C       0.118245     1.163899     0.347047      69.84
 H      -0.330970     2.088746     0.184879      18.96
 C       1.479786     0.834725    -0.032470      14.29
 O       2.344782     1.830431    -0.123006     218.70
 C       1.968865     3.177238     0.011818     131.26
 H       2.844246     3.713794    -0.391518      26.27
 H       0.932376     3.392578    -0.490376      22.80
 H       1.786746     3.409162     0.999212      27.57
 C       1.860123    -0.526139    -0.212427      17.09
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 O       3.255170    -0.625326    -0.386268     154.33
 C       0.988448    -1.558489     0.144777      64.06
 H       1.156596    -2.575686    -0.121284      18.06
 C      -0.801776     0.110908     0.663797      28.41
 C      -2.112216     0.451123     1.138070     106.73
 H      -2.627423    -0.387529     1.606783      23.96
 O      -2.094948     1.488929     2.188095     238.91
 H      -1.806435     0.988049     3.001120      25.84
 C      -2.976968     0.938127    -0.072188      82.63
 H      -2.524590     1.739701    -0.730905      22.59
 O      -3.075284    -0.268753    -0.906203     216.63
 H      -3.392179    -0.046356    -1.864188      24.00
 C      -4.334669     1.439682     0.384745      85.26
 O      -4.692933     2.546116    -0.591150     252.12
 H      -4.990215     3.328333    -0.085397      26.34
 H      -4.448435     1.674187     1.543083      24.98
 H      -5.139947     0.564352     0.129966      24.71
55
name = lig-etoh-Waterframe_352
 C       5.823894    -1.695720     1.964760      50.12
 H       5.971669    -0.652343     1.710244      19.80
 C       5.363830    -3.911671     1.111833      70.66
 H       4.995365    -4.563826     0.263556      16.41
 C       5.598643    -4.524989     2.419648      31.60
 O       5.674346    -5.865977     2.668199     282.82
 C       4.869101    -6.899343     2.074640     117.82
 H       5.509809    -7.321908     1.229327      28.84
 H       3.887669    -6.528122     1.536395      27.83
 H       4.777937    -7.715155     2.830228      24.80
 C       6.100964    -3.668905     3.505399      -7.80
 O       6.565232    -4.159714     4.678705     214.28
 H       6.226641    -5.082434     4.954118      24.50
 C       6.123588    -2.244547     3.308133      52.05
 H       6.603879    -1.452953     3.986063      25.16
 C       5.436326    -2.492820     0.960350      41.02
 C       5.301668    -1.986515    -0.523334     103.28
 H       5.676852    -2.742215    -1.035722      26.00
 O       6.040480    -0.768962    -0.945592     303.91
 H       5.661830    -0.086244    -0.369880      26.51
 C       3.749013    -1.973780    -0.886666      76.89
 H       3.308169    -2.812556    -0.316941      18.91
 C       3.303602    -2.095251    -2.332593      74.39
 O       3.475045    -3.379768    -2.993979     251.45
 H       4.476489    -3.368349    -3.487458      22.25
 H       3.869056    -1.231484    -2.831422      19.26
 H       2.145887    -1.888423    -2.353836      21.42
 C      -0.350191    -1.276017     0.586430      49.62
 H      -0.851840    -2.175839     0.878895      23.84
 C       0.097042     1.137146     0.342742      51.35
 H      -0.250227     2.071236     0.309442      14.88
 C       1.382196     0.855778    -0.052814      16.31
 O       2.454405     1.804822    -0.137750     174.27
 C       1.909043     3.220499     0.002536      92.53
 H       2.830824     3.828848    -0.277802      22.38
 H       0.924721     3.521577    -0.723607      20.36
 H       1.913723     3.507056     1.230989      21.45
 C       1.879544    -0.455901    -0.222239      21.55
 O       3.269687    -0.642091    -0.422608     176.21
 C       0.939354    -1.499691     0.173666      61.63
 H       1.196514    -2.610975    -0.046961      13.44
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 C      -0.760238     0.050104     0.653582      36.04
 C      -2.151337     0.436719     1.151568      83.43
 H      -2.588973    -0.537156     1.531174      21.54
 O      -2.079550     1.520365     2.217063     223.56
 H      -1.900685     1.020520     3.155206      22.96
 C      -2.996674     0.971976    -0.026562      78.45
 H      -2.333405     1.657199    -0.602130      20.04
 O      -3.113820    -0.287158    -0.924411     187.90
 H      -3.465140     0.085687    -1.820570      23.36
 C      -4.307379     1.414391     0.375325      96.54
 O      -4.710712     2.502143    -0.526743     301.99
 H      -4.783525     3.357861    -0.006794      26.13
 H      -4.453974     1.698897     1.544519      24.77
 H      -4.994367     0.582855     0.124643      25.49
55
name = lig-etoh-Waterframe_353
 C       5.767087    -1.696725     2.038569      48.13
 H       5.996157    -0.623419     1.976835      23.09
 C       5.359398    -3.935977     1.114993      31.58
 H       5.008840    -4.610539     0.290769      12.84
 C       5.589046    -4.495678     2.358750      47.53
 O       5.676941    -5.866294     2.670871     303.79
 C       4.909726    -6.872400     2.017957     123.15
 H       5.444073    -7.322037     1.094656      29.64
 H       3.867503    -6.438447     1.696825      28.16
 H       4.684693    -7.581912     2.746501      24.61
 C       6.059652    -3.683201     3.450881     -18.17
 O       6.567509    -4.175391     4.666065     245.19
 H       6.207557    -5.113013     4.873743      26.54
 C       6.122822    -2.260147     3.238906      51.80
 H       6.720340    -1.617239     4.005246      21.96
 C       5.445259    -2.496600     0.866260      27.09
 C       5.306466    -2.043800    -0.575862     103.38
 H       5.916311    -2.730149    -1.253002      23.42
 O       6.017783    -0.840506    -0.917367     274.85
 H       5.621144    -0.059060    -0.525652      24.77
 C       3.783699    -1.962755    -0.882958      75.96
 H       3.293351    -2.832678    -0.316847      15.91
 C       3.333569    -2.040401    -2.307405      73.31
 O       3.469831    -3.424645    -2.979677     245.62
 H       4.463027    -3.391884    -3.415413      22.80
 H       3.736578    -1.212185    -3.015418      20.23
 H       2.221417    -1.875105    -2.318477      22.19
 C      -0.364729    -1.294299     0.587626      26.97
 H      -1.059561    -2.052769     0.889680      17.84
 C       0.053954     1.098602     0.317107      80.75
 H      -0.206881     2.070830     0.661147      14.78
 C       1.425639     0.886085    -0.069202       8.31
 O       2.480796     1.845799    -0.171815     197.88
 C       1.990213     3.253225     0.011590      89.75
 H       2.663357     4.034467    -0.426948      22.87
 H       1.062952     3.392861    -0.718721      24.31
 H       1.361212     3.386484     1.131965      21.84
 C       1.872929    -0.474298    -0.160798      25.12
 O       3.237312    -0.669362    -0.463207     193.66
 C       1.009633    -1.488185     0.104917      77.24
 H       1.515081    -2.562542     0.288868      18.00
 C      -0.762238     0.033431     0.694016      27.35
 C      -2.176629     0.430601     1.211919      76.38
 H      -2.769010    -0.455267     1.639260      17.90
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 O      -2.083131     1.512640     2.210960     246.98
 H      -1.709362     0.847453     3.077073      19.06
 C      -2.899102     0.871299    -0.005112      75.36
 H      -2.449528     1.787535    -0.414064      22.24
 O      -3.163900    -0.252292    -0.928390     249.36
 H      -3.354271     0.112009    -1.875640      23.00
 C      -4.406122     1.433705     0.344735     101.16
 O      -4.756876     2.461667    -0.463198     335.74
 H      -4.498842     3.374839    -0.155725      28.65
 H      -4.266485     1.813830     1.399050      25.43
 H      -5.008864     0.646319     0.306296      28.29
55
name = lig-etoh-Waterframe_354
 C       5.744425    -1.672035     2.013955      56.65
 H       5.812556    -0.561530     1.963604      24.41
 C       5.324111    -3.915933     1.088307      66.89
 H       5.171596    -4.628164     0.271985      24.03
 C       5.629209    -4.491998     2.363709      -0.37
 O       5.693774    -5.848653     2.691769     294.78
 C       4.896122    -6.838981     1.938956     118.14
 H       5.405329    -7.285964     1.050557      24.64
 H       3.936301    -6.397513     1.675324      29.57
 H       4.728008    -7.617782     2.607815      24.21
 C       6.031869    -3.668121     3.418750      15.69
 O       6.555083    -4.177340     4.623339     241.63
 H       6.215552    -5.111533     4.844365      21.59
 C       6.150440    -2.344112     3.210921      38.97
 H       6.501743    -1.840313     4.156462      19.57
 C       5.486064    -2.568387     0.858104      14.41
 C       5.300823    -2.061168    -0.609161      72.20
 H       5.509535    -3.052913    -1.416726      17.48
 O       6.006433    -0.887383    -0.890108     323.32
 H       5.648445    -0.093199    -0.481372      24.37
 C       3.783228    -1.973083    -0.893733      65.69
 H       3.280755    -2.799341    -0.285464      17.30
 C       3.311664    -2.066408    -2.404095      92.63
 O       3.462047    -3.412271    -2.924099     261.05
 H       4.256216    -3.492678    -3.453044      27.89
 H       3.901306    -1.386311    -3.080396      21.86
 H       2.286621    -1.896356    -2.329981      23.96
 C      -0.297022    -1.307810     0.564493      33.36
 H      -0.976707    -2.096425     0.872188      19.16
 C       0.131679     1.114894     0.319119      85.64
 H      -0.316672     2.117826     0.737259      15.56
 C       1.492110     0.909199    -0.057021       6.39
 O       2.447247     1.924718    -0.203472     228.83
 C       1.979369     3.237883    -0.050543     121.19
 H       2.847709     3.900840    -0.025628      24.84
 H       1.258955     3.304486    -0.709333      28.39
 H       1.615815     3.480147     1.023253      25.07
 C       1.909510    -0.473499    -0.123012      15.74
 O       3.220102    -0.666869    -0.475094     160.14
 C       1.003859    -1.573825     0.115488      68.50
 H       1.554986    -2.580927     0.305687      21.59
 C      -0.816573     0.008984     0.758543      60.59
 C      -2.153148     0.379608     1.265044      96.42
 H      -2.663868    -0.430346     1.814480      20.02
 O      -2.084188     1.456259     2.197349     262.91
 H      -1.546679     1.062005     3.105412      23.91
 C      -2.996101     0.843813    -0.016394      83.45
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 H      -2.369983     1.593767    -0.538753      22.71
 O      -3.179974    -0.207245    -0.936888     278.35
 H      -3.106563     0.164957    -1.895983      24.81
 C      -4.373011     1.407345     0.432717     107.75
 O      -4.848850     2.471516    -0.504646     277.78
 H      -4.570805     3.345673    -0.057426      27.17
 H      -4.376362     1.795417     1.393693      28.27
 H      -5.224055     0.709476     0.414459      26.30
55
name = lig-etoh-Waterframe_355
 C       5.768588    -1.723714     1.931730      62.48
 H       5.648395    -0.634702     1.760974      22.91
 C       5.331313    -3.978808     1.092697      70.39
 H       5.222607    -4.578972     0.212667      25.50
 C       5.653159    -4.542959     2.346055       2.96
 O       5.695957    -5.858023     2.687176     324.38
 C       4.876775    -6.792878     1.879597     118.47
 H       5.457385    -6.981658     0.996465      24.93
 H       3.990680    -6.404529     1.515394      31.50
 H       4.794429    -7.703864     2.514049      23.77
 C       6.055272    -3.732148     3.428745       7.88
 O       6.537560    -4.163545     4.574760     348.01
 H       6.179724    -5.063755     4.883338      24.68
 C       6.143377    -2.293909     3.206122      45.06
 H       6.246939    -1.668575     4.059742      20.63
 C       5.519578    -2.547884     0.885763      20.11
 C       5.207751    -2.094807    -0.575624      89.11
 H       5.732387    -2.917551    -1.312844      18.45
 O       6.035342    -0.919363    -0.901797     298.73
 H       5.631046    -0.284571    -0.308890      25.59
 C       3.708383    -1.957001    -0.946809      74.75
 H       3.254958    -2.813572    -0.423493      18.26
 C       3.308768    -2.105568    -2.462433     102.62
 O       3.437342    -3.435498    -2.886010     263.11
 H       4.321850    -3.435301    -3.281238      26.01
 H       3.903984    -1.389016    -2.993591      24.49
 H       2.339457    -1.777973    -2.615356      26.21
 C      -0.283375    -1.313336     0.579985      50.78
 H      -0.753520    -2.264154     0.844769      24.44
 C       0.161604     1.083063     0.424064      71.61
 H      -0.146736     2.256019     0.283083      16.66
 C       1.474476     0.882342     0.003812       5.29
 O       2.433607     1.919117    -0.234770     209.47
 C       1.966435     3.279238    -0.065511     122.31
 H       2.930733     3.779517    -0.177928      24.78
 H       1.354545     3.761546    -0.849012      25.85
 H       1.596365     3.385106     0.816178      28.68
 C       1.927912    -0.497433    -0.118027      10.65
 O       3.261430    -0.646701    -0.472969     157.79
 C       1.047040    -1.592898     0.164143      55.36
 H       1.209621    -2.651758     0.041732      16.25
 C      -0.678694     0.009066     0.726975      41.96
 C      -2.163581     0.301415     1.269050      91.78
 H      -2.496417    -0.633317     1.669222      23.79
 O      -2.074313     1.446131     2.193023     258.25
 H      -1.678386     0.948917     3.080106      23.91
 C      -3.109635     0.865412     0.027391      83.29
 H      -2.477602     1.653451    -0.401099      21.81
 O      -3.194389    -0.213924    -0.976013     289.57
 H      -2.923494     0.157593    -1.900616      25.28
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 C      -4.382320     1.427088     0.510850      89.46
 O      -4.917515     2.476340    -0.540348     208.51
 H      -4.987772     3.388890    -0.034662      26.35
 H      -4.325183     1.831436     1.469294      28.10
 H      -5.196009     0.505068     0.409023      24.30
55
name = lig-etoh-Waterframe_356
 C       5.825206    -1.760404     1.918047      40.53
 H       5.783536    -0.668756     1.799803      13.75
 C       5.396642    -4.015333     1.084599      22.83
 H       5.095012    -4.655308     0.285302      11.10
 C       5.674958    -4.577366     2.322210      53.62
 O       5.657149    -5.925943     2.675102     323.63
 C       4.918722    -6.743244     1.797731     140.39
 H       5.469842    -6.916802     0.890953      34.21
 H       3.935109    -6.346852     1.624355      30.08
 H       4.715866    -7.785011     2.347960      24.61
 C       6.099913    -3.638478     3.368805      12.93
 O       6.544166    -4.170238     4.608416     273.79
 H       6.147453    -5.074356     4.857352      27.83
 C       6.067889    -2.247400     3.188509      58.79
 H       6.209768    -1.545233     3.931909      26.58
 C       5.455744    -2.633945     0.830582      80.70
 C       5.209646    -2.115202    -0.558160     156.61
 H       5.632920    -2.834933    -1.123869      28.37
 O       6.029081    -0.957573    -0.905443     251.96
 H       5.898675    -0.086098    -0.451091      23.60
 C       3.631320    -1.954627    -0.988801      88.31
 H       3.057787    -2.672703    -0.473958      21.03
 C       3.324016    -2.039186    -2.461743      91.57
 O       3.445894    -3.499810    -2.898809     245.48
 H       4.415388    -3.609950    -3.115925      26.82
 H       4.028434    -1.519154    -3.066478      24.11
 H       2.290289    -1.748179    -2.729238      25.33
 C      -0.214477    -1.336120     0.611332      32.45
 H      -1.043921    -2.043602     0.878129      15.31
 C       0.208971     1.098880     0.486399      79.69
 H      -0.386018     2.087592     0.249920      15.89
 C       1.491888     0.802920     0.071683       9.71
 O       2.381697     1.852595    -0.285523     152.61
 C       2.021038     3.337742    -0.083929      92.73
 H       2.964896     3.923961    -0.128931      23.26
 H       1.283120     3.822183    -1.075594      21.19
 H       1.422059     3.482060     0.823772      23.45
 C       1.954050    -0.520749    -0.110707      18.80
 O       3.307089    -0.636919    -0.471968     176.12
 C       1.088431    -1.574815     0.182997      68.98
 H       1.324410    -2.485694    -0.185485      19.66
 C      -0.677918     0.014352     0.726601      56.87
 C      -2.128999     0.286990     1.170679     101.19
 H      -2.561909    -0.613174     1.625751      22.97
 O      -2.069603     1.388902     2.201887     245.61
 H      -1.876671     0.891862     3.036740      27.06
 C      -3.057688     0.852431     0.087733      84.06
 H      -2.670404     1.807929    -0.249339      22.41
 O      -3.221118    -0.216245    -0.999816     274.85
 H      -2.950888     0.150775    -1.930400      24.47
 C      -4.509174     1.480420     0.492076      89.75
 O      -4.952867     2.441586    -0.502338     231.09
 H      -5.052014     3.326560     0.045891      26.13
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 H      -4.298532     1.948909     1.476966      26.75
 H      -5.263242     0.511543     0.640331      24.96
55
name = lig-etoh-Waterframe_357
 C       5.826563    -1.775919     1.838803      49.95
 H       5.990480    -0.719092     1.688505      19.81
 C       5.432713    -4.080398     1.030792      38.64
 H       4.997498    -4.758552     0.318727      13.88
 C       5.742787    -4.543429     2.370086       1.59
 O       5.634222    -5.956319     2.681907     265.12
 C       4.924831    -6.750660     1.691535      98.51
 H       5.348797    -6.893707     0.670495      29.25
 H       3.897275    -6.269066     1.551750      27.67
 H       4.852574    -7.827000     2.197256      24.61
 C       6.137701    -3.645457     3.375065     -12.40
 O       6.549836    -4.124815     4.625790     240.13
 H       6.203382    -5.066646     4.761886      25.90
 C       6.008870    -2.233591     3.181044      59.59
 H       6.351144    -1.644404     4.010681      24.16
 C       5.401586    -2.667802     0.840481      47.09
 C       5.206189    -2.125283    -0.602811     128.28
 H       5.458799    -2.866170    -1.273876      25.63
 O       6.032718    -1.000930    -0.926434     273.13
 H       5.641141    -0.139617    -0.503231      22.82
 C       3.667645    -1.942656    -0.963802      86.34
 H       3.125421    -2.709841    -0.472509      20.79
 C       3.380645    -2.034590    -2.516128      73.82
 O       3.458603    -3.516206    -2.910861     231.92
 H       4.432687    -3.610644    -3.317033      24.59
 H       4.111671    -1.460297    -3.121290      21.16
 H       2.252125    -1.728684    -2.687223      23.08
 C      -0.214193    -1.282511     0.664414      37.38
 H      -0.911520    -2.182326     0.788150      13.19
 C       0.168849     1.076721     0.498237      64.98
 H      -0.162560     2.098339     0.581349      18.12
 C       1.530578     0.839148     0.123106       9.18
 O       2.350168     1.833832    -0.332061     201.83
 C       2.057132     3.321527    -0.137595      82.11
 H       3.007500     3.842326     0.064353      23.09
 H       1.374072     3.379266    -1.178189      20.32
 H       1.393505     3.614197     0.896084      22.69
 C       2.011159    -0.501614    -0.072249      14.93
 O       3.305103    -0.632915    -0.480824     186.76
 C       1.114373    -1.599785     0.157583      58.25
 H       1.445630    -2.555967    -0.054606      20.63
 C      -0.702323    -0.010805     0.750485      53.96
 C      -2.099766     0.327406     1.118965     101.78
 H      -2.621782    -0.580166     1.557191      23.76
 O      -2.076730     1.299717     2.203163     274.87
 H      -1.833017     0.819268     2.935247      29.15
 C      -3.061012     0.870816     0.050943      77.81
 H      -2.488987     1.654564    -0.487351      22.20
 O      -3.237741    -0.180915    -0.975932     263.60
 H      -3.109448     0.218846    -1.918986      24.66
 C      -4.564658     1.443913     0.502748     105.87
 O      -4.988539     2.394090    -0.436522     265.79
 H      -4.748258     3.326643    -0.036424      26.19
 H      -4.472814     2.071045     1.492065      25.02
 H      -5.461072     0.860408     0.682249      25.80
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name = lig-etoh-Waterframe_358
 C       5.796754    -1.777994     1.818677      57.29
 H       5.996547    -0.800155     1.433541      23.14
 C       5.426116    -4.110855     1.075224      40.38
 H       5.131779    -4.778466     0.253015      14.96
 C       5.778139    -4.578640     2.328341      10.32
 O       5.642798    -5.930770     2.664761     240.94
 C       4.903891    -6.773386     1.606626     106.22
 H       5.491420    -6.666061     0.655986      28.05
 H       3.801722    -6.434021     1.414068      27.23
 H       4.915323    -7.799625     2.022786      24.83
 C       6.139579    -3.674296     3.430825      -7.67
 O       6.553971    -4.054228     4.633211     225.21
 H       6.338581    -5.021725     4.848711      27.49
 C       6.027022    -2.281512     3.144586      59.34
 H       6.407506    -1.594813     3.967385      22.01
 C       5.411552    -2.682722     0.794372      26.30
 C       5.181458    -2.178394    -0.661367      96.59
 H       5.557097    -3.055244    -1.464916      21.16
 O       6.030722    -1.027572    -0.953565     247.65
 H       5.459915    -0.265111    -0.546585      23.37
 C       3.774761    -1.927549    -0.974745      84.81
 H       3.304698    -2.799547    -0.477333      20.64
 C       3.439093    -2.100751    -2.531522      83.28
 O       3.489564    -3.457467    -2.941283     249.16
 H       4.370121    -3.488785    -3.552727      23.08
 H       4.073067    -1.375499    -3.138557      22.15
 H       2.355068    -1.679013    -2.742651      23.43
 C      -0.181383    -1.330463     0.650949      40.71
 H      -0.742379    -2.273110     0.873693      16.31
 C       0.187149     1.068904     0.502746      55.92
 H      -0.048911     1.979310     0.802385      20.34
 C       1.494899     0.884889     0.151346      11.15
 O       2.389832     1.864930    -0.338497     237.96
 C       2.055710     3.204419    -0.206294     121.82
 H       3.010613     3.723685    -0.272863      24.42
 H       1.658144     3.795619    -0.961100      26.64
 H       1.307882     3.425235     0.758335      24.17
 C       1.991999    -0.490988    -0.005118      16.42
 O       3.303712    -0.627602    -0.499754     169.34
 C       1.112730    -1.555446     0.164326      73.87
 H       1.310607    -2.642324     0.286213      22.14
 C      -0.703653     0.008278     0.756864      45.70
 C      -2.168288     0.329697     1.154111      81.62
 H      -2.584370    -0.711367     1.370433      22.81
 O      -2.085131     1.236331     2.207929     300.76
 H      -1.671053     0.755938     2.893094      28.98
 C      -3.123598     0.901188    -0.042833      79.32
 H      -2.622277     1.791482    -0.532246      22.33
 O      -3.256655    -0.162254    -0.942572     267.24
 H      -3.297997     0.225399    -1.897799      23.88
 C      -4.522118     1.408553     0.572099      95.35
 O      -5.035235     2.393547    -0.427492     272.11
 H      -4.631645     3.300540    -0.216107      28.36
 H      -4.354684     1.822733     1.655356      25.68
 H      -5.144933     0.613325     0.569689      28.72
55
name = lig-etoh-Waterframe_359
 C       5.753890    -1.825707     1.796125      47.08
 H       5.871315    -0.743564     1.686260      21.27
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 C       5.397299    -4.048094     1.087341      53.91
 H       5.294267    -4.795806     0.258907      20.40
 C       5.775916    -4.625062     2.332799      13.56
 O       5.624951    -5.942768     2.604132     288.20
 C       4.941879    -6.767049     1.573766     119.73
 H       5.538671    -6.709714     0.630372      24.38
 H       3.864650    -6.462399     1.453965      27.14
 H       5.013705    -7.730979     1.863556      24.29
 C       6.084566    -3.673412     3.364934      13.02
 O       6.574507    -4.014627     4.698600     223.89
 H       6.322264    -4.986546     4.861572      23.36
 C       6.106722    -2.317182     3.076305      42.82
 H       6.314594    -1.498567     3.861319      21.56
 C       5.474248    -2.725155     0.747625      33.07
 C       5.268969    -2.231409    -0.682680      79.27
 H       5.693941    -3.212670    -1.420085      20.37
 O       6.014533    -1.056491    -0.985424     278.48
 H       5.743216    -0.106641    -0.671419      21.68
 C       3.768241    -1.967583    -1.048559      81.71
 H       3.097441    -2.697471    -0.487992      21.09
 C       3.465964    -2.061544    -2.499159      96.94
 O       3.536819    -3.403962    -3.012948     240.82
 H       4.519521    -3.587321    -3.390909      23.72
 H       4.220465    -1.522179    -3.132079      22.43
 H       2.406002    -1.768986    -2.615138      25.25
 C      -0.216485    -1.331966     0.620176       8.15
 H      -0.897222    -2.083859     0.961221      17.14
 C       0.183046     1.112269     0.554147      77.89
 H      -0.289097     2.043147     0.694080      18.41
 C       1.535233     0.840125     0.092755      11.45
 O       2.433251     1.824718    -0.335435     227.63
 C       2.064541     3.217427    -0.272651     124.62
 H       3.008233     3.704245    -0.044608      24.85
 H       1.485263     3.615236    -1.056043      26.01
 H       1.591256     3.378975     0.702283      25.86
 C       1.986793    -0.462516     0.006013      23.32
 O       3.311985    -0.623946    -0.510770     154.97
 C       1.110861    -1.535326     0.251808      63.71
 H       1.681346    -2.582086     0.233491      20.04
 C      -0.717822    -0.035624     0.732148      69.67
 C      -2.214730     0.274038     1.101321      87.09
 H      -2.761377    -0.617930     1.464342      22.89
 O      -2.113003     1.212020     2.246041     232.96
 H      -1.629555     0.724347     3.041557      28.45
 C      -3.131251     0.957186    -0.002100      92.89
 H      -2.715514     1.875329    -0.477850      22.22
 O      -3.292924    -0.179600    -0.952765     242.34
 H      -3.435754     0.080341    -1.943071      23.94
 C      -4.423840     1.367374     0.558328      95.76
 O      -5.083681     2.358908    -0.407271     246.25
 H      -4.861775     3.276352    -0.025800      28.08
 H      -4.354399     1.706670     1.605796      27.97
 H      -4.957349     0.404788     0.486237      27.78
55
name = lig-etoh-Waterframe_360
 C       5.745320    -1.835390     1.791178      59.69
 H       5.594565    -0.734477     1.726415      22.21
 C       5.408723    -4.080350     1.055197      42.47
 H       5.188912    -4.775371     0.193699      18.07
 C       5.709484    -4.583806     2.339469       7.98
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 O       5.609260    -6.003736     2.549539     317.33
 C       5.020588    -6.766250     1.553845     123.14
 H       5.376008    -6.711897     0.509789      25.89
 H       4.001721    -6.436862     1.437917      29.43
 H       5.059664    -7.732728     1.937298      23.70
 C       6.100289    -3.711162     3.391523      -7.14
 O       6.557970    -3.995924     4.701052     314.48
 H       6.277763    -4.947921     4.943676      27.26
 C       6.156918    -2.314082     2.997167      49.29
 H       6.337516    -1.671260     3.912844      21.07
 C       5.537679    -2.695147     0.726344      34.55
 C       5.312916    -2.234999    -0.670546      98.52
 H       5.698165    -2.948437    -1.412246      22.32
 O       6.063577    -1.084994    -1.056982     278.10
 H       5.614784    -0.330371    -0.488507      22.03
 C       3.723492    -2.014995    -1.024468      67.41
 H       3.096136    -2.880428    -0.598395      19.14
 C       3.479205    -1.988199    -2.538612     101.36
 O       3.581270    -3.400308    -3.073673     252.33
 H       4.561062    -3.437040    -3.292769      23.65
 H       4.120264    -1.224861    -3.014288      23.91
 H       2.526762    -1.651299    -2.709171      26.90
 C      -0.287857    -1.329137     0.622388      42.50
 H      -0.923347    -2.147521     0.800595      19.74
 C       0.161528     1.083655     0.574970      72.60
 H      -0.261339     2.149255     0.337992      19.00
 C       1.496854     0.877473     0.048878       0.04
 O       2.489220     1.760532    -0.338178     154.18
 C       2.080911     3.263913    -0.252991      97.36
 H       3.010161     3.935782    -0.345791      24.24
 H       1.346795     3.203647    -1.198694      22.58
 H       1.535597     3.466540     0.543200      27.99
 C       2.020974    -0.506630    -0.047535      10.68
 O       3.331867    -0.639967    -0.521597     154.58
 C       1.166879    -1.539095     0.356856      47.15
 H       1.556143    -2.670927     0.191065      17.98
 C      -0.739529    -0.000343     0.687014      36.18
 C      -2.194084     0.263290     1.092472      93.88
 H      -2.743646    -0.613137     1.386208      23.51
 O      -2.148772     1.208149     2.258470     190.92
 H      -1.847864     0.510391     3.113620      22.55
 C      -3.020718     0.944912     0.025423      89.28
 H      -2.409724     1.675828    -0.498315      22.82
 O      -3.331041    -0.200011    -0.966406     250.70
 H      -3.391614     0.179536    -1.927260      25.38
 C      -4.432568     1.338506     0.495969      98.44
 O      -5.119697     2.292786    -0.342394     293.38
 H      -5.115901     3.138972     0.141921      29.65
 H      -4.404800     1.785410     1.434770      27.81
 H      -5.281331     0.480505     0.589064      25.09
55
name = lig-etoh-Waterframe_361
 C       5.764199    -1.772766     1.781326      42.82
 H       5.557664    -0.703096     1.530908      20.53
 C       5.457115    -4.092244     1.000278      60.18
 H       5.074493    -4.793534     0.233728      14.02
 C       5.624725    -4.614667     2.330477      42.15
 O       5.652282    -5.982898     2.545609     268.07
 C       5.017911    -6.811175     1.492337     135.06
 H       5.614552    -6.728907     0.571416      33.58
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 H       3.990114    -6.590064     1.402772      31.11
 H       5.049332    -7.905145     1.890747      25.51
 C       6.156025    -3.702294     3.397104      18.55
 O       6.508788    -4.009801     4.663790     149.80
 H       6.276724    -4.955361     4.927947      21.94
 C       6.174232    -2.368752     3.068007      54.67
 H       6.452640    -1.636559     3.828686      22.12
 C       5.556801    -2.720494     0.727036      27.46
 C       5.269856    -2.230781    -0.726372     112.32
 H       5.517616    -2.984316    -1.277662      26.04
 O       6.104905    -1.086432    -1.104946     253.16
 H       5.833269    -0.227660    -0.559674      24.11
 C       3.746611    -2.031170    -1.000111      74.55
 H       3.234347    -2.891415    -0.518334      19.67
 C       3.461626    -1.943267    -2.589693      94.54
 O       3.629128    -3.332814    -3.109120     265.20
 H       4.480321    -3.478797    -3.549453      27.31
 H       4.195645    -1.265987    -3.004794      23.78
 H       2.485563    -1.650383    -2.839727      25.95
 C      -0.225877    -1.310118     0.624582      47.36
 H      -0.836494    -2.177527     0.680374      19.22
 C       0.199105     1.079939     0.461762      62.45
 H      -0.246950     2.229950     0.424226      16.13
 C       1.476702     0.822792     0.037974      10.69
 O       2.525959     1.793008    -0.300617     176.09
 C       2.078850     3.195936    -0.288488     107.14
 H       2.897424     3.815618    -0.726398      23.48
 H       1.269442     3.547688    -1.274107      21.98
 H       1.520364     3.550456     0.591043      24.80
 C       1.995593    -0.526420    -0.073406       7.45
 O       3.339892    -0.708285    -0.519679     147.94
 C       1.132158    -1.562050     0.410903      52.69
 H       1.289668    -2.674643     0.417956      17.58
 C      -0.763241     0.004152     0.680557      39.46
 C      -2.154753     0.291421     1.151176      90.21
 H      -2.509454    -0.726592     1.320443      23.00
 O      -2.192140     1.175306     2.243356     236.80
 H      -1.845774     0.635116     3.205006      21.71
 C      -2.977390     0.835793    -0.046679      85.98
 H      -2.429078     1.659493    -0.475450      23.05
 O      -3.332997    -0.202500    -0.968003     285.12
 H      -3.195545     0.203063    -1.906276      24.75
 C      -4.486711     1.366350     0.504447      80.26
 O      -5.177347     2.245023    -0.322737     314.16
 H      -5.036368     3.131265     0.057359      29.48
 H      -4.300343     1.759856     1.470631      26.52
 H      -4.993386     0.256508     0.620141      25.32
55
name = lig-etoh-Waterframe_362
 C       5.819527    -1.821843     1.789746      49.76
 H       5.909735    -0.722439     1.696335      20.55
 C       5.485182    -4.100688     1.007310      59.40
 H       5.182471    -4.742870     0.196997      13.67
 C       5.631694    -4.613074     2.305649      29.80
 O       5.673161    -5.971513     2.554604     271.34
 C       5.026266    -6.872331     1.472937      98.39
 H       5.638978    -6.754483     0.571499      31.30
 H       3.997653    -6.590294     1.199127      30.06
 H       5.198187    -8.015723     1.872656      25.91
 C       6.137780    -3.733536     3.294777     -23.10
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 O       6.466309    -4.072921     4.658608     153.18
 H       6.250943    -5.050818     4.746013      23.16
 C       6.149956    -2.280100     3.085482      51.34
 H       6.542356    -1.682503     3.868023      23.67
 C       5.529140    -2.687108     0.729414      44.95
 C       5.237961    -2.215331    -0.742081     110.95
 H       5.517863    -3.111176    -1.417191      23.08
 O       6.134862    -1.100594    -1.147811     260.19
 H       5.923747    -0.158750    -0.762961      23.41
 C       3.764150    -1.996180    -1.059328      86.07
 H       3.234334    -2.754171    -0.556186      19.18
 C       3.486994    -1.973700    -2.584140      91.56
 O       3.643103    -3.264379    -3.145851     267.35
 H       4.563984    -3.279012    -3.549535      25.92
 H       4.232550    -1.350877    -3.066623      20.94
 H       2.406697    -1.632909    -2.780991      23.31
 C      -0.199988    -1.261928     0.646883      54.02
 H      -0.898983    -2.073269     0.920479      21.60
 C       0.171981     1.072610     0.320503      73.66
 H      -0.117382     2.169415     0.667635      17.49
 C       1.583655     0.769295    -0.002987       2.42
 O       2.477081     1.833366    -0.244154     178.57
 C       2.050242     3.147221    -0.413828     105.97
 H       3.040008     3.585106    -0.495108      23.18
 H       1.091567     3.255133    -1.023583      23.70
 H       1.937274     3.591729     0.760693      23.18
 C       1.975898    -0.585599    -0.057463      16.89
 O       3.301463    -0.767013    -0.472119     194.33
 C       1.118507    -1.594461     0.376485      60.42
 H       1.548524    -2.514272     0.491716      18.23
 C      -0.664498     0.027529     0.687937      32.63
 C      -2.130581     0.242248     1.144076      71.50
 H      -2.595793    -0.716185     1.562496      19.47
 O      -2.240054     1.170538     2.256801     245.98
 H      -1.647455     0.680260     3.029643      21.68
 C      -3.079275     0.817378    -0.058602      83.03
 H      -2.596886     1.645697    -0.587212      22.15
 O      -3.292425    -0.223378    -0.999931     288.61
 H      -3.014025    -0.074521    -1.979233      24.74
 C      -4.395022     1.310885     0.561563      89.83
 O      -5.256470     2.227770    -0.344451     302.51
 H      -4.885147     3.084296    -0.169063      30.78
 H      -4.327063     1.742221     1.605558      24.19
 H      -5.063688     0.398277     0.579388      25.05
55
name = lig-etoh-Waterframe_363
 C       5.903816    -1.815914     1.805110      56.34
 H       6.153665    -0.781528     1.583358      22.28
 C       5.462642    -4.046315     0.982028      43.97
 H       5.379623    -4.723723     0.174177      15.06
 C       5.718155    -4.607817     2.258721      32.07
 O       5.639400    -6.013807     2.536215     281.34
 C       5.105099    -6.880192     1.491848     116.66
 H       5.559957    -6.808092     0.505871      30.23
 H       4.005253    -6.611634     1.312671      26.78
 H       5.124710    -7.949269     2.004030      24.63
 C       6.091100    -3.682042     3.312973       5.27
 O       6.412109    -4.166208     4.590028     202.61
 H       6.251780    -5.139120     4.756097      27.94
 C       6.131846    -2.307265     3.076572      71.15
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 H       6.466667    -1.688205     3.861777      23.40
 C       5.485282    -2.673645     0.716901      57.31
 C       5.277660    -2.187414    -0.704296     112.59
 H       5.702131    -3.048363    -1.548590      21.35
 O       6.156347    -1.128399    -1.196057     239.05
 H       5.642652    -0.347265    -0.777363      24.13
 C       3.746356    -1.975467    -1.095322      79.70
 H       3.244134    -2.881698    -0.821181      19.58
 C       3.518450    -1.957599    -2.572323      92.47
 O       3.650764    -3.254781    -3.191247     248.93
 H       4.659338    -3.357090    -3.440385      24.46
 H       4.061761    -1.136407    -3.072893      22.01
 H       2.394866    -1.549369    -2.684507      23.37
 C      -0.215977    -1.303853     0.707351      48.60
 H      -0.932801    -2.007083     1.240332      21.85
 C       0.255130     1.078721     0.228929      79.87
 H      -0.052633     2.083287     0.432867      20.24
 C       1.543689     0.802785    -0.027593      19.11
 O       2.450776     1.749522    -0.208757     219.17
 C       2.059642     3.153081    -0.414388     110.09
 H       2.803970     3.676614    -1.037079      24.65
 H       1.279234     3.212132    -0.967736      29.70
 H       1.701770     3.668365     0.624525      23.90
 C       2.016469    -0.600930    -0.062693      14.92
 O       3.288189    -0.781508    -0.408310     190.50
 C       1.149981    -1.642466     0.307961      58.12
 H       1.568349    -2.552857     0.456731      20.59
 C      -0.646810     0.061517     0.689924      50.07
 C      -2.139703     0.229347     1.095161      74.08
 H      -2.581930    -0.792730     1.396316      21.24
 O      -2.246773     1.181978     2.267551     252.39
 H      -1.759075     0.783622     3.032723      25.04
 C      -3.117848     0.838782    -0.022176      76.50
 H      -2.587762     1.696657    -0.502139      22.01
 O      -3.262066    -0.303978    -1.052419     260.27
 H      -2.874236     0.035899    -1.940778      24.96
 C      -4.424694     1.247169     0.558601     103.80
 O      -5.268244     2.180818    -0.345706     293.05
 H      -4.938179     3.055751    -0.231303      32.34
 H      -4.247421     1.814536     1.571440      23.71
 H      -5.089786     0.529282     0.743137      28.09
55
name = lig-etoh-Waterframe_364
 C       5.959501    -1.778041     1.730780      53.53
 H       6.163267    -0.748075     1.488710      21.50
 C       5.435036    -4.042668     0.952828      48.42
 H       5.313399    -4.684718     0.108867      21.02
 C       5.791474    -4.603579     2.209405      15.70
 O       5.630658    -5.995655     2.507904     322.13
 C       5.129779    -6.871915     1.533652     125.53
 H       5.688031    -6.931918     0.608466      24.39
 H       4.022362    -6.662995     1.435842      26.67
 H       5.226665    -7.855053     1.927727      21.81
 C       6.018709    -3.749316     3.363238      20.87
 O       6.367108    -4.237275     4.527793     259.35
 H       6.113789    -5.205723     4.571318      31.19
 C       6.148981    -2.354110     3.093867      44.69
 H       6.361032    -1.645750     3.888795      23.40
 C       5.505154    -2.618351     0.746302      36.27
 C       5.327628    -2.199916    -0.743422      86.28
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 H       5.593688    -3.273337    -1.237632      19.61
 O       6.128977    -1.118425    -1.196093     253.57
 H       5.863337    -0.181160    -0.913640      24.01
 C       3.800861    -2.020800    -1.071697      68.40
 H       3.236702    -2.931187    -0.692500      19.21
 C       3.495731    -1.850820    -2.615389      82.10
 O       3.667599    -3.251944    -3.208519     233.54
 H       4.617758    -3.401906    -3.619263      25.19
 H       4.173469    -1.137195    -3.149517      22.44
 H       2.356320    -1.804777    -2.747871      23.87
 C      -0.176009    -1.310151     0.773360      44.94
 H      -0.781806    -2.163224     1.220081      17.87
 C       0.179259     1.100260     0.236640      56.39
 H      -0.086747     2.027093    -0.000094      19.22
 C       1.523689     0.732824    -0.056519       7.31
 O       2.527165     1.728721    -0.210842     181.07
 C       2.036175     3.144317    -0.423303     110.66
 H       2.737725     3.598624    -1.131920      25.41
 H       1.091878     3.112427    -1.077813      25.06
 H       1.848607     3.776569     0.433369      26.64
 C       1.965962    -0.577654    -0.068376      18.19
 O       3.363597    -0.786513    -0.368737     129.36
 C       1.112380    -1.655545     0.282736      51.46
 H       1.381771    -2.719987     0.293024      22.19
 C      -0.687633     0.002828     0.657149      37.88
 C      -2.145564     0.293798     1.081868      95.21
 H      -2.471001    -0.743243     1.229447      24.35
 O      -2.235969     1.176176     2.253668     272.00
 H      -1.948191     0.722301     2.970279      29.30
 C      -3.068143     0.766650    -0.028256      74.71
 H      -2.641140     1.721587    -0.458032      23.44
 O      -3.227908    -0.328918    -1.064699     272.47
 H      -2.957935     0.072690    -1.963499      25.78
 C      -4.558996     1.259436     0.535711     104.09
 O      -5.231429     2.100837    -0.343045     289.86
 H      -5.019145     2.947951     0.016742      32.44
 H      -4.164964     1.854958     1.435231      25.74
 H      -5.060142     0.401500     0.866717      28.86
55
name = lig-etoh-Waterframe_365
 C       6.004185    -1.772034     1.774988      61.15
 H       6.093712    -0.702672     1.662296      21.54
 C       5.439466    -4.036146     0.955000      26.77
 H       5.054740    -4.642925     0.140522      14.76
 C       5.763022    -4.619488     2.153588      23.48
 O       5.681325    -5.913033     2.510821     323.20
 C       5.115725    -6.909460     1.562921     132.05
 H       5.661714    -6.744689     0.607421      26.14
 H       4.097467    -6.720316     1.201666      30.12
 H       5.285988    -7.788477     1.992580      22.13
 C       5.979686    -3.769141     3.262345      -1.90
 O       6.329158    -4.317514     4.542937     338.27
 H       6.099276    -5.303717     4.687318      31.05
 C       6.155401    -2.347271     3.040808      53.49
 H       6.356726    -1.765856     3.981027      21.59
 C       5.565089    -2.615916     0.708445      45.83
 C       5.314933    -2.240674    -0.740795     103.55
 H       5.703535    -2.920720    -1.423208      23.55
 O       6.131896    -1.100251    -1.213417     223.48
 H       5.795160    -0.269748    -0.737727      24.63
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 C       3.854037    -2.020011    -1.070002      76.31
 H       3.270345    -2.871628    -0.547213      16.66
 C       3.471801    -1.883357    -2.635657      95.72
 O       3.683814    -3.233904    -3.211896     256.92
 H       4.610128    -3.120057    -3.598115      24.14
 H       4.120482    -1.113709    -3.128919      23.54
 H       2.479390    -1.500846    -2.825006      24.53
 C      -0.148181    -1.308106     0.809603      49.05
 H      -0.852552    -2.126235     1.044730      17.46
 C       0.073289     1.033804     0.241997      56.00
 H      -0.407167     1.898783    -0.094713      17.56
 C       1.533038     0.749636    -0.058793     -17.31
 O       2.572505     1.752182    -0.227885     163.19
 C       2.025488     3.084158    -0.497959     105.81
 H       2.921337     3.523803    -0.973653      23.81
 H       0.827110     3.034167    -0.978866      20.96
 H       2.026785     3.568168     0.371236      27.87
 C       1.997946    -0.653875    -0.096581       7.81
 O       3.413725    -0.786474    -0.332326     145.01
 C       1.062266    -1.631020     0.283490      59.58
 H       1.390338    -2.746281     0.071936      19.45
 C      -0.724896    -0.004396     0.630053      42.35
 C      -2.139732     0.276418     1.094957      96.40
 H      -2.607692    -0.583904     1.517127      22.56
 O      -2.223333     1.156672     2.220677     278.90
 H      -1.961493     0.670084     2.922792      29.38
 C      -3.109621     0.732969    -0.077003      85.78
 H      -2.701260     1.591808    -0.652175      23.05
 O      -3.177956    -0.303085    -1.030341     295.84
 H      -3.189888    -0.121626    -2.014669      25.69
 C      -4.512950     1.203339     0.556417      96.70
 O      -5.222870     2.062600    -0.374736     273.49
 H      -5.159750     2.896275     0.062315      32.49
 H      -4.437231     1.765623     1.495971      26.75
 H      -5.259174     0.262031     0.822908      25.40
55
name = lig-etoh-Waterframe_366
 C       6.006311    -1.780759     1.796738      55.79
 H       6.077169    -0.688861     1.749181      21.32
 C       5.430949    -3.994857     0.892010      41.73
 H       4.961396    -4.650332     0.146145      12.79
 C       5.677653    -4.591372     2.157750      55.48
 O       5.707667    -5.918080     2.505856     334.70
 C       5.142091    -6.888358     1.552027     151.38
 H       5.764825    -6.899517     0.594768      36.68
 H       4.068322    -6.731573     1.438377      31.09
 H       5.247487    -7.852785     2.053290      26.21
 C       6.039527    -3.760359     3.223943       9.08
 O       6.279818    -4.318028     4.521116     190.46
 H       6.091344    -5.301965     4.667893      26.16
 C       6.152467    -2.405688     3.050573      55.72
 H       6.449482    -1.764662     3.947305      21.80
 C       5.657511    -2.662916     0.676662      52.72
 C       5.355374    -2.218898    -0.786208     107.91
 H       5.647183    -2.954750    -1.417389      26.20
 O       6.130732    -1.062231    -1.205118     230.98
 H       5.826883    -0.340518    -0.598730      26.51
 C       3.809876    -1.973408    -1.077125      72.98
 H       3.303226    -2.928577    -0.756295      18.01
 C       3.483462    -1.930000    -2.580230     110.45
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 O       3.693478    -3.185077    -3.210358     253.91
 H       4.636252    -3.375607    -3.506602      25.74
 H       4.203579    -1.225096    -3.017393      24.47
 H       2.540092    -1.553298    -2.696802      25.82
 C      -0.239798    -1.315821     0.791527      35.94
 H      -0.944256    -2.082704     1.030077      18.17
 C       0.136918     0.979515     0.157876      75.05
 H      -0.465832     1.986979     0.190832      16.41
 C       1.521152     0.762083    -0.032176      10.70
 O       2.505829     1.706541    -0.263777     196.34
 C       2.076496     3.030700    -0.515221     108.48
 H       2.676396     3.591233    -1.268320      24.26
 H       1.021008     3.197498    -1.226768      22.45
 H       1.867958     3.492116     0.480600      24.83
 C       2.052235    -0.602305    -0.105732       9.00
 O       3.413431    -0.803301    -0.314246     159.72
 C       1.121046    -1.638045     0.251527      41.60
 H       1.351662    -2.826889     0.199473      18.93
 C      -0.752024    -0.063838     0.673156      38.74
 C      -2.203620     0.198581     1.101111      78.29
 H      -2.609893    -0.798011     1.423157      21.96
 O      -2.198616     1.176967     2.199210     266.02
 H      -1.772235     0.798562     3.010018      25.91
 C      -3.158228     0.777756    -0.082768      92.56
 H      -2.735301     1.690571    -0.496867      23.73
 O      -3.148943    -0.349018    -0.992776     272.10
 H      -3.327453     0.028445    -1.885884      24.95
 C      -4.448566     1.101891     0.567866      85.56
 O      -5.233115     2.053599    -0.417899     232.31
 H      -5.154980     2.934160    -0.069105      32.25
 H      -4.345815     1.477005     1.537302      27.33
 H      -5.227650     0.129769     0.519592      25.03
55
name = lig-etoh-Waterframe_367
 C       5.981013    -1.844223     1.757906      56.33
 H       6.133501    -0.752663     1.606922      22.69
 C       5.419261    -4.039584     0.879343      61.99
 H       5.186654    -4.652457    -0.025611      17.21
 C       5.606822    -4.557968     2.160688      41.17
 O       5.708212    -5.966497     2.475885     302.34
 C       5.177893    -6.875184     1.568787     110.02
 H       5.649199    -7.008192     0.541171      30.70
 H       4.109315    -6.623022     1.447156      31.08
 H       5.265201    -7.954657     2.113593      26.14
 C       6.109170    -3.810168     3.281999     -24.30
 O       6.241370    -4.258333     4.483266      92.38
 H       6.039949    -5.240376     4.415515      15.27
 C       6.176052    -2.397036     3.078785      38.54
 H       6.485954    -1.747377     3.949569      20.59
 C       5.726721    -2.611574     0.643302      32.19
 C       5.386274    -2.161671    -0.816245      80.75
 H       5.611560    -3.143638    -1.403993      19.96
 O       6.128732    -1.013591    -1.180397     287.72
 H       6.010822    -0.220812    -0.635576      26.43
 C       3.797966    -2.004232    -1.044200      79.45
 H       3.266532    -2.838148    -0.635930      20.19
 C       3.555982    -1.881820    -2.527382      98.55
 O       3.681030    -3.199547    -3.202135     243.87
 H       4.660324    -3.333245    -3.348342      24.70
 H       4.178768    -1.136467    -3.020608      25.09
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 H       2.484600    -1.803971    -2.695096      25.34
 C      -0.237827    -1.411154     0.674717      48.91
 H      -0.816806    -2.196632     1.075621      24.41
 C       0.151298     0.944320     0.144001      81.08
 H       0.140778     2.160811     0.299203      17.88
 C       1.505123     0.709011    -0.030281      20.36
 O       2.433777     1.653874    -0.334509     186.77
 C       2.061604     3.049336    -0.559148     109.25
 H       2.953027     3.502020    -1.062774      24.20
 H       1.201500     2.902761    -1.080130      26.75
 H       1.782583     3.798522     0.386536      23.68
 C       1.998862    -0.589108    -0.048583      20.14
 O       3.389753    -0.809842    -0.322026     156.22
 C       1.121007    -1.621192     0.265261      52.57
 H       1.574486    -2.673128     0.354714      20.02
 C      -0.744516    -0.058182     0.677244      24.15
 C      -2.232028     0.171750     1.106315      80.75
 H      -2.658777    -0.878922     1.303113      21.84
 O      -2.183329     1.196382     2.184395     237.36
 H      -1.598597     0.801059     2.994172      23.62
 C      -3.088130     0.765529     0.010423      92.41
 H      -2.656065     1.679641    -0.371858      24.36
 O      -3.148869    -0.371150    -0.975709     246.62
 H      -3.303909    -0.059469    -1.896609      25.11
 C      -4.526958     1.045206     0.473643      90.20
 O      -5.222930     2.031570    -0.410361     285.61
 H      -4.841055     2.848849    -0.063993      31.09
 H      -4.372453     1.372399     1.463406      27.00
 H      -4.989049     0.010829     0.458030      26.76
55
name = lig-etoh-Waterframe_368
 C       5.998147    -1.862392     1.752987      52.36
 H       6.173954    -0.776628     1.584349      22.21
 C       5.463791    -4.025355     0.880091      74.40
 H       5.459892    -4.779651     0.046599      22.25
 C       5.618164    -4.619610     2.164357      51.37
 O       5.721695    -5.946493     2.459299     259.65
 C       5.140254    -6.927621     1.561825     130.64
 H       5.693636    -6.841195     0.631748      30.30
 H       4.101227    -6.718489     1.245053      28.29
 H       5.257096    -7.994802     2.129289      25.32
 C       6.082204    -3.718292     3.211624       2.00
 O       6.227299    -4.264360     4.531232      93.70
 H       6.161162    -5.259539     4.652718      21.56
 C       6.215170    -2.371893     3.046592      67.17
 H       6.443249    -1.726776     3.886306      20.69
 C       5.688533    -2.677221     0.609914      34.79
 C       5.369634    -2.127263    -0.733314      81.11
 H       5.882439    -2.767421    -1.679167      18.97
 O       6.154431    -0.961556    -1.192434     257.42
 H       5.853473    -0.267754    -0.595304      25.81
 C       3.855711    -2.031518    -0.967811      79.20
 H       3.392715    -2.887936    -0.553602      21.10
 C       3.549919    -1.870638    -2.530483      85.78
 O       3.705763    -3.224077    -3.164335     237.83
 H       4.632502    -3.295149    -3.545697      24.96
 H       4.089971    -1.042307    -2.992602      23.72
 H       2.417660    -1.489108    -2.663699      24.00
 C      -0.217904    -1.432351     0.549558      55.61
 H      -0.828183    -2.241790     0.917941      24.51
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 C       0.147677     0.956133     0.250508      60.99
 H      -0.324494     2.072390     0.274764      16.83
 C       1.493405     0.654024    -0.070573      10.16
 O       2.425559     1.647001    -0.386088     189.79
 C       2.018332     3.054589    -0.616188     110.06
 H       3.020337     3.361390    -0.945902      23.96
 H       1.272204     3.198073    -1.300515      27.19
 H       1.833342     3.613562     0.447831      23.74
 C       1.992344    -0.666157    -0.010368      25.08
 O       3.337751    -0.786190    -0.327800     160.29
 C       1.112446    -1.664852     0.322110      70.56
 H       1.578417    -2.584678     0.429151      22.50
 C      -0.729235    -0.091546     0.614921      42.10
 C      -2.143342     0.191479     1.138494      94.21
 H      -2.653366    -0.664400     1.654058      21.15
 O      -2.175539     1.186323     2.174676     228.99
 H      -1.697866     0.653409     3.049406      23.32
 C      -3.040502     0.704181     0.028463      86.05
 H      -2.497370     1.544856    -0.440493      22.87
 O      -3.147387    -0.357636    -0.965528     296.65
 H      -3.092728    -0.078569    -1.901262      26.40
 C      -4.588514     1.003108     0.388025     102.59
 O      -5.186166     1.997032    -0.370259     318.64
 H      -4.743904     2.845499    -0.202079      30.68
 H      -4.821553     1.402753     1.451140      25.05
 H      -5.170506     0.180534     0.291644      27.60
55
name = lig-etoh-Waterframe_369
 C       6.033045    -1.826307     1.693444      59.79
 H       6.127506    -0.737467     1.567882      20.58
 C       5.546377    -4.109248     0.877032      28.22
 H       5.344264    -4.768606     0.001817      15.60
 C       5.711560    -4.598092     2.156625      27.98
 O       5.704164    -5.946729     2.470760     297.97
 C       5.115765    -6.956623     1.516431     138.28
 H       5.778934    -7.071171     0.699993      27.92
 H       4.049139    -6.770248     1.345181      28.45
 H       5.230853    -7.947148     2.047049      23.89
 C       5.990205    -3.769633     3.239323      14.39
 O       6.233707    -4.235792     4.573369     353.51
 H       6.155534    -5.241018     4.640514      27.64
 C       6.242225    -2.327946     2.984097      48.83
 H       6.464328    -1.708178     3.810151      22.34
 C       5.647774    -2.707418     0.679091      38.54
 C       5.423686    -2.087279    -0.744696      88.12
 H       5.605443    -3.046164    -1.455196      21.55
 O       6.151161    -0.891603    -1.143223     308.05
 H       5.840883    -0.088423    -0.725258      25.68
 C       3.883062    -1.992222    -0.968410      67.84
 H       3.480985    -2.939696    -0.594536      19.65
 C       3.515944    -1.903349    -2.498194      90.76
 O       3.737753    -3.215172    -3.117302     253.56
 H       4.520675    -3.169559    -3.710933      27.08
 H       4.324551    -1.299489    -2.921100      21.58
 H       2.377015    -1.527063    -2.602163      22.65
 C      -0.272152    -1.431353     0.496614      43.22
 H      -1.029392    -2.238924     0.607706      18.38
 C       0.127206     0.962293     0.370159      76.06
 H      -0.442656     1.853681     0.236994      17.78
 C       1.449922     0.688644    -0.103148       3.60
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 O       2.413070     1.638493    -0.450804     194.73
 C       2.038093     3.025272    -0.637325     116.83
 H       2.900265     3.593527    -0.957475      24.08
 H       1.317222     3.519754    -1.512277      22.97
 H       1.609080     3.346535     0.310953      25.26
 C       2.007921    -0.684587    -0.012855      10.60
 O       3.325989    -0.784926    -0.325691     152.23
 C       1.159785    -1.794091     0.363461      53.26
 H       1.353779    -2.769916     0.448383      20.43
 C      -0.710660    -0.156805     0.560231      42.34
 C      -2.078974     0.185371     1.199496      87.66
 H      -2.362985    -0.801144     1.581939      22.21
 O      -2.134678     1.195851     2.193303     259.84
 H      -1.923151     0.786801     3.247562      23.64
 C      -3.090180     0.644054    -0.007802      84.00
 H      -2.673083     1.619616    -0.423023      21.90
 O      -3.127476    -0.368512    -0.984409     309.62
 H      -2.854339     0.039542    -1.808654      26.17
 C      -4.599017     0.966320     0.408391      87.45
 O      -5.167145     2.018823    -0.420117     279.52
 H      -4.835515     2.920944    -0.164056      29.13
 H      -4.725616     1.031301     1.610027      26.03
 H      -5.162128     0.155146     0.032107      26.10
55
name = lig-etoh-Waterframe_370
 C       6.058380    -1.790822     1.675757      48.28
 H       6.117737    -0.747941     1.394475      19.31
 C       5.620763    -4.130342     0.841178      32.66
 H       5.219818    -4.764288     0.054325      12.53
 C       5.799959    -4.640744     2.162968      32.52
 O       5.660845    -6.006965     2.480514     299.98
 C       5.145851    -6.964962     1.526149     129.20
 H       5.612612    -7.123213     0.547338      30.68
 H       4.115845    -6.654210     1.238859      31.97
 H       5.107768    -7.789232     2.109109      24.70
 C       5.971409    -3.723901     3.341022      27.60
 O       6.233567    -4.189335     4.571706     293.94
 H       6.004259    -5.167785     4.598434      31.56
 C       6.224532    -2.389286     2.980794      65.26
 H       6.541336    -1.729981     3.754429      23.67
 C       5.652726    -2.670514     0.672133      42.73
 C       5.415380    -2.097262    -0.740973     112.43
 H       5.791375    -2.785731    -1.415208      24.79
 O       6.153613    -0.867386    -1.078757     300.03
 H       5.738194    -0.119195    -0.644966      25.81
 C       3.872371    -1.947260    -1.007132      84.91
 H       3.382820    -2.832846    -0.479184      16.90
 C       3.556799    -1.938524    -2.445535     101.18
 O       3.740118    -3.227425    -3.073989     274.62
 H       4.574928    -3.126924    -3.576780      25.69
 H       4.165500    -1.162337    -2.973967      22.13
 H       2.517036    -1.678977    -2.721937      23.58
 C      -0.243965    -1.538015     0.471021      40.32
 H      -1.035609    -2.329853     0.525470      17.59
 C       0.152944     0.956924     0.394070      51.93
 H      -0.092577     1.908685     0.397744      17.06
 C       1.425512     0.696564    -0.083889       7.67
 O       2.396877     1.626832    -0.559029     189.88
 C       2.039796     3.055307    -0.638619     103.96
 H       2.984327     3.587158    -0.577182      22.90
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 H       1.153702     2.856850    -1.534878      20.00
 H       1.508819     3.400805     0.134655      26.91
 C       1.945052    -0.702946    -0.010351       5.04
 O       3.370025    -0.790861    -0.318524     169.07
 C       1.115067    -1.821253     0.344918      44.34
 H       1.490047    -2.843977     0.274922      15.38
 C      -0.722375    -0.129986     0.598130      44.77
 C      -2.107642     0.124910     1.176635      86.23
 H      -2.457113    -0.829676     1.537946      21.49
 O      -2.082838     1.228156     2.227629     239.98
 H      -1.829232     0.712894     3.207721      22.58
 C      -3.147033     0.627729     0.056881      85.45
 H      -2.809090     1.617758    -0.354105      19.86
 O      -3.087278    -0.391331    -1.045304     274.89
 H      -2.811263    -0.093725    -1.913243      24.91
 C      -4.584257     0.882077     0.406114      77.57
 O      -5.145621     2.069903    -0.464572     194.02
 H      -4.886602     2.886314     0.099852      27.26
 H      -4.659971     1.041639     1.544962      26.17
 H      -5.104937    -0.116058     0.041069      24.20
55
name = lig-etoh-Waterframe_371
 C       6.051552    -1.843815     1.706491      69.73
 H       6.289958    -0.794466     1.622628      21.66
 C       5.663901    -4.062013     0.880104      23.99
 H       5.390898    -4.744838     0.112252      13.88
 C       5.829636    -4.677602     2.178493      38.40
 O       5.652131    -6.033451     2.495882     374.71
 C       5.121890    -6.957619     1.539936     137.17
 H       5.872838    -7.017351     0.646676      29.07
 H       4.125796    -6.589746     1.184362      28.24
 H       4.980865    -7.873576     2.011570      20.78
 C       6.011576    -3.727555     3.261717      39.17
 O       6.222754    -4.163866     4.607062     349.56
 H       5.952054    -5.119248     4.730901      37.39
 C       6.202748    -2.361621     3.010333      55.42
 H       6.566436    -1.754176     3.853970      22.36
 C       5.709688    -2.672953     0.606260      53.08
 C       5.403945    -2.101444    -0.743267     139.19
 H       5.862367    -2.625364    -1.480357      24.73
 O       6.145066    -0.870769    -1.003583     272.59
 H       5.778243    -0.167112    -0.440428      22.44
 C       3.865925    -1.960213    -0.964629      78.30
 H       3.366497    -2.915763    -0.562610      15.77
 C       3.554708    -1.917431    -2.494953      99.36
 O       3.769718    -3.265750    -3.044751     269.72
 H       4.672267    -3.461652    -3.367166      25.87
 H       4.105899    -1.096252    -3.002149      22.70
 H       2.551747    -1.734615    -2.519421      25.07
 C      -0.276355    -1.534064     0.491742      46.44
 H      -0.872412    -2.448763     0.726758      21.48
 C       0.178776     0.960322     0.369817      60.64
 H      -0.054843     1.945685     0.716930      16.37
 C       1.525665     0.615949    -0.061453       5.91
 O       2.385667     1.585151    -0.618374     168.37
 C       1.959037     2.994341    -0.625443     116.73
 H       2.907383     3.539950    -0.781180      24.52
 H       1.542863     3.408438    -1.673732      23.29
 H       1.385808     3.380942     0.205831      25.42
 C       1.938982    -0.683476    -0.033993      19.75
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 O       3.364445    -0.763710    -0.292573     184.47
 C       1.099203    -1.765995     0.238669      49.82
 H       1.676408    -2.778686     0.128740      13.79
 C      -0.715095    -0.187854     0.676040      35.65
 C      -2.188731     0.117627     1.149341      93.46
 H      -2.617090    -0.696044     1.727179      21.15
 O      -2.036549     1.200290     2.230819     268.85
 H      -1.582749     0.701282     3.023418      24.13
 C      -3.110092     0.618855     0.058280      83.13
 H      -2.639648     1.548178    -0.268936      21.38
 O      -3.046653    -0.414008    -1.085450     256.79
 H      -2.942625     0.014688    -1.927158      25.45
 C      -4.610383     0.830015     0.360366      97.70
 O      -5.097745     2.048390    -0.436049     204.29
 H      -4.842374     2.901541     0.128265      25.39
 H      -4.828380     1.226305     1.278585      27.33
 H      -5.433284    -0.068460     0.229224      24.60
55
name = lig-etoh-Waterframe_372
 C       6.054430    -1.867029     1.754126      68.65
 H       6.297988    -0.817617     1.641085      23.84
 C       5.675869    -4.064750     0.919466      25.36
 H       5.630326    -4.673790     0.057740      22.13
 C       5.803495    -4.651376     2.174938      43.85
 O       5.667658    -6.011938     2.545447     340.44
 C       5.095029    -6.924911     1.511568     130.46
 H       5.974697    -7.104476     0.776123      27.89
 H       4.170079    -6.555294     1.005762      26.49
 H       4.964408    -7.977887     1.970200      23.90
 C       6.096808    -3.817061     3.239854     -11.82
 O       6.195691    -4.137011     4.619197     196.90
 H       6.057647    -5.128001     4.700725      25.31
 C       6.187214    -2.349909     3.036834      54.51
 H       6.424128    -1.694980     3.930625      22.90
 C       5.807113    -2.696845     0.634142      58.95
 C       5.431580    -2.077368    -0.750542      93.65
 H       5.635485    -2.971312    -1.584097      18.27
 O       6.128597    -0.867984    -0.926316     286.88
 H       5.890281    -0.105511    -0.331070      21.05
 C       3.884814    -1.984397    -0.954830      66.66
 H       3.431868    -2.921005    -0.586230      18.77
 C       3.530676    -1.917101    -2.515423      97.82
 O       3.790971    -3.312718    -3.023450     239.04
 H       4.735230    -3.356864    -3.303216      24.48
 H       4.214791    -1.278139    -3.090202      23.56
 H       2.484744    -1.778749    -2.619980      24.18
 C      -0.273286    -1.496844     0.546082      30.86
 H      -0.994942    -2.293569     0.819369      17.54
 C       0.204476     0.837503     0.381917      67.62
 H      -0.286206     1.887247     0.699846      16.72
 C       1.503644     0.667785    -0.046612      15.68
 O       2.366331     1.555195    -0.649483     223.61
 C       1.932542     2.969750    -0.685940     117.25
 H       2.942740     3.484733    -0.508788      23.78
 H       1.413699     3.357231    -1.419118      27.83
 H       1.314144     3.178330     0.324945      23.51
 C       2.042413    -0.695129    -0.086563      26.47
 O       3.342818    -0.772431    -0.271031     163.85
 C       1.108845    -1.702070     0.102115      75.89
 H       1.343481    -2.874564     0.207278      20.42
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 C      -0.715741    -0.210126     0.726367      42.10
 C      -2.183497     0.127897     1.230264      88.41
 H      -2.617824    -0.832976     1.642014      21.45
 O      -2.005834     1.152569     2.190072     342.46
 H      -1.607224     0.754518     2.938979      30.12
 C      -3.077756     0.565419    -0.029128      76.81
 H      -2.696358     1.517651    -0.347568      22.81
 O      -3.004522    -0.404635    -1.083997     289.94
 H      -3.094402     0.091111    -1.877655      25.34
 C      -4.669780     0.920293     0.347847      90.67
 O      -5.057805     1.970560    -0.420498     297.57
 H      -4.651381     2.869509    -0.020052      25.36
 H      -4.690706     1.051018     1.413063      27.45
 H      -5.315326     0.008504    -0.005506      24.93
55
name = lig-etoh-Waterframe_373
 C       6.082124    -1.821558     1.777079      44.68
 H       6.059696    -0.759978     1.533772      21.55
 C       5.694068    -4.120288     0.866195      42.66
 H       5.593626    -4.799177     0.017678      18.99
 C       5.779724    -4.663195     2.209764      51.79
 O       5.654077    -5.989415     2.557205     244.62
 C       5.142259    -6.893897     1.486805     102.39
 H       5.819707    -7.157778     0.655974      30.88
 H       4.291889    -6.439937     0.964897      29.94
 H       4.769643    -7.793853     2.198813      26.11
 C       6.172879    -3.753594     3.332677      10.50
 O       6.165879    -4.157312     4.602491      75.77
 H       6.213584    -5.144636     4.704525      20.50
 C       6.179642    -2.451249     3.078625      65.90
 H       6.224216    -1.721480     3.937703      23.34
 C       5.863902    -2.703096     0.702361      46.37
 C       5.443378    -2.099998    -0.670243      91.67
 H       5.951892    -2.839806    -1.610768      17.94
 O       6.158210    -0.875343    -0.913081     266.11
 H       5.641394    -0.207327    -0.336768      20.82
 C       3.898090    -1.975567    -0.987039      92.58
 H       3.454534    -2.799802    -0.495406      20.11
 C       3.541278    -2.001555    -2.484429      95.18
 O       3.800922    -3.344899    -3.001371     255.39
 H       4.647732    -3.273364    -3.506314      24.63
 H       4.209124    -1.308454    -3.021231      24.31
 H       2.511392    -1.642813    -2.882484      22.86
 C      -0.214104    -1.473649     0.578744      51.47
 H      -0.872444    -2.324917     0.689126      18.40
 C       0.158633     0.789399     0.448024      61.14
 H      -0.258235     1.922333     0.153382      17.25
 C       1.466544     0.642011    -0.068254       8.99
 O       2.337003     1.579291    -0.687509     196.32
 C       1.956388     2.943826    -0.650238     108.61
 H       2.831769     3.650473    -0.460970      23.67
 H       1.225099     3.035365    -1.472678      24.82
 H       1.221005     3.073490     0.338088      21.83
 C       1.995501    -0.670532    -0.115323       7.45
 O       3.420458    -0.832163    -0.286469     147.04
 C       1.042038    -1.727229     0.043190      53.13
 H       1.466667    -2.819318     0.020855      21.17
 C      -0.732038    -0.209584     0.759618      40.35
 C      -2.092311     0.080767     1.222123      95.04
 H      -2.535094    -0.879942     1.620536      22.86
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 O      -2.018590     1.140365     2.175657     325.76
 H      -1.821970     0.793157     2.969961      31.14
 C      -3.101500     0.564054    -0.029631      80.34
 H      -2.696332     1.491330    -0.457256      22.01
 O      -2.962513    -0.399770    -1.075816     289.66
 H      -3.156580    -0.130217    -1.955096      26.37
 C      -4.588110     0.890738     0.366053      99.96
 O      -5.063316     1.969280    -0.461146     275.30
 H      -4.696582     2.888098    -0.127763      26.06
 H      -4.718864     0.901961     1.527760      26.79
 H      -5.099824     0.074826    -0.000232      27.40
55
name = lig-etoh-Waterframe_374
 C       6.085433    -1.850061     1.804697      53.29
 H       5.946746    -0.756792     1.813487      19.64
 C       5.741442    -4.165625     0.903990      19.74
 H       5.390851    -4.801107     0.046884      12.53
 C       5.822152    -4.624808     2.220609      39.02
 O       5.637747    -5.979415     2.523188     289.48
 C       5.154130    -6.843409     1.510092     110.10
 H       5.912750    -7.225261     0.898143      32.64
 H       4.327352    -6.331229     1.068339      34.38
 H       4.678866    -7.791811     2.031152      25.95
 C       6.145821    -3.803785     3.307460     -40.46
 O       6.159527    -4.223478     4.660892     225.89
 H       6.166016    -5.226311     4.695608      23.21
 C       6.194828    -2.348911     3.088697      71.22
 H       6.195427    -1.817476     4.059051      22.95
 C       5.834044    -2.720637     0.719726      81.83
 C       5.523375    -2.140566    -0.632223     103.21
 H       6.002339    -2.821736    -1.382991      24.43
 O       6.183647    -0.891139    -0.918761     275.53
 H       5.795619     0.022695    -0.551292      19.76
 C       3.907150    -2.039472    -0.967874      77.50
 H       3.469541    -2.935236    -0.552199      20.02
 C       3.612714    -2.048111    -2.493556      88.99
 O       3.803650    -3.376965    -2.997465     261.67
 H       4.593654    -3.475097    -3.582277      26.43
 H       4.328792    -1.337037    -2.902155      23.49
 H       2.445910    -1.721850    -2.568664      22.74
 C      -0.205766    -1.548888     0.574178      47.08
 H      -0.802229    -2.424489     0.701497      16.56
 C       0.161542     0.911475     0.402681      64.29
 H      -0.405354     1.920715     0.154693      16.11
 C       1.460803     0.593134    -0.110012       3.11
 O       2.325301     1.573197    -0.685211     183.66
 C       1.893828     2.934368    -0.560299     106.78
 H       2.681409     3.604119    -0.841162      24.09
 H       1.311994     3.295220    -1.700068      21.65
 H       1.263635     3.264819     0.327573      23.31
 C       1.942804    -0.711701    -0.139091      15.33
 O       3.447881    -0.841233    -0.311480     125.81
 C       1.090909    -1.762467     0.033976      56.93
 H       1.460399    -2.737912    -0.216817      22.40
 C      -0.676828    -0.224859     0.767302      36.66
 C      -2.102442     0.046277     1.153791     103.79
 H      -2.469386    -0.827670     1.702878      23.17
 O      -2.068766     1.155938     2.189536     266.42
 H      -1.961958     0.743030     3.041434      28.05
 C      -3.043831     0.605723     0.023582      87.64
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 H      -2.571920     1.590852    -0.273984      21.26
 O      -2.929976    -0.451795    -1.066869     269.48
 H      -3.187051    -0.090439    -1.901310      25.50
 C      -4.479237     0.774046     0.362367     102.10
 O      -5.089766     1.979884    -0.509470     204.16
 H      -4.840713     2.810503    -0.021808      26.80
 H      -4.798305     1.255818     1.375103      25.66
 H      -5.060052    -0.029805     0.153515      28.21
55
name = lig-etoh-Waterframe_375
 C       6.040534    -1.868353     1.850706      58.51
 H       6.046039    -0.768207     1.624663      21.84
 C       5.772257    -4.086669     0.950887      11.38
 H       5.423422    -4.784764     0.126424      14.12
 C       5.887793    -4.661956     2.214515      59.00
 O       5.642753    -5.963794     2.535202     318.76
 C       5.114140    -6.826743     1.530484     141.64
 H       5.958765    -7.123301     0.934513      28.68
 H       4.429934    -6.414785     0.781396      27.48
 H       4.726613    -7.686408     2.030201      23.80
 C       6.086602    -3.774527     3.337022      49.93
 O       6.168351    -4.288967     4.682046     248.47
 H       6.002604    -5.273150     4.783399      29.22
 C       6.213446    -2.374100     3.168041      57.59
 H       6.342534    -1.641529     3.959776      23.49
 C       5.790697    -2.749427     0.742690      58.07
 C       5.555727    -2.154117    -0.650768     103.66
 H       5.825922    -2.833633    -1.279252      28.35
 O       6.242847    -0.919423    -0.961676     251.88
 H       5.847089    -0.107964    -0.384293      21.86
 C       3.996042    -2.145108    -0.921902      60.63
 H       3.471109    -3.049146    -0.497840      19.11
 C       3.711174    -2.048538    -2.444297      90.24
 O       3.790961    -3.429488    -3.027010     240.14
 H       4.721572    -3.417960    -3.414326      23.85
 H       4.257712    -1.354823    -3.083856      24.18
 H       2.595039    -1.831507    -2.589056      24.44
 C      -0.199417    -1.608427     0.539740      47.82
 H      -0.925526    -2.344643     0.834373      22.77
 C       0.159858     0.935473     0.302666      68.86
 H      -0.233543     1.896104     0.463069      18.13
 C       1.438655     0.659773    -0.152207      -1.13
 O       2.310045     1.557539    -0.636286     205.65
 C       1.835638     2.996157    -0.593756     112.53
 H       2.813654     3.384821    -0.596436      23.58
 H       0.894290     3.237781    -1.353323      22.97
 H       1.511486     3.241260     0.335559      27.88
 C       2.043759    -0.754193    -0.179923       5.05
 O       3.370034    -0.838994    -0.348049     109.29
 C       1.137885    -1.849711     0.059038      56.95
 H       1.396919    -2.794616    -0.136960      21.68
 C      -0.583994    -0.223573     0.721282      32.78
 C      -2.132674     0.072691     1.197584      84.57
 H      -2.586205    -0.859923     1.509896      20.88
 O      -2.143923     1.158226     2.190927     286.67
 H      -1.807758     0.666869     3.070431      24.27
 C      -2.915275     0.557603     0.031005      78.09
 H      -2.534599     1.589548    -0.273862      21.08
 O      -2.904559    -0.461186    -1.032959     270.30
 H      -3.158054    -0.003660    -1.814328      25.93
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 C      -4.492554     0.823295     0.324926      75.54
 O      -5.096897     1.887524    -0.542839     276.11
 H      -4.858486     2.714443    -0.081403      29.23
 H      -4.400296     1.121095     1.447492      25.03
 H      -5.056612    -0.164489     0.226111      26.21
55
name = lig-etoh-Waterframe_376
 C       5.987750    -1.877646     1.879215      64.85
 H       6.253957    -0.819366     1.647366      20.46
 C       5.762124    -4.097083     0.972694      57.37
 H       5.709641    -4.742104     0.052018      25.06
 C       5.930229    -4.635015     2.267491      12.01
 O       5.635754    -5.954549     2.573994     283.56
 C       5.117608    -6.858375     1.497749     110.42
 H       5.990030    -7.243490     0.858636      21.60
 H       4.319918    -6.339773     0.851828      25.50
 H       4.675884    -7.583807     2.053656      23.51
 C       6.050328    -3.786755     3.459922      40.73
 O       6.177249    -4.298880     4.661298     230.16
 H       6.069321    -5.308098     4.679199      29.22
 C       6.211957    -2.413814     3.203827      56.68
 H       6.510212    -1.747188     3.989339      22.74
 C       5.797319    -2.649341     0.792495      34.38
 C       5.535264    -2.170532    -0.641307      81.75
 H       5.941902    -2.962299    -1.451510      19.91
 O       6.299647    -0.984577    -1.003522     273.02
 H       5.910891    -0.246814    -0.364353      21.72
 C       4.072816    -2.131850    -0.926522      73.00
 H       3.604650    -3.011914    -0.360750      19.00
 C       3.730973    -2.103627    -2.411885     100.29
 O       3.811873    -3.443625    -3.063419     242.94
 H       4.737983    -3.600183    -3.463057      23.54
 H       4.407545    -1.404904    -2.945497      24.74
 H       2.767054    -1.738803    -2.537510      26.39
 C      -0.165334    -1.541171     0.508107      59.66
 H      -0.835699    -2.350915     0.825859      23.80
 C       0.150752     0.850237     0.252969      68.13
 H      -0.052806     1.754846     0.550103      19.96
 C       1.475860     0.583340    -0.197570       4.81
 O       2.306879     1.626453    -0.604419     203.02
 C       1.833033     2.998191    -0.573500     118.41
 H       2.662267     3.693750    -0.840931      25.09
 H       1.037190     3.131102    -1.190149      28.57
 H       1.592847     3.137956     0.428147      27.64
 C       1.981942    -0.750639    -0.186546       4.99
 O       3.366157    -0.871686    -0.408995     105.89
 C       1.164622    -1.904977     0.097255      60.12
 H       1.528562    -2.867860     0.143012      24.60
 C      -0.629981    -0.244279     0.687686      26.66
 C      -2.042890     0.083649     1.243017      82.54
 H      -2.485150    -0.857327     1.598017      21.76
 O      -2.220614     1.116797     2.204971     275.74
 H      -1.613551     0.848183     3.114365      23.26
 C      -2.928756     0.543242    -0.036084      74.33
 H      -2.384896     1.395549    -0.497107      22.71
 O      -2.868915    -0.446401    -1.005333     288.04
 H      -3.077050    -0.106744    -1.856677      27.47
 C      -4.434074     0.899659     0.327762      89.01
 O      -5.082756     1.752829    -0.543922     306.30
 H      -4.831333     2.654401    -0.294483      30.76
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 H      -4.572668     1.150770     1.376691      26.38
 H      -5.075301    -0.139301     0.121918      24.38
55
name = lig-etoh-Waterframe_377
 C       6.003771    -1.816668     1.971886      55.74
 H       6.225107    -0.750795     2.003744      19.68
 C       5.777963    -4.071180     1.009921      40.01
 H       5.876198    -4.746490     0.167940      24.99
 C       5.879134    -4.594151     2.311862       6.99
 O       5.634092    -5.974792     2.584803     265.74
 C       5.133758    -6.862786     1.504308     104.50
 H       5.942341    -7.364760     0.803410      22.02
 H       4.318219    -6.232428     1.006011      26.74
 H       4.650276    -7.690446     2.001107      23.64
 C       6.045231    -3.791670     3.427926      41.29
 O       6.194397    -4.303683     4.717820     174.01
 H       6.231215    -5.314263     4.694172      24.87
 C       6.194510    -2.414261     3.218245      41.03
 H       6.523434    -1.889918     4.092927      23.63
 C       5.803424    -2.680888     0.788262      26.68
 C       5.582331    -2.172165    -0.607781      61.80
 H       6.070401    -3.163124    -1.338906      19.02
 O       6.336563    -1.053089    -1.026622     254.89
 H       6.122468    -0.121174    -0.665018      22.60
 C       4.012938    -2.078874    -0.936279      78.53
 H       3.656916    -3.017968    -0.434562      21.79
 C       3.753754    -2.168157    -2.441953     115.81
 O       3.829575    -3.445187    -3.074520     260.87
 H       4.668239    -3.505100    -3.671988      23.38
 H       4.564982    -1.489835    -2.781810      24.97
 H       2.809229    -1.787258    -2.577553      25.87
 C      -0.147306    -1.548137     0.511615      53.10
 H      -0.776093    -2.430481     0.771327      20.49
 C       0.201688     0.749315     0.250433      62.64
 H      -0.134104     1.766732     0.368705      17.67
 C       1.481637     0.530843    -0.238607      -1.65
 O       2.364036     1.667348    -0.603013     205.70
 C       1.843935     2.975523    -0.503542     107.31
 H       2.411278     3.693672    -1.165899      23.97
 H       0.963458     3.042689    -1.105689      26.76
 H       1.483568     3.428100     0.563506      23.95
 C       1.965706    -0.815040    -0.219164       4.26
 O       3.428640    -0.889473    -0.466196     142.73
 C       1.156049    -1.838339     0.148125      70.86
 H       1.643946    -2.826487     0.362293      23.70
 C      -0.695175    -0.229379     0.664398      54.02
 C      -2.022341     0.046739     1.207349      96.07
 H      -2.333883    -0.880729     1.737258      22.89
 O      -2.250684     1.097135     2.226029     236.80
 H      -1.761062     0.749293     3.228316      23.19
 C      -2.941386     0.605278    -0.036068      90.07
 H      -2.451633     1.496050    -0.378320      23.41
 O      -2.846501    -0.500430    -1.035513     271.83
 H      -2.995274    -0.144435    -1.904164      26.03
 C      -4.360380     0.859993     0.378735     101.76
 O      -5.083161     1.701989    -0.596499     295.94
 H      -4.795736     2.600288    -0.329418      31.22
 H      -4.588257     1.288260     1.265131      28.42
 H      -4.867403    -0.210832     0.277521      25.74
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name = lig-etoh-Waterframe_378
 C       6.040617    -1.778843     2.013965      51.71
 H       5.959827    -0.715202     1.880373      23.21
 C       5.823406    -4.040958     1.050164      55.00
 H       5.751191    -4.716456     0.241252      14.88
 C       5.757410    -4.663002     2.313673      53.59
 O       5.659731    -6.000782     2.573154     281.62
 C       5.120333    -6.835153     1.548344     122.56
 H       5.954671    -7.057942     0.812728      29.70
 H       4.407941    -6.389152     0.824801      30.26
 H       4.689815    -7.774781     2.067859      25.24
 C       6.069039    -3.806835     3.422873       8.40
 O       6.223697    -4.275137     4.770816     124.32
 H       6.101136    -5.287990     4.843768      22.92
 C       6.180763    -2.406049     3.277255      55.89
 H       6.370051    -1.776928     4.154982      22.83
 C       5.832645    -2.644867     0.879430      59.24
 C       5.599289    -2.182407    -0.571267      89.48
 H       5.852086    -3.058491    -1.285871      22.23
 O       6.405812    -1.091971    -1.069737     233.34
 H       5.966168    -0.272625    -0.682752      26.02
 C       3.984195    -2.139699    -0.938395      74.44
 H       3.420670    -2.929271    -0.469909      20.39
 C       3.794798    -2.149035    -2.489859      96.42
 O       3.843364    -3.472832    -3.083991     257.24
 H       4.716004    -3.503552    -3.630053      22.70
 H       4.469724    -1.481468    -3.086238      24.69
 H       2.778193    -1.748930    -2.809414      23.73
 C      -0.222133    -1.593861     0.570063      40.02
 H      -0.930136    -2.433802     0.798476      18.96
 C       0.240614     0.766491     0.262676      58.38
 H      -0.260425     1.829688     0.059621      13.22
 C       1.541269     0.556199    -0.277331       0.24
 O       2.425038     1.599772    -0.576462     180.74
 C       1.757403     2.992590    -0.506433      74.50
 H       2.620339     3.507019    -1.031183      21.58
 H       0.616514     2.869059    -0.870914      20.46
 H       1.948858     3.450502     0.684234      21.87
 C       2.119478    -0.776857    -0.298286      11.17
 O       3.444902    -0.869407    -0.490376     166.08
 C       1.168222    -1.789861     0.210649      39.77
 H       1.570078    -2.913417     0.334928      18.04
 C      -0.632365    -0.285183     0.630455      37.97
 C      -2.126093     0.048952     1.178354      79.51
 H      -2.539046    -0.971046     1.419851      20.93
 O      -2.224381     1.077208     2.244157     249.76
 H      -2.018818     0.510269     3.184066      22.14
 C      -2.885041     0.590222     0.023303      88.14
 H      -2.529118     1.559403    -0.280249      21.08
 O      -2.853059    -0.519312    -1.068409     255.55
 H      -2.944803    -0.117129    -1.935585      25.16
 C      -4.370797     0.787310     0.397306      87.30
 O      -5.070126     1.674373    -0.661588     295.57
 H      -4.880246     2.575291    -0.297073      30.94
 H      -4.230591     1.264093     1.382629      25.87
 H      -4.849803    -0.142353     0.553296      28.40
55
name = lig-etoh-Waterframe_379
 C       6.043861    -1.775295     2.022243      45.85
 H       5.877760    -0.727080     1.846153      20.82
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 C       5.827647    -4.060464     1.085839      57.52
 H       5.586901    -4.518492     0.165360      13.80
 C       5.704888    -4.665126     2.350128      59.25
 O       5.660857    -6.016416     2.574185     265.76
 C       5.126897    -6.832559     1.519574     126.69
 H       5.958392    -7.128871     0.951881      32.34
 H       4.261711    -6.386528     1.084725      32.92
 H       4.789291    -7.825701     2.086181      25.22
 C       6.083554    -3.830144     3.510634      -8.55
 O       6.248077    -4.230873     4.780838     179.57
 H       6.009053    -5.215130     4.847291      22.94
 C       6.168324    -2.380127     3.322324      52.17
 H       6.185103    -1.770172     4.265578      22.15
 C       5.878184    -2.583842     0.944973      56.43
 C       5.549106    -2.249309    -0.560465     105.58
 H       5.888360    -2.992550    -1.059679      26.26
 O       6.420903    -1.112339    -1.087804     221.10
 H       6.082747    -0.268321    -0.708772      25.22
 C       4.037986    -2.162315    -0.984385      74.03
 H       3.485688    -2.953515    -0.538970      18.85
 C       3.802917    -2.102588    -2.569471      79.93
 O       3.861324    -3.504136    -3.094091     268.26
 H       4.747116    -3.742576    -3.476741      24.84
 H       4.575111    -1.443598    -3.033682      22.48
 H       2.665011    -1.702411    -2.665863      22.62
 C      -0.187766    -1.628682     0.608467      40.59
 H      -0.883557    -2.447268     0.892115      20.17
 C       0.261370     0.783026     0.222405      60.18
 H      -0.286283     1.901983     0.208773      12.32
 C       1.603138     0.569100    -0.261031      16.11
 O       2.435937     1.559045    -0.552848     199.40
 C       1.812951     2.937936    -0.485897      88.13
 H       2.252800     3.646697    -1.254536      24.06
 H       0.641627     3.170818    -0.830307      19.79
 H       1.909181     3.166651     0.639641      23.13
 C       2.078743    -0.734048    -0.271669      20.66
 O       3.492886    -0.843749    -0.509237     149.97
 C       1.219153    -1.763149     0.228501      51.06
 H       1.613137    -2.901267     0.215099      15.11
 C      -0.634090    -0.274687     0.659589      27.23
 C      -2.114989     0.043395     1.146634      80.14
 H      -2.655605    -0.901050     1.410316      19.42
 O      -2.186069     0.996718     2.241696     282.54
 H      -1.917219     0.591105     3.168895      24.20
 C      -2.934807     0.518810    -0.031605      85.64
 H      -2.448766     1.443680    -0.442427      20.14
 O      -2.861679    -0.472753    -1.061394     304.40
 H      -2.955972    -0.049070    -1.926342      24.81
 C      -4.387961     0.789551     0.378493     103.84
 O      -5.027994     1.608433    -0.654946     307.69
 H      -4.999265     2.538282    -0.309184      29.24
 H      -4.376621     1.447012     1.405401      24.06
 H      -5.019245     0.013039     0.491175      27.94
55
name = lig-etoh-Waterframe_380
 C       6.022182    -1.756493     2.090118      52.68
 H       6.069417    -0.657577     2.097579      22.03
 C       5.768568    -4.004342     1.123223      42.24
 H       5.571260    -4.688769     0.279654      13.46
 C       5.776659    -4.600169     2.418161      59.84
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 O       5.637056    -6.012039     2.610622     313.43
 C       5.132884    -6.883636     1.510037     120.42
 H       5.741899    -7.119323     0.673216      32.45
 H       4.276424    -6.396630     1.102651      30.75
 H       4.808620    -7.833642     2.051599      25.50
 C       6.056519    -3.749806     3.512715      33.38
 O       6.262596    -4.230528     4.820471     155.80
 H       6.198192    -5.238110     4.924052      23.24
 C       6.134569    -2.392671     3.340477      51.48
 H       6.189659    -1.778693     4.281410      22.39
 C       5.873024    -2.665101     0.895679      76.69
 C       5.568232    -2.253872    -0.549518     113.35
 H       6.038602    -3.131840    -1.064620      26.29
 O       6.371960    -1.139122    -1.081432     233.02
 H       6.183114    -0.280547    -0.697377      25.98
 C       4.094898    -2.094224    -1.054380      81.81
 H       3.643299    -3.004466    -0.645941      19.44
 C       3.835932    -2.123163    -2.571397      87.28
 O       3.852480    -3.502564    -3.087894     272.78
 H       4.719891    -3.509162    -3.578905      23.78
 H       4.549106    -1.447521    -3.049390      23.89
 H       2.741910    -1.739257    -2.779703      23.70
 C      -0.055501    -1.568762     0.627957      52.81
 H      -0.559542    -2.467955     0.958581      21.66
 C       0.216090     0.755025     0.201753      78.53
 H      -0.041795     1.887273     0.445628      16.21
 C       1.521762     0.571431    -0.174077       2.47
 O       2.446007     1.619419    -0.588750     219.01
 C       1.901774     2.900189    -0.465538     126.09
 H       2.429681     3.570000    -1.123526      25.21
 H       0.766938     2.697518    -0.719845      22.55
 H       1.889332     3.318373     0.405680      31.61
 C       2.043352    -0.763186    -0.184715      -0.35
 O       3.518460    -0.844382    -0.518643     122.78
 C       1.235774    -1.798609     0.210292      56.49
 H       1.819091    -2.784689     0.192098      17.72
 C      -0.630286    -0.253941     0.692671      43.61
 C      -2.027893    -0.015058     1.144627      89.64
 H      -2.323600    -0.971892     1.579595      22.50
 O      -2.147329     0.926414     2.227389     322.29
 H      -1.688673     0.582137     2.957070      28.31
 C      -3.003728     0.508125    -0.092016      77.89
 H      -2.567530     1.511773    -0.478468      21.40
 O      -2.880948    -0.456064    -1.073882     298.76
 H      -3.043595    -0.072658    -1.961574      24.59
 C      -4.420333     0.853134     0.359403     103.16
 O      -5.012447     1.570023    -0.657514     290.14
 H      -4.934357     2.529853    -0.378245      29.22
 H      -4.581506     1.432909     1.409937      24.56
 H      -4.974665    -0.132352     0.428582      26.37
55
name = lig-etoh-Waterframe_381
 C       5.993246    -1.803453     2.075734      56.57
 H       6.228233    -0.713258     1.987142      22.19
 C       5.681840    -4.033127     1.183694      62.71
 H       5.648506    -4.821188     0.372941      28.77
 C       5.866066    -4.589252     2.431487      18.59
 O       5.624400    -5.979812     2.640138     246.75
 C       5.098932    -6.887212     1.521649     107.46
 H       5.843501    -6.939135     0.667998      25.20
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 H       4.149638    -6.491655     1.088102      26.70
 H       4.925028    -7.835025     1.996193      22.61
 C       6.026784    -3.774165     3.573127      26.50
 O       6.273617    -4.232505     4.860815     235.48
 H       6.294399    -5.236640     4.857424      30.29
 C       6.093336    -2.338989     3.356457      52.06
 H       6.352341    -1.725184     4.240601      23.10
 C       5.819566    -2.605655     0.917831      47.66
 C       5.648426    -2.209484    -0.585564      72.83
 H       5.904581    -3.189559    -1.407513      17.28
 O       6.339287    -1.139410    -1.069129     265.78
 H       5.993053    -0.422627    -0.552512      25.46
 C       4.108890    -2.056003    -1.052896      69.02
 H       3.513270    -2.918476    -0.621712      21.06
 C       3.863747    -2.126321    -2.568667     103.56
 O       3.875856    -3.466786    -3.087654     290.83
 H       4.533922    -3.567989    -3.806946      27.06
 H       4.510290    -1.586225    -3.223325      24.41
 H       2.907536    -1.694940    -2.746735      24.98
 C       0.015777    -1.532053     0.677607      42.19
 H      -0.597195    -2.330973     1.048393      20.18
 C       0.168771     0.815026     0.258249      64.29
 H      -0.249190     1.780961     0.455762      19.12
 C       1.544402     0.565783    -0.127419       4.12
 O       2.452957     1.585495    -0.595485     193.52
 C       1.926035     2.915039    -0.476816     123.36
 H       2.567634     3.413693    -1.133185      25.33
 H       0.949086     3.022266    -0.914111      25.72
 H       1.979970     3.433561     0.545735      25.55
 C       2.154655    -0.735224    -0.148213      14.30
 O       3.472074    -0.847701    -0.504819     119.59
 C       1.330720    -1.855014     0.174541      63.32
 H       1.637125    -2.863240     0.355836      22.64
 C      -0.560826    -0.296692     0.675457      35.86
 C      -2.008484    -0.082749     1.138958      88.37
 H      -2.354140    -1.091766     1.378541      22.92
 O      -2.098643     0.892319     2.209258     322.02
 H      -1.679510     0.621585     2.941929      31.70
 C      -2.958160     0.548478     0.002155      71.82
 H      -2.539368     1.540704    -0.336692      22.73
 O      -2.924594    -0.491681    -1.133028     240.74
 H      -3.131776    -0.131606    -2.045612      23.83
 C      -4.457779     0.809735     0.390111      80.92
 O      -5.065181     1.615961    -0.721037     257.44
 H      -4.761361     2.554271    -0.461071      30.45
 H      -4.383328     1.267381     1.385265      26.36
 H      -4.941215    -0.283627     0.474997      26.26
55
name = lig-etoh-Waterframe_382
 C       6.090086    -1.549751     1.530034      63.40
 H       6.195378    -0.570541     1.094670      24.85
 C       5.573802    -3.823093     0.924360      72.02
 H       5.307176    -4.679845     0.227535      17.32
 C       5.907477    -4.173316     2.192373      28.72
 O       5.887366    -5.498310     2.611423     251.01
 C       5.493868    -6.499995     1.649721     115.96
 H       6.027525    -6.585278     0.771152      32.48
 H       4.426113    -6.265174     1.207123      26.39
 H       5.499040    -7.525482     2.341969      25.83
 C       6.518437    -3.285706     3.138530      23.60
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 O       7.015937    -3.658115     4.330423     188.07
 H       6.658713    -4.450552     4.754532      21.59
 C       6.580822    -1.939112     2.795207      38.44
 H       7.131647    -1.102785     3.388847      21.35
 C       5.728486    -2.494144     0.543194       1.51
 C       5.307964    -2.124099    -0.911926      62.55
 H       5.908426    -3.051560    -1.639555      17.05
 O       6.055683    -0.971589    -1.330811     259.80
 H       5.595250    -0.137729    -1.074699      28.25
 C       3.758921    -2.083937    -1.148984      84.90
 H       3.348073    -2.887855    -0.578401      21.74
 C       3.408097    -1.925935    -2.637261     102.22
 O       3.553766    -3.232843    -3.356951     260.86
 H       4.443631    -3.304814    -3.814515      25.43
 H       4.014765    -1.226658    -3.148749      25.42
 H       2.331407    -1.734463    -2.758448      25.76
 C      -0.245522    -1.751392     0.292659      39.04
 H      -0.915824    -2.741439     0.407314      18.47
 C       0.045749     0.659048     0.397611      66.42
 H      -0.288661     1.690022     0.468466      20.18
 C       1.397430     0.556877     0.096819      14.18
 O       2.234951     1.647417    -0.182202     179.95
 C       1.585380     2.910502    -0.175235     101.29
 H       2.470768     3.566357    -0.573217      23.32
 H       0.483460     3.161243    -0.902158      21.69
 H       1.374261     3.138580     0.774201      27.78
 C       2.045764    -0.685949    -0.129693      11.49
 O       3.376714    -0.806660    -0.507522     175.08
 C       1.172572    -1.850089     0.082009      49.42
 H       1.632440    -2.875873    -0.058282      19.92
 C      -0.844278    -0.503941     0.330725      44.88
 C      -2.362766    -0.399707     0.740698      68.42
 H      -2.835034    -1.432407     0.764252      24.91
 O      -2.594982     0.337537     1.927571     198.71
 H      -2.024671    -0.229130     2.777713      22.97
 C      -3.201064     0.283215    -0.476728      74.51
 H      -2.543198     1.107075    -1.078311      22.25
 O      -3.545871    -0.769821    -1.343570     209.09
 H      -3.584338    -0.478713    -2.375934      23.78
 C      -4.523025     0.910261     0.182380     107.57
 O      -5.202459     1.831443    -0.715526     287.74
 H      -5.149813     2.673618    -0.120537      26.66
 H      -4.370301     1.397139     1.135239      26.05
 H      -5.196477     0.146738     0.319014      28.40
55
name = lig-etoh-Waterframe_383
 C       5.981616    -1.812106     2.013817      43.51
 H       6.043092    -0.714959     1.915071      20.30
 C       5.622185    -4.046196     1.169740      25.25
 H       5.268179    -4.724010     0.360888      11.89
 C       5.775653    -4.587735     2.472946      32.44
 O       5.587485    -5.976094     2.713353     285.40
 C       5.157118    -6.756283     1.639448     106.53
 H       5.683374    -6.676783     0.611937      30.09
 H       4.147149    -6.388554     1.215778      29.40
 H       5.051434    -7.741497     2.043608      26.25
 C       6.049386    -3.757033     3.601818     -13.03
 O       6.290354    -4.254427     4.944288     242.35
 H       6.079921    -5.236239     4.984970      30.44
 C       6.086812    -2.340899     3.335129      58.63
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 H       6.239585    -1.708062     4.190957      25.13
 C       5.671419    -2.676062     0.898588      69.92
 C       5.515767    -2.213233    -0.555334      87.09
 H       5.954134    -2.914063    -1.138806      26.56
 O       6.380329    -0.987340    -1.011239     205.29
 H       6.027798    -0.169473    -0.681344      26.69
 C       4.050101    -2.099880    -1.019565      79.26
 H       3.529292    -2.971099    -0.562059      20.28
 C       3.902392    -2.024059    -2.567509      92.27
 O       3.896985    -3.429923    -3.118853     280.24
 H       4.791572    -3.560011    -3.511123      24.49
 H       4.749388    -1.349655    -2.927772      23.98
 H       2.941788    -1.563627    -2.955215      24.63
 C       0.059595    -1.620531     0.707080      53.00
 H      -0.457470    -2.551312     0.898931      19.05
 C       0.323904     0.814415     0.357988      65.70
 H       0.002865     1.773511     0.026385      15.38
 C       1.589204     0.561258    -0.059347      13.32
 O       2.416547     1.565400    -0.589171     207.31
 C       2.045783     2.990026    -0.576015      95.68
 H       2.928158     3.463631    -0.967289      23.39
 H       1.034645     3.080316    -0.988791      23.83
 H       1.962016     3.433423     0.631740      22.62
 C       2.139682    -0.739414    -0.088077       6.84
 O       3.592990    -0.778483    -0.514056     126.56
 C       1.415808    -1.853948     0.314885      48.25
 H       1.922878    -2.730250     0.160342      19.39
 C      -0.507906    -0.331528     0.669262      50.74
 C      -1.997005    -0.144624     1.107452      93.93
 H      -2.272349    -1.157899     1.516240      23.31
 O      -2.028951     0.840211     2.188342     265.19
 H      -1.918995     0.322578     3.052417      25.78
 C      -2.930838     0.396108    -0.031535     101.45
 H      -2.522875     1.329139    -0.335494      23.42
 O      -3.000765    -0.471596    -1.074744     285.16
 H      -2.981589     0.022408    -1.975296      23.35
 C      -4.427106     0.767004     0.334658      91.83
 O      -5.092331     1.678042    -0.677819     247.82
 H      -4.876998     2.609188    -0.273137      28.57
 H      -4.633181     1.229396     1.272799      27.24
 H      -4.919686    -0.237280     0.267075      26.72
55
name = lig-etoh-Waterframe_384
 C       5.939547    -1.832278     2.020752      47.15
 H       5.919322    -0.756296     1.940686      21.50
 C       5.566945    -4.094338     1.165176      39.49
 H       5.233914    -4.834907     0.460120      10.17
 C       5.666649    -4.558442     2.492606      45.11
 O       5.602988    -5.931592     2.788862     230.06
 C       5.137870    -6.722687     1.638153     128.21
 H       5.893996    -6.689535     0.840256      32.42
 H       4.122325    -6.386338     1.508602      28.47
 H       5.052016    -7.825850     1.940630      25.55
 C       6.074559    -3.764999     3.581408     -15.38
 O       6.277366    -4.225512     4.920631     209.35
 H       6.215307    -5.241083     4.940663      26.12
 C       6.127528    -2.363165     3.290112      61.42
 H       6.134637    -1.704055     4.148615      24.19
 C       5.662204    -2.644560     0.921119      60.41
 C       5.515101    -2.131384    -0.523523     104.04
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 H       5.849497    -2.886315    -1.149587      25.19
 O       6.358056    -0.991549    -0.939756     261.45
 H       5.945216    -0.199304    -0.545624      26.14
 C       4.026566    -2.043791    -1.049485      88.04
 H       3.434670    -2.845930    -0.675074      21.88
 C       3.915983    -2.030967    -2.527126      91.95
 O       3.930140    -3.353057    -3.131857     282.54
 H       4.767123    -3.631179    -3.579182      25.31
 H       4.814489    -1.522301    -3.000007      23.59
 H       2.923031    -1.445249    -2.902034      23.05
 C       0.053103    -1.649421     0.676769      49.93
 H      -0.739832    -2.439908     0.800550      17.19
 C       0.315788     0.701720     0.365326      55.10
 H      -0.143702     1.837574     0.356928      14.78
 C       1.672759     0.578624    -0.053723      11.53
 O       2.445429     1.614238    -0.614810     216.02
 C       2.095766     2.948445    -0.525689     127.39
 H       2.862182     3.437955    -1.158127      23.72
 H       1.209732     3.172074    -1.363500      23.36
 H       1.890226     3.437426     0.327626      28.62
 C       2.239715    -0.713453    -0.076293      14.07
 O       3.581410    -0.784902    -0.494630     175.46
 C       1.445007    -1.817765     0.392668      59.48
 H       1.754750    -2.912488     0.336835      16.96
 C      -0.505620    -0.355957     0.709935      29.25
 C      -1.947275    -0.155058     1.135951      82.21
 H      -2.282666    -1.165667     1.509532      20.03
 O      -2.025340     0.809845     2.176083     255.34
 H      -1.795482     0.397130     3.173256      23.74
 C      -2.979675     0.428619    -0.035310      82.37
 H      -2.460638     1.363503    -0.382750      21.12
 O      -3.012535    -0.527656    -1.096085     272.51
 H      -2.954664    -0.143201    -2.061346      23.06
 C      -4.461487     0.771196     0.286426     101.57
 O      -5.041591     1.679963    -0.600840     323.00
 H      -4.998031     2.598418    -0.112583      26.87
 H      -4.403304     1.038785     1.444086      25.28
 H      -4.930098    -0.139842     0.192427      27.87
55
name = lig-etoh-Waterframe_385
 C       5.882969    -1.822740     2.013264      53.34
 H       5.905648    -0.766166     1.841740      21.70
 C       5.480245    -4.045459     1.182650      75.16
 H       5.366502    -4.609448     0.296838      21.73
 C       5.618328    -4.592711     2.502228      60.37
 O       5.613784    -5.903666     2.835104     275.81
 C       5.100285    -6.728185     1.678788     153.02
 H       5.818780    -6.609978     0.926528      33.47
 H       4.158603    -6.434329     1.265165      28.59
 H       5.182190    -7.823057     2.094196      26.00
 C       6.080112    -3.728736     3.600862      19.07
 O       6.262728    -4.175364     4.833512     -16.59
 H       6.225518    -5.188446     4.936859      18.86
 C       6.160282    -2.397289     3.337601      54.49
 H       6.325861    -1.646172     4.123728      21.68
 C       5.661109    -2.680701     0.927554      33.60
 C       5.526533    -2.120460    -0.545151      86.26
 H       6.006918    -3.132920    -1.174161      19.16
 O       6.306354    -1.019153    -0.841524     271.12
 H       6.048477    -0.133585    -0.425340      22.21
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 C       4.060327    -1.979912    -0.993828      83.52
 H       3.500708    -2.797340    -0.649420      20.62
 C       3.974417    -1.998586    -2.601926      93.60
 O       3.928615    -3.321465    -3.124402     283.85
 H       4.736366    -3.352540    -3.711121      24.31
 H       4.787191    -1.363957    -2.993195      24.23
 H       2.928459    -1.503296    -2.733661      23.22
 C       0.055198    -1.658431     0.637620      49.97
 H      -0.585816    -2.584022     0.836213      23.50
 C       0.334909     0.704882     0.351100      62.12
 H      -0.271210     1.717948     0.755513      15.44
 C       1.700012     0.611200    -0.057675       0.88
 O       2.510504     1.571512    -0.601723     183.59
 C       2.080903     2.987187    -0.609621     112.91
 H       2.999466     3.476622    -0.945410      24.25
 H       1.044804     3.234989    -1.203304      23.35
 H       1.878800     3.297430     0.348618      27.89
 C       2.299550    -0.730096    -0.023475      16.77
 O       3.531584    -0.782680    -0.472126     196.73
 C       1.438022    -1.790110     0.418413      53.48
 H       1.856082    -2.917986     0.601886      18.79
 C      -0.502001    -0.399492     0.727287      30.88
 C      -1.978793    -0.164707     1.139762      82.36
 H      -2.514013    -1.093038     1.345257      20.92
 O      -2.038751     0.815606     2.195248     248.95
 H      -1.567300     0.498065     3.202085      22.16
 C      -2.946425     0.485256    -0.024158      61.95
 H      -2.437291     1.451912    -0.417590      19.25
 O      -3.004182    -0.638918    -1.155409     227.40
 H      -2.971718    -0.110990    -2.064532      22.13
 C      -4.431027     0.679334     0.337660      95.43
 O      -5.018759     1.716814    -0.537380     295.80
 H      -4.820463     2.639800    -0.068581      25.41
 H      -4.593616     1.150699     1.471391      23.06
 H      -5.119935    -0.105275     0.220644      25.61
55
name = lig-etoh-Waterframe_386
 C       5.865830    -1.822989     2.053775      66.30
 H       6.009256    -0.767653     1.897144      21.66
 C       5.413416    -4.023814     1.207783      70.55
 H       5.366552    -4.663263     0.363823      24.57
 C       5.644676    -4.543436     2.493709      15.38
 O       5.561652    -5.931524     2.807695     324.04
 C       5.125896    -6.751137     1.747161     123.48
 H       5.756665    -6.706290     0.882964      27.72
 H       4.148684    -6.474781     1.329857      27.54
 H       5.022709    -7.814412     2.187773      24.28
 C       6.015123    -3.722787     3.521987       1.63
 O       6.275179    -4.152886     4.819599     143.10
 H       6.072597    -5.153765     4.873923      25.84
 C       6.164285    -2.281868     3.317165      36.33
 H       6.617923    -1.755886     4.191744      23.69
 C       5.632411    -2.659837     0.936658      39.69
 C       5.527855    -2.225507    -0.490272      80.17
 H       6.084181    -2.967924    -1.381119      18.37
 O       6.319386    -1.015899    -0.770217     247.74
 H       5.865352    -0.218731    -0.267692      20.77
 C       4.131188    -2.005073    -1.002171      80.12
 H       3.584426    -2.875480    -0.625867      21.00
 C       3.975201    -1.885207    -2.588492      91.46
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 O       3.944970    -3.306403    -3.136993     272.35
 H       4.690162    -3.484760    -3.799165      25.04
 H       4.695254    -1.283184    -3.089128      24.85
 H       3.051698    -1.491361    -2.927146      25.22
 C       0.070303    -1.699785     0.629746      63.45
 H      -0.347589    -2.673112     0.938103      23.36
 C       0.333443     0.752110     0.404783      61.35
 H       0.055244     1.876678     0.459670      18.59
 C       1.643806     0.568231    -0.045355       0.97
 O       2.564858     1.544872    -0.593835     141.96
 C       2.026323     2.992985    -0.641390      92.99
 H       2.937358     3.545641    -0.917593      24.08
 H       1.105760     3.067185    -1.246077      24.04
 H       1.854331     3.171067     0.584169      22.37
 C       2.162605    -0.706008     0.064679      18.30
 O       3.561091    -0.754927    -0.457777     121.48
 C       1.467234    -1.804792     0.415723      53.80
 H       2.155171    -2.757599     0.598230      20.96
 C      -0.515114    -0.404888     0.694589      22.09
 C      -2.042382    -0.130646     1.093722      92.15
 H      -2.436294    -1.099076     1.405586      22.61
 O      -2.057789     0.850622     2.219625     210.68
 H      -1.606982     0.280990     3.109529      22.78
 C      -2.888827     0.390124    -0.053045      76.17
 H      -2.589925     1.391608    -0.500934      19.68
 O      -2.972672    -0.665523    -1.140976     248.65
 H      -2.983408    -0.244716    -2.109287      22.56
 C      -4.421295     0.677880     0.408720      75.55
 O      -5.003896     1.741332    -0.491362     299.96
 H      -4.669946     2.599248    -0.039672      26.62
 H      -4.546491     0.952294     1.517964      25.11
 H      -4.910457    -0.381552     0.271720      24.67
55
name = lig-etoh-Waterframe_387
 C       5.899753    -1.734991     2.041164      57.13
 H       6.103824    -0.679069     1.832845      21.98
 C       5.396630    -4.035860     1.202097      44.51
 H       5.127272    -4.809245     0.483814      19.34
 C       5.649856    -4.558343     2.454956      39.51
 O       5.514336    -5.910322     2.771847     327.30
 C       5.106009    -6.820686     1.757810     138.66
 H       5.893980    -7.005862     0.946843      28.52
 H       4.058043    -6.480646     1.546462      24.10
 H       5.008558    -7.797991     2.223650      22.38
 C       5.976125    -3.621179     3.537214      49.77
 O       6.286948    -4.138144     4.807566     159.39
 H       6.200962    -5.160731     4.915237      26.58
 C       6.155183    -2.287473     3.317169      55.36
 H       6.620375    -1.617492     4.091336      22.13
 C       5.569281    -2.657952     0.986366      39.23
 C       5.593107    -2.226531    -0.498040      92.72
 H       5.965449    -3.120195    -0.992385      19.83
 O       6.358230    -1.019956    -0.694290     263.48
 H       5.776352    -0.195618    -0.353661      18.01
 C       4.110470    -2.023532    -1.065771      58.70
 H       3.433498    -2.908369    -0.820016      18.75
 C       3.966554    -1.837861    -2.574312      96.02
 O       3.959257    -3.273388    -3.150567     268.50
 H       4.784192    -3.438885    -3.732906      24.01
 H       4.817547    -1.356148    -3.003045      23.35
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 H       3.054362    -1.394916    -2.764822      25.57
 C       0.100583    -1.731720     0.673658      35.83
 H      -0.641409    -2.458365     0.954636      18.85
 C       0.301537     0.801533     0.443859      62.78
 H      -0.149427     1.691560     0.240405      17.97
 C       1.612668     0.595967    -0.047698       3.14
 O       2.534270     1.542143    -0.576319     187.06
 C       2.001318     2.872412    -0.581514     111.47
 H       2.636582     3.624691    -1.131643      23.98
 H       1.266241     2.962906    -1.239495      27.27
 H       1.512393     3.503503     0.467162      22.30
 C       2.219349    -0.691545     0.032683      13.27
 O       3.560998    -0.744261    -0.402330     118.49
 C       1.486330    -1.860148     0.426280      55.15
 H       1.981006    -2.847573     0.491961      18.60
 C      -0.540018    -0.355441     0.653840      16.76
 C      -2.000140    -0.113698     1.081619      95.35
 H      -2.374880    -1.056300     1.498164      21.64
 O      -2.081677     0.858827     2.185736     232.88
 H      -1.898045     0.419506     3.175860      23.85
 C      -2.942771     0.309411    -0.109447      91.72
 H      -2.405953     1.173425    -0.514789      22.08
 O      -2.924602    -0.663348    -1.072363     280.00
 H      -2.970383    -0.259717    -2.021986      23.23
 C      -4.372293     0.681966     0.421681      88.96
 O      -4.980713     1.690187    -0.426271     329.18
 H      -4.866442     2.535610     0.052015      28.01
 H      -4.340130     0.864103     1.407848      28.35
 H      -4.984297    -0.343065     0.150551      24.36
55
name = lig-etoh-Waterframe_388
 C       5.938234    -1.712619     1.975685      48.38
 H       6.145855    -0.650484     1.711461      17.98
 C       5.387839    -4.052950     1.202217      44.62
 H       4.945869    -4.561105     0.302725       7.67
 C       5.624968    -4.549583     2.478435      25.23
 O       5.510380    -5.869028     2.773929     251.16
 C       5.040731    -6.922584     1.777093     113.03
 H       5.812591    -6.954863     0.878158      27.51
 H       4.125514    -6.689975     1.114201      29.45
 H       5.011229    -7.740547     2.394757      24.81
 C       5.968503    -3.659914     3.591277      24.92
 O       6.303348    -4.101994     4.805427     225.66
 H       6.306345    -5.117987     4.776393      29.07
 C       6.146849    -2.243263     3.303520      55.96
 H       6.397264    -1.567893     4.154838      24.87
 C       5.517657    -2.607052     1.006985      71.50
 C       5.568540    -2.187545    -0.480419     122.19
 H       6.080906    -2.888125    -0.935937      28.36
 O       6.412339    -1.053715    -0.645633     257.42
 H       5.948979    -0.103430    -0.535355      19.58
 C       4.081374    -1.999096    -1.079446      64.18
 H       3.393318    -2.869458    -0.763213      18.46
 C       3.993895    -1.871556    -2.591572      97.31
 O       3.957415    -3.208874    -3.149865     298.10
 H       4.799296    -3.202755    -3.711428      24.87
 H       4.845425    -1.238059    -2.966141      23.22
 H       3.060142    -1.294691    -2.789385      24.39
 C       0.051493    -1.609161     0.732178      45.74
 H      -0.586990    -2.461120     0.881467      17.10
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 C       0.245315     0.810507     0.390852      71.20
 H      -0.334270     1.614325     0.321874      15.30
 C       1.638350     0.594731    -0.031567       1.71
 O       2.458250     1.561292    -0.512393     201.84
 C       1.913309     2.844688    -0.604376      98.73
 H       2.811729     3.399510    -0.994190      21.75
 H       0.990361     2.737137    -1.208157      23.97
 H       1.628163     3.176410     0.470262      24.84
 C       2.279532    -0.744456    -0.024649       6.48
 O       3.576250    -0.781312    -0.356225     163.99
 C       1.467536    -1.881937     0.421003      47.88
 H       1.774360    -2.838475     0.434291      17.92
 C      -0.478817    -0.362031     0.657520      52.94
 C      -1.945176    -0.157531     1.125931      90.56
 H      -2.355473    -1.146125     1.441502      23.11
 O      -2.116471     0.885445     2.118276     279.20
 H      -1.933241     0.518434     3.025759      27.30
 C      -2.935088     0.349515    -0.066859      92.26
 H      -2.528980     1.244878    -0.464532      23.31
 O      -2.881313    -0.733347    -1.056439     268.62
 H      -2.988099    -0.286260    -1.962513      23.82
 C      -4.321660     0.624669     0.362066     114.11
 O      -4.985821     1.641176    -0.365084     319.31
 H      -4.825299     2.453517     0.129806      30.16
 H      -4.265577     0.939908     1.353587      27.66
 H      -5.106013    -0.190898     0.367240      25.59
55
name = lig-etoh-Waterframe_389
 C       5.965840    -1.750523     1.988556      50.80
 H       6.149443    -0.683558     1.724184      19.72
 C       5.353117    -3.933878     1.212273      45.01
 H       5.050320    -4.659478     0.368244      15.28
 C       5.572362    -4.509283     2.493619      31.86
 O       5.481642    -5.904856     2.776970     254.12
 C       5.025790    -6.943772     1.779761     121.92
 H       5.951056    -7.144142     1.143597      28.80
 H       4.009217    -6.746799     1.311171      27.65
 H       4.898091    -7.821630     2.354584      26.22
 C       5.986854    -3.628851     3.523745       8.38
 O       6.331573    -4.089154     4.843712     264.92
 H       6.195830    -5.090452     5.002072      28.82
 C       6.108404    -2.227394     3.279122      64.45
 H       6.255984    -1.631490     4.162050      23.34
 C       5.503717    -2.609094     0.957349      62.62
 C       5.486556    -2.144866    -0.452551     117.03
 H       6.029463    -2.891365    -1.199026      23.03
 O       6.485817    -1.053694    -0.643228     160.50
 H       6.035309    -0.118050    -0.421235      21.37
 C       4.108312    -1.967899    -1.016598      87.44
 H       3.571114    -2.883682    -0.665954      18.96
 C       4.003752    -1.843363    -2.587489      85.71
 O       3.969859    -3.143105    -3.165083     295.72
 H       4.634152    -3.434646    -3.872143      26.02
 H       4.881866    -1.253238    -3.048669      23.04
 H       3.022581    -1.339431    -3.031071      22.24
 C       0.100451    -1.586878     0.752963      53.58
 H      -0.503730    -2.456911     0.953400      20.46
 C       0.286743     0.769382     0.272111      84.76
 H      -0.069410     1.821995     0.426864      17.44
 C       1.611994     0.520065     0.004931      13.84
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 O       2.426159     1.536248    -0.444156     188.61
 C       1.817110     2.855043    -0.609309     107.15
 H       2.599037     3.545931    -1.024410      24.83
 H       0.769182     2.985096    -1.274740      23.19
 H       1.658325     3.159486     0.268041      29.80
 C       2.173844    -0.795078    -0.017751      15.14
 O       3.630669    -0.833872    -0.350423     195.67
 C       1.398008    -1.810924     0.391222      62.81
 H       1.781587    -2.744673     0.474927      20.52
 C      -0.508693    -0.310168     0.738591      52.97
 C      -1.958195    -0.178821     1.115868      92.54
 H      -2.309854    -1.170810     1.513689      20.89
 O      -2.132817     0.908054     2.073669     307.02
 H      -1.792503     0.635653     2.864435      29.13
 C      -2.828713     0.323216    -0.024276      80.77
 H      -2.588647     1.293925    -0.439018      22.54
 O      -2.842496    -0.789289    -1.066869     253.69
 H      -2.938351    -0.455526    -2.000412      24.56
 C      -4.350196     0.551936     0.408742      86.73
 O      -5.024013     1.645986    -0.353911     288.46
 H      -4.636764     2.424845     0.074698      30.28
 H      -4.251610     0.988015     1.519741      23.89
 H      -4.767204    -0.401937     0.444816      27.77
55
name = lig-etoh-Waterframe_390
 C       5.949416    -1.757577     1.988404      53.39
 H       6.128279    -0.674030     1.876494      23.67
 C       5.282099    -3.937342     1.245751      62.74
 H       5.202148    -4.722699     0.435039      20.31
 C       5.514918    -4.506337     2.481060      28.74
 O       5.433392    -5.932333     2.781081     269.17
 C       5.055115    -6.928547     1.832164     107.45
 H       5.760811    -7.213984     1.074265      28.90
 H       4.166834    -6.527962     1.339249      29.30
 H       4.789433    -7.856597     2.437931      25.72
 C       6.015279    -3.645839     3.535798      15.06
 O       6.349077    -4.053705     4.850294     160.19
 H       6.035416    -4.997330     4.999223      26.35
 C       6.068258    -2.268777     3.299321      56.55
 H       6.337590    -1.583303     4.064896      21.70
 C       5.561712    -2.567572     0.925268      45.27
 C       5.548624    -2.105244    -0.518438      74.70
 H       5.731341    -3.242954    -1.127328      19.08
 O       6.525093    -1.037041    -0.665075     186.73
 H       6.136595    -0.170175    -0.243537      22.75
 C       4.119154    -1.948094    -1.000185      76.94
 H       3.646798    -2.865067    -0.798217      22.58
 C       4.027987    -1.784078    -2.606708      86.58
 O       3.955842    -3.163677    -3.194717     273.39
 H       4.731617    -3.242087    -3.865640      23.59
 H       4.944187    -1.220631    -2.932561      24.20
 H       3.019782    -1.204359    -2.732728      23.53
 C       0.039583    -1.599168     0.792549      54.73
 H      -0.596904    -2.388571     1.188706      22.64
 C       0.277970     0.717717     0.241785      78.61
 H       0.108482     1.927345     0.297508      16.99
 C       1.618158     0.480416    -0.029944      20.94
 O       2.418217     1.538159    -0.418615     157.32
 C       1.750142     2.894195    -0.588913      99.13
 H       2.428399     3.503270    -1.169880      25.31
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 H       0.765952     2.816223    -1.365572      22.23
 H       1.435000     3.492516     0.380100      24.44
 C       2.204529    -0.741896    -0.042808      27.33
 O       3.555804    -0.827953    -0.310141     183.72
 C       1.384459    -1.840010     0.364761      50.00
 H       1.881968    -2.829895     0.498259      21.13
 C      -0.526487    -0.283699     0.790555      42.31
 C      -1.979094    -0.145699     1.119535      95.65
 H      -2.376008    -1.080580     1.568655      21.64
 O      -2.130485     0.933852     2.076628     318.15
 H      -1.725252     0.707721     2.825151      30.14
 C      -2.837615     0.237193    -0.079523      70.23
 H      -2.204366     1.122766    -0.490800      20.73
 O      -2.799505    -0.798191    -1.059997     294.01
 H      -2.811647    -0.340600    -1.918076      25.75
 C      -4.325741     0.520107     0.490487      78.65
 O      -5.046995     1.606502    -0.345067     265.51
 H      -4.740455     2.459778     0.043751      28.61
 H      -4.425145     0.782576     1.719131      24.11
 H      -4.825349    -0.371603     0.227287      26.88
55
name = lig-etoh-Waterframe_391
 C       5.908641    -1.728398     2.008716      54.56
 H       6.104518    -0.667922     1.878531      22.28
 C       5.249086    -3.989983     1.223617      61.95
 H       5.058170    -4.569468     0.332332      23.27
 C       5.492451    -4.560812     2.528743      23.72
 O       5.421134    -5.888596     2.820271     272.61
 C       5.028191    -6.888371     1.845275     106.45
 H       5.780215    -7.094473     1.133876      26.92
 H       4.222516    -6.582575     1.222653      30.34
 H       4.714214    -7.803569     2.523306      24.77
 C       5.995306    -3.698171     3.599505       8.34
 O       6.348620    -4.028992     4.830741     113.34
 H       6.194630    -5.009617     5.001058      25.95
 C       6.063164    -2.300471     3.307989      41.08
 H       6.451233    -1.668720     4.098208      21.13
 C       5.619720    -2.579573     0.932935      21.21
 C       5.621692    -2.139565    -0.535107      67.44
 H       6.270263    -2.837537    -1.229520      21.73
 O       6.540690    -1.041864    -0.732174     211.78
 H       6.163510    -0.219278    -0.279899      23.13
 C       4.128815    -1.924702    -1.067291      73.43
 H       3.563694    -2.777208    -0.804226      22.86
 C       4.038358    -1.754650    -2.554590     102.09
 O       3.936648    -3.144488    -3.212210     271.01
 H       4.726892    -3.228258    -3.858990      23.46
 H       4.839538    -1.207591    -3.016920      25.18
 H       3.168697    -1.166000    -2.834350      25.22
 C      -0.018739    -1.616498     0.836108      47.10
 H      -0.580446    -2.430073     1.312223      21.40
 C       0.262491     0.707788     0.292750      71.04
 H      -0.459938     1.726066     0.118705      14.12
 C       1.604696     0.559880    -0.110566       9.37
 O       2.413891     1.637037    -0.409720     210.88
 C       1.717121     2.891290    -0.627816      94.25
 H       2.497522     3.382880    -1.121304      25.46
 H       0.831683     2.575256    -1.146186      25.81
 H       1.306266     3.485597     0.501733      23.15
 C       2.192257    -0.804271    -0.044401      22.51
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 O       3.506212    -0.792056    -0.277092     180.77
 C       1.379520    -1.873099     0.366404      54.15
 H       1.804807    -2.998015     0.430410      21.50
 C      -0.517562    -0.352220     0.780166      50.60
 C      -1.989262    -0.115380     1.184757      98.98
 H      -2.366040    -1.061352     1.584348      23.72
 O      -2.130428     0.988014     2.101462     305.31
 H      -1.778857     0.636203     2.963460      26.85
 C      -2.873894     0.213092    -0.076195      76.60
 H      -2.461976     1.216783    -0.574532      20.18
 O      -2.768235    -0.791118    -1.067834     305.99
 H      -2.782575    -0.410485    -1.948964      26.63
 C      -4.313959     0.517249     0.433614      98.05
 O      -5.036221     1.538326    -0.297299     281.80
 H      -4.939349     2.414281     0.184494      28.58
 H      -4.386968     0.612174     1.598200      27.19
 H      -5.024730    -0.304789     0.163298      25.54
55
name = lig-etoh-Waterframe_392
 C       5.885808    -1.736505     2.048368      53.53
 H       6.094925    -0.714411     1.826682      21.04
 C       5.292824    -3.984401     1.210678      50.21
 H       4.874057    -4.602005     0.483610      20.36
 C       5.494587    -4.544701     2.527473      31.09
 O       5.404863    -5.871881     2.885385     321.04
 C       4.987286    -6.835100     1.831475     127.63
 H       5.959949    -7.065645     1.379706      26.25
 H       4.094670    -6.569397     1.267813      27.65
 H       4.740728    -7.823754     2.409799      23.93
 C       5.914267    -3.674681     3.541687      31.23
 O       6.357293    -4.069862     4.871143     221.27
 H       6.345607    -5.050545     5.064142      23.86
 C       6.087775    -2.315722     3.302947      47.29
 H       6.424279    -1.756626     4.202723      21.35
 C       5.624538    -2.681826     0.960064      18.81
 C       5.694533    -2.158391    -0.535780      86.31
 H       5.968196    -2.907182    -1.148524      24.18
 O       6.537134    -1.008163    -0.803894     292.83
 H       6.177130    -0.156929    -0.467559      22.32
 C       4.166758    -1.922232    -1.065811      64.92
 H       3.571619    -2.825772    -0.783343      21.53
 C       4.027262    -1.742853    -2.605053     102.27
 O       3.912056    -3.078662    -3.188073     307.27
 H       4.558644    -3.313930    -3.907025      26.11
 H       4.898463    -1.285820    -2.994643      23.79
 H       3.150912    -1.294788    -2.894222      25.91
 C       0.055612    -1.711812     0.855138      46.29
 H      -0.579439    -2.532970     1.230373      17.06
 C       0.216020     0.719255     0.317762      55.52
 H      -0.432703     1.652925     0.132854      15.85
 C       1.539804     0.591692    -0.127975      -2.28
 O       2.423771     1.698536    -0.398788     214.23
 C       1.694247     2.871503    -0.668785     123.32
 H       2.235414     3.651377    -1.157624      26.22
 H       0.882420     2.868550    -1.226403      29.27
 H       1.425367     3.301639     0.443126      24.39
 C       2.058160    -0.782598    -0.030289       0.16
 O       3.577936    -0.788305    -0.300627     108.57
 C       1.300570    -1.892279     0.403365      59.35
 H       1.768895    -2.998011     0.380790      20.51
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 C      -0.555295    -0.411863     0.768469      41.11
 C      -1.984287    -0.100721     1.206579      93.93
 H      -2.378470    -0.991973     1.697888      22.01
 O      -2.120483     1.037592     2.142706     244.27
 H      -1.916397     0.660360     3.158406      24.38
 C      -2.904917     0.286058    -0.031040      85.31
 H      -2.750253     1.303146    -0.402430      23.18
 O      -2.742404    -0.798084    -1.080592     268.03
 H      -2.868518    -0.455461    -1.959196      26.42
 C      -4.373210     0.440391     0.338450     101.73
 O      -5.032592     1.530983    -0.249944     292.72
 H      -4.890109     2.341694     0.346249      28.89
 H      -4.259463     0.713771     1.296240      28.80
 H      -4.825816    -0.636445     0.276790      26.02
55
name = lig-etoh-Waterframe_393
 C       5.898250    -1.814184     2.019681      54.67
 H       6.069424    -0.777349     1.832093      21.92
 C       5.339429    -4.050321     1.235441      38.67
 H       4.953475    -4.698132     0.499941      17.88
 C       5.495771    -4.515858     2.507051      24.16
 O       5.342819    -5.882065     2.927138     293.85
 C       5.001150    -6.806074     1.880478     109.91
 H       5.816011    -7.001449     1.022493      27.08
 H       4.209697    -6.369244     1.190472      28.07
 H       4.672502    -7.715239     2.388802      24.46
 C       5.896586    -3.671536     3.589754      11.85
 O       6.349330    -4.107778     4.867921     295.30
 H       6.125449    -5.082390     4.912333      28.62
 C       6.104799    -2.293710     3.328986      48.95
 H       6.347139    -1.617937     4.200258      22.37
 C       5.642103    -2.636126     0.956611      30.52
 C       5.638642    -2.154721    -0.527358      81.60
 H       5.872047    -3.058755    -1.074627      22.06
 O       6.533749    -0.989628    -0.866798     280.35
 H       6.031469    -0.226988    -0.591580      24.92
 C       4.191113    -1.916389    -1.012174      55.37
 H       3.693743    -2.944785    -0.806547      21.13
 C       4.034696    -1.741161    -2.670077      91.59
 O       3.863358    -3.061898    -3.157595     301.74
 H       4.568359    -3.126722    -3.843454      24.43
 H       4.902001    -1.182644    -3.039791      23.51
 H       3.141228    -1.107310    -2.767031      24.63
 C      -0.016101    -1.732002     0.883040      40.38
 H      -0.676724    -2.603884     1.118992      14.71
 C       0.125304     0.706192     0.311299      61.34
 H      -0.134869     1.662245     0.353649      17.61
 C       1.511508     0.566790    -0.078205       1.80
 O       2.400766     1.655892    -0.426612     178.25
 C       1.656218     2.956104    -0.665280     107.94
 H       2.401702     3.681759    -1.105706      23.54
 H       0.746807     2.805736    -1.350343      25.20
 H       1.303969     3.333647     0.162631      28.40
 C       2.094105    -0.688916    -0.065376       1.42
 O       3.570961    -0.800796    -0.329827     121.98
 C       1.351401    -1.897661     0.391401      39.34
 H       1.903272    -2.888587     0.406715      20.93
 C      -0.559875    -0.428863     0.774554      33.85
 C      -2.015023    -0.083027     1.212770      82.99
 H      -2.483373    -0.959165     1.704270      22.44
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 O      -2.104838     1.069439     2.172540     225.96
 H      -1.761728     0.635341     3.205226      21.17
 C      -2.918050     0.318423    -0.047514      93.07
 H      -2.452806     1.185702    -0.370330      24.15
 O      -2.708728    -0.759402    -1.056134     272.67
 H      -2.875313    -0.336712    -1.889368      26.08
 C      -4.392819     0.331830     0.378292      88.71
 O      -5.077455     1.554120    -0.252972     240.59
 H      -4.726356     2.288222     0.375070      27.56
 H      -4.419933     0.515744     1.418671      27.99
 H      -5.023310    -0.620327     0.089976      25.23
55
name = lig-etoh-Waterframe_394
 C       5.958707    -1.822687     2.011478      47.84
 H       6.077228    -0.755798     1.832937      22.07
 C       5.391394    -4.045906     1.207421      64.61
 H       5.273652    -4.727063     0.343723      16.68
 C       5.508639    -4.558043     2.587402      37.99
 O       5.286788    -5.860189     2.933792     231.48
 C       4.989049    -6.773651     1.877261     108.45
 H       5.907778    -6.962922     1.166626      29.16
 H       4.040213    -6.352038     1.387562      27.11
 H       4.667525    -7.653466     2.290644      26.20
 C       5.954300    -3.630843     3.677256       9.08
 O       6.305010    -4.151096     4.822151     114.74
 H       6.093544    -5.129688     5.038344      27.40
 C       6.080629    -2.292845     3.364580      62.95
 H       6.350971    -1.498014     4.097510      24.62
 C       5.634729    -2.651419     0.908697      61.59
 C       5.556666    -2.127966    -0.512709      98.94
 H       6.210738    -2.926530    -1.206286      20.48
 O       6.494507    -1.028957    -0.906165     201.08
 H       6.137727    -0.195105    -0.616859      26.76
 C       4.163310    -1.913644    -1.051078      68.03
 H       3.541503    -2.827009    -0.766057      17.94
 C       4.040658    -1.701281    -2.569486      81.00
 O       3.809123    -3.063354    -3.162528     265.19
 H       4.538572    -3.366122    -3.804491      23.63
 H       4.891131    -1.267366    -3.193469      23.20
 H       3.086356    -1.014251    -2.791740      22.62
 C      -0.027033    -1.696613     0.822472      45.98
 H      -0.709750    -2.516325     1.122865      21.39
 C       0.160340     0.694541     0.299967      77.36
 H      -0.266301     1.567368     0.576662      18.53
 C       1.515848     0.586177    -0.033112      -1.09
 O       2.298885     1.608384    -0.460917     151.14
 C       1.633866     3.016292    -0.666163      79.52
 H       2.605158     3.511195    -1.072419      22.68
 H       0.820432     2.632287    -1.539241      22.01
 H       1.175274     3.469725     0.148962      25.15
 C       2.197955    -0.769919    -0.076335      17.45
 O       3.501153    -0.786170    -0.342177     192.64
 C       1.408127    -1.805342     0.372861      59.82
 H       1.903040    -2.697320     0.458932      20.73
 C      -0.635351    -0.404046     0.819702      25.86
 C      -2.062923    -0.074089     1.231795      80.00
 H      -2.516264    -1.007317     1.676671      20.46
 O      -2.080886     1.063128     2.173126     262.19
 H      -1.576927     0.633116     3.110706      20.59
 C      -2.882781     0.256706    -0.024924      85.10
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 H      -2.555509     1.231289    -0.445043      22.38
 O      -2.676751    -0.692622    -1.028699     276.48
 H      -2.756702    -0.350404    -1.921144      25.02
 C      -4.440408     0.349225     0.410898      74.83
 O      -5.109760     1.538626    -0.224890     215.74
 H      -4.767981     2.427334     0.183046      27.21
 H      -4.728803     0.084358     1.564945      25.72
 H      -4.956457    -0.403779    -0.222729      25.50
55
name = lig-etoh-Waterframe_395
 C       5.998778    -1.809524     2.011352      51.96
 H       6.146850    -0.737747     1.807485      21.90
 C       5.472502    -4.032832     1.235411      61.01
 H       5.470274    -4.793210     0.382412      15.78
 C       5.536041    -4.494424     2.580935      14.23
 O       5.255587    -5.834453     2.963248     244.37
 C       4.930250    -6.754637     1.863750     125.30
 H       5.848935    -6.825496     1.302555      29.24
 H       4.079355    -6.466710     1.188204      28.02
 H       4.812759    -7.679154     2.343573      26.34
 C       5.956399    -3.678390     3.601377     -15.85
 O       6.284957    -4.180834     4.887446     217.16
 H       6.161848    -5.224606     4.936126      24.68
 C       6.068329    -2.239767     3.342789      57.33
 H       6.399529    -1.618424     4.180075      25.32
 C       5.637352    -2.684243     0.937422      52.38
 C       5.587543    -2.111763    -0.543020      91.44
 H       5.791606    -3.129447    -1.287284      20.14
 O       6.438466    -1.058282    -0.916406     262.04
 H       6.256437    -0.233962    -0.485645      26.42
 C       4.075264    -1.913449    -1.074873      73.59
 H       3.458122    -2.790502    -0.896054      21.73
 C       4.022646    -1.707720    -2.529379      88.65
 O       3.720712    -3.067393    -3.146448     250.18
 H       4.533866    -3.304849    -3.736586      21.82
 H       5.017280    -1.250148    -2.895088      24.42
 H       3.030317    -1.143140    -2.828031      23.13
 C       0.018599    -1.595633     0.721477      63.20
 H      -0.418293    -2.506265     1.078054      26.30
 C       0.190536     0.681705     0.372393      58.34
 H      -0.332890     1.727253     0.427177      16.28
 C       1.529146     0.528868    -0.024884      16.02
 O       2.204356     1.639278    -0.481028     209.18
 C       1.661554     2.923304    -0.717357     104.78
 H       2.488905     3.686404    -1.041323      24.36
 H       0.860585     3.196051    -1.624411      23.46
 H       1.161986     3.490307     0.262125      23.14
 C       2.147149    -0.734516    -0.043690      22.24
 O       3.513081    -0.754267    -0.371332     181.54
 C       1.358011    -1.792673     0.405338      67.75
 H       1.737339    -2.705510     0.543655      22.11
 C      -0.618731    -0.400136     0.823772      40.32
 C      -2.059851    -0.098363     1.262375      91.71
 H      -2.510374    -0.986091     1.771607      20.86
 O      -2.058927     1.027394     2.147910     311.17
 H      -1.743274     0.738583     3.077718      26.50
 C      -2.928136     0.280298     0.058864      74.83
 H      -2.813551     1.389165    -0.272996      21.33
 O      -2.639461    -0.686197    -1.035087     252.70
 H      -2.705828    -0.215190    -1.894297      23.82
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 C      -4.506632     0.377712     0.314479      88.62
 O      -5.128582     1.519151    -0.159123     237.90
 H      -4.796200     2.371464     0.348309      26.99
 H      -4.780137     0.199303     1.525442      25.34
 H      -4.785206    -0.436407    -0.252903      27.05
55
name = lig-etoh-Waterframe_396
 C       5.993934    -1.777935     2.000090      54.72
 H       6.200136    -0.716677     1.733983      22.33
 C       5.556349    -4.038972     1.246817      63.23
 H       5.321561    -4.822237     0.436874      14.79
 C       5.541904    -4.503984     2.526216      27.85
 O       5.213618    -5.793441     2.960046     249.14
 C       4.931040    -6.745945     1.865360     122.13
 H       5.710319    -6.820030     1.188607      32.17
 H       4.102374    -6.488481     1.210464      31.60
 H       4.751926    -7.744759     2.392053      26.24
 C       5.973215    -3.652124     3.610685     -13.54
 O       6.265009    -4.145553     4.911907     190.71
 H       6.073800    -5.162698     5.067105      22.60
 C       6.101328    -2.284918     3.335688      66.10
 H       6.383312    -1.666726     4.165588      24.18
 C       5.693511    -2.636980     0.951019      58.37
 C       5.516908    -2.211431    -0.565858      99.99
 H       5.890695    -3.038029    -1.173607      24.46
 O       6.418752    -1.083437    -0.923812     251.26
 H       6.026716    -0.390667    -0.379586      26.25
 C       4.012929    -1.915222    -0.984972      79.87
 H       3.501834    -2.788829    -0.718632      23.68
 C       3.950768    -1.754631    -2.582899      96.56
 O       3.658485    -3.058205    -3.106414     285.36
 H       4.359616    -3.296406    -3.844263      23.10
 H       4.899026    -1.277127    -2.880624      25.61
 H       3.237850    -0.956972    -2.836516      24.69
 C       0.020025    -1.621826     0.696223      54.18
 H      -0.569833    -2.460989     1.002758      22.59
 C       0.179009     0.723251     0.479380      74.54
 H      -0.107724     1.831035     0.074999      17.11
 C       1.453942     0.557569    -0.037261       5.31
 O       2.195026     1.664542    -0.536334     195.98
 C       1.653911     2.945846    -0.764416     110.46
 H       2.590502     3.507931    -0.864542      23.75
 H       0.890657     2.947887    -1.492124      26.40
 H       1.153619     3.233791     0.385349      21.56
 C       2.127597    -0.672937    -0.010506      14.33
 O       3.521020    -0.715688    -0.394075     141.20
 C       1.356697    -1.822820     0.417682      52.10
 H       1.733073    -2.826157     0.541251      20.75
 C      -0.590314    -0.333036     0.786709      42.94
 C      -2.028897    -0.139316     1.291008      94.79
 H      -2.392734    -1.049458     1.785679      23.82
 O      -2.060223     1.016822     2.142278     321.92
 H      -1.853643     0.741213     2.967369      32.34
 C      -3.026731     0.340223     0.102683      79.00
 H      -2.459797     1.313708    -0.145220      21.30
 O      -2.611859    -0.660531    -1.025853     231.79
 H      -2.748395    -0.198801    -1.907543      24.68
 C      -4.515760     0.299354     0.250654     108.53
 O      -5.165716     1.560903    -0.114252     237.21
 H      -4.882581     2.171160     0.671134      27.25
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 H      -4.706979     0.270314     1.344582      26.99
 H      -5.038329    -0.514668    -0.172272      27.74
55
name = lig-etoh-Waterframe_397
 C       5.985346    -1.749173     2.002050      53.25
 H       6.155084    -0.656230     1.886857      21.80
 C       5.590300    -4.023957     1.193363      52.57
 H       5.167812    -4.612634     0.342113      11.04
 C       5.574785    -4.533445     2.568934      44.80
 O       5.170237    -5.779556     2.905339     255.36
 C       4.941786    -6.744528     1.875508      98.61
 H       5.807277    -6.900627     1.207856      32.48
 H       4.035916    -6.406203     1.458438      33.54
 H       4.644209    -7.787725     2.413367      24.58
 C       5.981173    -3.657845     3.662825      12.29
 O       6.235856    -4.061177     4.900197     157.92
 H       6.000661    -5.006188     5.082251      26.14
 C       6.170343    -2.308359     3.327913      51.81
 H       6.384761    -1.591743     4.093196      22.31
 C       5.747903    -2.637879     0.903170      50.44
 C       5.482673    -2.280570    -0.539129     109.29
 H       5.826894    -2.996405    -1.096640      26.79
 O       6.373054    -1.131726    -0.910274     256.64
 H       6.025393    -0.217077    -0.605725      21.26
 C       4.003935    -1.946405    -0.955443      69.14
 H       3.371022    -2.695733    -0.541561      21.02
 C       3.892563    -1.761760    -2.562276      97.93
 O       3.603523    -3.070091    -3.089231     296.73
 H       4.252959    -3.330534    -3.836143      24.77
 H       4.820791    -1.593806    -3.027283      25.04
 H       3.157739    -1.097532    -2.831527      24.79
 C      -0.060443    -1.664488     0.742264      39.97
 H      -0.770389    -2.463057     0.892129      19.33
 C       0.201746     0.878668     0.472556      63.54
 H      -0.573823     1.808565     0.499796      17.13
 C       1.463682     0.657620    -0.067725       5.56
 O       2.245546     1.599113    -0.607623     173.03
 C       1.631353     2.971514    -0.716450     123.28
 H       2.395581     3.608706    -1.020911      26.54
 H       1.006661     2.923124    -1.476155      28.10
 H       1.071931     3.452208     0.139480      25.50
 C       2.149423    -0.696108     0.020810      15.28
 O       3.471248    -0.665338    -0.379254     144.87
 C       1.413943    -1.803022     0.389501      51.39
 H       1.982794    -2.828711     0.441069      18.90
 C      -0.619733    -0.359017     0.778909      22.66
 C      -2.044252    -0.149030     1.271161      95.60
 H      -2.299878    -1.082319     1.751723      24.19
 O      -2.079974     1.015956     2.178236     330.35
 H      -1.798244     0.766395     3.001507      31.75
 C      -2.955533     0.264158     0.046954      83.08
 H      -2.752753     1.366642    -0.170115      21.95
 O      -2.604272    -0.599128    -0.991128     267.92
 H      -2.850732    -0.318678    -1.947509      23.76
 C      -4.548416     0.265907     0.302694      85.63
 O      -5.204035     1.588258    -0.078280     231.27
 H      -4.998567     2.360867     0.590380      27.59
 H      -4.666232     0.017165     1.264496      28.79
 H      -5.117871    -0.510046    -0.337745      25.91
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name = lig-etoh-Waterframe_398
 C       5.998171    -1.779535     2.014381      54.90
 H       5.983128    -0.689529     1.885058      21.42
 C       5.570733    -4.011890     1.216274      40.55
 H       5.259900    -4.664152     0.435877      18.85
 C       5.625714    -4.490491     2.531139      33.33
 O       5.160160    -5.796625     2.899654     271.19
 C       4.898569    -6.762856     1.883307     114.61
 H       5.849702    -6.888413     1.190208      25.69
 H       4.123351    -6.528558     1.123247      26.36
 H       4.766859    -7.746510     2.521862      21.83
 C       5.980832    -3.660593     3.589780      18.84
 O       6.203517    -4.000049     4.955055     272.59
 H       6.108223    -4.967215     5.021511      30.13
 C       6.225111    -2.259017     3.280270      47.10
 H       6.462442    -1.622748     4.134714      23.92
 C       5.770523    -2.665706     0.922910      32.55
 C       5.487284    -2.203569    -0.508959      85.00
 H       5.652013    -3.154057    -1.213783      20.34
 O       6.336333    -1.191839    -0.918024     280.95
 H       5.915887    -0.247160    -0.677116      20.54
 C       3.999055    -1.937693    -0.974643      63.73
 H       3.304356    -2.804056    -0.763567      22.89
 C       3.871539    -1.808165    -2.488852     101.76
 O       3.524435    -3.143380    -3.088340     274.54
 H       4.320246    -3.300017    -3.674865      22.52
 H       4.797388    -1.339029    -2.876403      24.59
 H       3.025361    -1.182588    -2.725765      25.59
 C      -0.041592    -1.641022     0.755076      45.02
 H      -0.619503    -2.561495     0.837083      18.95
 C       0.116653     0.869586     0.458808      58.92
 H      -0.286523     1.870272     0.792483      17.29
 C       1.487171     0.669966    -0.044473      -7.89
 O       2.320450     1.635202    -0.677882     169.30
 C       1.637391     2.978942    -0.723808     113.81
 H       2.352992     3.675225    -1.061992      25.88
 H       0.821502     2.964529    -1.589184      24.41
 H       1.222009     3.242569     0.141729      28.45
 C       2.088994    -0.631052     0.033483      15.76
 O       3.443004    -0.651146    -0.359999     114.39
 C       1.342467    -1.773777     0.393213      35.70
 H       1.943604    -2.822109     0.483521      21.04
 C      -0.559918    -0.352355     0.791064      35.55
 C      -2.051672    -0.107185     1.235839      97.61
 H      -2.500585    -0.980703     1.696394      24.53
 O      -2.120999     0.998001     2.218765     307.86
 H      -1.712033     0.688079     3.082388      27.80
 C      -2.948270     0.240569     0.026565      91.86
 H      -2.864506     1.249177    -0.249649      23.66
 O      -2.579999    -0.597705    -1.012162     269.11
 H      -2.945517    -0.188611    -1.892736      22.95
 C      -4.577562     0.304211     0.358708      73.23
 O      -5.231160     1.552970    -0.027086     277.78
 H      -4.757510     2.310330     0.458030      27.95
 H      -4.876588    -0.071512     1.363634      26.80
 H      -4.910469    -0.412106    -0.538064      24.67
55
name = lig-etoh-Waterframe_399
 C       6.018285    -1.777876     1.971957      61.56
 H       5.936018    -0.736598     1.693181      23.67
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 C       5.536600    -4.037755     1.226076      46.37
 H       5.407241    -4.767630     0.502991      20.54
 C       5.624157    -4.531722     2.516650      88.09
 O       5.169615    -5.770816     2.903680     222.13
 C       4.905778    -6.803440     1.852768     125.10
 H       5.913849    -6.996854     1.320260      25.16
 H       4.037538    -6.642102     1.126982      22.58
 H       4.637481    -7.715714     2.367835      23.25
 C       6.043343    -3.580238     3.574732      44.16
 O       6.154722    -3.967671     4.962847      53.34
 H       6.157627    -4.929900     5.118512      24.71
 C       6.250811    -2.272210     3.294759      60.88
 H       6.541727    -1.595694     4.132141      24.47
 C       5.735101    -2.661299     0.952216      38.14
 C       5.428608    -2.181519    -0.493716      60.71
 H       5.749725    -3.228092    -1.203737      17.66
 O       6.347678    -1.197145    -0.965815     209.80
 H       5.988088    -0.295819    -0.482702      22.82
 C       3.960445    -1.906077    -0.943753      75.86
 H       3.429215    -2.897687    -0.605132      21.52
 C       3.819967    -1.846006    -2.448383      90.32
 O       3.517906    -3.195392    -3.065961     268.71
 H       4.188029    -3.476721    -3.735081      23.72
 H       4.665558    -1.267514    -2.957725      23.54
 H       2.877995    -1.152117    -2.591283      24.11
 C       0.016949    -1.601805     0.731097      57.13
 H      -0.653492    -2.449186     0.992858      22.96
 C       0.168034     0.782332     0.440399      66.67
 H      -0.124121     1.741493     0.610639      19.07
 C       1.470421     0.687498    -0.014671      -7.39
 O       2.341260     1.712706    -0.712257     144.30
 C       1.675477     2.961624    -0.784436     104.26
 H       2.487964     3.721059    -0.975078      23.41
 H       0.539896     2.901929    -1.421124      22.16
 H       1.425014     3.106667     0.235315      26.58
 C       2.032831    -0.574773     0.012463      10.92
 O       3.424483    -0.693902    -0.344592     131.40
 C       1.292848    -1.718680     0.409740      58.99
 H       1.725199    -2.798533     0.512915      18.80
 C      -0.601107    -0.288256     0.845430      42.11
 C      -2.044240    -0.052067     1.234501      86.05
 H      -2.419573    -1.032161     1.604243      20.44
 O      -2.167344     0.973537     2.241015     266.73
 H      -1.793326     0.549267     3.177271      23.41
 C      -3.018773     0.350598     0.085621      78.51
 H      -2.590761     1.265330    -0.258684      23.21
 O      -2.567932    -0.641127    -1.060878     237.29
 H      -2.786217    -0.237770    -2.020713      22.95
 C      -4.556291     0.300126     0.320097      88.05
 O      -5.229570     1.499431     0.031638     279.90
 H      -4.835837     2.266458     0.515933      28.78
 H      -4.975681     0.006895     1.439573      24.82
 H      -5.047894    -0.536310    -0.323618      24.60
55
name = lig-etoh-Waterframe_400
 C       6.033655    -1.747001     1.945301      58.45
 H       6.172841    -0.694646     1.773252      23.83
 C       5.524912    -4.082424     1.207495      57.66
 H       5.351737    -4.696996     0.344569      18.50
 C       5.612606    -4.521650     2.577861      18.68
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 O       5.171891    -5.786014     2.893136     237.81
 C       4.945250    -6.846182     1.851127      94.95
 H       5.837477    -7.092397     1.273739      29.10
 H       4.142737    -6.346573     1.236734      29.77
 H       4.594243    -7.607272     2.386127      28.45
 C       6.081445    -3.638951     3.630839     -17.55
 O       6.111640    -3.935344     4.926993      39.61
 H       5.946227    -4.926464     4.990884      22.90
 C       6.272184    -2.218138     3.279591      33.93
 H       6.580201    -1.505647     4.103388      20.14
 C       5.639200    -2.667096     0.921991      24.40
 C       5.406269    -2.225430    -0.493329      55.49
 H       5.693426    -3.117317    -1.178993      22.42
 O       6.367081    -1.166414    -1.006750     168.70
 H       6.378354    -0.223119    -0.545706      23.20
 C       3.933698    -1.946633    -0.863658      76.68
 H       3.321937    -2.750600    -0.347391      21.37
 C       3.712303    -1.867381    -2.472279      81.44
 O       3.552628    -3.223050    -3.005149     268.09
 H       4.202632    -3.244396    -3.759343      24.21
 H       4.611803    -1.528981    -3.066306      23.82
 H       2.683118    -1.325024    -2.716215      23.02
 C      -0.121045    -1.499464     0.774726      53.37
 H      -0.662026    -2.411401     1.148245      23.36
 C       0.228564     0.837048     0.435626      62.18
 H      -0.330502     1.668010     0.286559      19.75
 C       1.562264     0.724562    -0.081699       2.34
 O       2.303192     1.689032    -0.703536     204.09
 C       1.700270     2.977383    -0.749212     105.52
 H       2.338219     3.752102    -1.380197      24.08
 H       0.743335     3.033379    -1.492001      23.63
 H       1.394480     3.529649     0.294671      23.91
 C       2.098289    -0.622972    -0.038178      20.98
 O       3.402572    -0.729183    -0.319692     172.22
 C       1.348334    -1.678235     0.401712      65.16
 H       1.870263    -2.636746     0.420643      22.30
 C      -0.637046    -0.270544     0.860110      31.93
 C      -2.081376    -0.049367     1.267788      82.67
 H      -2.329561    -1.095624     1.619757      22.81
 O      -2.217917     0.955042     2.271077     256.38
 H      -1.908448     0.644249     3.334006      22.97
 C      -2.994409     0.394409     0.033726      68.88
 H      -2.780046     1.536722    -0.217840      20.59
 O      -2.593335    -0.647408    -1.024994     253.22
 H      -2.599678    -0.315046    -2.029638      23.56
 C      -4.536185     0.253943     0.320954      87.01
 O      -5.256333     1.476781     0.044506     282.65
 H      -5.034155     2.212415     0.619973      30.69
 H      -4.390437     0.006556     1.474722      26.09
 H      -4.964626    -0.545982    -0.217141      27.20
55
name = lig-etoh-Waterframe_401
 C       6.039249    -1.754141     1.957883      57.66
 H       6.330520    -0.738906     1.735752      24.29
 C       5.525664    -4.031914     1.225373      63.85
 H       5.168857    -4.771469     0.448367      14.99
 C       5.600844    -4.500841     2.558043      33.04
 O       5.202947    -5.840607     2.909130     272.20
 C       4.963920    -6.797509     1.877106     111.87
 H       5.804555    -7.116541     1.332591      30.71
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 H       4.280047    -6.463108     1.052228      32.06
 H       4.540123    -7.626435     2.407861      27.53
 C       6.063322    -3.595749     3.566914      -5.16
 O       6.075447    -3.955638     4.939087      78.65
 H       5.873372    -4.960726     5.075946      22.29
 C       6.275376    -2.233394     3.231317      55.74
 H       6.588371    -1.519897     4.023525      20.87
 C       5.585872    -2.679392     0.929943      29.13
 C       5.434437    -2.209530    -0.548816      76.16
 H       5.591372    -2.959885    -1.122959      27.25
 O       6.392381    -1.186824    -1.047919     240.70
 H       6.087560    -0.348968    -0.499378      25.02
 C       3.895381    -1.988862    -0.863966      65.89
 H       3.364353    -2.879474    -0.564382      23.17
 C       3.603299    -1.931134    -2.453517     101.21
 O       3.595882    -3.257038    -2.950809     281.35
 H       4.298917    -3.393492    -3.688329      22.59
 H       4.412863    -1.255984    -2.775247      25.65
 H       2.722695    -1.305653    -2.726763      24.74
 C      -0.079431    -1.508974     0.829062      47.50
 H      -0.751474    -2.359118     1.141545      19.77
 C       0.239682     0.935034     0.401198      67.76
 H      -0.297145     1.861076     0.031188      19.83
 C       1.544081     0.675796    -0.111638      -1.85
 O       2.283916     1.680909    -0.679884     168.82
 C       1.692680     3.084654    -0.787151      96.97
 H       2.546853     3.469123    -1.445786      23.64
 H       0.834172     2.918578    -1.219015      26.89
 H       1.474721     3.644877     0.305211      23.43
 C       2.118802    -0.623200    -0.059409      28.27
 O       3.485265    -0.728399    -0.306569     135.99
 C       1.251761    -1.666683     0.420124      54.90
 H       1.665232    -2.580524     0.521388      24.84
 C      -0.602925    -0.153222     0.832153      15.90
 C      -2.102226    -0.039859     1.274492      80.31
 H      -2.563840    -0.982430     1.604680      23.15
 O      -2.295309     0.969847     2.317608     220.71
 H      -1.799882     0.543672     3.275063      22.17
 C      -2.937812     0.342020    -0.058474      86.37
 H      -2.872831     1.490354    -0.374565      20.85
 O      -2.619458    -0.605075    -0.946636     282.85
 H      -2.689235    -0.217092    -1.899270      24.72
 C      -4.436867     0.244087     0.383087      96.02
 O      -5.319554     1.421336     0.039851     274.11
 H      -4.972006     2.153698     0.570317      30.12
 H      -4.599718     0.087024     1.439954      28.48
 H      -4.837354    -0.518410    -0.147623      28.25
55
name = lig-etoh-Waterframe_402
 C       6.036783    -1.785163     1.905761      60.07
 H       6.250629    -0.754706     1.608553      22.01
 C       5.467735    -4.004614     1.253770      53.02
 H       5.095471    -4.764958     0.462345      17.02
 C       5.590695    -4.522814     2.524783      47.43
 O       5.261551    -5.815247     2.920565     260.87
 C       4.972612    -6.769774     1.865963     127.82
 H       5.963429    -7.098913     1.576716      24.52
 H       4.258447    -6.491235     1.093813      26.60
 H       4.447010    -7.726546     2.377944      22.80
 C       5.982177    -3.593571     3.550198      20.81
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 O       6.046937    -3.962746     4.932061      35.42
 H       6.123549    -5.028663     4.973166      22.34
 C       6.281096    -2.271305     3.227074      61.52
 H       6.640790    -1.635047     4.025059      27.19
 C       5.626652    -2.606870     0.915704      26.86
 C       5.440198    -2.229639    -0.619706      77.71
 H       5.731459    -3.157690    -1.183692      22.73
 O       6.358616    -1.222028    -1.041485     300.52
 H       6.006742    -0.290629    -0.781830      23.87
 C       3.889825    -2.017082    -0.955062      74.78
 H       3.452319    -2.828625    -0.458073      23.82
 C       3.566489    -1.911075    -2.369507     116.26
 O       3.627786    -3.302008    -2.923004     267.72
 H       4.377104    -3.489593    -3.601871      23.49
 H       4.291432    -1.278612    -2.859591      26.21
 H       2.572886    -1.628464    -2.498451      26.44
 C      -0.044332    -1.412233     0.880973      50.12
 H      -0.675701    -2.271987     1.127957      20.49
 C       0.183695     0.960092     0.327508      64.20
 H      -0.083426     2.150940     0.280853      21.30
 C       1.466305     0.657131    -0.114596       0.03
 O       2.296889     1.719261    -0.649176     183.60
 C       1.724130     3.092064    -0.837274     116.33
 H       2.439912     3.679044    -1.407119      26.16
 H       0.790670     3.137435    -1.253716      27.65
 H       1.790644     3.595963     0.174740      25.66
 C       2.053635    -0.613415    -0.016575      -1.88
 O       3.549647    -0.742419    -0.285902      57.66
 C       1.230764    -1.701083     0.425844      32.52
 H       1.494517    -2.673237     0.572248      25.26
 C      -0.577154    -0.090966     0.837603      20.67
 C      -2.059242     0.084360     1.220608      89.64
 H      -2.269689    -1.007119     1.446372      24.56
 O      -2.368715     0.973754     2.339939     241.72
 H      -1.806120     0.629638     3.229660      23.28
 C      -2.951490     0.384622     0.042773      95.35
 H      -2.519599     1.237530    -0.476321      24.70
 O      -2.609472    -0.618773    -0.968911     249.28
 H      -2.870428    -0.332563    -1.911625      26.44
 C      -4.432354     0.275458     0.434420     100.30
 O      -5.351332     1.332371     0.038151     295.50
 H      -4.995362     2.208183     0.328237      30.50
 H      -4.607896     0.121435     1.424619      28.59
 H      -4.800210    -0.648746    -0.077002      26.65
55
name = lig-etoh-Waterframe_403
 C       6.075606    -1.743949     1.888031      43.11
 H       6.210976    -0.651754     1.731937      18.90
 C       5.371241    -3.982181     1.209854      55.89
 H       5.139848    -4.618521     0.293301      21.10
 C       5.570324    -4.506430     2.531251      32.11
 O       5.296635    -5.768168     2.910520     271.83
 C       4.999395    -6.796498     1.873366      86.87
 H       5.958148    -7.159177     1.325158      22.40
 H       4.436534    -6.277144     1.122326      25.91
 H       4.452214    -7.655295     2.557884      21.07
 C       5.904382    -3.630912     3.605624      29.13
 O       6.040208    -3.964042     4.879345     135.85
 H       6.072409    -5.014384     5.023157      24.23
 C       6.269280    -2.287476     3.217787      44.21
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 H       6.653611    -1.670329     3.995556      24.82
 C       5.654615    -2.647244     0.823764      26.47
 C       5.433100    -2.287560    -0.633138      78.05
 H       5.889934    -3.316016    -1.278921      19.62
 O       6.307781    -1.229641    -1.051264     308.45
 H       6.003435    -0.288801    -0.909916      23.21
 C       3.976594    -2.020132    -0.912321      81.70
 H       3.365421    -2.774290    -0.428856      23.44
 C       3.527660    -1.942628    -2.391692     111.42
 O       3.633993    -3.330690    -2.887848     267.16
 H       4.361093    -3.328915    -3.570197      24.46
 H       4.023788    -1.281479    -3.099756      26.20
 H       2.480989    -1.743650    -2.363228      25.75
 C      -0.066034    -1.292829     0.913919      48.11
 H      -0.697658    -2.054740     1.294814      24.41
 C       0.152159     0.983463     0.267879      53.25
 H      -0.258281     2.056791     0.652553      20.59
 C       1.474922     0.758515    -0.155026     -15.73
 O       2.303424     1.741873    -0.634330     200.18
 C       1.811064     3.073730    -0.835584     123.28
 H       2.401399     3.565862    -1.527694      27.86
 H       0.732433     3.289861    -1.414418      24.05
 H       1.752396     3.560543     0.042929      28.88
 C       2.088268    -0.650415     0.017085     -22.39
 O       3.484048    -0.754008    -0.254675      95.96
 C       1.283554    -1.705783     0.439226      51.90
 H       1.697647    -2.747906     0.429052      23.78
 C      -0.597417    -0.024856     0.857727      40.41
 C      -1.986307     0.131073     1.236829     100.22
 H      -2.268044    -0.880693     1.567317      24.65
 O      -2.416387     0.979177     2.332252     285.89
 H      -1.951308     0.725922     3.180879      27.19
 C      -2.942252     0.473499     0.089363      70.52
 H      -2.768918     1.482133    -0.220085      26.53
 O      -2.596391    -0.683056    -1.008898     178.79
 H      -2.980331    -0.320013    -1.860180      25.23
 C      -4.486316     0.301773     0.485933      85.13
 O      -5.377642     1.265725     0.004303     264.12
 H      -5.027655     2.145096     0.361331      30.04
 H      -4.356595     0.195495     1.586746      25.75
 H      -4.791862    -0.743513    -0.035736      24.66
55
name = lig-etoh-Waterframe_404
 C       6.105874    -1.764510     1.884673      49.97
 H       6.348361    -0.687083     1.747237      20.43
 C       5.318483    -3.975798     1.155850      71.06
 H       5.117752    -4.744002     0.418546      23.04
 C       5.506158    -4.432010     2.486559      27.96
 O       5.326559    -5.795807     2.885379     298.25
 C       5.035083    -6.770790     1.893750     117.17
 H       5.917133    -7.257908     1.320213      24.33
 H       4.280007    -6.436924     1.167807      26.32
 H       4.457693    -7.635906     2.390951      23.34
 C       5.877475    -3.575382     3.542450      19.97
 O       6.048869    -3.988893     4.889826     217.75
 H       5.814789    -4.943845     5.035869      27.22
 C       6.222560    -2.281033     3.179711      53.98
 H       6.575686    -1.623822     3.946800      20.80
 C       5.692320    -2.675603     0.842288      32.36
 C       5.481459    -2.292567    -0.604201      83.25
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 H       5.549487    -3.209970    -1.430767      18.51
 O       6.282353    -1.217610    -1.102591     326.42
 H       5.849519    -0.469605    -0.661262      25.15
 C       3.977242    -1.992203    -0.861644      52.57
 H       3.438000    -2.961667    -0.579507      20.98
 C       3.468392    -2.019235    -2.425516     103.15
 O       3.620678    -3.322064    -2.867945     276.39
 H       4.282272    -3.603586    -3.562979      24.29
 H       3.927178    -1.202516    -3.032369      25.09
 H       2.366695    -1.666884    -2.354298      24.44
 C      -0.019033    -1.314949     0.926094      48.36
 H      -0.655495    -1.979349     1.432332      23.43
 C       0.185113     1.067644     0.269557      64.95
 H      -0.240672     2.096736     0.242943      20.74
 C       1.512967     0.773330    -0.154233      -8.60
 O       2.342560     1.742240    -0.646098     210.22
 C       1.872768     3.112223    -0.857848     101.03
 H       2.691514     3.400182    -1.482145      24.24
 H       0.731634     2.726692    -1.355246      20.90
 H       1.730621     3.702970     0.016933      26.24
 C       2.112509    -0.578327     0.003949      12.64
 O       3.421374    -0.750114    -0.233471     127.59
 C       1.257992    -1.609229     0.484784      42.30
 H       1.678373    -2.734162     0.512718      20.20
 C      -0.555339     0.010220     0.858889      36.67
 C      -2.051307     0.097480     1.322077      89.27
 H      -2.380955    -0.879503     1.605147      23.73
 O      -2.428487     1.034968     2.335370     312.49
 H      -2.022192     0.762117     3.078814      29.51
 C      -2.959874     0.468671     0.037440      73.74
 H      -2.987411     1.513125    -0.280549      23.52
 O      -2.612537    -0.649755    -0.988915     232.98
 H      -2.866397    -0.311955    -1.885249      25.20
 C      -4.436802     0.255160     0.533542      73.83
 O      -5.409946     1.258978    -0.035341     211.33
 H      -5.219198     2.077758     0.552207      28.52
 H      -4.645237     0.404352     1.720657      24.11
 H      -4.900789    -0.812561     0.206940      24.76
55
name = lig-etoh-Waterframe_405
 C       6.130655    -1.822459     1.840609      60.38
 H       6.517407    -0.846566     1.509363      24.06
 C       5.320573    -4.026047     1.159854      52.13
 H       5.024925    -4.697337     0.413226      20.71
 C       5.414784    -4.443756     2.457868      34.45
 O       5.362465    -5.796730     2.854368     263.73
 C       5.003071    -6.795677     1.873106     143.65
 H       5.988427    -7.067586     1.454538      28.05
 H       4.231113    -6.491421     1.133598      29.31
 H       4.701668    -7.577188     2.439316      25.98
 C       5.875557    -3.558756     3.517938      -5.68
 O       6.043265    -3.970691     4.863143     153.45
 H       5.931499    -4.934353     4.934836      25.68
 C       6.179685    -2.213482     3.189130      65.40
 H       6.490963    -1.542202     4.004226      25.69
 C       5.725823    -2.659321     0.852532      51.61
 C       5.455594    -2.241931    -0.629938      88.97
 H       5.688884    -3.104628    -1.136892      24.03
 O       6.261466    -1.184174    -1.140877     299.58
 H       6.150319    -0.373190    -0.648896      27.93
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 C       3.860831    -1.992340    -0.899427      67.61
 H       3.437386    -2.858465    -0.241313      20.77
 C       3.453351    -1.983088    -2.362416      92.95
 O       3.573067    -3.361125    -2.887797     259.78
 H       4.353943    -3.394826    -3.551356      23.42
 H       4.131480    -1.329997    -2.988934      24.59
 H       2.281557    -1.877043    -2.458017      23.85
 C      -0.021869    -1.295762     0.964536      47.83
 H      -0.496705    -2.174952     1.394994      20.80
 C       0.233628     1.107151     0.300848      67.62
 H      -0.090296     1.949848    -0.127810      21.20
 C       1.547730     0.776855    -0.115440      11.06
 O       2.447768     1.727429    -0.641812     194.37
 C       1.898893     3.049314    -0.906013     114.17
 H       2.602774     3.665538    -1.578631      25.32
 H       0.969355     3.289747    -1.633150      23.80
 H       1.766484     3.748835     0.040563      25.18
 C       2.025127    -0.492390    -0.000621      30.71
 O       3.458090    -0.750283    -0.236595     127.32
 C       1.271205    -1.504446     0.515970      49.69
 H       1.652161    -2.613101     0.748824      21.00
 C      -0.552247     0.007102     0.879041      35.67
 C      -2.124615     0.101088     1.302464      85.21
 H      -2.274286    -0.930874     1.595170      25.21
 O      -2.412860     1.112819     2.346232     287.29
 H      -1.968064     0.839733     3.131885      26.43
 C      -3.023556     0.341402     0.037268      90.26
 H      -2.699679     1.304014    -0.480818      22.05
 O      -2.649847    -0.545360    -0.945963     292.01
 H      -2.724779    -0.228242    -1.849793      27.63
 C      -4.466489     0.244058     0.549412      85.63
 O      -5.417573     1.255535    -0.063212     241.80
 H      -5.394463     2.061885     0.569755      28.75
 H      -4.469337     0.405616     1.739791      25.48
 H      -4.768516    -0.788099     0.314246      27.44
55
name = lig-etoh-Waterframe_406
 C       6.187424    -1.808986     1.807583      49.32
 H       6.553388    -0.831410     1.499509      24.18
 C       5.339423    -4.017090     1.133503      67.67
 H       4.978813    -4.584302     0.330067      17.43
 C       5.392745    -4.487792     2.510980      25.44
 O       5.364492    -5.774371     2.844795     236.17
 C       5.011204    -6.846227     1.861322     108.50
 H       5.820422    -7.014355     1.188798      28.19
 H       4.227149    -6.480897     1.139260      31.77
 H       4.776104    -7.646788     2.443676      26.62
 C       5.863403    -3.547580     3.528041      -1.93
 O       6.028704    -3.934568     4.792856     153.10
 H       6.146368    -4.881381     4.983419      22.15
 C       6.142564    -2.186701     3.219473      53.83
 H       6.487269    -1.463946     4.017461      25.58
 C       5.675426    -2.709324     0.780463      54.75
 C       5.384729    -2.190935    -0.636860      94.96
 H       5.771457    -2.951830    -1.205323      24.50
 O       6.261741    -1.137289    -1.179336     246.75
 H       6.256897    -0.308297    -0.738894      28.25
 C       3.797468    -2.002984    -0.850939      70.95
 H       3.171880    -2.802153    -0.353853      20.00
 C       3.431786    -2.007129    -2.315573     100.08
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 O       3.531849    -3.375841    -2.924425     255.63
 H       4.345257    -3.418601    -3.561016      21.66
 H       4.083404    -1.267644    -2.848158      25.58
 H       2.434498    -1.477692    -2.504050      24.59
 C      -0.039198    -1.231943     1.015986      42.67
 H      -0.683510    -2.106666     1.364084      19.88
 C       0.241193     1.049524     0.331714      72.48
 H      -0.257558     1.889890     0.001402      23.42
 C       1.587541     0.872665    -0.086811      -8.04
 O       2.515668     1.735824    -0.662079     173.44
 C       1.942240     3.073590    -0.989213     101.43
 H       2.882475     3.586580    -1.509493      23.45
 H       1.119509     3.066984    -1.510738      28.12
 H       1.680579     3.455713     0.134491      22.74
 C       2.103068    -0.504082    -0.003741     -11.90
 O       3.474908    -0.708721    -0.255275     121.63
 C       1.279365    -1.483307     0.581751      53.11
 H       1.902038    -2.407619     0.737908      21.68
 C      -0.636010     0.049981     0.895100      48.36
 C      -2.079959     0.129574     1.262554      99.07
 H      -2.332359    -0.814534     1.813460      24.00
 O      -2.386036     1.162995     2.318389     238.45
 H      -1.847414     0.816200     3.172149      24.17
 C      -3.052948     0.331087     0.102473      81.76
 H      -2.859352     1.493464    -0.067997      22.18
 O      -2.673317    -0.548730    -0.972615     294.62
 H      -2.798528    -0.007168    -1.747204      27.14
 C      -4.540543     0.279041     0.532694     111.45
 O      -5.411995     1.218629    -0.072281     278.52
 H      -5.245489     2.082164     0.482548      29.09
 H      -4.421636     0.415178     1.596380      28.44
 H      -4.910280    -0.610579     0.304373      29.51
55
name = lig-etoh-Waterframe_407
 C       6.194585    -1.812923     1.801554      60.46
 H       6.447330    -0.781372     1.635516      25.26
 C       5.330619    -4.013063     1.138021      42.70
 H       4.978637    -4.753896     0.424494      16.66
 C       5.450945    -4.419961     2.460320      11.89
 O       5.344205    -5.839676     2.860970     224.32
 C       5.032059    -6.829239     1.833323     107.88
 H       5.790109    -7.056908     1.104831      28.14
 H       3.996672    -6.596685     1.465274      28.24
 H       4.762045    -7.816779     2.365720      23.96
 C       5.821251    -3.534586     3.477847       6.30
 O       6.032707    -3.907261     4.805114     192.93
 H       6.009953    -4.911193     4.924666      25.84
 C       6.129626    -2.190677     3.129570      63.01
 H       6.509119    -1.545988     3.975180      25.25
 C       5.659468    -2.653645     0.789488      58.61
 C       5.336789    -2.192799    -0.645479      71.56
 H       5.437334    -3.016179    -1.581939      19.37
 O       6.247669    -1.090489    -1.200346     233.05
 H       5.964868    -0.329041    -0.734894      27.48
 C       3.810051    -2.006090    -0.793076      66.07
 H       3.331567    -2.850726    -0.362637      22.84
 C       3.436031    -1.996519    -2.353937     102.47
 O       3.483354    -3.319738    -2.939338     263.22
 H       4.199242    -3.500939    -3.644555      23.73
 H       4.226518    -1.403969    -2.789432      25.94
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 H       2.449650    -1.626576    -2.445307      26.29
 C      -0.044310    -1.194165     1.055147      37.24
 H      -0.769697    -1.988798     1.469574      18.25
 C       0.199958     1.056811     0.326579      67.61
 H      -0.285157     2.110000     0.405605      19.00
 C       1.645197     0.844970    -0.064559       2.94
 O       2.517493     1.753897    -0.702030     164.03
 C       2.021505     3.059513    -0.993540     106.32
 H       2.938028     3.634063    -1.433742      24.15
 H       1.189062     2.802116    -1.620861      26.93
 H       1.630024     3.714172    -0.127476      25.54
 C       2.157568    -0.451522     0.060452      20.93
 O       3.468156    -0.659923    -0.292295     145.26
 C       1.323992    -1.467118     0.649859      53.89
 H       1.600334    -2.454397     0.859791      22.76
 C      -0.604684     0.041530     0.874744      33.63
 C      -2.064085     0.165608     1.326069      82.05
 H      -2.297856    -0.865121     1.794233      21.18
 O      -2.332217     1.207550     2.261431     254.38
 H      -1.843898     0.796340     3.221032      22.32
 C      -3.068121     0.429228     0.183992      67.93
 H      -3.076179     1.491201    -0.139431      22.68
 O      -2.705772    -0.542630    -1.029235     241.78
 H      -2.904011    -0.132389    -1.868132      25.84
 C      -4.583354     0.255804     0.550731     108.38
 O      -5.418003     1.232968    -0.081901     266.33
 H      -5.094620     2.191108     0.183435      29.10
 H      -4.777892     0.407098     1.544939      28.76
 H      -5.042402    -0.678179     0.267457      27.09
55
name = lig-etoh-Waterframe_408
 C       6.136423    -1.767411     1.754939      44.61
 H       6.394733    -0.742473     1.512304      21.05
 C       5.319502    -3.972987     1.124822      62.36
 H       5.046892    -4.768509     0.361803      20.01
 C       5.516704    -4.477953     2.420500      28.15
 O       5.342130    -5.858186     2.866949     286.52
 C       4.978963    -6.820605     1.838833     123.39
 H       5.753132    -6.787166     1.018780      29.91
 H       3.999059    -6.604572     1.337176      26.93
 H       5.131119    -7.858755     2.480658      20.30
 C       5.807845    -3.518410     3.473516      35.03
 O       6.031948    -3.887382     4.820207     253.02
 H       5.778201    -4.871805     4.910943      31.86
 C       6.152120    -2.246972     3.084269      61.24
 H       6.511184    -1.550562     3.864111      21.77
 C       5.667253    -2.628193     0.769529      47.27
 C       5.344380    -2.194705    -0.693296      68.49
 H       5.540849    -3.339500    -1.295916      16.59
 O       6.172064    -1.082790    -1.176386     271.15
 H       5.846192    -0.245250    -0.881600      24.78
 C       3.845647    -1.963074    -0.830618      83.73
 H       3.449992    -2.659809    -0.170102      20.14
 C       3.480684    -1.962519    -2.365077     107.16
 O       3.432459    -3.277063    -2.954429     279.55
 H       4.145397    -3.268432    -3.659135      24.35
 H       4.144873    -1.324143    -2.937362      24.94
 H       2.499142    -1.640079    -2.482912      24.83
 C       0.028460    -1.218974     1.061544      50.82
 H      -0.458028    -2.083192     1.575145      19.82
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 C       0.250783     1.131978     0.315719      67.37
 H       0.038859     2.322385     0.475193      15.40
 C       1.573221     0.847952    -0.047637       1.08
 O       2.502564     1.731696    -0.686906     196.47
 C       2.050672     3.060238    -1.008654     116.61
 H       2.831160     3.577363    -1.558152      24.84
 H       1.240467     3.202919    -2.044730      22.94
 H       1.665318     3.649414    -0.277088      27.83
 C       2.134433    -0.454415     0.188212      10.12
 O       3.474803    -0.643879    -0.331408     141.93
 C       1.319133    -1.455557     0.738888      61.71
 H       1.609290    -2.418352     0.843483      21.14
 C      -0.554389     0.062038     0.847076      56.14
 C      -2.076062     0.192288     1.348274      82.29
 H      -2.326780    -0.833114     1.719280      21.77
 O      -2.257039     1.261069     2.241901     262.40
 H      -1.899451     1.013539     3.311705      22.44
 C      -3.111327     0.467391     0.152701      86.46
 H      -2.849827     1.371431    -0.290503      23.02
 O      -2.763348    -0.484885    -1.020704     237.22
 H      -3.028817    -0.147298    -1.860166      25.39
 C      -4.627294     0.235073     0.601904      69.76
 O      -5.443766     1.284366    -0.139442     256.82
 H      -4.983924     2.183774     0.162643      27.45
 H      -4.844901     0.203848     1.719159      26.75
 H      -4.827923    -0.854621     0.057969      24.05
55
name = lig-etoh-Waterframe_409
 C       6.054426    -1.719446     1.711117      50.63
 H       6.399969    -0.709003     1.430215      20.13
 C       5.343282    -3.971665     1.106627      58.00
 H       5.070129    -4.551563     0.146929      17.94
 C       5.544045    -4.551380     2.447559       4.71
 O       5.339670    -5.797455     2.849831     299.77
 C       4.975105    -6.802419     1.840855      98.56
 H       5.667368    -6.620788     0.966721      27.48
 H       3.957535    -6.741438     1.470625      31.31
 H       5.140649    -7.914087     2.284748      20.49
 C       5.842030    -3.585932     3.477991      23.30
 O       6.003286    -3.864968     4.802906     217.06
 H       5.879816    -4.863413     5.052190      26.15
 C       6.205757    -2.225252     3.072262      48.00
 H       6.501080    -1.560306     3.863728      21.54
 C       5.652681    -2.638557     0.722446      27.66
 C       5.399458    -2.208270    -0.664635      97.17
 H       5.839530    -2.927215    -1.367553      21.17
 O       6.102534    -1.115517    -1.167069     279.40
 H       5.784480    -0.266360    -0.883613      24.40
 C       3.871713    -1.908530    -0.911960      80.30
 H       3.235559    -2.689409    -0.434457      20.61
 C       3.460427    -1.906286    -2.357494     104.74
 O       3.417692    -3.244003    -2.990819     267.43
 H       4.156638    -3.449682    -3.639808      24.00
 H       4.102002    -1.206739    -2.932389      24.67
 H       2.480909    -1.339436    -2.395272      24.32
 C       0.023417    -1.196199     1.082790      43.76
 H      -0.580861    -1.955186     1.548152      19.60
 C       0.296446     1.191228     0.371455      67.79
 H      -0.187494     2.261163     0.115624      17.64
 C       1.572091     0.850985    -0.055583       8.94
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 O       2.443771     1.704998    -0.653935     186.80
 C       2.069277     3.103042    -1.109663      98.33
 H       3.022518     3.390762    -1.313329      23.87
 H       1.015004     3.076758    -1.858893      21.41
 H       1.756378     3.524112    -0.215106      26.70
 C       2.150054    -0.456641     0.236646      13.95
 O       3.458989    -0.613600    -0.339025     125.80
 C       1.423519    -1.489923     0.793952      58.63
 H       1.956531    -2.397559     0.866480      21.06
 C      -0.564830     0.092030     0.861948      46.37
 C      -2.047299     0.202289     1.263390      98.44
 H      -2.329943    -0.646640     1.847079      23.42
 O      -2.204102     1.351844     2.254542     227.38
 H      -1.733615     0.830077     3.122497      23.48
 C      -3.106843     0.445747     0.094145      93.45
 H      -2.952468     1.502226    -0.100582      21.82
 O      -2.840126    -0.424767    -0.960814     284.25
 H      -3.103265     0.068903    -1.707703      25.29
 C      -4.626094     0.285441     0.533751      63.50
 O      -5.448311     1.290296    -0.161066     253.91
 H      -5.143056     2.184689     0.310297      27.54
 H      -4.702688     0.198961     1.732061      26.15
 H      -4.977388    -0.825691     0.064260      24.33
55
name = lig-etoh-Waterframe_410
 C       6.013070    -1.727099     1.756946      55.15
 H       6.281961    -0.676378     1.510426      21.58
 C       5.399531    -4.013266     1.094626      21.14
 H       5.018530    -4.779978     0.349914      12.35
 C       5.534549    -4.462674     2.395910      61.90
 O       5.317425    -5.806955     2.842942     333.95
 C       4.987164    -6.775042     1.812080     140.70
 H       5.553051    -6.698433     0.857262      37.63
 H       3.943367    -6.679873     1.745370      33.34
 H       5.205978    -7.756989     2.258723      25.09
 C       5.939058    -3.574028     3.413388      28.11
 O       5.967772    -3.857256     4.811458     119.61
 H       6.158705    -4.881991     4.988396      18.64
 C       6.218842    -2.212002     3.040614      72.27
 H       6.520117    -1.590206     3.840248      21.61
 C       5.638507    -2.655173     0.777823      57.85
 C       5.386731    -2.222930    -0.698278      98.38
 H       5.553971    -2.951971    -1.339528      22.48
 O       6.110582    -1.073037    -1.177239     255.01
 H       5.851049    -0.307491    -0.635095      23.80
 C       3.849982    -1.931350    -0.956227      48.19
 H       3.223345    -2.866380    -0.644543      19.37
 C       3.450639    -1.798470    -2.439156      89.31
 O       3.402262    -3.197597    -3.006207     250.95
 H       4.206571    -3.385489    -3.558367      23.15
 H       4.236308    -1.238230    -3.008463      23.41
 H       2.290942    -1.513715    -2.460191      23.31
 C       0.029523    -1.162872     1.116220      37.28
 H      -0.699298    -1.838784     1.423664      18.65
 C       0.232727     1.169352     0.425927      62.86
 H      -0.301098     1.971256    -0.068754      19.75
 C       1.596554     0.843572    -0.023587       3.36
 O       2.405329     1.711223    -0.676004     176.22
 C       2.066070     3.056197    -1.098776     112.55
 H       2.929688     3.448362    -1.546159      25.48
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 H       1.317863     3.048777    -1.894200      25.97
 H       1.787675     3.790077    -0.194655      24.40
 C       2.202923    -0.435017     0.190687      23.18
 O       3.462063    -0.585855    -0.327270     117.46
 C       1.483117    -1.480567     0.830577      46.92
 H       1.924368    -2.470427     1.112354      19.48
 C      -0.539408     0.101229     0.881853      33.07
 C      -2.035256     0.266854     1.221312     103.55
 H      -2.261325    -0.653515     1.737529      24.37
 O      -2.142406     1.393742     2.237412     244.66
 H      -1.720746     1.055900     3.106427      26.51
 C      -3.098163     0.479021     0.155721      91.23
 H      -3.132589     1.593341    -0.135796      21.13
 O      -2.901665    -0.378382    -0.970013     290.75
 H      -3.001990     0.001683    -1.816193      26.68
 C      -4.590036     0.326964     0.443390     104.62
 O      -5.443543     1.288779    -0.141835     255.62
 H      -5.380779     2.206408     0.284741      29.90
 H      -4.765199     0.578906     1.547047      25.81
 H      -5.113405    -0.595778     0.197250      26.45
55
name = lig-etoh-Waterframe_411
 C       6.003144    -1.752572     1.783696      51.95
 H       6.057595    -0.662158     1.593408      23.27
 C       5.441838    -4.052752     1.064928      42.98
 H       5.089198    -4.799037     0.357239      12.01
 C       5.530114    -4.438790     2.411389      42.18
 O       5.330311    -5.778544     2.817868     278.90
 C       4.968167    -6.768306     1.812906     122.51
 H       5.409036    -6.626090     0.829444      33.86
 H       3.891585    -6.742327     1.569653      33.10
 H       5.270232    -7.610606     2.238773      27.19
 C       6.035227    -3.515601     3.409370       0.72
 O       5.955042    -3.857570     4.775554      71.50
 H       6.141029    -4.884863     4.904834      18.16
 C       6.222780    -2.216360     3.092113      56.96
 H       6.567676    -1.521650     3.833526      26.88
 C       5.609336    -2.664240     0.759186      70.76
 C       5.289469    -2.210199    -0.728752      84.44
 H       5.457497    -3.258214    -1.314465      21.31
 O       6.155572    -1.027327    -1.181219     187.00
 H       6.083904    -0.287880    -0.521163      26.87
 C       3.809237    -1.934911    -0.998550      64.95
 H       3.235757    -2.703809    -0.353713      16.50
 C       3.457904    -1.770365    -2.532670      95.36
 O       3.407649    -3.139742    -3.007495     281.85
 H       4.182951    -3.308361    -3.592708      25.48
 H       4.045376    -1.040372    -3.145735      24.53
 H       2.395090    -1.293172    -2.727705      23.59
 C       0.108628    -1.168013     1.143176      52.57
 H      -0.417163    -2.048306     1.444330      21.60
 C       0.245198     1.117541     0.370612      75.57
 H      -0.163188     1.981999     0.085269      22.11
 C       1.540982     0.868081     0.043224      -4.67
 O       2.413129     1.737507    -0.727323     199.77
 C       2.061427     3.018941    -1.088620     121.56
 H       2.845246     3.412708    -1.767011      24.33
 H       1.302455     3.036595    -1.734605      28.61
 H       1.637209     3.863977    -0.273719      23.41
 C       2.197169    -0.446721     0.167936      -1.91
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 O       3.514864    -0.615296    -0.323450     118.27
 C       1.394631    -1.382881     0.861659      52.61
 H       1.830540    -2.434472     1.143099      18.66
 C      -0.542122     0.073481     0.904629      36.06
 C      -2.014084     0.319215     1.295770      94.68
 H      -2.358856    -0.680825     1.675521      22.44
 O      -2.091465     1.412124     2.192269     298.88
 H      -1.822798     1.105107     3.032345      28.38
 C      -3.128570     0.600928     0.138694      77.93
 H      -2.843632     1.627629    -0.317092      21.41
 O      -2.914570    -0.383592    -1.035881     254.62
 H      -2.847940     0.072669    -1.852348      26.27
 C      -4.608694     0.398724     0.532073     100.98
 O      -5.482944     1.327207    -0.191933     310.11
 H      -5.192611     2.179010     0.249118      28.99
 H      -4.676486     0.458199     1.588253      28.17
 H      -4.750298    -0.533620     0.235891      29.39
55
name = lig-etoh-Waterframe_412
 C       5.975813    -1.780217     1.753101      50.25
 H       5.947483    -0.701940     1.574113      23.71
 C       5.461293    -4.035048     1.053737      48.71
 H       5.236498    -4.615370     0.219205      16.43
 C       5.576703    -4.456700     2.426368      31.62
 O       5.351112    -5.726313     2.795075     266.81
 C       4.941574    -6.755891     1.806728     121.48
 H       5.579825    -6.555522     0.950173      31.81
 H       3.805278    -6.827969     1.592434      29.90
 H       5.225234    -7.688864     2.156703      26.39
 C       6.032637    -3.566898     3.456482      -2.90
 O       5.980594    -3.868223     4.735527      60.49
 H       5.849943    -4.868346     4.986622      17.57
 C       6.256508    -2.144937     3.126484      59.53
 H       6.547094    -1.433348     3.940822      25.70
 C       5.570326    -2.648597     0.700582      50.31
 C       5.244385    -2.180892    -0.705417      73.52
 H       5.834399    -2.934031    -1.571156      19.29
 O       6.190061    -1.073032    -1.183780     180.46
 H       6.050806    -0.273373    -0.576532      26.98
 C       3.767814    -1.835182    -1.018244      79.29
 H       3.091755    -2.658838    -0.690295      21.91
 C       3.432025    -1.752263    -2.567832     102.54
 O       3.431524    -3.099024    -3.046640     285.79
 H       4.137962    -3.366524    -3.667730      25.94
 H       4.269429    -1.198482    -3.015936      24.85
 H       2.463624    -1.284556    -2.621552      25.60
 C       0.046889    -1.171990     1.194412      51.45
 H      -0.414149    -2.049356     1.694560      22.11
 C       0.228341     1.097674     0.306109      66.13
 H      -0.076350     2.091237     0.352059      20.20
 C       1.651917     0.875256    -0.008983       6.58
 O       2.425016     1.702465    -0.722692     149.89
 C       1.970527     3.068673    -1.159919      90.84
 H       2.978483     3.436229    -1.589797      23.23
 H       0.875771     2.956505    -1.659786      23.82
 H       1.982769     3.572530    -0.127921      24.48
 C       2.163396    -0.401914     0.169011      16.90
 O       3.522674    -0.648265    -0.304418     200.84
 C       1.445162    -1.329269     0.831231      54.51
 H       1.882585    -2.424108     0.981836      20.00
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 C      -0.582095     0.028752     0.926227      22.40
 C      -2.033561     0.296293     1.306610      89.99
 H      -2.475629    -0.546484     1.945318      21.50
 O      -2.060912     1.446450     2.183870     302.51
 H      -1.887303     1.099982     2.968366      30.36
 C      -3.057886     0.683302     0.037629      68.68
 H      -2.834004     1.736913    -0.299633      22.26
 O      -2.914028    -0.375150    -1.061674     259.73
 H      -2.766293     0.109122    -1.850481      26.31
 C      -4.595448     0.485421     0.627506      81.80
 O      -5.507896     1.358358    -0.217579     290.27
 H      -5.276658     2.277910    -0.006368      30.76
 H      -4.776677     0.474338     1.676448      27.85
 H      -4.707841    -0.543862     0.256302      26.52
55
name = lig-etoh-Waterframe_413
 C       5.947823    -1.743903     1.757622      45.58
 H       6.048744    -0.708534     1.473044      21.52
 C       5.470956    -3.971052     1.041491      38.05
 H       5.279405    -4.731991     0.353146      19.34
 C       5.651899    -4.423931     2.341879      23.99
 O       5.348218    -5.763176     2.813406     266.01
 C       4.968581    -6.727128     1.803855     113.30
 H       5.511109    -6.644142     0.829575      28.41
 H       3.828179    -6.528665     1.605854      25.78
 H       5.191485    -7.744710     2.308451      21.92
 C       5.982600    -3.513158     3.406071      32.45
 O       6.021918    -3.898714     4.795064     217.33
 H       5.806037    -4.888744     4.934538      25.08
 C       6.246827    -2.188345     3.066606      56.45
 H       6.449599    -1.408714     3.867830      20.61
 C       5.553586    -2.636713     0.722809      27.88
 C       5.325371    -2.126155    -0.748632      78.80
 H       5.338983    -3.105437    -1.451378      20.16
 O       6.195513    -1.123152    -1.154244     286.74
 H       5.916680    -0.188063    -0.811282      23.88
 C       3.738473    -1.809304    -1.061805      70.01
 H       3.159445    -2.644438    -0.812628      23.76
 C       3.482315    -1.702265    -2.541460     108.51
 O       3.425524    -3.106247    -3.108737     270.81
 H       4.249636    -3.188421    -3.631412      24.76
 H       4.283717    -1.192019    -3.072098      25.37
 H       2.560858    -1.318945    -2.762478      26.75
 C       0.045360    -1.196309     1.231351      41.40
 H      -0.670914    -1.866114     1.849851      19.37
 C       0.251435     1.052889     0.299044      62.73
 H      -0.195521     2.118267     0.396289      18.76
 C       1.607661     0.890143    -0.089421       5.51
 O       2.468107     1.713695    -0.765578     193.78
 C       1.921616     3.055040    -1.102290     105.86
 H       2.596909     3.526320    -1.972943      23.44
 H       0.822321     3.178599    -1.796695      23.27
 H       1.845473     3.694409    -0.287350      26.61
 C       2.216356    -0.380710     0.153581       9.31
 O       3.468748    -0.625774    -0.257062     185.85
 C       1.425746    -1.394795     0.822843      40.44
 H       2.031715    -2.362037     0.915122      19.89
 C      -0.585580     0.048609     0.900702      37.33
 C      -2.080688     0.308831     1.249933      84.93
 H      -2.500667    -0.595664     1.777049      21.50
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 O      -2.047070     1.502198     2.199501     275.67
 H      -1.833478     1.183035     3.023643      29.64
 C      -3.003815     0.640777     0.049740      93.41
 H      -2.864159     1.637345    -0.297393      23.61
 O      -2.914040    -0.311005    -1.034925     290.47
 H      -2.830251    -0.068117    -1.945956      26.34
 C      -4.528342     0.592970     0.567382      79.33
 O      -5.511334     1.347612    -0.209367     272.60
 H      -5.369667     2.263387     0.112531      29.84
 H      -4.690909     0.960838     1.641733      24.96
 H      -5.110567    -0.484224     0.413422      23.60
55
name = lig-etoh-Waterframe_414
 C       5.936509    -1.676064     1.729003      44.47
 H       6.212824    -0.648492     1.554516      21.18
 C       5.466281    -3.990346     1.020275      49.74
 H       5.181015    -4.730916     0.262910      18.64
 C       5.692664    -4.439288     2.358631      12.55
 O       5.393625    -5.754848     2.808069     273.58
 C       4.973637    -6.694588     1.806411     108.41
 H       5.560576    -6.771045     0.854148      27.64
 H       3.915054    -6.515139     1.488848      29.27
 H       4.982098    -7.793630     2.340510      21.86
 C       5.930397    -3.520603     3.416462      29.99
 O       6.065375    -3.883056     4.792270     250.40
 H       6.111365    -4.869550     4.915445      27.78
 C       6.191642    -2.203496     2.996661      59.04
 H       6.483371    -1.489278     3.821608      19.29
 C       5.561174    -2.553540     0.716637      26.95
 C       5.270065    -2.169710    -0.757328      93.39
 H       5.494750    -2.985928    -1.262132      24.28
 O       6.215045    -1.131382    -1.150212     256.60
 H       5.802094    -0.202645    -0.931116      23.18
 C       3.808991    -1.833499    -1.036651      73.71
 H       3.285953    -2.605753    -0.536412      22.19
 C       3.532045    -1.667183    -2.591161      95.24
 O       3.434166    -3.083963    -3.144512     282.27
 H       4.245642    -3.333101    -3.682230      24.63
 H       4.230894    -1.025945    -3.137664      24.57
 H       2.592827    -1.159092    -2.841301      25.09
 C       0.072371    -1.173253     1.222832      41.15
 H      -0.459865    -2.047153     1.774178      18.56
 C       0.245917     1.068265     0.325996      55.63
 H      -0.306729     2.094417    -0.064621      15.93
 C       1.533311     0.826998    -0.144208      -1.69
 O       2.461859     1.803364    -0.848111     180.80
 C       1.878499     3.078806    -1.109012     100.51
 H       2.516602     3.492731    -1.939954      23.95
 H       0.764482     2.718477    -1.388792      23.34
 H       1.758143     3.764183    -0.388366      28.31
 C       2.106564    -0.425380     0.187521      17.87
 O       3.458427    -0.592586    -0.241543     125.40
 C       1.383870    -1.450561     0.814021      59.07
 H       1.811073    -2.362509     1.138536      21.06
 C      -0.535880     0.040463     0.864512      43.59
 C      -2.036350     0.359749     1.224717      93.40
 H      -2.394467    -0.577386     1.633177      24.41
 O      -2.066517     1.526395     2.186681     240.21
 H      -1.695140     1.109838     3.019966      26.59
 C      -3.059846     0.623954     0.060830     101.92
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 H      -2.735813     1.583813    -0.267393      24.55
 O      -2.900081    -0.306929    -0.998954     266.80
 H      -2.981541     0.167629    -1.831688      25.59
 C      -4.505063     0.696377     0.503528      86.70
 O      -5.503747     1.361218    -0.219902     292.64
 H      -5.418541     2.268449     0.168010      29.77
 H      -4.232277     1.243478     1.496272      23.97
 H      -4.716608    -0.528787     0.790161      25.01
55
name = lig-etoh-Waterframe_415
 C       5.957719    -1.621460     1.693938      50.00
 H       6.177811    -0.558273     1.536396      21.31
 C       5.467694    -3.955050     1.042488      15.65
 H       5.108359    -4.559159     0.151339       4.77
 C       5.646804    -4.477457     2.380191      56.53
 O       5.478038    -5.738753     2.776241     373.98
 C       4.943084    -6.703908     1.793133     127.97
 H       5.775871    -6.763940     1.105831      32.96
 H       4.034351    -6.403756     1.390797      34.01
 H       4.867612    -7.738211     2.369200      23.69
 C       5.926121    -3.551680     3.435353      17.67
 O       6.121128    -3.823832     4.726804     224.59
 H       6.113095    -4.754081     4.988200      28.96
 C       6.124490    -2.171206     3.025411      91.22
 H       6.570888    -1.533460     3.792989      29.02
 C       5.551185    -2.577887     0.689331      78.41
 C       5.270899    -2.205148    -0.705744     101.68
 H       5.665008    -2.937185    -1.373864      26.15
 O       6.217518    -1.116532    -1.179960     133.09
 H       5.907158    -0.176854    -0.800943      25.02
 C       3.848869    -1.819456    -0.993642      58.45
 H       3.162625    -2.684485    -0.687454      18.96
 C       3.554386    -1.687181    -2.644416      87.96
 O       3.452296    -3.022694    -3.150266     288.12
 H       4.188812    -3.309932    -3.771555      24.55
 H       4.455547    -1.179433    -3.033720      21.71
 H       2.489338    -1.204292    -2.616096      23.09
 C       0.063363    -1.170286     1.191595      44.51
 H      -0.518471    -2.000193     1.674791      18.22
 C       0.219522     1.123882     0.267517      49.80
 H      -0.378869     2.053030    -0.198448      15.82
 C       1.561610     0.827152    -0.200015      -4.47
 O       2.396575     1.791773    -0.854855     191.85
 C       1.762712     3.078440    -1.158777     111.35
 H       2.307524     3.547006    -1.900966      26.27
 H       0.803301     3.021316    -1.480892      28.10
 H       1.878489     3.676114    -0.179910      24.67
 C       2.068055    -0.481659     0.144578      11.89
 O       3.459381    -0.578983    -0.252781     135.65
 C       1.354958    -1.481294     0.828642      58.87
 H       1.781906    -2.354320     1.121894      19.48
 C      -0.551557     0.059861     0.859045      42.18
 C      -1.971746     0.368147     1.241419      99.49
 H      -2.305771    -0.434510     1.876484      23.63
 O      -2.092925     1.493490     2.149504     208.89
 H      -1.630735     1.099218     3.052364      24.48
 C      -3.042441     0.711564     0.015825      85.52
 H      -2.747928     1.706124    -0.409108      23.34
 O      -2.876558    -0.350084    -1.001802     260.25
 H      -3.048690     0.139436    -1.815859      25.20
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 C      -4.408162     0.760429     0.605341      98.65
 O      -5.503964     1.379069    -0.254601     267.23
 H      -5.409333     2.364735    -0.110051      29.71
 H      -4.473606     1.356176     1.555144      25.40
 H      -4.769233    -0.249511     0.907921      26.96
55
name = lig-etoh-Waterframe_416
 C       5.968605    -1.670752     1.723002      55.95
 H       6.034621    -0.612734     1.411479      22.80
 C       5.442672    -3.922648     1.082370      34.70
 H       5.184464    -4.734131     0.319735      14.06
 C       5.569835    -4.415771     2.354104      34.76
 O       5.538947    -5.796507     2.757018     280.74
 C       4.975834    -6.704201     1.791301     122.97
 H       5.670622    -6.978282     0.983519      31.05
 H       4.178067    -6.275868     1.270640      33.98
 H       4.691651    -7.579281     2.372671      26.27
 C       5.949298    -3.478978     3.339082      10.81
 O       6.191702    -3.773198     4.713072     159.64
 H       5.866065    -4.683555     4.897298      22.84
 C       6.080958    -2.120888     3.048004      65.72
 H       6.453568    -1.501872     3.817085      28.70
 C       5.588396    -2.593644     0.758430      83.82
 C       5.367949    -2.162555    -0.705894      81.57
 H       5.388810    -3.177620    -1.510481      21.17
 O       6.192731    -1.088409    -1.208350     135.40
 H       6.135909    -0.244383    -0.565782      24.16
 C       3.805201    -1.808191    -1.036595      58.39
 H       3.078312    -2.701118    -0.770214      19.01
 C       3.610039    -1.709774    -2.547415      96.85
 O       3.448615    -2.996195    -3.157057     280.47
 H       4.267909    -3.115626    -3.708996      24.37
 H       4.360238    -1.112239    -3.141798      23.47
 H       2.622543    -1.088183    -2.858068      22.97
 C      -0.030258    -1.174526     1.160609      40.33
 H      -0.734004    -1.780004     1.648692      22.08
 C       0.217027     1.101202     0.144868      72.12
 H      -0.249810     2.087252     0.065537      19.48
 C       1.529394     0.856637    -0.200727      11.82
 O       2.298705     1.716292    -0.866263     169.55
 C       1.667512     3.087113    -1.183748     105.11
 H       2.311528     3.524314    -1.876747      26.16
 H       0.759932     3.218734    -1.559616      28.45
 H       1.714218     3.711948    -0.072721      23.30
 C       2.143798    -0.465108     0.035995       1.57
 O       3.448633    -0.618735    -0.280566     192.48
 C       1.380138    -1.468659     0.816538      37.92
 H       1.877634    -2.367448     0.938127      18.88
 C      -0.538598     0.128720     0.843701      27.81
 C      -1.992615     0.366185     1.252398      82.72
 H      -2.444701    -0.580380     1.674550      21.32
 O      -2.095923     1.481337     2.125950     230.49
 H      -1.728400     1.191190     3.153122      22.74
 C      -2.911046     0.750017     0.016730      65.22
 H      -2.724487     1.755858    -0.490489      21.90
 O      -2.878444    -0.361714    -1.001553     259.63
 H      -2.956969    -0.243167    -1.974596      24.50
 C      -4.439753     0.856130     0.730196      92.36
 O      -5.468478     1.366968    -0.290399     289.07
 H      -5.238922     2.349028    -0.270879      28.32
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 H      -4.443523     1.453502     1.623629      26.50
 H      -4.788858    -0.032644     0.817289      29.69
55
name = lig-etoh-Waterframe_417
 C       5.951983    -1.687707     1.751973      52.40
 H       6.047917    -0.600210     1.532155      21.97
 C       5.381383    -3.983491     1.067306      93.74
 H       5.277915    -4.715731     0.213091      20.39
 C       5.542741    -4.397083     2.404250      58.42
 O       5.597727    -5.801147     2.724006     253.29
 C       5.002582    -6.715775     1.760243     149.97
 H       5.679203    -7.207036     1.025804      27.42
 H       4.090527    -6.207802     1.266311      24.53
 H       4.526621    -7.446452     2.272191      26.91
 C       5.972139    -3.409503     3.365546      21.81
 O       6.244904    -3.734356     4.668051     173.13
 H       5.983712    -4.713703     4.919501      25.20
 C       6.083693    -2.044740     3.069068      49.05
 H       6.207560    -1.377170     3.878713      24.26
 C       5.632686    -2.576052     0.729848      87.77
 C       5.337123    -2.120158    -0.729346      82.56
 H       5.786998    -3.165662    -1.353542      21.25
 O       6.185882    -1.077299    -1.234370     154.43
 H       6.163834    -0.322917    -0.492598      24.66
 C       3.822846    -1.844588    -1.059221      79.62
 H       3.258920    -2.695646    -0.582294      18.80
 C       3.623285    -1.635046    -2.524565      97.02
 O       3.450375    -2.997262    -3.156294     276.45
 H       4.258550    -3.429485    -3.597562      24.02
 H       4.524405    -1.110664    -2.936276      24.22
 H       2.677471    -1.065793    -2.707340      24.50
 C      -0.027230    -1.136900     1.092606      56.53
 H      -0.575496    -1.833600     1.612352      24.55
 C       0.165381     1.076703     0.107145      72.43
 H      -0.045724     2.040509     0.128772      21.20
 C       1.504007     0.786428    -0.197288      10.40
 O       2.200846     1.737468    -0.947579     155.47
 C       1.663981     3.072756    -1.168581      93.35
 H       2.509576     3.483825    -1.740543      23.77
 H       0.588057     2.818317    -1.654915      22.68
 H       1.443028     3.793593    -0.170364      23.63
 C       2.080489    -0.447236     0.027942      18.15
 O       3.470615    -0.659012    -0.333851     169.94
 C       1.367971    -1.376400     0.737895      50.88
 H       1.761279    -2.401089     0.934760      19.19
 C      -0.541993     0.116641     0.838960      27.36
 C      -2.011395     0.374404     1.175854      81.13
 H      -2.432505    -0.637133     1.502325      21.74
 O      -2.104656     1.507400     2.144276     205.32
 H      -1.762597     0.955803     3.107401      20.86
 C      -2.903568     0.733833     0.038039      72.21
 H      -2.394738     1.690439    -0.355734      22.50
 O      -2.887702    -0.368333    -0.952695     268.20
 H      -2.814994     0.097900    -1.851286      23.83
 C      -4.468447     0.942529     0.691254      89.72
 O      -5.376294     1.361791    -0.285797     315.99
 H      -5.375866     2.373856    -0.367719      28.42
 H      -4.346442     1.515360     1.579657      26.46
 H      -4.645628    -0.114569     0.969872      28.32
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name = lig-etoh-Waterframe_418
 C       5.922736    -1.610230     1.722383      56.52
 H       6.085590    -0.537819     1.522668      22.35
 C       5.365915    -3.956338     1.031305      84.95
 H       5.205496    -4.658686     0.215454      25.75
 C       5.578392    -4.407665     2.407671      25.44
 O       5.655432    -5.764875     2.695565     325.83
 C       4.964688    -6.728406     1.742878     139.55
 H       5.832833    -7.101936     1.136000      26.22
 H       4.203164    -6.121509     1.015897      22.44
 H       4.543287    -7.456464     2.363250      24.69
 C       5.956962    -3.411876     3.435339      44.96
 O       6.298249    -3.718771     4.668982     234.08
 H       6.286780    -4.740539     4.931728      21.35
 C       6.082940    -2.016602     3.109447      48.30
 H       6.144747    -1.234853     3.873260      18.62
 C       5.614921    -2.615547     0.678908      39.91
 C       5.352338    -2.153090    -0.728311      99.50
 H       5.636821    -2.881290    -1.424184      24.18
 O       6.195397    -1.058562    -1.242398     184.73
 H       6.100423    -0.132008    -0.729242      20.55
 C       3.884863    -1.918489    -1.007903      67.17
 H       3.330557    -2.783116    -0.741053      22.25
 C       3.631097    -1.635753    -2.574399     103.22
 O       3.436169    -2.993168    -3.137213     285.71
 H       4.297492    -3.343273    -3.548266      24.75
 H       4.529814    -1.121274    -2.873270      23.94
 H       2.761631    -1.120902    -2.673683      26.69
 C       0.048584    -1.124942     1.038580      37.50
 H      -0.379512    -1.965883     1.545324      19.32
 C       0.152671     1.071372     0.159308      51.37
 H      -0.236616     2.003384     0.017602      18.40
 C       1.468134     0.818420    -0.285751       7.62
 O       2.167778     1.747501    -1.002996     227.72
 C       1.643504     3.017835    -1.160966     107.93
 H       2.329114     3.720600    -1.773637      22.93
 H       0.668829     2.998694    -2.046845      22.35
 H       1.328499     3.476363    -0.278313      27.39
 C       2.112583    -0.459386     0.013003      19.93
 O       3.458120    -0.638337    -0.360015     154.54
 C       1.287389    -1.367356     0.673232      61.13
 H       1.770661    -2.387802     0.999413      19.62
 C      -0.638110     0.094933     0.806050      63.71
 C      -2.014032     0.362139     1.157992     101.74
 H      -2.354511    -0.446253     1.812289      23.08
 O      -2.109571     1.480682     2.178921     174.23
 H      -1.673403     0.989637     3.116549      23.25
 C      -2.977689     0.742118     0.058770     102.02
 H      -2.607355     1.629907    -0.482829      23.79
 O      -2.904038    -0.324551    -0.898688     281.62
 H      -2.779542     0.150576    -1.788596      24.22
 C      -4.338200     0.978667     0.595559      94.15
 O      -5.330670     1.371257    -0.308802     293.60
 H      -5.372812     2.392619    -0.160761      27.80
 H      -4.384406     1.734113     1.408939      24.92
 H      -4.747789    -0.117142     1.168968      25.36
55
name = lig-etoh-Waterframe_419
 C       5.890730    -1.605261     1.708531      36.66
 H       6.019749    -0.602985     1.327919      21.18
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 C       5.403564    -3.911172     1.063415      12.90
 H       5.104572    -4.619429     0.354004      21.55
 C       5.648488    -4.351524     2.341562      43.23
 O       5.676873    -5.738194     2.674747     334.38
 C       4.992316    -6.682361     1.751397     142.96
 H       5.761250    -7.202095     1.113395      25.00
 H       4.195177    -6.250508     0.984329      23.02
 H       4.488971    -7.482560     2.373229      22.99
 C       5.922808    -3.418617     3.390291      15.24
 O       6.382407    -3.729579     4.761051     424.75
 H       6.109166    -4.751811     4.936668      32.75
 C       6.029293    -2.023811     3.030421      79.13
 H       6.358202    -1.336850     3.875584      22.97
 C       5.602140    -2.555099     0.729586      53.04
 C       5.404132    -2.169646    -0.760131      87.59
 H       5.510458    -2.952536    -1.416020      22.55
 O       6.222167    -1.033090    -1.236052     216.75
 H       5.785796    -0.106065    -0.976437      20.77
 C       3.883692    -1.913696    -1.033102      59.58
 H       3.265478    -2.702794    -0.730943      20.54
 C       3.652987    -1.719527    -2.547227     109.52
 O       3.431608    -2.989815    -3.127705     291.30
 H       4.202103    -3.175679    -3.758386      24.64
 H       4.345230    -1.187738    -3.182395      23.14
 H       2.798408    -1.139355    -2.749550      24.41
 C      -0.040187    -1.145498     1.048646      31.01
 H      -0.670419    -1.954919     1.573830      15.32
 C       0.147902     1.097642     0.206765      82.00
 H      -0.497096     1.929168    -0.212168      16.67
 C       1.435134     0.825977    -0.359332       7.94
 O       2.212985     1.722829    -1.062129     199.51
 C       1.570355     3.041187    -1.235476      96.12
 H       2.475580     3.736775    -1.468380      22.13
 H       0.590421     3.104329    -1.902322      23.43
 H       1.224806     3.286993    -0.344947      28.54
 C       2.132565    -0.403584    -0.049228      14.19
 O       3.441861    -0.617318    -0.361432     145.64
 C       1.384966    -1.429863     0.590535      48.72
 H       1.865986    -2.455976     0.959357      16.96
 C      -0.632689     0.056579     0.735833      35.01
 C      -2.068887     0.377206     1.302779      79.91
 H      -2.491769    -0.564900     1.668580      22.82
 O      -2.091267     1.451384     2.214861     256.84
 H      -1.575638     1.088177     3.098868      25.05
 C      -2.980031     0.769476     0.032039     102.62
 H      -2.798232     1.732290    -0.379722      23.32
 O      -2.935832    -0.295483    -0.887711     265.71
 H      -2.877522    -0.172572    -1.899947      22.71
 C      -4.282080     0.987233     0.624145      80.59
 O      -5.334292     1.416463    -0.389462     248.22
 H      -5.392079     2.425062    -0.166949      29.45
 H      -4.053390     1.832543     1.361244      24.26
 H      -4.795220    -0.015120     1.138773      25.66
55
name = lig-etoh-Waterframe_420
 C       5.866889    -1.585043     1.685238      45.89
 H       6.029649    -0.538624     1.476615      19.03
 C       5.446511    -3.858964     1.059256      19.15
 H       5.157259    -4.533128     0.308525      18.15
 C       5.720495    -4.352549     2.362182      22.61
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 O       5.664123    -5.706845     2.642770     344.13
 C       5.045810    -6.650684     1.754251     100.29
 H       5.716378    -7.222410     1.122633      22.63
 H       4.260240    -6.160248     1.258432      30.06
 H       4.437072    -7.375743     2.484540      21.80
 C       5.965221    -3.395822     3.410514      11.71
 O       6.419264    -3.727603     4.752506     327.79
 H       6.117394    -4.610567     5.142992      31.34
 C       5.993219    -2.077177     3.001015      81.03
 H       6.486173    -1.392901     3.773980      27.83
 C       5.578359    -2.503852     0.705197      46.75
 C       5.393995    -2.126254    -0.760339      81.80
 H       5.822806    -3.218338    -1.336351      21.17
 O       6.240920    -1.039766    -1.226209     217.06
 H       5.675146    -0.186091    -1.045855      22.04
 C       3.877187    -1.822403    -1.084583      75.78
 H       3.305924    -2.625318    -0.609700      18.69
 C       3.623959    -1.741430    -2.559528      95.33
 O       3.427369    -3.058741    -3.150062     289.10
 H       4.085589    -3.296269    -3.869144      26.01
 H       4.512731    -1.252624    -3.040883      22.37
 H       2.600813    -1.163078    -2.599997      22.42
 C      -0.012458    -1.241095     1.004711      33.62
 H      -0.757146    -1.954688     1.577559      15.05
 C       0.141995     1.105994     0.143201      71.24
 H      -0.393477     2.119426    -0.259916      14.45
 C       1.431666     0.824539    -0.382108       5.73
 O       2.230853     1.721549    -1.146670     189.26
 C       1.543510     3.071413    -1.244624      95.27
 H       2.384914     3.778409    -1.483898      23.89
 H       0.848234     2.929661    -1.956240      26.64
 H       1.107645     3.377271    -0.167190      22.42
 C       2.043199    -0.426981    -0.077753      10.20
 O       3.485432    -0.594151    -0.384303     148.48
 C       1.358950    -1.443810     0.574839      49.93
 H       1.974539    -2.388467     0.722048      16.06
 C      -0.623164     0.034728     0.768437      56.54
 C      -2.074260     0.369604     1.302871      78.91
 H      -2.541116    -0.564217     1.641701      22.32
 O      -2.058547     1.439892     2.282194     259.39
 H      -1.633037     1.015163     3.079155      26.57
 C      -2.921667     0.806654     0.025761      87.43
 H      -2.434485     1.705312    -0.349733      23.67
 O      -2.962853    -0.336630    -0.915092     250.47
 H      -2.935045     0.140028    -1.844641      23.04
 C      -4.399013     1.028982     0.651808      95.47
 O      -5.320334     1.481227    -0.434964     268.16
 H      -5.385570     2.506341    -0.350125      29.17
 H      -4.250861     1.771584     1.482117      26.34
 H      -4.670779     0.160360     1.143377      29.96
55
name = lig-etoh-Waterframe_421
 C       5.851133    -1.541565     1.713465      44.83
 H       6.035266    -0.473360     1.633996      21.79
 C       5.492921    -3.836120     1.045332       0.95
 H       5.366578    -4.555630     0.231636      19.13
 C       5.747240    -4.352278     2.370709      39.51
 O       5.686296    -5.681116     2.659329     313.37
 C       5.029097    -6.617138     1.769992     115.45
 H       5.752143    -7.035066     1.100731      25.16
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 H       4.347628    -6.154229     1.195651      33.09
 H       4.657101    -7.439166     2.523972      22.83
 C       6.044744    -3.450389     3.451527      26.52
 O       6.430704    -3.679639     4.693411     253.87
 H       6.299624    -4.641394     4.855225      31.90
 C       6.036787    -2.062403     3.039790      67.81
 H       6.302535    -1.276810     3.787253      26.75
 C       5.545548    -2.470711     0.652881      73.49
 C       5.362145    -2.086992    -0.748714      90.84
 H       5.784015    -3.028565    -1.573701      21.21
 O       6.246022    -1.054707    -1.219789     232.51
 H       6.060646    -0.086041    -0.911424      23.41
 C       3.903422    -1.796847    -1.074449      71.54
 H       3.320873    -2.726580    -0.687267      19.59
 C       3.570566    -1.742926    -2.616085      83.11
 O       3.403561    -3.160487    -3.171655     249.09
 H       4.283239    -3.257991    -3.655990      24.02
 H       4.436978    -1.126235    -3.024796      23.40
 H       2.558959    -1.121085    -2.892992      23.39
 C       0.005086    -1.265286     0.941709      51.16
 H      -0.365300    -2.218319     1.468984      22.53
 C       0.126795     1.035853     0.042464      68.08
 H      -0.285892     2.176143     0.097591      17.68
 C       1.467115     0.839402    -0.398729      -0.44
 O       2.189509     1.740774    -1.183802     204.33
 C       1.595967     3.055632    -1.235445     109.41
 H       2.200909     3.809318    -1.689390      25.98
 H       0.869397     3.039213    -1.879053      30.09
 H       1.013136     3.545603    -0.169001      22.74
 C       2.028884    -0.464438    -0.125244       5.12
 O       3.481951    -0.551903    -0.414837     137.89
 C       1.293523    -1.464174     0.574666      55.95
 H       1.747772    -2.400958     0.718602      20.45
 C      -0.578168     0.045708     0.831575      36.75
 C      -2.007471     0.331689     1.200196      93.63
 H      -2.422973    -0.462913     1.817162      22.13
 O      -2.025122     1.413742     2.351676     253.15
 H      -1.762537     0.915161     3.044156      26.64
 C      -2.936613     0.801268     0.130466      78.84
 H      -2.378560     1.563696    -0.486352      22.25
 O      -2.975096    -0.320974    -0.938451     211.69
 H      -2.946448     0.148226    -1.882810      23.23
 C      -4.451607     1.122538     0.602044     108.75
 O      -5.305398     1.545982    -0.444156     283.32
 H      -5.191182     2.555177    -0.285047      26.96
 H      -4.693390     1.807002     1.399420      26.15
 H      -4.805723     0.212035     0.859058      29.64
55
name = lig-etoh-Waterframe_422
 C       5.833912    -1.554473     1.777983      50.23
 H       5.864951    -0.488313     1.504869      21.26
 C       5.552352    -3.837131     1.036015      47.32
 H       5.534297    -4.639061     0.237754      17.76
 C       5.746388    -4.300155     2.334158      58.14
 O       5.726383    -5.678664     2.719330     308.96
 C       5.036160    -6.594051     1.776910     152.21
 H       5.789957    -6.919581     1.052706      29.31
 H       4.133936    -6.228693     1.211941      25.82
 H       4.682834    -7.513500     2.289086      24.42
 C       6.104364    -3.380243     3.336041      30.14
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 O       6.451451    -3.684405     4.686305     317.16
 H       6.433709    -4.636798     4.912408      24.92
 C       6.103094    -2.011121     3.066042      58.13
 H       6.129561    -1.375353     3.917505      23.84
 C       5.561024    -2.449070     0.732095      76.17
 C       5.348930    -2.023409    -0.813584     106.28
 H       5.412409    -2.889074    -1.382796      24.52
 O       6.283305    -1.028757    -1.229181     278.52
 H       6.194079    -0.260505    -0.601681      26.48
 C       3.852995    -1.808882    -1.108692      57.95
 H       3.237687    -2.676443    -0.634692      18.88
 C       3.531833    -1.751744    -2.661961      90.24
 O       3.420301    -3.200812    -3.172282     252.72
 H       4.311965    -3.493265    -3.514683      25.05
 H       4.244731    -1.356722    -3.399289      24.65
 H       2.514564    -1.291881    -2.943105      24.39
 C      -0.031854    -1.246561     0.930485      43.06
 H      -0.632801    -2.038679     1.395204      22.86
 C       0.143837     0.966064     0.037248      86.08
 H      -0.336590     1.983002     0.134110      18.64
 C       1.466615     0.796778    -0.418617       5.95
 O       2.151059     1.761211    -1.167035     194.71
 C       1.599697     3.085068    -1.276174     105.23
 H       2.429543     3.612455    -1.653832      24.53
 H       0.554439     3.078846    -1.737997      25.35
 H       1.503886     3.441791    -0.101554      24.98
 C       2.099734    -0.450056    -0.178728      22.83
 O       3.413296    -0.538261    -0.446838     153.39
 C       1.353152    -1.480927     0.494314      51.38
 H       1.647664    -2.408769     0.733005      21.24
 C      -0.525542     0.033477     0.799594      46.71
 C      -1.943579     0.325847     1.269682      75.73
 H      -2.305487    -0.702653     1.574562      21.56
 O      -1.994544     1.368140     2.362115     294.82
 H      -1.728455     0.894626     3.132945      25.98
 C      -2.987839     0.785718     0.135573      75.38
 H      -2.690540     1.836417    -0.291475      22.51
 O      -2.997307    -0.265725    -0.910898     231.62
 H      -2.888049     0.021596    -1.932189      21.39
 C      -4.452369     1.127157     0.566473      87.05
 O      -5.295016     1.665450    -0.490527     263.82
 H      -5.329794     2.682290    -0.456955      28.48
 H      -4.431395     1.700759     1.506043      26.46
 H      -4.974415     0.029105     0.733099      25.97
55
name = lig-etoh-Waterframe_423
 C       5.808558    -1.524520     1.786655      51.40
 H       5.641796    -0.440598     1.597905      20.89
 C       5.614487    -3.848248     0.999070      68.03
 H       5.462238    -4.563735     0.115757      13.91
 C       5.772037    -4.309384     2.330760      51.91
 O       5.732537    -5.662695     2.756026     277.23
 C       5.074698    -6.591518     1.767574     125.19
 H       5.717252    -6.814328     0.851114      31.16
 H       4.047243    -5.993614     1.492852      23.77
 H       4.855497    -7.428921     2.336138      26.00
 C       6.169670    -3.327251     3.318516       5.39
 O       6.477409    -3.694733     4.651730     250.79
 H       6.117877    -4.595526     4.938818      25.90
 C       6.149738    -1.939612     3.099104      47.78
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 H       6.246937    -1.347749     3.963010      23.93
 C       5.588356    -2.462078     0.745405      45.66
 C       5.328681    -2.021733    -0.780647      92.26
 H       5.628515    -2.869188    -1.270973      26.54
 O       6.314408    -1.004184    -1.239795     249.26
 H       6.181770    -0.259169    -0.620325      27.21
 C       3.797657    -1.748992    -1.184202      75.99
 H       3.279306    -2.613776    -0.735405      22.30
 C       3.490148    -1.845208    -2.736228     113.05
 O       3.433160    -3.227944    -3.135513     275.18
 H       4.265057    -3.457406    -3.638758      25.27
 H       4.232385    -1.259902    -3.277274      26.25
 H       2.528812    -1.481753    -2.731612      26.96
 C       0.029522    -1.260210     0.910536      42.17
 H      -0.674828    -1.861284     1.315712      19.50
 C       0.188530     1.009635     0.080019      64.77
 H      -0.246895     1.875923    -0.233889      19.12
 C       1.430768     0.775625    -0.461708      17.09
 O       2.132519     1.728583    -1.146064     209.91
 C       1.639805     3.114524    -1.212810     102.32
 H       2.317407     3.607309    -1.944135      24.68
 H       0.465488     3.205974    -1.724496      22.38
 H       1.703753     3.585668    -0.356198      28.16
 C       2.072488    -0.455983    -0.170456      23.46
 O       3.406371    -0.558698    -0.521157     173.92
 C       1.340602    -1.489700     0.422258      59.35
 H       1.920676    -2.375469     0.572636      20.65
 C      -0.563558     0.010806     0.733341      40.83
 C      -1.953596     0.336339     1.348368      76.16
 H      -2.352952    -0.671402     1.659372      23.44
 O      -1.974615     1.290781     2.331908     255.96
 H      -1.551310     0.909731     3.247585      24.23
 C      -3.027200     0.820112     0.083975      87.27
 H      -2.603793     1.818757    -0.207679      23.36
 O      -3.016020    -0.209498    -0.867345     248.46
 H      -2.729439     0.220810    -1.789397      22.77
 C      -4.453537     1.035033     0.550944      79.30
 O      -5.280973     1.792316    -0.545716     228.92
 H      -5.238256     2.766691    -0.227579      26.35
 H      -4.253403     1.630054     1.471342      26.37
 H      -5.106467    -0.001549     0.953447      25.50
55
name = lig-etoh-Waterframe_424
 C       5.778406    -1.467387     1.779883      38.59
 H       5.568995    -0.388797     1.643780      22.59
 C       5.660402    -3.859123     0.985496      51.93
 H       5.371009    -4.532760     0.136185       9.71
 C       5.854762    -4.310945     2.340157      47.03
 O       5.740257    -5.634181     2.751701     289.81
 C       5.106619    -6.538471     1.807687     129.93
 H       5.628727    -6.638772     0.800884      32.13
 H       4.006612    -6.087185     1.522133      26.51
 H       5.043206    -7.433618     2.309892      26.72
 C       6.209531    -3.342392     3.376318      -6.73
 O       6.496288    -3.715154     4.614534     228.09
 H       5.922247    -4.513837     4.813181      25.99
 C       6.170492    -1.906072     3.084066      46.78
 H       6.479457    -1.160463     3.808956      24.35
 C       5.595516    -2.432254     0.703306      51.86
 C       5.339519    -2.048115    -0.722616      70.71
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 H       5.851771    -2.961233    -1.438345      21.61
 O       6.307550    -0.992063    -1.223409     203.65
 H       6.132699    -0.078629    -0.980114      27.48
 C       3.858395    -1.785047    -1.235212      88.00
 H       3.316851    -2.589062    -0.861714      23.43
 C       3.449255    -1.884921    -2.727495     110.49
 O       3.460287    -3.279198    -3.117835     279.27
 H       4.147266    -3.354053    -3.822218      25.29
 H       4.063704    -1.187141    -3.298423      26.52
 H       2.493603    -1.510989    -2.915735      25.96
 C       0.048893    -1.263951     0.881857      49.22
 H      -0.309648    -2.155432     1.326556      20.61
 C       0.149043     1.100487     0.094994      66.98
 H      -0.290860     1.921679    -0.265971      19.04
 C       1.414441     0.778587    -0.464719      14.88
 O       2.145456     1.721238    -1.153141     197.25
 C       1.708939     3.130521    -1.184331     102.27
 H       2.140757     3.586442    -2.116776      25.32
 H       0.442865     3.174643    -1.397257      21.90
 H       1.793367     3.732546    -0.334443      26.75
 C       2.008477    -0.450927    -0.184558      21.62
 O       3.412195    -0.560970    -0.617086     133.05
 C       1.333736    -1.521007     0.383523      51.50
 H       1.917814    -2.513978     0.530337      19.03
 C      -0.605763     0.013193     0.690990      27.71
 C      -2.031044     0.285497     1.272954      89.67
 H      -2.407930    -0.539466     1.859247      23.53
 O      -1.950616     1.277200     2.343876     185.94
 H      -1.516685     0.671423     3.229076      22.46
 C      -3.005715     0.830662     0.145532     101.51
 H      -2.592649     1.660106    -0.349554      24.53
 O      -3.012189    -0.171972    -0.887157     242.37
 H      -2.657589     0.181715    -1.815309      24.07
 C      -4.477280     1.039211     0.547226      96.64
 O      -5.230790     1.856364    -0.516768     254.06
 H      -5.106407     2.786524    -0.215944      27.12
 H      -4.640406     1.724849     1.390338      26.14
 H      -5.052178     0.036764     0.705234      26.84
55
name = lig-etoh-Waterframe_425
 C       5.760669    -1.469910     1.750159      46.93
 H       5.737339    -0.410391     1.490604      19.86
 C       5.680903    -3.801627     1.026968      31.01
 H       5.486033    -4.581672     0.314616      17.39
 C       5.947208    -4.247817     2.316638      18.78
 O       5.766821    -5.594209     2.743976     307.75
 C       5.111626    -6.479713     1.833273     150.59
 H       5.750910    -6.504451     0.937450      28.87
 H       4.044826    -6.356305     1.641467      29.82
 H       5.153754    -7.511558     2.219311      24.03
 C       6.208110    -3.290390     3.325063      20.04
 O       6.513148    -3.754877     4.646859     249.04
 H       6.251250    -4.709545     4.959952      24.17
 C       6.181289    -1.940531     3.008464      56.02
 H       6.560544    -1.189098     3.748876      23.42
 C       5.587018    -2.412138     0.732537      40.26
 C       5.416080    -2.020294    -0.785807      68.38
 H       5.538824    -3.154420    -1.446066      19.27
 O       6.292709    -0.986519    -1.209924     250.50
 H       5.794988    -0.198839    -1.070897      24.72
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 C       3.904889    -1.884665    -1.213723      62.91
 H       3.376480    -2.671306    -0.717140      23.27
 C       3.442235    -1.852572    -2.712685      92.94
 O       3.501330    -3.339063    -3.136706     255.19
 H       4.136351    -3.520840    -3.868573      25.01
 H       4.083393    -1.457608    -3.509007      25.36
 H       2.339983    -1.520897    -2.816633      24.70
 C       0.021366    -1.263442     0.841161      43.80
 H      -0.493482    -2.109268     1.455457      22.65
 C       0.059175     1.091042     0.075216      66.88
 H      -0.451378     2.074420     0.120951      19.61
 C       1.374245     0.855522    -0.408384     -14.41
 O       2.189663     1.756633    -1.172198     178.07
 C       1.711635     3.113031    -1.195310     112.72
 H       2.275677     3.602031    -2.040922      24.14
 H       0.637198     3.158469    -1.143225      26.69
 H       2.207977     3.622056    -0.110045      24.82
 C       2.072340    -0.476254    -0.279163       5.37
 O       3.369564    -0.537657    -0.704809     107.72
 C       1.349504    -1.513317     0.359635      47.14
 H       1.638596    -2.647959     0.583803      20.92
 C      -0.630981    -0.004529     0.687584      29.98
 C      -2.075124     0.249893     1.214525      86.99
 H      -2.439567    -0.746711     1.436660      24.89
 O      -1.919499     1.289070     2.355117     173.68
 H      -1.647760     0.701149     3.328876      21.03
 C      -2.983517     0.821100     0.196755      91.09
 H      -2.630472     1.790929    -0.081072      25.57
 O      -3.009976    -0.189195    -0.936737     222.77
 H      -2.766997     0.188406    -1.900443      22.72
 C      -4.542158     1.145817     0.526401     113.98
 O      -5.165700     1.858287    -0.455215     313.88
 H      -5.051759     2.794984    -0.426126      30.42
 H      -4.705500     1.422440     1.603695      27.81
 H      -4.893556     0.250563     0.401494      30.55
55
name = lig-etoh-Waterframe_426
 C       5.791084    -1.475621     1.695584      57.25
 H       5.941341    -0.429609     1.473423      20.22
 C       5.682671    -3.753374     1.042843      51.48
 H       5.610132    -4.443106     0.254980      21.41
 C       5.977130    -4.223635     2.319561      11.18
 O       5.804913    -5.518435     2.756434     257.40
 C       5.150458    -6.484018     1.821634     101.55
 H       5.575243    -6.468493     0.835672      25.36
 H       4.189557    -6.222520     1.740867      34.12
 H       5.370763    -7.484988     2.394051      22.21
 C       6.223606    -3.325231     3.357279      20.44
 O       6.537563    -3.746934     4.673778     238.06
 H       6.470665    -4.769386     4.625151      24.33
 C       6.201910    -1.935593     2.974017      42.14
 H       6.423286    -1.254889     3.868847      22.90
 C       5.572509    -2.419363     0.685668      31.84
 C       5.406652    -2.067846    -0.842893      90.22
 H       5.871129    -2.899771    -1.362717      21.82
 O       6.267484    -0.986171    -1.223725     257.11
 H       5.895081    -0.160769    -0.942342      25.15
 C       3.910381    -1.886131    -1.185209      66.04
 H       3.414528    -2.744267    -0.610047      20.80
 C       3.500421    -1.960517    -2.731018      85.53
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 O       3.502846    -3.387599    -3.154488     255.95
 H       4.300972    -3.449052    -3.747027      23.37
 H       4.141541    -1.200555    -3.318165      23.87
 H       2.384556    -1.531910    -2.605699      24.35
 C      -0.018763    -1.237022     0.795720      50.81
 H      -0.793879    -1.927437     1.380071      22.68
 C       0.019824     1.036592     0.062207      74.81
 H      -0.344093     2.131939     0.385289      20.57
 C       1.402418     0.885203    -0.389686      -7.57
 O       2.195732     1.752716    -1.169305     178.21
 C       1.775609     3.118221    -1.145456     120.90
 H       2.135560     3.706993    -2.017786      25.88
 H       0.847639     3.306068    -1.173728      31.39
 H       2.243643     3.664582    -0.054071      24.44
 C       2.031461    -0.456423    -0.335662       4.01
 O       3.359983    -0.537368    -0.798982     108.56
 C       1.306980    -1.483167     0.351671      63.24
 H       1.856796    -2.503081     0.430619      21.37
 C      -0.647093    -0.025280     0.682735      29.59
 C      -2.018837     0.225476     1.249348      79.51
 H      -2.436857    -0.752668     1.500144      24.57
 O      -1.926081     1.251131     2.323064     242.89
 H      -1.625194     0.767528     3.244260      23.54
 C      -3.035987     0.873626     0.145146      75.64
 H      -2.491707     1.839389    -0.114959      23.71
 O      -3.007243    -0.186094    -0.952056     201.51
 H      -2.967171     0.286799    -1.894167      22.37
 C      -4.515502     1.108456     0.568101      98.53
 O      -5.149998     1.915448    -0.455690     292.54
 H      -4.931323     2.834699    -0.257950      29.75
 H      -4.626404     1.390485     1.652448      27.03
 H      -5.015214     0.116138     0.394444      26.97
55
name = lig-etoh-Waterframe_427
 C       5.885322    -1.463805     1.675353      47.04
 H       5.902138    -0.392110     1.501879      21.06
 C       5.675861    -3.777115     0.989192      34.89
 H       5.595498    -4.481916     0.196190      14.95
 C       5.943537    -4.212053     2.343977      32.40
 O       5.860945    -5.498074     2.745459     299.57
 C       5.219516    -6.469153     1.847112     117.33
 H       5.575441    -6.521173     0.844579      29.92
 H       4.174312    -6.212927     1.882436      30.29
 H       5.317082    -7.538422     2.386796      24.00
 C       6.268912    -3.283619     3.402921      21.48
 O       6.560820    -3.717582     4.646676     215.00
 H       6.422014    -4.737472     4.705687      27.18
 C       6.208865    -1.946235     3.019701      56.76
 H       6.291348    -1.098996     3.759220      23.46
 C       5.586767    -2.399304     0.613177      48.35
 C       5.408936    -2.092113    -0.824200     105.83
 H       5.770628    -2.816000    -1.378796      27.27
 O       6.249125    -0.962718    -1.265562     223.30
 H       6.168087    -0.176778    -0.757035      27.26
 C       3.883173    -1.876912    -1.219618      87.00
 H       3.257739    -2.686716    -0.631641      20.34
 C       3.551654    -2.082220    -2.645711      96.53
 O       3.516755    -3.385622    -3.196698     267.77
 H       4.325044    -3.580069    -3.756231      24.22
 H       4.158079    -1.335003    -3.249354      24.89
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 H       2.473822    -1.777207    -2.945784      24.75
 C      -0.068479    -1.274477     0.770875      53.57
 H      -0.430436    -2.295453     1.147451      20.36
 C       0.132438     1.044614     0.073600      69.64
 H      -0.302267     2.178176     0.086835      18.80
 C       1.415693     0.836374    -0.425621      14.65
 O       2.165849     1.745813    -1.146712     218.49
 C       1.852276     3.192544    -1.075490     119.39
 H       2.335669     3.565202    -1.963916      24.88
 H       0.677162     3.285203    -1.154247      24.88
 H       2.046914     3.745410    -0.147266      27.56
 C       1.931969    -0.416161    -0.330690      14.92
 O       3.358575    -0.566856    -0.872585     126.84
 C       1.275936    -1.440495     0.309303      59.02
 H       1.813236    -2.369824     0.459108      21.46
 C      -0.653322     0.010148     0.643752      50.03
 C      -2.012827     0.268660     1.266767      93.44
 H      -2.348564    -0.619181     1.880789      24.13
 O      -1.944385     1.205344     2.279187     295.30
 H      -1.583360     0.814733     3.023951      28.86
 C      -3.025794     0.837386     0.112332      87.08
 H      -2.642280     1.781546    -0.455619      22.41
 O      -3.007823    -0.132640    -0.937013     226.81
 H      -3.076625     0.233058    -1.908179      23.47
 C      -4.449956     1.000560     0.578822      87.25
 O      -5.151094     2.007526    -0.450050     205.46
 H      -5.033043     2.908566    -0.039638      27.04
 H      -4.545074     1.657902     1.442702      25.88
 H      -5.149514    -0.044792     0.737098      25.19
55
name = lig-etoh-Waterframe_428
 C       5.978547    -1.499839     1.678595      58.12
 H       5.796292    -0.431800     1.539355      20.83
 C       5.671314    -3.804869     0.971613      47.22
 H       5.458018    -4.633457     0.287008      15.70
 C       5.892883    -4.146246     2.303882      22.66
 O       5.942766    -5.547748     2.735971     217.60
 C       5.247062    -6.461039     1.914171     134.49
 H       5.771044    -6.482674     0.964261      29.61
 H       4.065194    -6.305360     1.799444      25.57
 H       5.410293    -7.502042     2.358626      25.30
 C       6.275458    -3.248077     3.345504      -0.33
 O       6.595997    -3.693747     4.649317     225.67
 H       6.189086    -4.582352     4.959531      25.26
 C       6.193420    -1.864905     3.021862      58.33
 H       6.384038    -1.115193     3.793943      25.59
 C       5.673953    -2.404701     0.666892      48.03
 C       5.392912    -2.011610    -0.829896      83.47
 H       5.542450    -3.037979    -1.497924      21.57
 O       6.249584    -0.953978    -1.322968     248.39
 H       6.035293    -0.281011    -0.675716      28.01
 C       3.817711    -1.910526    -1.181873      76.94
 H       3.306632    -2.708392    -0.561747      21.01
 C       3.550304    -2.100012    -2.694813     104.52
 O       3.552283    -3.456698    -3.237808     259.29
 H       4.333919    -3.545098    -3.894928      24.00
 H       4.320397    -1.664659    -3.283567      24.88
 H       2.579777    -1.652609    -2.750565      25.48
 C      -0.054077    -1.328961     0.718076      44.56
 H      -0.616422    -2.176910     1.110211      19.80
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 C       0.191698     1.089563     0.116319      63.29
 H      -0.314121     2.055359    -0.216034      16.71
 C       1.407027     0.853215    -0.500479      14.00
 O       2.161248     1.786232    -1.108792     211.89
 C       1.864921     3.227263    -1.037321      96.76
 H       2.553585     3.649514    -1.751958      25.15
 H       0.587098     3.409317    -1.380182      21.42
 H       2.094007     3.575626    -0.176377      29.29
 C       2.026390    -0.466676    -0.365565      25.04
 O       3.295038    -0.577492    -0.900401     145.83
 C       1.241175    -1.450119     0.271582      67.33
 H       1.629699    -2.366335     0.483138      23.02
 C      -0.630776    -0.000435     0.622659      36.14
 C      -2.044153     0.299637     1.211176      90.93
 H      -2.435448    -0.773237     1.416923      24.28
 O      -1.954217     1.265430     2.283470     294.32
 H      -1.591954     0.854941     2.975613      30.62
 C      -2.998223     0.747860     0.097025      95.93
 H      -2.727983     1.838537    -0.091638      23.87
 O      -3.005914    -0.148084    -0.959154     250.80
 H      -2.967161     0.324706    -1.876276      22.47
 C      -4.450783     1.076593     0.566467      79.44
 O      -5.143690     2.020725    -0.413671     237.15
 H      -5.160385     2.938999     0.028936      27.45
 H      -4.290094     1.535865     1.545908      26.48
 H      -5.055540    -0.011750     0.717965      25.80
55
name = lig-etoh-Waterframe_429
 C       6.021162    -1.476256     1.690664      44.98
 H       5.925193    -0.418306     1.381484      21.01
 C       5.653797    -3.795837     0.988506      44.71
 H       5.312573    -4.522895     0.188704      14.75
 C       5.893166    -4.204497     2.322449      27.75
 O       6.014351    -5.524595     2.748930     266.20
 C       5.290503    -6.518218     1.940348     136.85
 H       5.717061    -6.576367     0.921728      31.34
 H       4.129540    -6.188598     1.735448      24.81
 H       5.417817    -7.409808     2.461099      25.30
 C       6.240022    -3.233650     3.319214      -3.71
 O       6.620109    -3.642865     4.638605     259.03
 H       6.026982    -4.437765     4.798077      29.21
 C       6.218785    -1.828089     3.040669      56.98
 H       6.479107    -1.158973     3.813340      25.28
 C       5.764621    -2.452617     0.657949      42.73
 C       5.334191    -1.986891    -0.823573      84.17
 H       5.824589    -3.038362    -1.469203      21.42
 O       6.222043    -0.962595    -1.359411     236.75
 H       6.008070    -0.039739    -1.007279      25.19
 C       3.827508    -1.944330    -1.131706      79.49
 H       3.367520    -2.697026    -0.557450      20.61
 C       3.555405    -2.093538    -2.779938      92.80
 O       3.559594    -3.553409    -3.245565     272.76
 H       4.284676    -3.532570    -3.958972      23.23
 H       4.300852    -1.450956    -3.203591      24.98
 H       2.676720    -1.586169    -3.005165      25.99
 C      -0.104124    -1.261866     0.663659      36.51
 H      -0.753452    -1.922963     1.107275      20.73
 C       0.143940     1.084224     0.119797      70.29
 H      -0.336191     2.000905     0.006010      18.08
 C       1.429392     0.825585    -0.518678       9.71
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 O       2.205543     1.856150    -1.110540     202.77
 C       1.865789     3.219515    -1.024716      97.93
 H       2.608749     3.808191    -1.575118      23.86
 H       0.809572     3.733680    -1.492311      22.26
 H       1.922697     3.502564     0.098978      23.77
 C       2.034088    -0.468949    -0.386755      21.06
 O       3.267449    -0.599393    -0.912591     152.11
 C       1.292705    -1.551300     0.219096      55.42
 H       1.689272    -2.501685     0.328040      20.84
 C      -0.592279    -0.000402     0.628336      44.48
 C      -2.029183     0.244371     1.109278      87.19
 H      -2.481481    -0.698565     1.519027      23.63
 O      -1.977991     1.328351     2.279822     210.88
 H      -1.631739     0.837989     3.061341      25.87
 C      -3.029308     0.822322     0.124674      87.68
 H      -2.479345     1.681843    -0.231798      23.64
 O      -2.986962    -0.202693    -1.032774     223.42
 H      -2.750508     0.293106    -1.899211      22.80
 C      -4.443897     1.175609     0.569826     115.97
 O      -5.132599     1.975666    -0.340184     306.06
 H      -4.962756     2.981347    -0.068974      26.09
 H      -4.415925     1.485810     1.610907      27.37
 H      -5.099123     0.350146     0.496157      26.97
55
name = lig-etoh-Waterframe_430
 C       6.035785    -1.431609     1.650732      43.89
 H       6.246180    -0.384028     1.347243      21.39
 C       5.626455    -3.801363     1.020761      59.53
 H       5.335841    -4.506255     0.166354      21.01
 C       5.942238    -4.237810     2.354836      -2.99
 O       6.055475    -5.516652     2.761255     264.80
 C       5.338213    -6.561624     1.946632     123.19
 H       5.800255    -6.793794     0.961912      25.50
 H       4.268243    -6.184986     1.982317      27.80
 H       5.283307    -7.387867     2.518296      24.34
 C       6.209068    -3.213713     3.350420      25.16
 O       6.600675    -3.588820     4.586951     231.17
 H       6.272170    -4.488797     4.881890      23.24
 C       6.272972    -1.865132     3.022244      56.87
 H       6.504585    -1.156203     3.758547      23.18
 C       5.786241    -2.399798     0.641480      22.81
 C       5.394229    -2.036235    -0.774972      84.83
 H       5.678911    -2.864396    -1.506577      19.95
 O       6.176475    -0.957066    -1.394413     275.18
 H       5.788064    -0.015794    -1.234400      21.57
 C       3.842372    -1.956298    -1.212519      84.91
 H       3.346728    -2.688786    -0.684734      22.00
 C       3.579064    -2.123784    -2.780320      86.83
 O       3.556267    -3.548215    -3.234993     281.07
 H       4.249212    -3.823345    -3.895700      24.56
 H       4.401335    -1.549550    -3.295695      24.29
 H       2.603454    -1.828564    -3.191455      24.82
 C      -0.041977    -1.275018     0.612552      53.18
 H      -0.582711    -2.080580     1.010770      24.91
 C       0.152420     1.088968     0.043060      73.64
 H      -0.146605     2.016254     0.271642      21.87
 C       1.404403     0.863305    -0.465207      -5.81
 O       2.248551     1.854160    -1.142503     177.66
 C       1.873983     3.287140    -0.962194     100.17
 H       2.797989     3.810123    -1.309494      24.58
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 H       1.036326     3.362952    -1.506109      28.30
 H       1.504556     3.635619     0.240843      24.53
 C       1.927468    -0.498188    -0.373875      -3.51
 O       3.319667    -0.630686    -0.920458     119.87
 C       1.256081    -1.587562     0.168889      65.25
 H       1.690336    -2.604972     0.152471      20.98
 C      -0.625876     0.062780     0.628438      40.71
 C      -2.016376     0.241292     1.151873      92.65
 H      -2.306139    -0.597466     1.724701      23.46
 O      -2.005338     1.337315     2.218716     221.51
 H      -1.655554     0.802936     3.136492      22.21
 C      -2.973096     0.895471     0.047488      73.01
 H      -2.586033     1.702624    -0.520729      23.98
 O      -2.977785    -0.215943    -1.063039     212.72
 H      -2.709568     0.073703    -2.000646      22.97
 C      -4.445154     1.170548     0.605007     108.52
 O      -5.145061     2.012778    -0.301962     323.48
 H      -4.751236     2.978832    -0.292394      27.67
 H      -4.550972     1.672022     1.585699      25.88
 H      -4.870198     0.249568     0.627411      28.67
55
name = lig-etoh-Waterframe_431
 C       6.095147    -1.418786     1.629708      51.48
 H       6.355616    -0.373709     1.417236      22.74
 C       5.629160    -3.760709     1.060097      55.29
 H       5.474155    -4.611637     0.356664      21.43
 C       5.975404    -4.171026     2.315751       4.16
 O       6.089378    -5.577036     2.770436     250.79
 C       5.351427    -6.570964     2.018004     121.15
 H       5.886857    -6.790371     1.053079      25.27
 H       4.396394    -6.277471     1.734210      32.44
 H       5.377956    -7.457861     2.664991      22.48
 C       6.193000    -3.237778     3.332750      21.96
 O       6.582463    -3.554406     4.614125     280.47
 H       6.509603    -4.529518     4.781873      26.54
 C       6.308402    -1.864514     2.920981      54.56
 H       6.588039    -1.175839     3.704914      21.50
 C       5.722383    -2.371754     0.671263      29.45
 C       5.452192    -2.089273    -0.849716      91.44
 H       5.697469    -2.925698    -1.260274      22.89
 O       6.132440    -0.947727    -1.429775     312.88
 H       5.586815    -0.174114    -0.973784      19.83
 C       3.854579    -1.957466    -1.306949      67.40
 H       3.317192    -2.784172    -0.818941      21.73
 C       3.641923    -2.193017    -2.794469      89.13
 O       3.537515    -3.530936    -3.200717     273.11
 H       4.335619    -3.621478    -3.794961      22.76
 H       4.412070    -1.691507    -3.502605      22.40
 H       2.570491    -1.614761    -2.814090      22.89
 C      -0.053202    -1.293064     0.610838      46.17
 H      -0.618613    -2.193947     0.932497      21.00
 C       0.130955     1.150096     0.026206      79.52
 H      -0.090101     2.192466     0.223855      17.96
 C       1.476076     0.879446    -0.463034     -12.64
 O       2.264627     1.806665    -1.105628     183.63
 C       1.855359     3.295277    -0.904954     101.80
 H       2.726723     3.979662    -1.099448      25.12
 H       1.199330     3.438608    -1.620121      29.33
 H       1.505678     3.508227     0.252569      26.15
 C       1.978886    -0.493810    -0.448375      14.13
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 O       3.311044    -0.643596    -0.891532     141.34
 C       1.199098    -1.546202     0.086980      57.45
 H       1.546445    -2.661582     0.106184      20.45
 C      -0.594957     0.004211     0.599966      30.24
 C      -2.007950     0.371834     1.220895      80.86
 H      -2.442849    -0.612284     1.413098      22.71
 O      -2.027411     1.329020     2.158349     241.73
 H      -1.552825     0.889408     3.130142      20.38
 C      -2.910293     0.846694    -0.051183      80.70
 H      -2.580460     1.862301    -0.338087      24.09
 O      -2.983517    -0.204804    -1.037196     256.26
 H      -2.900935     0.105336    -1.971973      23.31
 C      -4.398325     1.154828     0.601067      75.48
 O      -5.191766     2.032261    -0.333624     282.40
 H      -4.874875     3.008164    -0.022222      25.74
 H      -4.172872     1.613606     1.624529      24.27
 H      -4.837574     0.072319     0.816340      25.95
55
name = lig-etoh-Waterframe_432
 C       6.156380    -1.415925     1.586473      45.94
 H       6.224917    -0.367353     1.307406      15.98
 C       5.650281    -3.715859     1.037906      54.33
 H       5.475875    -4.434903     0.261294      18.89
 C       5.989816    -4.221119     2.353960      17.48
 O       6.104349    -5.549770     2.764814     260.76
 C       5.369388    -6.587780     2.054901     121.04
 H       5.999023    -6.877625     1.173685      27.50
 H       4.422065    -6.339891     1.715438      32.43
 H       5.323679    -7.544756     2.778838      23.35
 C       6.241058    -3.201872     3.310573      15.87
 O       6.563132    -3.535287     4.666270     218.35
 H       6.453900    -4.509735     4.668337      28.09
 C       6.347525    -1.877968     2.910446      59.93
 H       6.760455    -1.150020     3.657545      28.45
 C       5.628146    -2.375601     0.637302      20.47
 C       5.416917    -2.114906    -0.927608      88.60
 H       5.949653    -3.084024    -1.404517      24.47
 O       6.079926    -0.959287    -1.438466     276.88
 H       5.970007    -0.066410    -0.852704      24.42
 C       3.938049    -2.004224    -1.309571      70.96
 H       3.309001    -2.837897    -0.788436      21.23
 C       3.657678    -2.135850    -2.810105      88.47
 O       3.524601    -3.543202    -3.175183     285.22
 H       4.184604    -3.784695    -3.911036      24.70
 H       4.361946    -1.532277    -3.457599      24.46
 H       2.635418    -1.577862    -3.079639      24.13
 C      -0.132190    -1.286267     0.602704      33.53
 H      -0.885999    -2.084570     1.005965      16.45
 C       0.198160     1.106711     0.069417      67.67
 H      -0.403556     2.123634    -0.074128      16.75
 C       1.487379     0.849058    -0.474402      14.37
 O       2.296674     1.835321    -1.036693     199.96
 C       1.863597     3.219279    -0.863340     107.54
 H       2.787435     3.811779    -0.957319      23.10
 H       1.041700     3.763774    -1.616305      23.54
 H       1.417186     3.293146     0.068046      28.51
 C       2.036459    -0.477233    -0.518821      23.72
 O       3.329499    -0.663441    -0.877650     122.17
 C       1.194932    -1.495892    -0.022389      53.19
 H       1.604013    -2.600225     0.006491      21.29
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 C      -0.573168     0.047206     0.590395      48.46
 C      -1.986916     0.368670     1.069513      83.07
 H      -2.589859    -0.544359     1.499340      22.25
 O      -2.036784     1.377990     2.185243     184.58
 H      -1.461434     0.855521     3.038786      21.98
 C      -2.940034     0.831066    -0.027185      99.36
 H      -2.409732     1.748779    -0.510369      22.41
 O      -2.971509    -0.179943    -1.013276     251.61
 H      -3.048944     0.225211    -1.883621      25.43
 C      -4.274598     1.137776     0.524419      91.96
 O      -5.213980     2.001139    -0.324330     247.28
 H      -5.311881     2.905780     0.105939      27.94
 H      -4.063468     1.695423     1.488586      24.70
 H      -5.162611     0.284814     0.692560      23.65
55
name = lig-etoh-Waterframe_433
 C       6.137808    -1.449390     1.515097      51.28
 H       6.205090    -0.389561     1.303514      17.77
 C       5.664377    -3.770651     1.014393      49.05
 H       5.389544    -4.411250     0.234730      18.60
 C       5.971058    -4.206481     2.340113      19.70
 O       6.099735    -5.500202     2.771310     203.18
 C       5.406241    -6.626326     2.051824     102.70
 H       5.973775    -7.047736     1.207851      27.65
 H       4.379318    -6.223763     1.835960      27.66
 H       5.198179    -7.425122     2.949926      24.47
 C       6.331842    -3.206847     3.353382       0.59
 O       6.529650    -3.525801     4.666631     195.27
 H       6.271842    -4.426103     4.958281      25.10
 C       6.422309    -1.832711     2.901878      55.64
 H       6.857855    -1.094463     3.665075      26.67
 C       5.614923    -2.356314     0.593437      31.33
 C       5.383354    -2.094911    -0.901465      77.62
 H       5.848507    -2.920689    -1.811769      21.26
 O       6.077624    -0.963558    -1.456668     276.96
 H       6.042352    -0.134518    -0.778323      24.54
 C       3.923565    -2.052114    -1.306715      72.52
 H       3.385534    -2.915794    -0.708070      21.09
 C       3.641714    -2.040165    -2.862984      91.93
 O       3.519861    -3.542897    -3.174355     287.09
 H       4.062065    -3.822603    -3.976845      26.13
 H       4.519280    -1.643042    -3.308513      25.36
 H       2.687934    -1.708254    -3.145210      25.68
 C      -0.114976    -1.232978     0.520581      49.22
 H      -0.731459    -2.116502     0.975978      18.21
 C       0.274111     1.038012     0.084068      59.08
 H      -0.285484     2.049529    -0.299610      16.82
 C       1.492913     0.845918    -0.506228      17.01
 O       2.318690     1.870477    -0.988515     217.34
 C       1.882520     3.166015    -0.798368      99.51
 H       2.759787     3.813941    -0.860942      23.55
 H       0.933803     3.454667    -1.721093      22.87
 H       1.456916     3.307968     0.096830      28.95
 C       1.999335    -0.498213    -0.521974       2.35
 O       3.428575    -0.687506    -0.888081      90.82
 C       1.124152    -1.503616    -0.066406      57.45
 H       1.618197    -2.508802    -0.121797      22.65
 C      -0.598494     0.086714     0.604260      50.15
 C      -1.997533     0.327948     0.994658      91.51
 H      -2.227291    -0.627108     1.588976      22.70
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 O      -2.016653     1.415696     2.201513     170.13
 H      -1.550903     0.813331     2.983328      22.38
 C      -2.933293     0.880182    -0.037738      96.89
 H      -2.578490     1.802544    -0.607253      23.13
 O      -2.960194    -0.199995    -1.044331     240.88
 H      -3.037396     0.143777    -1.930096      24.84
 C      -4.317069     1.223464     0.475350     100.16
 O      -5.221378     1.940063    -0.324048     302.38
 H      -5.137821     2.855475     0.076487      28.94
 H      -4.237870     1.728161     1.433224      26.09
 H      -4.608733     0.069539     0.718218      26.46
55
name = lig-etoh-Waterframe_434
 C       6.103834    -1.466193     1.538962      40.42
 H       6.263324    -0.430001     1.243756      23.07
 C       5.643807    -3.803400     0.976929      64.27
 H       5.382169    -4.680787     0.405123      20.53
 C       5.970395    -4.113771     2.303331      11.71
 O       6.087215    -5.503230     2.774740     182.37
 C       5.398686    -6.603999     2.099781     121.45
 H       5.920836    -7.048669     1.275711      28.31
 H       4.377859    -6.246845     1.584671      24.85
 H       5.302552    -7.394577     2.918822      24.74
 C       6.380028    -3.190129     3.314563      10.31
 O       6.508106    -3.511444     4.686654     209.81
 H       6.068159    -4.348354     4.930737      26.05
 C       6.502357    -1.842683     2.852780      44.39
 H       6.823242    -0.984988     3.525969      20.49
 C       5.687504    -2.448116     0.569227      11.70
 C       5.384659    -2.055766    -0.936571      76.98
 H       5.677794    -3.118060    -1.272619      21.75
 O       6.114356    -0.950860    -1.461422     294.92
 H       5.733520    -0.092784    -0.917615      19.87
 C       3.812813    -2.005790    -1.325497      76.86
 H       3.287622    -2.878978    -0.879286      25.54
 C       3.651402    -2.089934    -2.862485     113.18
 O       3.509896    -3.494625    -3.213940     288.71
 H       4.215409    -3.551730    -3.934618      23.88
 H       4.452659    -1.644794    -3.403400      26.88
 H       2.867170    -1.445713    -3.065553      27.30
 C      -0.099179    -1.217830     0.453467      54.01
 H      -0.608570    -2.127225     0.828448      22.69
 C       0.258223     1.081761     0.024486      71.66
 H      -0.001778     2.214243     0.051484      18.33
 C       1.578065     0.806404    -0.533002       6.42
 O       2.364545     1.818039    -0.948933     209.50
 C       1.858615     3.200193    -0.743085      94.28
 H       2.541943     3.967557    -1.034592      25.34
 H       1.059321     3.292248    -1.620053      24.65
 H       1.429991     3.442650     0.339531      24.91
 C       2.037872    -0.520044    -0.532825      12.76
 O       3.434162    -0.716063    -0.868866     125.52
 C       1.139407    -1.544953    -0.112839      57.24
 H       1.281010    -2.594331    -0.078846      25.85
 C      -0.571681     0.068965     0.570997      43.30
 C      -1.983716     0.383881     1.124099      77.68
 H      -2.506280    -0.589182     1.253298      23.09
 O      -1.982021     1.386741     2.167040     293.93
 H      -1.707213     0.938072     2.982104      26.38
 C      -2.915526     0.948945    -0.146743      72.63
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 H      -2.411936     1.849597    -0.450064      24.81
 O      -2.967248    -0.227740    -1.096840     257.93
 H      -2.877706    -0.009687    -2.006591      26.22
 C      -4.357852     1.199211     0.542516     104.09
 O      -5.242844     1.905201    -0.359538     317.57
 H      -4.932416     2.812081    -0.249354      32.88
 H      -4.259444     1.682107     1.469813      27.56
 H      -4.750776     0.274802     0.696653      29.64
55
name = lig-etoh-Waterframe_435
 C       6.099789    -1.518347     1.540056      47.40
 H       6.209713    -0.495027     1.171895      20.26
 C       5.626050    -3.832939     0.972834      49.36
 H       5.394072    -4.684885     0.258938      20.14
 C       6.006056    -4.145190     2.322254       5.58
 O       6.058890    -5.467498     2.769667     228.72
 C       5.378641    -6.561693     2.117764     132.13
 H       6.089609    -6.911414     1.402676      25.54
 H       4.304356    -6.354885     1.691695      27.28
 H       5.191235    -7.303282     2.787275      25.76
 C       6.380209    -3.148367     3.275955      14.49
 O       6.493431    -3.479777     4.671642     227.01
 H       6.118777    -4.371936     4.723958      23.49
 C       6.556072    -1.855417     2.808421      56.65
 H       6.860988    -1.075171     3.515147      22.45
 C       5.751754    -2.477570     0.552291      29.00
 C       5.351607    -2.128753    -0.917108      83.77
 H       5.749229    -2.819888    -1.533359      24.91
 O       6.143853    -0.955406    -1.446868     242.46
 H       5.659384    -0.043677    -1.335977      22.38
 C       3.821351    -1.961468    -1.340782      89.94
 H       3.205502    -2.668079    -0.911873      25.81
 C       3.659157    -2.099921    -2.834416      97.96
 O       3.502930    -3.421761    -3.311815     280.87
 H       4.259559    -3.680653    -3.927347      24.20
 H       4.528456    -1.676022    -3.380056      26.67
 H       2.737848    -1.464010    -3.181219      25.00
 C      -0.097589    -1.274170     0.397661      44.84
 H      -0.807627    -1.964542     0.722617      23.40
 C       0.277549     1.137750    -0.034134      84.93
 H       0.012341     2.048127     0.408293      19.18
 C       1.550343     0.777057    -0.484987     -11.38
 O       2.464929     1.812057    -0.905413     147.13
 C       1.820815     3.237258    -0.763575      94.49
 H       2.688042     3.797164    -1.049851      24.35
 H       0.970746     3.365800    -1.161655      30.66
 H       1.477749     3.411331     0.482469      24.25
 C       2.092873    -0.581253    -0.549324      28.34
 O       3.358136    -0.717473    -0.831178     170.87
 C       1.195919    -1.591582    -0.157182      57.00
 H       1.422691    -2.598669    -0.212721      24.94
 C      -0.556515     0.105500     0.520472      31.16
 C      -1.979765     0.441748     1.124071      88.12
 H      -2.594379    -0.366587     1.481569      22.04
 O      -1.952580     1.346868     2.149382     324.94
 H      -1.711150     0.916266     2.879297      30.46
 C      -2.902134     0.940940    -0.140763      76.19
 H      -2.469426     1.749013    -0.689023      25.04
 O      -2.976773    -0.202749    -1.121897     261.49
 H      -2.781682     0.033046    -2.002895      28.30
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 C      -4.344716     1.135129     0.547488     100.10
 O      -5.269139     1.896909    -0.402517     289.83
 H      -4.982517     2.792372    -0.529088      34.03
 H      -4.192395     1.713696     1.449545      26.22
 H      -4.989479     0.341975     0.691956      27.73
55
name = lig-etoh-Waterframe_436
 C       6.146736    -1.530012     1.444013      42.34
 H       6.136384    -0.460283     1.190551      20.55
 C       5.661183    -3.854336     1.005726      55.81
 H       5.377510    -4.558119     0.147579      20.42
 C       6.019089    -4.210578     2.290999      10.68
 O       6.013274    -5.429519     2.823626     281.47
 C       5.359259    -6.536547     2.108769     112.64
 H       5.985963    -6.923553     1.260021      24.68
 H       4.436795    -6.128995     1.688671      31.77
 H       5.236720    -7.212204     2.858517      24.71
 C       6.363201    -3.171404     3.282895      12.31
 O       6.481297    -3.441990     4.589896     200.43
 H       6.396547    -4.378943     4.870195      22.69
 C       6.571106    -1.843205     2.808768      54.36
 H       6.940725    -1.132047     3.493773      22.85
 C       5.737478    -2.508700     0.538207      36.50
 C       5.359488    -2.156771    -0.924821      82.75
 H       5.672792    -2.833776    -1.728992      22.79
 O       6.162078    -0.989278    -1.436202     231.51
 H       5.731014    -0.088504    -1.219823      22.00
 C       3.891050    -1.999158    -1.294567      77.64
 H       3.405536    -2.808416    -0.816708      23.25
 C       3.677922    -2.001843    -2.885737      80.11
 O       3.489895    -3.418944    -3.408778     256.90
 H       4.229459    -3.600445    -4.082228      23.26
 H       4.618060    -1.483510    -3.297237      23.99
 H       2.592699    -1.595399    -3.180000      24.03
 C      -0.125913    -1.262921     0.334136      60.13
 H      -0.771971    -2.034350     0.576763      23.96
 C       0.272002     1.117643     0.019833      73.45
 H       0.083557     2.074442     0.235976      18.76
 C       1.579424     0.812853    -0.463776      -1.47
 O       2.483245     1.835636    -0.846612     194.10
 C       1.870716     3.188524    -0.740342     101.39
 H       2.613332     3.925471    -1.152270      25.41
 H       0.942649     3.333549    -1.195437      29.41
 H       1.959082     3.448833     0.425842      25.79
 C       1.963037    -0.560132    -0.518942       4.99
 O       3.376966    -0.679598    -0.829095     125.53
 C       1.179078    -1.656805    -0.163874      71.38
 H       1.634611    -2.590663    -0.318692      24.32
 C      -0.543887     0.055051     0.453006      35.20
 C      -1.957462     0.408402     0.968524      91.45
 H      -2.176236    -0.525316     1.449784      24.55
 O      -1.912065     1.388228     2.190205     274.57
 H      -1.566831     0.828918     2.809191      28.09
 C      -2.946602     0.845186    -0.084608     100.64
 H      -2.754055     1.797440    -0.615988      24.37
 O      -2.988331    -0.167628    -1.103452     265.23
 H      -2.880696     0.198390    -1.961529      26.30
 C      -4.343343     1.178127     0.428640      85.95
 O      -5.280424     1.865440    -0.439057     286.41
 H      -4.927284     2.752805    -0.373934      32.71
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 H      -4.223564     1.757866     1.417809      24.84
 H      -4.773486     0.036411     0.763838      25.77
55
name = lig-etoh-Waterframe_437
 C       6.231174    -1.505195     1.412387      47.09
 H       6.228611    -0.453070     1.072974      20.46
 C       5.703755    -3.861358     0.951415      67.42
 H       5.400628    -4.780196     0.370905      15.49
 C       6.026685    -4.178433     2.295449      22.29
 O       5.974319    -5.470553     2.903162     290.39
 C       5.337395    -6.485121     2.096017     108.94
 H       5.924920    -6.928861     1.186838      27.43
 H       4.427813    -6.128250     1.737548      31.76
 H       5.154226    -7.335271     2.845805      24.30
 C       6.345282    -3.190277     3.192765      23.21
 O       6.494164    -3.411829     4.565938     195.10
 H       6.459836    -4.364641     4.835382      24.98
 C       6.529450    -1.862569     2.760170      65.29
 H       6.894046    -1.109437     3.383205      28.06
 C       5.705863    -2.519931     0.524642      41.80
 C       5.431294    -2.124150    -0.979209      85.55
 H       5.675284    -3.293809    -1.339392      24.13
 O       6.179229    -1.029253    -1.424336     230.33
 H       5.891697    -0.318900    -0.820521      29.34
 C       3.911063    -2.008829    -1.286824      68.91
 H       3.459531    -2.949740    -0.835029      21.58
 C       3.667950    -1.976840    -2.901291      84.51
 O       3.511873    -3.399944    -3.486424     265.88
 H       4.144960    -3.433802    -4.273255      24.44
 H       4.395079    -1.346566    -3.507560      23.95
 H       2.791243    -1.228261    -2.991146      24.15
 C      -0.149082    -1.339758     0.266692      29.81
 H      -0.808833    -2.159369     0.534515      18.68
 C       0.326564     1.099336     0.093338      59.39
 H      -0.106627     2.056838    -0.021833      15.95
 C       1.574955     0.869925    -0.433827      11.70
 O       2.452779     1.840881    -0.803976     245.57
 C       2.024591     3.162269    -0.680084     109.49
 H       2.541320     3.825321    -1.436866      24.17
 H       0.880986     3.145612    -1.277621      23.35
 H       1.887844     3.544770     0.255930      29.38
 C       1.965461    -0.509414    -0.511325      12.14
 O       3.388071    -0.672584    -0.831081     100.50
 C       1.116790    -1.623530    -0.164385      52.72
 H       1.381466    -2.712554    -0.172779      20.24
 C      -0.560073     0.044731     0.370805      69.93
 C      -1.895372     0.341647     0.938436      84.31
 H      -2.326424    -0.700784     1.204077      25.10
 O      -1.862762     1.393416     2.169636     191.83
 H      -1.423353     0.840154     2.893100      25.18
 C      -3.006127     0.848312    -0.095534      94.70
 H      -2.446989     1.824798    -0.366305      23.82
 O      -3.013285    -0.168918    -1.098140     250.26
 H      -3.070111     0.183701    -1.990648      24.41
 C      -4.376911     1.153754     0.406056      90.94
 O      -5.254808     1.832690    -0.480661     261.52
 H      -5.175008     2.745345    -0.228425      31.52
 H      -4.286125     1.793681     1.371262      25.65
 H      -4.903244     0.007555     0.696457      25.57
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name = lig-etoh-Waterframe_438
 C       6.262067    -1.529100     1.376252      63.69
 H       6.511736    -0.500563     1.085983      21.37
 C       5.732760    -3.895810     0.927356      49.08
 H       5.427353    -4.671825     0.214451      12.12
 C       6.007716    -4.211729     2.294635      18.07
 O       5.945060    -5.494147     2.934543     255.82
 C       5.285152    -6.471976     2.097244     122.55
 H       6.058787    -6.673080     1.281376      31.06
 H       4.313453    -6.181273     1.751877      29.78
 H       5.042215    -7.505428     2.718437      25.34
 C       6.362698    -3.143620     3.189516      -0.30
 O       6.526075    -3.382148     4.552893     198.53
 H       6.249507    -4.337347     4.693846      25.59
 C       6.485965    -1.848887     2.681491      70.48
 H       6.792053    -1.139892     3.438970      24.79
 C       5.730847    -2.471203     0.511075      58.83
 C       5.446959    -2.194868    -0.932240     104.17
 H       5.960157    -2.996516    -1.778239      23.13
 O       6.220290    -1.067535    -1.419354     221.41
 H       6.113656    -0.309801    -0.846269      28.57
 C       3.928012    -1.984402    -1.385785      80.65
 H       3.192251    -2.760817    -0.897077      21.34
 C       3.639865    -1.974560    -2.888918     103.64
 O       3.525263    -3.303249    -3.530344     280.46
 H       4.174513    -3.452598    -4.277208      25.76
 H       4.501238    -1.580989    -3.408836      25.64
 H       2.676300    -1.568832    -3.036556      25.50
 C      -0.226024    -1.345817     0.224968      24.72
 H      -0.952040    -2.164798     0.550681      18.34
 C       0.297998     1.105749     0.124924      74.03
 H      -0.252145     2.115799     0.109903      16.85
 C       1.587140     0.832161    -0.386432       5.77
 O       2.482426     1.802785    -0.771374     208.97
 C       2.070016     3.204877    -0.721907      98.11
 H       2.894200     3.676616    -1.341200      22.53
 H       0.818834     3.316427    -1.010075      21.19
 H       2.022968     3.635535     0.224684      27.62
 C       2.080542    -0.528317    -0.509949      23.84
 O       3.374973    -0.711653    -0.822389     152.69
 C       1.128538    -1.541981    -0.194994      54.77
 H       1.463596    -2.666627    -0.174378      20.11
 C      -0.578664    -0.009787     0.336350      50.87
 C      -1.948184     0.295865     1.010216      83.04
 H      -2.512504    -0.597814     1.521650      22.53
 O      -1.809282     1.311953     2.062226     227.05
 H      -1.483090     0.823861     2.992631      24.60
 C      -2.932467     0.912624    -0.098797      75.59
 H      -2.515285     1.822347    -0.686403      23.51
 O      -3.058732    -0.187612    -1.127012     240.12
 H      -3.141401     0.124868    -2.060970      25.19
 C      -4.430071     1.091978     0.487863      99.30
 O      -5.238587     1.826378    -0.548237     244.04
 H      -5.397650     2.698874    -0.237540      31.62
 H      -4.335213     1.637604     1.445343      28.13
 H      -5.051201     0.237415     0.636897      28.86
55
name = lig-etoh-Waterframe_439
 C       6.269250    -1.511641     1.306533      49.18
 H       6.567161    -0.520391     0.965867      22.39
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 C       5.730338    -3.877915     0.941613      62.35
 H       5.478559    -4.486792     0.124170      17.71
 C       5.987018    -4.244839     2.290441      24.63
 O       5.894415    -5.477381     2.932461     249.55
 C       5.247584    -6.496754     2.083558     125.72
 H       5.835443    -6.691994     1.193756      31.39
 H       4.295793    -6.059994     1.643155      27.45
 H       5.257701    -7.462905     2.782924      25.79
 C       6.357228    -3.139766     3.205840      19.51
 O       6.557766    -3.358155     4.522926     164.96
 H       6.221704    -4.232844     4.913186      24.43
 C       6.483846    -1.833087     2.718074      47.07
 H       6.761335    -0.971303     3.414526      22.41
 C       5.793983    -2.564547     0.479655      48.87
 C       5.450955    -2.205872    -0.987044     105.03
 H       5.746691    -3.039313    -1.626680      25.17
 O       6.285035    -1.071389    -1.420643     238.95
 H       5.961629    -0.239498    -1.106653      26.23
 C       3.887212    -1.995782    -1.418808      79.17
 H       3.326542    -2.925583    -0.993081      21.81
 C       3.643893    -1.980844    -2.939598     114.60
 O       3.517382    -3.249525    -3.538691     292.82
 H       4.329355    -3.424255    -4.086054      24.36
 H       4.373547    -1.270398    -3.308131      27.26
 H       2.727769    -1.517843    -3.130881      27.29
 C      -0.210352    -1.308830     0.169728      59.80
 H      -0.859283    -2.234487     0.443942      24.90
 C       0.225481     1.042645     0.101893      65.91
 H       0.107345     2.178406     0.497312      18.98
 C       1.599786     0.787925    -0.335246     -11.34
 O       2.518788     1.772771    -0.741718     137.58
 C       2.091945     3.249035    -0.743476     102.30
 H       2.820521     3.795062    -1.382414      25.75
 H       1.181914     3.583953    -1.289675      26.50
 H       2.441045     3.565447     0.345207      25.02
 C       2.066801    -0.559327    -0.467487      15.51
 O       3.441066    -0.743915    -0.833708     136.35
 C       1.158258    -1.542800    -0.221003      68.62
 H       1.669303    -2.572564    -0.348017      22.84
 C      -0.673209    -0.026643     0.408866      17.55
 C      -2.029502     0.316316     1.032376      94.40
 H      -2.399589    -0.641553     1.473991      24.29
 O      -1.760651     1.245261     1.971901     253.88
 H      -1.536312     0.589824     2.892854      22.59
 C      -2.947339     0.857635    -0.102275      86.06
 H      -2.761841     1.827589    -0.565591      26.06
 O      -3.109199    -0.201650    -1.139079     254.64
 H      -3.000556     0.200970    -2.064458      25.28
 C      -4.439831     1.101565     0.508918     100.10
 O      -5.225911     1.822545    -0.590622     224.54
 H      -5.277589     2.693600    -0.234646      31.62
 H      -4.511187     1.620701     1.419913      29.22
 H      -4.759448     0.177013     0.628013      31.51
55
name = lig-etoh-Waterframe_440
 C       6.281715    -1.541939     1.332794      56.72
 H       6.318477    -0.587620     0.829508      21.60
 C       5.700054    -3.904211     0.947804      51.90
 H       5.471154    -4.772525     0.383947      24.42
 C       5.982618    -4.181500     2.316387      18.51
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 O       5.831964    -5.465989     2.882648     259.94
 C       5.248203    -6.506500     2.053044     140.95
 H       5.755398    -6.807057     1.202744      29.71
 H       4.113815    -6.256258     1.887109      24.02
 H       5.116157    -7.361156     2.708019      24.76
 C       6.314696    -3.174163     3.170096      20.82
 O       6.597477    -3.328291     4.550837     234.89
 H       6.397827    -4.283107     4.905786      25.58
 C       6.486424    -1.794875     2.683422      50.74
 H       6.811297    -0.959371     3.427469      24.06
 C       5.869968    -2.571348     0.428301      39.90
 C       5.450928    -2.193362    -1.074541      98.42
 H       5.640838    -3.069002    -1.514463      24.04
 O       6.321580    -1.065825    -1.442592     271.99
 H       5.717324    -0.382185    -1.325083      27.16
 C       3.894750    -2.050417    -1.383804      79.81
 H       3.485251    -2.948300    -0.978033      23.26
 C       3.630409    -1.882614    -2.975238      89.12
 O       3.531779    -3.253190    -3.539342     276.79
 H       4.288997    -3.458659    -4.185631      23.85
 H       4.359989    -1.263769    -3.554998      25.22
 H       2.671609    -1.280001    -3.022570      25.69
 C      -0.135520    -1.336698     0.128507      40.82
 H      -0.761790    -2.277310     0.280887      25.99
 C       0.266701     0.983237     0.098443      69.63
 H       0.033322     2.033687     0.589246      19.73
 C       1.561329     0.780655    -0.300320      15.12
 O       2.503766     1.787475    -0.731234     165.76
 C       2.213708     3.251048    -0.766932     110.67
 H       2.960174     3.632971    -1.430108      24.51
 H       1.292517     3.383995    -1.049336      29.37
 H       2.055977     3.790363     0.407357      23.66
 C       2.074325    -0.531778    -0.447695       3.25
 O       3.476230    -0.764421    -0.832768      96.25
 C       1.166360    -1.624754    -0.240509      52.89
 H       1.325796    -2.709641    -0.397232      21.22
 C      -0.691514    -0.013277     0.434952      31.66
 C      -2.064766     0.255471     0.914384      99.32
 H      -2.540415    -0.626186     1.227735      25.19
 O      -1.745862     1.250594     2.007928     211.94
 H      -1.353913     0.693934     2.954313      22.77
 C      -3.092786     0.799191    -0.080237     106.87
 H      -2.522711     1.651576    -0.363895      26.46
 O      -3.158788    -0.189295    -1.125420     264.33
 H      -2.894858     0.187632    -2.046493      24.40
 C      -4.425981     1.111778     0.427149     103.51
 O      -5.203650     1.806647    -0.571247     250.45
 H      -5.008254     2.713864    -0.387103      32.30
 H      -4.475312     1.690370     1.329503      27.61
 H      -4.854876    -0.020426     0.627429      26.14
55
name = lig-etoh-Waterframe_441
 C       6.258332    -1.580291     1.301724      50.75
 H       6.239306    -0.524261     1.060011      21.63
 C       5.691417    -3.918106     0.939319      29.90
 H       5.354947    -4.804340     0.378791      19.49
 C       5.933348    -4.161523     2.291534      13.57
 O       5.786949    -5.459711     2.819874     242.50
 C       5.192262    -6.536345     2.070653     147.62
 H       5.789185    -6.736970     1.176700      30.82
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 H       4.109408    -6.318531     1.740140      26.93
 H       5.255258    -7.328634     2.682500      25.65
 C       6.331502    -3.072899     3.228982      20.30
 O       6.631983    -3.303677     4.567049     163.80
 H       6.528022    -4.308454     4.768404      27.29
 C       6.487757    -1.839969     2.666114      58.39
 H       6.827970    -1.052031     3.407842      22.96
 C       5.879405    -2.591697     0.385857      23.61
 C       5.497398    -2.216929    -1.072541      79.67
 H       5.874690    -3.106067    -1.912589      21.32
 O       6.286992    -1.073256    -1.499394     232.20
 H       5.877948    -0.236246    -1.417032      27.65
 C       3.980429    -2.029321    -1.408271      81.91
 H       3.384263    -2.760230    -1.011454      24.36
 C       3.621383    -1.833012    -2.953790      84.64
 O       3.520678    -3.249734    -3.519281     281.33
 H       4.121888    -3.267673    -4.333630      25.12
 H       4.499847    -1.441023    -3.514552      23.15
 H       2.518846    -1.449290    -3.106821      22.51
 C      -0.157614    -1.373208     0.142152      52.86
 H      -0.852312    -2.188763     0.255661      19.61
 C       0.266687     1.011747     0.185924      60.80
 H      -0.172425     2.007714     0.220343      19.88
 C       1.618652     0.793555    -0.325929      -6.80
 O       2.478202     1.797732    -0.700156     207.98
 C       2.252265     3.195125    -0.754348     111.76
 H       3.048618     3.605798    -1.321767      24.32
 H       1.198747     3.261182    -1.212822      23.82
 H       2.322605     3.821340     0.252429      24.30
 C       2.132687    -0.607589    -0.468479      13.65
 O       3.434582    -0.760968    -0.787647     145.28
 C       1.193807    -1.665878    -0.271321      63.14
 H       1.408743    -2.673603    -0.460457      23.81
 C      -0.572730    -0.117957     0.325140      37.48
 C      -2.065835     0.172013     0.912949      82.45
 H      -2.460149    -0.708257     1.403933      24.72
 O      -1.791611     1.260952     2.063849     178.34
 H      -1.378859     0.552834     2.828997      23.42
 C      -3.066265     0.805923    -0.107111      92.20
 H      -2.660866     1.732074    -0.586656      24.14
 O      -3.216331    -0.192375    -1.130469     254.26
 H      -2.986295     0.189492    -2.075223      23.58
 C      -4.476538     1.083864     0.394964      94.21
 O      -5.201067     1.820760    -0.560160     259.82
 H      -4.785437     2.662219    -0.639934      34.12
 H      -4.226661     1.644718     1.361698      26.35
 H      -5.392659     0.233435     0.678151      24.26
55
name = lig-etoh-Waterframe_442
 C       6.213129    -1.597943     1.255021      37.33
 H       6.315939    -0.552980     0.942462      21.84
 C       5.690108    -3.896226     0.905807      35.04
 H       5.284951    -4.587928     0.102999      13.42
 C       5.875001    -4.150787     2.298271      42.64
 O       5.754066    -5.426230     2.804637     240.58
 C       5.152384    -6.563351     2.058052     122.91
 H       5.804044    -6.712434     1.088604      31.59
 H       4.152035    -6.348887     1.704795      32.17
 H       5.295892    -7.407990     2.703567      26.70
 C       6.343547    -3.115795     3.255128      15.88
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 O       6.664573    -3.284647     4.564644      97.42
 H       6.482758    -4.241172     4.898596      24.60
 C       6.503169    -1.841956     2.668185      59.35
 H       6.800000    -0.970957     3.211878      23.61
 C       5.839416    -2.624483     0.369271      15.41
 C       5.550087    -2.215204    -1.077406      53.73
 H       5.945926    -3.135288    -1.931979      24.34
 O       6.254981    -1.063014    -1.585246     210.27
 H       5.957993    -0.276112    -1.077427      27.48
 C       3.991208    -1.954395    -1.450863      78.44
 H       3.449308    -2.854187    -1.092027      21.78
 C       3.651088    -1.926019    -2.918818      98.65
 O       3.472931    -3.224802    -3.474149     284.25
 H       4.200949    -3.387649    -4.207818      23.11
 H       4.334778    -1.160211    -3.374823      23.39
 H       2.725716    -1.228190    -3.095413      23.77
 C      -0.129189    -1.506777     0.134334      34.66
 H      -0.823663    -2.243186     0.353840      18.74
 C       0.338697     1.033949     0.184982      71.37
 H      -0.095912     1.929851     0.058474      19.87
 C       1.609215     0.766486    -0.317355       2.27
 O       2.522052     1.753952    -0.663805     194.98
 C       2.214073     3.160214    -0.742439     117.67
 H       3.004552     3.535692    -1.402964      24.58
 H       1.310997     3.680750    -1.478777      22.49
 H       2.313386     3.496455     0.166522      28.11
 C       2.090691    -0.646260    -0.474774      13.78
 O       3.460136    -0.750179    -0.745261     169.22
 C       1.211203    -1.689458    -0.300036      61.84
 H       1.666686    -2.596108    -0.452255      21.07
 C      -0.590875    -0.114371     0.295496      36.23
 C      -1.957343     0.195889     0.978842      82.76
 H      -2.359907    -0.776371     1.446969      22.13
 O      -1.871096     1.186581     2.063813     262.10
 H      -1.544925     0.702124     2.902040      25.74
 C      -3.008215     0.744662    -0.149845      78.55
 H      -2.846379     1.786572    -0.535439      23.20
 O      -3.262926    -0.235005    -1.188118     243.47
 H      -3.151176     0.144690    -2.177493      21.25
 C      -4.535446     1.109208     0.474845      81.35
 O      -5.229560     1.886409    -0.593747     254.55
 H      -4.688018     2.632558    -0.764065      33.59
 H      -4.456752     1.756578     1.422650      25.85
 H      -5.031043     0.059133     0.668582      26.15
55
name = lig-etoh-Waterframe_443
 C       6.201278    -1.595135     1.284414      59.54
 H       6.403868    -0.658885     0.768501      24.00
 C       5.656563    -3.881962     0.869594      55.07
 H       5.356568    -4.830893     0.288108      10.39
 C       5.833941    -4.153578     2.284454      56.11
 O       5.707721    -5.430625     2.836253     271.56
 C       5.171086    -6.533864     2.014420     129.42
 H       5.788603    -6.818501     1.039548      31.47
 H       4.147628    -6.398555     1.863768      31.28
 H       5.082921    -7.465988     2.750594      26.38
 C       6.333520    -3.183172     3.167154      -6.02
 O       6.690653    -3.286602     4.577029     196.31
 H       6.458573    -4.184781     4.973937      24.48
 C       6.495494    -1.811981     2.599446      69.22
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 H       6.819224    -1.039111     3.203610      26.18
 C       5.806352    -2.563220     0.364926      26.54
 C       5.523504    -2.188362    -1.149165      74.36
 H       5.751140    -3.133898    -1.594470      24.23
 O       6.252680    -1.027553    -1.643155     238.81
 H       6.056510    -0.395773    -0.919325      27.73
 C       3.969666    -1.961963    -1.404256      65.64
 H       3.558818    -2.969079    -0.946618      19.44
 C       3.677809    -1.886658    -2.913436      95.00
 O       3.434237    -3.219248    -3.437393     285.81
 H       4.243007    -3.523296    -3.961100      25.06
 H       4.491480    -1.474452    -3.564930      22.22
 H       2.687490    -1.458436    -2.896682      25.46
 C      -0.120336    -1.507278     0.132002      45.60
 H      -0.616316    -2.396723     0.380772      17.92
 C       0.325844     0.955848     0.103796      54.17
 H       0.108828     1.974355     0.241961      17.39
 C       1.631359     0.698959    -0.309979      16.62
 O       2.564469     1.677584    -0.664790     199.47
 C       2.210998     3.173563    -0.776253      95.29
 H       3.168588     3.518975    -1.225211      20.66
 H       1.038679     3.322892    -1.131432      22.11
 H       2.063667     3.573564     0.210783      25.82
 C       2.051529    -0.575414    -0.474417      14.81
 O       3.515874    -0.760375    -0.723058     135.19
 C       1.225253    -1.752598    -0.314514      55.37
 H       1.603197    -2.768519    -0.351413      16.42
 C      -0.562034    -0.116343     0.363587      72.38
 C      -1.881876     0.224586     0.978632      98.15
 H      -2.352057    -0.807295     1.233194      23.54
 O      -1.955660     1.109020     2.050651     298.83
 H      -1.643722     0.660407     2.778338      28.67
 C      -3.069825     0.711524    -0.106748      66.24
 H      -2.391348     1.515442    -0.544216      21.90
 O      -3.295313    -0.284071    -1.232021     201.48
 H      -3.177748     0.158576    -2.209880      20.78
 C      -4.485966     1.133489     0.496932     101.99
 O      -5.258982     1.911271    -0.608034     253.69
 H      -4.729768     2.687061    -0.651226      32.34
 H      -4.668648     1.705944     1.418734      26.71
 H      -4.940354     0.256047     0.580801      29.79
55
name = lig-etoh-Waterframe_444
 C       6.215010    -1.531001     1.240877      44.08
 H       6.460447    -0.505720     1.024056      21.45
 C       5.604222    -3.885076     0.887461      31.74
 H       5.423542    -4.771307     0.213034      15.52
 C       5.822596    -4.183395     2.238881      55.18
 O       5.660579    -5.466359     2.858340     254.47
 C       5.154579    -6.509906     2.018514     126.57
 H       5.791278    -6.713146     1.116027      32.53
 H       4.168192    -6.249678     1.641569      27.39
 H       5.271030    -7.463244     2.763440      24.76
 C       6.342431    -3.116869     3.120675      19.00
 O       6.688852    -3.292899     4.516624     108.52
 H       6.570836    -4.236823     4.788840      26.25
 C       6.484318    -1.879662     2.621630      57.50
 H       6.889876    -1.177456     3.303412      26.67
 C       5.760828    -2.543948     0.341779      33.00
 C       5.451143    -2.165287    -1.142682      82.82
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 H       5.705824    -2.910717    -1.771183      28.32
 O       6.265031    -1.034879    -1.667495     165.10
 H       6.116028    -0.102039    -1.293387      24.82
 C       4.000880    -2.006228    -1.338367      77.32
 H       3.312088    -2.835785    -0.914637      20.58
 C       3.653679    -1.868131    -2.902269      93.62
 O       3.401156    -3.267404    -3.390766     286.97
 H       4.154211    -3.474399    -4.031458      25.05
 H       4.464845    -1.406513    -3.488109      23.72
 H       2.793231    -1.317413    -3.131098      25.95
 C      -0.078363    -1.441106     0.143615      49.02
 H      -0.785939    -2.265666     0.389121      20.87
 C       0.298402     0.899630     0.027394      97.21
 H       0.030090     1.883575     0.568891      18.51
 C       1.668609     0.706419    -0.340664       4.54
 O       2.595946     1.657123    -0.675888     161.85
 C       2.171981     3.083790    -0.727365      97.59
 H       2.837896     3.778773    -1.366421      23.70
 H       1.366877     3.007531    -1.421008      26.29
 H       2.052205     3.693999     0.368886      22.75
 C       2.161191    -0.706926    -0.506963      12.33
 O       3.511976    -0.772659    -0.696835     182.82
 C       1.211840    -1.721653    -0.289739      61.25
 H       1.493062    -2.827766    -0.364426      18.81
 C      -0.503834    -0.168869     0.431309      38.04
 C      -1.998731     0.103188     0.901144      81.05
 H      -2.274518    -0.876616     1.338125      21.70
 O      -2.019587     1.064484     2.068483     301.46
 H      -1.639340     0.566196     2.707966      28.44
 C      -3.039188     0.714838    -0.092122      82.79
 H      -2.606947     1.572700    -0.703479      22.87
 O      -3.330598    -0.316871    -1.191885     210.48
 H      -3.107624     0.157091    -2.120932      22.26
 C      -4.446044     1.153305     0.402854     108.57
 O      -5.238076     1.900505    -0.573157     253.99
 H      -5.012105     2.818409    -0.506698      31.65
 H      -4.277303     1.631317     1.363363      27.20
 H      -5.111497     0.350534     0.544733      28.79
55
name = lig-etoh-Waterframe_445
 C       6.232060    -1.519852     1.238873      49.01
 H       6.303551    -0.478834     0.860187      22.92
 C       5.557089    -3.867536     0.874929      56.56
 H       5.291619    -4.509949     0.067809      18.55
 C       5.845042    -4.196261     2.258050      24.08
 O       5.632961    -5.440246     2.862837     258.45
 C       5.156772    -6.508670     2.010649     132.49
 H       5.866557    -6.579382     1.284121      32.01
 H       4.132098    -6.320648     1.539654      28.01
 H       5.058402    -7.510328     2.575066      23.45
 C       6.315387    -3.181057     3.137206      23.16
 O       6.672277    -3.309380     4.395311     156.69
 H       6.637153    -4.239430     4.703417      29.11
 C       6.494253    -1.856069     2.593922      63.01
 H       6.933673    -1.100539     3.301079      27.02
 C       5.754210    -2.517014     0.366803      44.76
 C       5.454107    -2.149199    -1.079414      74.81
 H       5.797820    -2.938310    -1.944088      23.98
 O       6.283333    -1.054163    -1.683933     175.44
 H       5.734564    -0.183412    -1.499254      26.82
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 C       3.912296    -1.981015    -1.374127      82.44
 H       3.496599    -2.927843    -0.966825      19.44
 C       3.616348    -1.906252    -2.879066     100.19
 O       3.386249    -3.305288    -3.347034     298.74
 H       4.003570    -3.477400    -4.102057      26.89
 H       4.503974    -1.418366    -3.256477      23.27
 H       2.837133    -1.194252    -3.127981      26.02
 C      -0.078309    -1.441689     0.195396      30.86
 H      -0.887480    -2.272982     0.270206      18.51
 C       0.367092     0.918995     0.042261     116.05
 H      -0.143891     1.984559     0.318784      16.72
 C       1.667118     0.627063    -0.394982       5.97
 O       2.648741     1.690696    -0.673791     217.77
 C       2.099036     2.981297    -0.745502     106.78
 H       2.935214     3.555617    -1.277469      22.74
 H       1.241790     3.075447    -1.261838      28.21
 H       1.822225     3.363053     0.449352      22.74
 C       2.189754    -0.726579    -0.498175      22.11
 O       3.525693    -0.808097    -0.679637     196.15
 C       1.249600    -1.718472    -0.266177      62.39
 H       1.484299    -2.844509    -0.490736      19.39
 C      -0.560784    -0.169408     0.436866      94.84
 C      -2.098839    -0.003475     0.895680      75.20
 H      -2.577234    -0.910756     1.192576      24.89
 O      -2.070577     0.996445     2.067240     256.89
 H      -1.576494     0.512747     2.856002      23.86
 C      -3.020752     0.673586    -0.210273      95.43
 H      -2.698102     1.660504    -0.531109      24.36
 O      -3.348480    -0.338299    -1.113096     243.35
 H      -3.088957    -0.127896    -2.112892      22.44
 C      -4.399802     1.152586     0.352455      91.83
 O      -5.190562     1.916262    -0.540877     248.76
 H      -5.170973     2.820505    -0.268785      31.80
 H      -4.095954     1.780460     1.180820      26.52
 H      -5.054816     0.142227     0.752924      26.19
55
name = lig-etoh-Waterframe_446
 C       6.229281    -1.519585     1.264982      65.56
 H       6.295119    -0.526557     0.784330      22.36
 C       5.533588    -3.806234     0.853459     114.12
 H       5.095969    -4.576415     0.309540      19.96
 C       5.828454    -4.197443     2.215898      39.15
 O       5.595162    -5.416739     2.880886     239.07
 C       5.172727    -6.519609     1.963032     145.00
 H       5.891083    -6.729174     1.218597      34.14
 H       4.134081    -6.222654     1.518960      23.30
 H       5.023406    -7.326976     2.588255      22.31
 C       6.286077    -3.167793     3.028275      26.62
 O       6.681216    -3.359498     4.366015     250.52
 H       6.494231    -4.219898     4.808058      27.86
 C       6.510391    -1.824820     2.555754      59.65
 H       6.880162    -0.997979     3.279606      24.31
 C       5.766564    -2.511295     0.418619      24.85
 C       5.483409    -2.165568    -1.120359      76.62
 H       5.738319    -3.382348    -1.433358      20.13
 O       6.258761    -1.067849    -1.666458     238.39
 H       5.715472    -0.181826    -1.421651      23.48
 C       3.902593    -2.016175    -1.400067      85.40
 H       3.490867    -2.866921    -0.963313      20.82
 C       3.611767    -1.947389    -2.868099      97.30
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 O       3.367321    -3.313852    -3.315724     291.26
 H       4.087625    -3.490787    -3.970600      26.74
 H       4.502222    -1.696419    -3.443075      22.60
 H       2.596573    -1.412219    -3.036758      23.87
 C      -0.086925    -1.492768     0.226992      33.43
 H      -0.653566    -2.499935     0.260781      18.54
 C       0.344046     0.907032     0.128021      66.49
 H       0.195819     1.986760    -0.236247      17.04
 C       1.680669     0.631893    -0.420204      14.13
 O       2.626278     1.619547    -0.675281     205.08
 C       2.033922     2.941412    -0.748218     120.70
 H       2.853143     3.597014    -0.955225      25.24
 H       1.001386     3.093126    -1.226166      24.06
 H       1.823457     3.238392     0.265614      26.79
 C       2.113023    -0.652261    -0.438311      17.50
 O       3.540522    -0.847167    -0.673297     177.17
 C       1.250193    -1.770112    -0.238276      46.89
 H       1.595313    -2.839655    -0.490997      18.85
 C      -0.632526    -0.131696     0.385420      40.56
 C      -2.105476     0.038264     0.921681      76.66
 H      -2.572260    -0.919396     1.027432      25.30
 O      -2.128693     0.889958     2.033329     214.82
 H      -1.592370     0.307944     2.921253      19.93
 C      -3.046260     0.677426    -0.250362      93.37
 H      -2.341020     1.312928    -0.769388      23.98
 O      -3.350112    -0.419335    -1.127438     232.55
 H      -3.072137    -0.204030    -2.089327      25.07
 C      -4.308296     1.149053     0.409245      89.88
 O      -5.167128     1.944631    -0.546289     245.23
 H      -5.029876     2.776548    -0.114951      29.38
 H      -4.184327     1.802442     1.272704      25.66
 H      -4.931449     0.125991     0.887205      24.86
55
name = lig-etoh-Waterframe_447
 C       6.214527    -1.475472     1.229094      74.96
 H       6.475008    -0.437886     0.973911      22.33
 C       5.496844    -3.836995     0.883718      13.83
 H       4.992685    -4.525540     0.232994      13.77
 C       5.784360    -4.154073     2.162338      33.70
 O       5.559691    -5.410319     2.838861     257.21
 C       5.170839    -6.504054     1.956811     119.08
 H       5.943415    -6.843755     1.142876      32.62
 H       4.241456    -6.199288     1.379960      28.30
 H       5.044648    -7.263338     2.617636      25.09
 C       6.324796    -3.102141     3.012306      43.48
 O       6.695318    -3.390061     4.360402     190.22
 H       6.339648    -4.260130     4.648167      32.12
 C       6.515173    -1.827377     2.594171      49.88
 H       6.857685    -1.063104     3.385156      20.21
 C       5.745011    -2.487755     0.365204      75.33
 C       5.465251    -2.257020    -1.081468     130.71
 H       5.932992    -2.979619    -1.889592      24.94
 O       6.212785    -1.113528    -1.642032     243.33
 H       5.927287    -0.179929    -1.200861      19.50
 C       4.003752    -2.084047    -1.358347      78.95
 H       3.394740    -2.872727    -1.017317      19.33
 C       3.595098    -2.014495    -2.897535      82.69
 O       3.358097    -3.365700    -3.308223     290.75
 H       4.168012    -3.619112    -3.809183      26.55
 H       4.212258    -1.363201    -3.593711      21.25
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 H       2.618400    -1.353303    -3.060980      22.23
 C      -0.085756    -1.529397     0.217463      31.85
 H      -0.790862    -2.318091     0.542095      17.03
 C       0.318762     0.885819     0.106042      69.68
 H      -0.241792     1.851301     0.063221      16.05
 C       1.603098     0.657798    -0.331440      16.14
 O       2.547643     1.557993    -0.712657     196.65
 C       2.003528     2.976672    -0.665536     110.73
 H       2.646745     3.685242    -1.101426      24.29
 H       1.303086     2.921136    -1.717679      21.10
 H       1.680739     3.195175     0.232523      27.52
 C       2.141520    -0.725415    -0.402614      10.29
 O       3.486513    -0.844237    -0.661803     177.96
 C       1.211835    -1.750215    -0.191379      67.00
 H       1.583362    -2.764557    -0.258475      18.41
 C      -0.612031    -0.186695     0.334189      50.36
 C      -2.062769     0.091322     0.836412      82.54
 H      -2.316293    -0.974677     1.129560      20.82
 O      -2.189292     0.794100     2.052222     220.16
 H      -1.596993     0.191455     2.872063      20.55
 C      -2.978146     0.652981    -0.212552      81.16
 H      -2.534371     1.348193    -0.968302      21.77
 O      -3.348781    -0.532367    -1.192892     205.32
 H      -3.170520    -0.137394    -2.073467      24.11
 C      -4.274212     1.202468     0.446920      97.62
 O      -5.130681     1.959425    -0.512840     307.19
 H      -4.930118     2.899025    -0.401845      30.34
 H      -3.987813     1.683233     1.397902      24.63
 H      -4.857289     0.289288     0.632604      26.90
55
name = lig-etoh-Waterframe_448
 C       6.225448    -1.460396     1.231407      56.01
 H       6.442016    -0.460798     0.834233      21.35
 C       5.438783    -3.814616     0.832996      56.19
 H       5.062034    -4.534973     0.060929      18.56
 C       5.762374    -4.113236     2.231516      43.74
 O       5.545593    -5.364873     2.752828     269.27
 C       5.155603    -6.493779     1.948935      81.89
 H       6.155939    -6.694588     1.291435      26.88
 H       4.265705    -6.370284     1.356974      32.90
 H       4.890558    -7.382405     2.571982      25.96
 C       6.362555    -3.144795     3.091380      -7.45
 O       6.697545    -3.394011     4.333758     183.42
 H       6.551677    -4.346626     4.590203      26.50
 C       6.490802    -1.787168     2.586348      71.92
 H       6.913504    -1.079120     3.321461      26.45
 C       5.742371    -2.507433     0.360484      59.21
 C       5.498845    -2.256127    -1.123231     123.12
 H       5.753180    -3.021244    -1.720381      25.06
 O       6.175631    -1.124822    -1.608008     305.05
 H       5.913852    -0.305792    -0.988792      21.97
 C       3.977097    -2.109077    -1.373977      61.68
 H       3.503917    -3.052255    -0.949992      13.70
 C       3.556133    -2.008371    -2.889706      79.16
 O       3.380315    -3.442069    -3.329152     277.84
 H       4.127993    -3.629768    -3.956993      26.45
 H       4.350731    -1.464464    -3.505619      19.55
 H       2.503057    -1.655091    -2.764009      22.26
 C      -0.172529    -1.514165     0.235666      46.88
 H      -0.785239    -2.288712     0.599775      21.66
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 C       0.192422     0.881354     0.051610     118.52
 H      -0.185239     1.750206     0.484042      18.23
 C       1.587560     0.566303    -0.234624       0.66
 O       2.480982     1.605451    -0.736089     146.08
 C       2.003114     2.967220    -0.702094      96.66
 H       2.943755     3.552731    -0.865924      22.84
 H       1.031220     3.040584    -1.477176      22.66
 H       1.336095     3.256584     0.174278      24.29
 C       2.116591    -0.744916    -0.369739      14.95
 O       3.460873    -0.851141    -0.664839     178.88
 C       1.227284    -1.789374    -0.131703      56.93
 H       1.498461    -2.767234    -0.041027      17.17
 C      -0.541569    -0.245340     0.318566      49.98
 C      -1.950651     0.000313     0.753392      73.12
 H      -2.534061    -1.011967     0.884416      19.58
 O      -2.222703     0.743879     2.106267     240.39
 H      -1.599127     0.329894     2.809441      22.84
 C      -2.970929     0.593903    -0.269107      64.04
 H      -2.651481     1.576213    -0.735102      20.93
 O      -3.322840    -0.568643    -1.217287     209.87
 H      -3.241707    -0.282784    -2.118426      23.74
 C      -4.275275     1.218273     0.410642     112.45
 O      -5.073834     1.976789    -0.461390     319.73
 H      -4.748507     2.889102    -0.470430      31.23
 H      -4.028335     1.816606     1.320069      23.48
 H      -4.852615     0.480089     0.644586      28.05
55
name = lig-etoh-Waterframe_449
 C       6.226487    -1.516791     1.234129      46.13
 H       6.346282    -0.532687     0.803199      18.80
 C       5.433818    -3.751023     0.859767      75.37
 H       5.188387    -4.673606     0.250488      20.26
 C       5.713866    -4.082592     2.184450      48.81
 O       5.516867    -5.334964     2.739228     278.64
 C       5.168512    -6.486767     1.905215      85.22
 H       6.052693    -6.852368     1.235711      27.50
 H       4.378179    -6.283987     1.249834      29.95
 H       4.994201    -7.318691     2.747589      24.81
 C       6.333247    -3.127392     3.033197       9.32
 O       6.729548    -3.406412     4.397909     153.04
 H       6.844651    -4.371770     4.657159      22.81
 C       6.471110    -1.793090     2.584724      69.79
 H       6.920090    -1.028460     3.135021      31.44
 C       5.759714    -2.513437     0.379800      58.93
 C       5.475746    -2.229453    -1.147503     108.37
 H       5.735777    -3.217113    -1.516972      20.93
 O       6.175052    -1.080794    -1.592571     306.78
 H       5.751863    -0.240036    -1.090981      21.53
 C       3.899193    -2.108822    -1.393096      69.06
 H       3.452702    -3.035769    -0.834566      12.63
 C       3.491157    -2.080258    -2.799473      92.92
 O       3.423165    -3.493110    -3.368042     285.26
 H       4.084310    -3.470483    -4.102777      26.06
 H       4.197152    -1.527328    -3.457118      20.81
 H       2.551488    -1.631505    -2.999711      23.68
 C      -0.113537    -1.622488     0.235732      42.64
 H      -0.765266    -2.413305     0.451306      21.30
 C       0.225418     0.872969     0.034762      74.42
 H       0.103753     1.832688     0.388926      16.69
 C       1.577560     0.613981    -0.233909       7.30
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 O       2.399839     1.613016    -0.704952     195.05
 C       1.934970     2.950782    -0.755852     113.39
 H       2.874774     3.610217    -0.688487      23.59
 H       1.374428     3.331393    -1.532258      26.48
 H       1.564900     3.295889     0.441439      21.96
 C       2.069460    -0.754549    -0.336002       2.28
 O       3.462349    -0.892540    -0.685333     184.34
 C       1.183876    -1.886735    -0.031808      43.51
 H       1.590895    -2.844837    -0.030511      15.53
 C      -0.634582    -0.220708     0.361407      30.51
 C      -2.023053    -0.103465     0.780718      70.37
 H      -2.396195    -1.178424     0.856778      20.11
 O      -2.207678     0.689899     2.078536     271.56
 H      -1.737169     0.337273     2.741889      27.91
 C      -3.007779     0.586561    -0.328942      71.63
 H      -2.346020     1.254316    -0.968966      19.85
 O      -3.278513    -0.522569    -1.211867     251.72
 H      -3.083670    -0.248321    -2.082997      26.22
 C      -4.263239     1.144698     0.395786      99.19
 O      -5.038271     2.006723    -0.485784     325.31
 H      -4.747089     2.921998    -0.128996      25.92
 H      -3.903162     1.813675     1.223827      20.40
 H      -4.936025     0.376918     0.956575      24.29
55
name = lig-etoh-Waterframe_450
 C       6.211466    -1.539330     1.216579      55.57
 H       6.387981    -0.511343     0.957800      20.36
 C       5.449209    -3.776594     0.885813      43.70
 H       5.100771    -4.543304     0.134897      17.18
 C       5.693996    -4.077268     2.190654      38.47
 O       5.488660    -5.326559     2.746203     269.62
 C       5.209604    -6.472922     1.867833      87.91
 H       5.980880    -6.826761     1.282074      30.51
 H       4.309290    -6.282878     1.284166      32.00
 H       4.870906    -7.297742     2.674172      26.19
 C       6.301588    -3.105852     3.070117      10.64
 O       6.767379    -3.388340     4.426441     202.19
 H       6.674804    -4.399202     4.527482      30.60
 C       6.481514    -1.817878     2.588560      70.71
 H       6.881389    -1.104288     3.231492      27.66
 C       5.732945    -2.472611     0.316249      89.09
 C       5.393790    -2.215495    -1.078249     122.81
 H       5.997162    -3.001217    -1.930875      21.30
 O       6.178360    -1.024531    -1.608531     219.21
 H       5.650496    -0.136959    -1.402820      20.43
 C       3.860015    -2.131483    -1.303178      74.66
 H       3.328359    -3.028246    -0.843815      14.49
 C       3.406902    -2.176636    -2.836175     101.53
 O       3.451970    -3.499575    -3.389113     287.96
 H       4.291264    -3.575267    -3.965684      25.41
 H       4.136295    -1.525354    -3.286606      21.90
 H       2.503888    -1.655442    -3.017415      25.10
 C      -0.149220    -1.634587     0.274567      44.43
 H      -0.827897    -2.480334     0.322274      19.47
 C       0.263938     0.832254     0.115689      76.87
 H      -0.159084     1.862716    -0.030265      17.26
 C       1.564067     0.581625    -0.313610      10.29
 O       2.371964     1.606693    -0.690919     210.08
 C       1.937165     3.026578    -0.705744     100.94
 H       2.901148     3.581981    -0.933105      22.37
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 H       1.415004     3.222976    -1.560364      26.24
 H       1.303211     3.258522     0.322818      21.00
 C       2.056874    -0.783554    -0.306690      10.70
 O       3.416274    -0.917166    -0.697278     200.56
 C       1.272312    -1.907250     0.017213      47.08
 H       1.645137    -2.955029    -0.109053      15.33
 C      -0.650545    -0.296658     0.378957      36.49
 C      -2.203225    -0.146230     0.862341      82.98
 H      -2.492490    -1.118029     1.121833      25.71
 O      -2.187380     0.629002     1.983481     272.43
 H      -1.715900     0.153894     2.748680      26.15
 C      -2.987777     0.521797    -0.297663      94.70
 H      -2.429151     1.345453    -0.821585      22.41
 O      -3.256597    -0.494862    -1.239516     265.03
 H      -3.012093    -0.198750    -2.108720      26.01
 C      -4.214645     1.124331     0.371198      83.99
 O      -5.010775     2.023453    -0.522445     232.30
 H      -5.168028     2.878531     0.031783      25.49
 H      -3.715683     1.649332     1.207229      22.50
 H      -4.887022     0.116511     0.892982      24.33
55
name = lig-etoh-Waterframe_451
 C       6.215935    -1.474989     1.234020      55.53
 H       6.422995    -0.484155     0.846121      21.10
 C       5.461186    -3.772093     0.798684      46.92
 H       4.963114    -4.533806     0.174766      14.75
 C       5.720019    -4.093366     2.274074      50.00
 O       5.470488    -5.352821     2.764218     247.28
 C       5.197506    -6.452653     1.875884     117.35
 H       6.047500    -6.604100     1.329983      33.47
 H       4.289166    -6.249607     1.179326      28.73
 H       4.942087    -7.355883     2.472563      24.70
 C       6.281422    -3.117588     3.173539      20.49
 O       6.774258    -3.378659     4.379594     220.26
 H       6.444173    -4.285840     4.727221      32.53
 C       6.500381    -1.842341     2.580477      59.58
 H       6.872150    -1.107648     3.297028      21.61
 C       5.698227    -2.504733     0.344915      25.73
 C       5.379730    -2.119732    -1.119902      82.68
 H       5.653569    -3.145555    -1.886423      21.57
 O       6.131486    -0.975959    -1.628588     267.82
 H       5.679874    -0.068693    -1.392088      23.05
 C       3.794926    -2.193933    -1.267546      69.78
 H       3.492522    -3.060611    -0.702176      17.24
 C       3.396259    -2.191172    -2.855942      93.48
 O       3.472875    -3.516758    -3.397660     266.74
 H       4.419050    -3.692074    -3.710139      25.19
 H       4.092872    -1.548432    -3.378591      22.93
 H       2.288891    -1.993253    -2.807632      23.83
 C      -0.138624    -1.637936     0.318321      42.96
 H      -0.848827    -2.507709     0.396730      20.01
 C       0.180948     0.722583     0.194274      66.03
 H      -0.450961     1.619184    -0.241215      18.04
 C       1.506931     0.515082    -0.351003      -5.81
 O       2.421387     1.618751    -0.698556     129.63
 C       1.940443     3.058903    -0.681345     103.99
 H       2.882203     3.621226    -0.755342      23.82
 H       1.076483     3.013690    -1.510317      22.64
 H       1.410140     3.454812     0.098441      26.85
 C       2.106024    -0.812763    -0.301704      21.75
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 O       3.359539    -0.904778    -0.697602     185.77
 C       1.269811    -1.856035     0.031136      57.79
 H       1.619767    -2.967758    -0.062747      18.57
 C      -0.656119    -0.402659     0.401587      33.13
 C      -2.197700    -0.217839     0.846462      87.30
 H      -2.797712    -1.073497     0.999576      25.53
 O      -2.179641     0.634302     1.975684     215.29
 H      -1.522358     0.154344     2.780296      22.27
 C      -2.978365     0.488435    -0.228407      99.28
 H      -2.449947     1.383905    -0.451691      24.45
 O      -3.252584    -0.518272    -1.299672     237.79
 H      -3.118277    -0.155620    -2.240230      22.75
 C      -4.198196     1.139959     0.328455     104.10
 O      -4.989635     1.963489    -0.538483     248.72
 H      -5.114332     2.864456    -0.045675      26.88
 H      -4.046466     1.703116     1.231734      24.98
 H      -4.987829     0.270651     0.552480      24.94
55
name = lig-etoh-Waterframe_452
 C       6.215444    -1.482415     1.257526      52.03
 H       6.428778    -0.500091     0.831820      23.86
 C       5.476809    -3.807212     0.892026      -9.70
 H       5.054905    -4.565743     0.260558      11.55
 C       5.722116    -4.102941     2.212096      45.97
 O       5.443906    -5.385740     2.828359     249.48
 C       5.185029    -6.433702     1.861314     129.44
 H       6.123367    -6.545826     1.184745      31.25
 H       4.335867    -6.173732     1.103941      24.72
 H       5.100619    -7.292698     2.408785      23.46
 C       6.239189    -3.133071     3.103016      18.08
 O       6.777795    -3.388955     4.404122     271.57
 H       6.457810    -4.240153     4.873477      30.62
 C       6.514181    -1.826951     2.589356      65.29
 H       6.982852    -1.004980     3.229375      23.27
 C       5.714975    -2.439101     0.377689       3.23
 C       5.345722    -2.092821    -1.157882      94.90
 H       5.711008    -2.890652    -1.615654      24.71
 O       6.046015    -0.948158    -1.655815     299.34
 H       5.734424    -0.178652    -1.093180      25.34
 C       3.826073    -2.165301    -1.323152      88.70
 H       3.492424    -2.987857    -0.773667      21.22
 C       3.381403    -2.216649    -2.761280      91.33
 O       3.497161    -3.567416    -3.381961     254.31
 H       4.386163    -3.625139    -3.906958      23.12
 H       3.691552    -1.389375    -3.433555      23.45
 H       2.218288    -1.969783    -2.899012      23.34
 C      -0.083679    -1.754102     0.365226      39.81
 H      -0.681816    -2.694495     0.631601      20.21
 C       0.108857     0.614423     0.134470      58.23
 H      -0.318367     1.732921     0.194561      16.78
 C       1.453155     0.537691    -0.301548       9.88
 O       2.432332     1.607296    -0.670508     176.75
 C       1.912410     2.994333    -0.678214     113.84
 H       2.692644     3.693004    -0.937702      24.48
 H       1.187361     3.377521    -1.691512      22.15
 H       1.608612     3.249497     0.285165      26.24
 C       2.046630    -0.751290    -0.300557      16.63
 O       3.374817    -0.912629    -0.720681     168.68
 C       1.193958    -1.857655     0.025456      62.53
 H       1.675390    -2.919738     0.084481      19.36
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 C      -0.738272    -0.479017     0.462633      50.78
 C      -2.101212    -0.287943     0.805162      80.58
 H      -2.582873    -1.311875     0.937399      22.70
 O      -2.175239     0.662461     2.015276     141.05
 H      -1.449726     0.338610     2.923305      20.70
 C      -2.954443     0.523111    -0.230953      73.82
 H      -2.253202     1.154140    -0.776267      21.78
 O      -3.251539    -0.524407    -1.314171     210.49
 H      -3.133293     0.003171    -2.226454      21.71
 C      -4.336336     1.094470     0.341858     114.94
 O      -4.983927     1.922043    -0.602222     310.36
 H      -4.646340     2.888427    -0.371392      27.09
 H      -4.143639     1.592003     1.276926      25.90
 H      -4.894302     0.341231     0.565977      29.58
55
name = lig-etoh-Waterframe_453
 C       6.226185    -1.498751     1.265390      42.92
 H       6.448790    -0.452985     1.011616      20.30
 C       5.479095    -3.757800     0.909928      58.60
 H       5.223080    -4.503061     0.205824      19.19
 C       5.708817    -4.171472     2.246136      41.21
 O       5.423270    -5.372726     2.853226     251.06
 C       5.214095    -6.420112     1.824965     111.10
 H       6.154878    -6.589439     1.055851      30.14
 H       4.209905    -6.276190     1.366219      25.70
 H       5.027584    -7.298307     2.343947      25.80
 C       6.278181    -3.104711     3.067836      19.06
 O       6.752406    -3.390985     4.419705      95.95
 H       6.539771    -4.378172     4.571347      32.89
 C       6.518087    -1.821067     2.614603      53.85
 H       7.092863    -1.111310     3.330171      26.74
 C       5.699532    -2.437377     0.380295      30.37
 C       5.388571    -2.141234    -1.094303      66.14
 H       5.876127    -2.875992    -1.723617      26.46
 O       5.940199    -0.922183    -1.667540     288.99
 H       5.820290    -0.159359    -1.093942      28.01
 C       3.868532    -2.094388    -1.363132      85.02
 H       3.440554    -2.986332    -0.908544      21.68
 C       3.282364    -2.243599    -2.760343      92.15
 O       3.533486    -3.587272    -3.348086     255.15
 H       4.216781    -3.479675    -4.079207      25.86
 H       3.843363    -1.442924    -3.358006      21.69
 H       2.146203    -2.097502    -2.548355      21.99
 C      -0.169029    -1.846581     0.455122      36.76
 H      -0.606370    -2.831680     0.768450      20.09
 C       0.073017     0.626277     0.069793     103.58
 H      -0.244957     1.522933     0.630815      17.10
 C       1.470320     0.585280    -0.239865       8.13
 O       2.356500     1.577469    -0.641266     179.95
 C       1.921579     2.952869    -0.694451      98.42
 H       2.850483     3.449247    -0.920609      23.28
 H       0.931618     3.077561    -1.369265      22.70
 H       1.504178     3.121333     0.453070      22.41
 C       1.963757    -0.745220    -0.334631      15.90
 O       3.372449    -0.890697    -0.733341     192.08
 C       1.269640    -1.892442    -0.008879      47.37
 H       1.797388    -2.875254     0.062311      17.81
 C      -0.657982    -0.567398     0.460698      37.39
 C      -2.117643    -0.261320     0.871085      69.02
 H      -2.486804    -1.318208     1.208115      19.73
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 O      -2.167261     0.667476     2.022249     245.11
 H      -1.680178     0.147494     2.854765      20.36
 C      -2.954153     0.470995    -0.282072      69.08
 H      -2.407601     1.344067    -0.836703      19.46
 O      -3.267521    -0.511919    -1.269132     242.87
 H      -3.064450    -0.188062    -2.285303      20.82
 C      -4.386590     1.014714     0.362569      86.67
 O      -4.987524     1.923829    -0.692551     274.78
 H      -4.523180     2.845569    -0.651551      28.60
 H      -4.165634     1.570887     1.287527      24.48
 H      -4.978326     0.128647     0.521951      26.89
55
name = lig-etoh-Waterframe_454
 C       6.253720    -1.459332     1.300071      54.05
 H       6.411894    -0.439341     0.908480      21.17
 C       5.468086    -3.749268     0.869292      72.95
 H       5.190704    -4.475170     0.136963      20.96
 C       5.720568    -4.091694     2.306371      22.74
 O       5.424470    -5.379260     2.819051     247.65
 C       5.192637    -6.449706     1.839592      73.40
 H       6.057258    -6.389938     1.023969      29.09
 H       4.317707    -6.207901     1.296973      30.97
 H       5.180811    -7.407119     2.431507      26.49
 C       6.350778    -3.154260     3.140557      -3.61
 O       6.692353    -3.408077     4.383443      69.00
 H       6.746452    -4.409400     4.548451      23.10
 C       6.534728    -1.835923     2.615836      63.73
 H       7.032405    -1.136434     3.355851      26.43
 C       5.702486    -2.458913     0.409522      25.11
 C       5.435729    -2.142216    -1.062297      54.93
 H       5.792169    -3.133469    -1.899376      21.56
 O       5.878770    -0.899626    -1.666846     333.66
 H       5.661483    -0.143123    -1.146239      28.14
 C       3.849130    -2.121049    -1.324605      59.45
 H       3.495344    -3.009824    -0.691520      17.09
 C       3.244780    -2.246685    -2.788024      94.29
 O       3.536013    -3.568309    -3.307308     250.18
 H       4.307796    -3.509108    -3.950523      26.40
 H       3.603717    -1.503309    -3.571642      22.24
 H       2.181670    -2.184491    -2.708611      24.38
 C      -0.075481    -1.910413     0.468776      32.01
 H      -0.850293    -2.652291     0.693066      18.02
 C       0.108314     0.659256     0.124775      65.36
 H      -0.443557     1.456414     0.456926      15.76
 C       1.443009     0.559359    -0.220720      16.03
 O       2.284687     1.522045    -0.617475     213.83
 C       1.880607     2.877748    -0.632617     118.77
 H       2.730618     3.486434    -0.998152      23.31
 H       1.122376     2.907240    -1.249770      27.79
 H       1.546149     3.599446     0.377691      22.00
 C       2.010669    -0.813094    -0.404203      19.55
 O       3.328157    -0.830917    -0.736327     180.47
 C       1.239334    -1.962361     0.014117      59.98
 H       1.824043    -2.817274    -0.093992      19.08
 C      -0.631050    -0.568993     0.446492      36.57
 C      -2.132060    -0.208409     0.949135      81.31
 H      -2.864145    -1.036988     1.203696      19.59
 O      -2.155237     0.658093     2.007796     303.48
 H      -1.747218     0.294641     2.761882      28.56
 C      -3.032292     0.408102    -0.244377      83.35
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 H      -2.528648     1.415172    -0.447515      20.05
 O      -3.288089    -0.549780    -1.248403     253.62
 H      -2.972178    -0.165670    -2.208902      20.13
 C      -4.335599     0.972843     0.277827      86.87
 O      -4.980907     1.878076    -0.755062     237.90
 H      -4.704430     2.841607    -0.449033      26.89
 H      -4.347255     1.541486     1.262619      24.11
 H      -5.270672     0.129646     0.313179      23.11
55
name = lig-etoh-Waterframe_455
 C       6.253779    -1.465944     1.307274      56.95
 H       6.460004    -0.456425     0.917687      24.52
 C       5.478196    -3.776037     0.924027      33.60
 H       5.027952    -4.549572     0.289566      15.79
 C       5.698562    -4.050317     2.216655      31.62
 O       5.445098    -5.369368     2.785563     245.24
 C       5.181105    -6.429222     1.840449     116.98
 H       5.982140    -6.484922     1.146872      33.32
 H       4.257947    -6.409961     1.298569      32.41
 H       5.287828    -7.463324     2.420294      27.08
 C       6.369699    -3.165695     3.104533      -1.18
 O       6.669867    -3.455442     4.442967      68.70
 H       6.711185    -4.426205     4.707846      18.92
 C       6.587183    -1.844963     2.644772      68.31
 H       6.928992    -1.050279     3.276504      23.42
 C       5.762006    -2.419092     0.433287     -11.66
 C       5.347102    -2.089454    -1.116289      74.34
 H       5.936068    -3.086848    -1.664331      21.78
 O       5.878844    -0.897534    -1.658539     321.37
 H       5.460220    -0.243356    -1.138174      26.25
 C       3.817779    -2.143376    -1.268904      69.13
 H       3.344194    -2.979638    -0.627617      19.40
 C       3.250019    -2.252631    -2.783322      96.01
 O       3.539014    -3.565329    -3.290919     266.21
 H       4.439606    -3.603750    -3.709063      26.81
 H       3.500201    -1.419966    -3.447060      24.36
 H       2.223479    -2.174242    -2.789553      26.20
 C      -0.062354    -1.810642     0.436478      42.27
 H      -0.631016    -2.721393     0.570230      17.99
 C       0.084110     0.614651     0.261049      72.81
 H      -0.281036     1.583248     0.005702      15.49
 C       1.411626     0.396076    -0.242429      10.46
 O       2.289899     1.500961    -0.565510     190.29
 C       1.815262     2.896980    -0.606256     108.92
 H       2.587313     3.413937    -1.229403      23.75
 H       1.014146     3.066203    -1.315712      26.06
 H       1.673972     3.189147     0.490610      24.20
 C       1.971888    -0.847742    -0.387466      17.74
 O       3.321729    -0.820176    -0.769282     183.64
 C       1.287564    -2.034964    -0.006974      60.78
 H       1.546704    -3.034825    -0.090325      20.72
 C      -0.687256    -0.538774     0.479541      51.39
 C      -2.176141    -0.257357     0.914960      89.93
 H      -2.556191    -1.248761     1.173457      25.25
 O      -2.136027     0.727333     2.032031     260.36
 H      -1.612155     0.375868     2.716100      29.92
 C      -3.062751     0.424316    -0.113140      95.07
 H      -2.461779     1.099204    -0.715654      23.45
 O      -3.279270    -0.606975    -1.257998     195.25
 H      -3.028977    -0.084761    -2.145553      23.51
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 C      -4.427321     0.956688     0.164979     101.16
 O      -4.929511     1.841837    -0.780100     261.68
 H      -5.147007     2.758699    -0.362820      24.88
 H      -4.271337     1.400181     1.203412      25.99
 H      -5.175766    -0.068772     0.369349      25.46
55
name = lig-etoh-Waterframe_456
 C       6.280029    -1.494816     1.318875      37.09
 H       6.490383    -0.459371     1.039738      21.34
 C       5.472036    -3.708094     0.877324      29.59
 H       4.911124    -4.477797     0.271477      13.38
 C       5.715752    -4.139257     2.223759      44.12
 O       5.457986    -5.325599     2.747743     212.80
 C       5.212301    -6.440163     1.825203     115.56
 H       5.894806    -6.530688     1.097382      38.49
 H       4.144501    -6.441476     1.474688      30.71
 H       5.191023    -7.338764     2.594876      25.87
 C       6.367205    -3.141871     3.097966      17.91
 O       6.660744    -3.498715     4.514706      84.48
 H       6.446871    -4.468490     4.546856      29.96
 C       6.636381    -1.835237     2.665821      66.74
 H       6.996668    -1.151488     3.360979      21.52
 C       5.759507    -2.428125     0.378967       3.87
 C       5.297942    -2.100544    -1.087109     111.59
 H       5.658352    -2.771631    -1.727925      24.09
 O       5.890705    -0.896723    -1.639501     342.63
 H       5.552949    -0.096253    -1.249699      25.93
 C       3.754262    -2.114077    -1.283776      88.57
 H       3.372456    -2.990522    -0.701221      19.63
 C       3.270466    -2.256383    -2.710296      98.32
 O       3.555400    -3.572193    -3.308241     256.59
 H       4.449920    -3.533112    -3.732704      26.10
 H       3.856548    -1.526647    -3.199240      22.35
 H       2.161939    -2.199024    -2.583130      22.93
 C      -0.099375    -1.732744     0.379377      38.27
 H      -0.581321    -2.649402     0.591798      19.41
 C       0.124366     0.570769     0.298784      75.84
 H      -0.253702     1.614255     0.037438      14.80
 C       1.370398     0.378914    -0.232720      19.20
 O       2.285094     1.452432    -0.528806     181.51
 C       1.762659     2.869006    -0.609916     109.48
 H       2.668099     3.424023    -0.974827      23.35
 H       0.551541     3.076571    -0.959184      21.76
 H       1.686671     3.167309     0.325121      28.17
 C       2.017911    -0.941015    -0.341286      13.91
 O       3.319190    -0.863907    -0.813398     206.69
 C       1.249751    -2.048078    -0.029378      65.23
 H       1.491636    -3.085379    -0.089180      19.82
 C      -0.781918    -0.492576     0.540209      79.35
 C      -2.186036    -0.324423     0.938081      91.77
 H      -2.470601    -1.278788     1.344898      25.72
 O      -2.141359     0.793043     2.024503     186.27
 H      -1.499899     0.302160     2.842839      23.31
 C      -3.041764     0.377289    -0.189550      79.15
 H      -2.459469     1.210673    -0.595452      23.21
 O      -3.254661    -0.671334    -1.246952     236.45
 H      -3.197856    -0.217114    -2.169850      22.92
 C      -4.510934     0.907976     0.222105     108.88
 O      -4.896770     1.834708    -0.829923     248.26
 H      -5.262200     2.659408    -0.355206      25.94
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 H      -4.524112     1.464236     1.154618      28.14
 H      -5.118613     0.030816     0.196018      28.56
55
name = lig-etoh-Waterframe_457
 C       6.345312    -1.496630     1.316085      58.43
 H       6.472115    -0.476082     0.987193      22.62
 C       5.437544    -3.702867     0.849825      31.85
 H       4.967468    -4.350173     0.049470      19.72
 C       5.808670    -4.060563     2.212175      16.86
 O       5.462904    -5.337702     2.726459     237.24
 C       5.197282    -6.478609     1.870803      96.39
 H       5.865652    -6.538504     1.000718      28.23
 H       4.162961    -6.220603     1.413693      27.14
 H       5.353445    -7.352069     2.550307      22.35
 C       6.350197    -3.184850     3.181779      12.65
 O       6.628266    -3.530024     4.487542     141.29
 H       6.389679    -4.484354     4.621091      31.37
 C       6.649094    -1.864857     2.659075      30.78
 H       7.146293    -1.210219     3.328992      22.61
 C       5.729524    -2.416005     0.354887       3.83
 C       5.298632    -2.093470    -1.060637     100.01
 H       5.572069    -2.882539    -1.746328      24.19
 O       5.907892    -0.892665    -1.629058     299.82
 H       5.704243    -0.084117    -1.070204      25.30
 C       3.780544    -2.158944    -1.255526      98.12
 H       3.418041    -2.938004    -0.643536      20.37
 C       3.332472    -2.278706    -2.667235      96.02
 O       3.567586    -3.561602    -3.334740     261.29
 H       4.334834    -3.509998    -3.959156      25.88
 H       3.772756    -1.503292    -3.300105      24.66
 H       2.175628    -1.958743    -2.856328      23.45
 C      -0.203732    -1.770395     0.354314      42.20
 H      -0.923808    -2.508929     0.626469      23.90
 C       0.112953     0.613066     0.254661      94.06
 H      -0.360958     1.580820     0.731944      17.62
 C       1.452391     0.385641    -0.192129      14.97
 O       2.239394     1.419665    -0.530342     202.67
 C       1.735857     2.793439    -0.506780     106.34
 H       2.349625     3.467559    -1.178912      25.78
 H       0.641808     2.799724    -1.230586      22.37
 H       1.647678     3.280848     0.461446      26.17
 C       2.038571    -0.916763    -0.296560      25.67
 O       3.275999    -0.908224    -0.831202     196.82
 C       1.132430    -2.006440    -0.037875      63.93
 H       1.596270    -3.016925    -0.106686      21.80
 C      -0.719364    -0.514733     0.553245      61.50
 C      -2.201703    -0.268543     1.033577      84.51
 H      -2.872909    -1.067968     1.417326      23.07
 O      -2.161324     0.806186     1.971167     253.24
 H      -1.838159     0.409337     2.999959      25.37
 C      -3.071321     0.283627    -0.261445      80.53
 H      -2.589924     1.222673    -0.449988      25.17
 O      -3.224615    -0.720702    -1.232514     250.65
 H      -3.220633    -0.328645    -2.139511      24.36
 C      -4.512083     0.852047     0.262970     105.82
 O      -4.888385     1.826159    -0.876167     220.49
 H      -5.032330     2.775095    -0.506803      26.10
 H      -4.670207     1.287620     1.217493      29.33
 H      -5.225298     0.160196     0.205571      30.76
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name = lig-etoh-Waterframe_458
 C       6.388074    -1.518740     1.278529      86.69
 H       6.657758    -0.508970     1.009788      24.31
 C       5.447450    -3.697671     0.871857      51.25
 H       5.107561    -4.589323     0.303116      18.87
 C       5.819162    -4.054606     2.144380      38.33
 O       5.499402    -5.338804     2.734359     224.41
 C       5.173908    -6.462498     1.885463     131.39
 H       6.015030    -6.545197     1.016915      25.16
 H       4.109820    -6.562185     1.442540      24.79
 H       5.247211    -7.373609     2.363878      23.96
 C       6.339880    -3.174130     3.169628      34.79
 O       6.592725    -3.563566     4.455160     139.67
 H       6.487906    -4.506452     4.694708      29.95
 C       6.657885    -1.927681     2.659193      21.81
 H       7.213223    -1.141392     3.215323      24.67
 C       5.730943    -2.371612     0.434557      17.32
 C       5.355386    -2.074221    -1.077941      78.82
 H       5.928799    -3.136032    -1.632765      19.61
 O       5.924220    -0.898258    -1.616320     259.94
 H       5.735239    -0.232836    -0.852874      25.71
 C       3.825512    -2.222092    -1.195002      83.41
 H       3.456021    -3.022025    -0.627165      22.43
 C       3.385391    -2.271552    -2.773073      87.45
 O       3.563758    -3.560989    -3.364233     249.69
 H       4.323734    -3.553980    -3.996477      25.53
 H       3.954761    -1.433097    -3.298750      24.21
 H       2.199869    -2.088504    -2.733076      23.97
 C      -0.324406    -1.872997     0.351057      52.47
 H      -0.955401    -2.789909     0.501908      22.57
 C       0.077222     0.624721     0.290343     101.39
 H      -0.016662     1.578792     0.908341      19.81
 C       1.443243     0.430692    -0.099367       8.86
 O       2.273405     1.464026    -0.548585     178.08
 C       1.682334     2.715427    -0.490008     113.07
 H       2.338288     3.273759    -1.159784      25.83
 H       0.686739     2.620334    -0.915477      25.70
 H       1.459856     3.161866     0.660986      24.04
 C       1.903151    -0.868200    -0.257261      23.46
 O       3.239048    -0.927797    -0.813237     167.68
 C       1.069844    -1.962837    -0.051769      52.32
 H       1.405705    -3.059487    -0.137399      21.41
 C      -0.686554    -0.511897     0.557423      26.53
 C      -2.228897    -0.177359     1.029133      81.82
 H      -2.660771    -1.175638     1.477154      22.11
 O      -2.228230     0.862867     1.942846     263.05
 H      -1.733883     0.333466     2.818299      20.72
 C      -3.131135     0.259900    -0.149536      74.84
 H      -2.614091     0.997403    -0.828086      22.15
 O      -3.192876    -0.779494    -1.241492     228.77
 H      -3.081798    -0.291220    -2.051858      26.73
 C      -4.509559     0.814603     0.179886      95.31
 O      -4.882426     1.814197    -0.869689     238.60
 H      -4.612634     2.733878    -0.552241      27.54
 H      -4.327951     1.239781     1.184465      26.25
 H      -5.404092    -0.011513     0.175419      25.67
55
name = lig-etoh-Waterframe_459
 C       6.441425    -1.529350     1.322061      66.44
 H       6.837536    -0.576384     0.991742      25.12
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 C       5.490122    -3.709954     0.904971      42.19
 H       5.062100    -4.434014     0.207263      17.77
 C       5.764965    -4.147334     2.201423      31.47
 O       5.531598    -5.340659     2.732841     210.64
 C       5.182064    -6.469272     1.865947     117.25
 H       5.965194    -6.518529     0.937174      29.39
 H       4.169333    -6.329515     1.453750      28.78
 H       5.307619    -7.233433     2.546850      26.13
 C       6.331514    -3.194633     3.080715       0.16
 O       6.572736    -3.580362     4.451166     132.86
 H       6.430271    -4.536883     4.430960      30.07
 C       6.697697    -1.907583     2.626291      51.83
 H       7.193883    -1.209961     3.408153      19.97
 C       5.725682    -2.376774     0.427186      18.10
 C       5.447253    -2.129079    -1.003136      79.81
 H       6.002527    -2.949978    -1.832214      22.70
 O       5.938984    -0.904804    -1.585095     242.58
 H       5.713664    -0.014599    -1.065708      24.14
 C       3.830541    -2.226524    -1.268545      72.88
 H       3.487555    -3.136503    -0.742401      21.15
 C       3.427397    -2.265794    -2.781927      95.60
 O       3.560720    -3.584479    -3.425617     241.32
 H       4.466912    -3.661606    -3.839490      26.25
 H       4.063297    -1.492585    -3.312198      24.55
 H       2.367421    -2.044658    -2.792920      26.23
 C      -0.338895    -1.868434     0.329848      40.98
 H      -0.941116    -2.847959     0.385632      20.19
 C       0.129487     0.618310     0.417180      62.83
 H      -0.348346     1.585884     0.629640      15.71
 C       1.402639     0.488872    -0.042927      17.35
 O       2.330842     1.448479    -0.528960     209.74
 C       1.591561     2.719610    -0.511973     116.92
 H       2.212103     3.506125    -0.854369      26.00
 H       0.660231     2.715050    -0.791277      28.27
 H       1.612014     3.064026     0.710460      23.89
 C       1.851101    -0.882892    -0.287684      13.14
 O       3.180814    -0.956539    -0.743509     146.52
 C       0.966606    -2.003553    -0.045074      52.71
 H       1.468710    -2.992119    -0.343593      20.40
 C      -0.841976    -0.520450     0.574008      71.31
 C      -2.206125    -0.185366     0.946884     109.06
 H      -2.448369    -1.136025     1.493094      25.13
 O      -2.289670     0.938005     1.984046     256.59
 H      -1.655311     0.684495     2.744158      29.54
 C      -3.147427     0.226823    -0.166800      73.75
 H      -2.561983     1.208628    -0.555430      22.01
 O      -3.172212    -0.859643    -1.233039     229.88
 H      -2.970957    -0.388005    -2.013328      26.65
 C      -4.500496     0.816436     0.092279      97.74
 O      -4.872438     1.795942    -0.835013     246.36
 H      -4.455099     2.618145    -0.451495      28.59
 H      -4.455778     1.389469     1.087462      26.28
 H      -5.368394    -0.153452     0.193289      24.45
55
name = lig-etoh-Waterframe_460
 C       6.484913    -1.501244     1.311015      56.95
 H       6.798808    -0.534414     0.894742      24.13
 C       5.493551    -3.738630     0.886058      62.45
 H       4.988781    -4.263642     0.120563      14.88
 C       5.722715    -4.131741     2.234041      37.64
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 O       5.550584    -5.410566     2.748302     245.02
 C       5.202980    -6.450807     1.851804     105.09
 H       5.893677    -6.618213     0.984991      32.53
 H       4.242263    -6.227689     1.500484      36.08
 H       5.245580    -7.373394     2.482458      28.27
 C       6.355661    -3.214158     3.092113       1.54
 O       6.552361    -3.583598     4.388922      98.43
 H       6.322171    -4.513675     4.578966      24.33
 C       6.733747    -1.920601     2.656872      48.65
 H       7.226941    -1.254725     3.466454      18.34
 C       5.801617    -2.441912     0.475399      25.69
 C       5.439091    -2.109742    -1.012498     104.98
 H       5.807500    -2.867214    -1.545680      27.70
 O       5.981595    -0.891713    -1.556464     262.90
 H       5.447131    -0.111683    -1.061579      23.82
 C       3.841792    -2.209286    -1.343803      74.80
 H       3.379069    -3.147761    -0.843477      18.66
 C       3.472191    -2.264205    -2.779507     106.39
 O       3.562043    -3.599338    -3.478423     254.21
 H       4.499320    -3.684045    -3.834816      25.40
 H       4.025598    -1.558785    -3.419548      24.73
 H       2.557694    -1.927256    -2.956684      28.04
 C      -0.392899    -1.773510     0.326418      36.94
 H      -1.152906    -2.619904     0.439545      19.22
 C       0.043139     0.590004     0.560450      70.21
 H      -0.490388     1.468237     0.407775      16.09
 C       1.454032     0.406003    -0.058641      -5.71
 O       2.301643     1.451621    -0.495060     161.00
 C       1.604891     2.797491    -0.442953      94.65
 H       2.091178     3.602030    -1.013507      24.46
 H       0.516027     2.745403    -1.067292      23.42
 H       1.368717     2.986446     0.622215      24.55
 C       1.820295    -0.924072    -0.313133      22.12
 O       3.151204    -1.022275    -0.671898     184.88
 C       0.996420    -2.012059    -0.098890      56.90
 H       1.287709    -3.056015    -0.377753      20.90
 C      -0.818025    -0.512809     0.549689      61.41
 C      -2.258414    -0.222990     1.021623      96.78
 H      -2.856714    -0.994132     1.441475      25.31
 O      -2.341782     0.996604     1.981486     278.56
 H      -1.789264     0.671482     2.672549      31.09
 C      -3.090938     0.212302    -0.274139      77.97
 H      -2.550793     1.121493    -0.612149      23.24
 O      -3.150753    -0.893248    -1.209827     274.87
 H      -2.976970    -0.600059    -2.063186      28.33
 C      -4.511149     0.782599     0.129511     100.25
 O      -4.876020     1.804488    -0.849534     260.61
 H      -4.728239     2.731992    -0.494185      27.61
 H      -4.660091     1.124512     1.192842      27.37
 H      -5.367194    -0.011814    -0.023879      25.85
55
name = lig-etoh-Waterframe_461
 C       6.509657    -1.522514     1.312257      68.72
 H       6.664117    -0.476876     0.978154      24.03
 C       5.465003    -3.770153     0.881698      55.04
 H       4.998777    -4.535590     0.311142      18.37
 C       5.706381    -4.118000     2.183325      40.03
 O       5.584491    -5.460913     2.785068     242.22
 C       5.193823    -6.468096     1.824500     142.21
 H       5.902094    -6.488570     1.101644      36.02
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 H       4.220255    -6.341669     1.376640      32.03
 H       5.033790    -7.543733     2.272998      26.58
 C       6.362134    -3.215108     3.109736      16.97
 O       6.556876    -3.584652     4.387078      74.42
 H       6.244171    -4.469916     4.638840      22.72
 C       6.759355    -1.936746     2.680832      42.57
 H       7.302598    -1.237582     3.344428      23.84
 C       5.894646    -2.435054     0.482143      29.89
 C       5.364049    -2.088222    -1.029460     105.57
 H       5.775077    -2.905901    -1.567067      23.85
 O       6.009199    -0.884218    -1.514683     227.29
 H       5.530846    -0.080826    -0.985726      23.49
 C       3.837746    -2.194092    -1.300890      75.12
 H       3.492107    -3.211774    -0.868080      20.22
 C       3.513562    -2.243200    -2.908673      91.62
 O       3.560353    -3.590100    -3.483018     258.14
 H       4.399007    -3.645684    -4.052533      25.23
 H       4.264612    -1.622606    -3.368085      23.65
 H       2.427269    -1.959575    -2.934252      24.62
 C      -0.367318    -1.778846     0.287600      39.08
 H      -1.116850    -2.562965     0.472957      19.99
 C       0.103839     0.595060     0.530096      60.45
 H      -0.212293     1.589430     0.676027      16.58
 C       1.334807     0.373755    -0.026806      16.65
 O       2.219502     1.484404    -0.447965     159.34
 C       1.588244     2.836216    -0.390353      99.25
 H       2.429218     3.404213    -0.911285      23.05
 H       0.558091     2.584060    -1.196553      21.33
 H       1.259764     3.214783     0.451014      27.15
 C       1.862996    -0.976233    -0.330985      21.86
 O       3.207471    -1.098200    -0.642647     194.55
 C       0.907074    -2.032929    -0.146323      59.23
 H       1.195427    -3.058447    -0.306651      21.44
 C      -0.820856    -0.471380     0.648524      64.29
 C      -2.378990    -0.178436     1.074181      84.85
 H      -2.869202    -1.048751     1.511739      23.28
 O      -2.376796     0.980417     1.936766     323.49
 H      -2.007421     0.654511     2.673020      34.03
 C      -3.052854     0.248426    -0.292965      84.28
 H      -2.604590     0.885217    -0.945485      24.61
 O      -3.130669    -0.918883    -1.198761     259.49
 H      -3.047421    -0.552141    -2.037656      29.26
 C      -4.552108     0.721320     0.118892     105.76
 O      -4.893731     1.840823    -0.867590     283.93
 H      -5.110341     2.684577    -0.393358      26.96
 H      -4.494463     0.956584     1.168759      28.36
 H      -5.112993    -0.012080    -0.125422      30.28
55
name = lig-etoh-Waterframe_462
 C       6.516191    -1.576750     1.355327      40.61
 H       6.689202    -0.509390     1.105771      22.33
 C       5.462938    -3.768216     0.890311      84.30
 H       5.083210    -4.495461     0.156175      24.24
 C       5.752585    -4.181915     2.230756      21.03
 O       5.587901    -5.457269     2.786256     220.24
 C       5.165497    -6.501333     1.763269     107.01
 H       5.936523    -6.524581     1.057269      29.79
 H       4.231563    -6.114050     1.232538      26.14
 H       5.199439    -7.453977     2.474345      22.79
 C       6.338329    -3.214287     3.086581      20.81
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 O       6.582455    -3.587994     4.464360     143.34
 H       6.302377    -4.521843     4.432524      29.19
 C       6.776111    -1.935585     2.662057      72.57
 H       7.268877    -1.316709     3.348095      24.77
 C       5.848895    -2.465233     0.366611      25.81
 C       5.371191    -2.091424    -0.986277      77.74
 H       5.863931    -2.923540    -1.920066      22.04
 O       6.005799    -0.878423    -1.476456     207.55
 H       5.907916     0.014989    -0.927332      23.96
 C       3.841886    -2.235258    -1.292153      75.63
 H       3.539913    -3.197085    -0.873143      19.94
 C       3.557794    -2.223547    -2.957601      77.20
 O       3.556313    -3.572381    -3.477745     259.53
 H       4.399352    -3.698482    -4.045462      25.51
 H       4.231960    -1.532629    -3.464000      22.96
 H       2.410715    -1.744221    -3.111789      22.58
 C      -0.441591    -1.754827     0.306496      48.21
 H      -0.921121    -2.695287     0.384032      22.68
 C       0.095074     0.634389     0.491900      84.95
 H       0.058133     1.548879     1.105914      21.25
 C       1.373265     0.352858    -0.070405       5.93
 O       2.110802     1.478934    -0.338187     197.60
 C       1.583099     2.787993    -0.437502     118.63
 H       2.465898     3.484721    -0.662635      25.18
 H       0.750263     3.121448    -1.163256      25.21
 H       1.313865     3.325034     0.505232      25.24
 C       1.846726    -0.997574    -0.325013      11.36
 O       3.257968    -1.121071    -0.615003     170.67
 C       0.905927    -2.054348    -0.211328      51.15
 H       1.194317    -3.048886    -0.328668      22.02
 C      -0.875799    -0.475614     0.776883      49.21
 C      -2.342000    -0.111216     1.009936      99.97
 H      -2.752050    -1.057194     1.479204      23.09
 O      -2.423182     0.951132     1.918850     342.07
 H      -2.116071     0.685337     2.708781      31.05
 C      -3.122592     0.255715    -0.267447      78.73
 H      -2.585737     1.151496    -0.652751      24.80
 O      -3.121555    -0.956333    -1.194188     217.60
 H      -3.114724    -0.537515    -2.020967      27.74
 C      -4.520482     0.716131    -0.008085     107.37
 O      -4.925986     1.851456    -0.832469     279.49
 H      -5.305994     2.530743    -0.251618      27.68
 H      -4.658733     1.086084     1.000869      27.04
 H      -5.160103    -0.231192    -0.104336      26.43
55
name = lig-etoh-Waterframe_463
 C       6.463041    -1.620768     1.275472      49.40
 H       6.843689    -0.631781     0.984491      21.77
 C       5.506240    -3.767888     0.892337      65.68
 H       5.099231    -4.439055     0.080777      20.55
 C       5.815902    -4.198631     2.239842      25.11
 O       5.560209    -5.454127     2.732440     225.00
 C       5.198503    -6.461658     1.754170     107.68
 H       5.959131    -6.740641     0.940342      27.21
 H       4.128348    -6.241832     1.316788      25.95
 H       4.962364    -7.420940     2.376651      22.85
 C       6.350935    -3.242970     3.171508      39.97
 O       6.593994    -3.593508     4.485291     183.95
 H       6.568843    -4.565584     4.672745      29.39
 C       6.756512    -1.993255     2.659108      53.93
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 H       7.180681    -1.337052     3.342339      22.57
 C       5.791335    -2.510968     0.422691      36.77
 C       5.441186    -2.084474    -1.037283      76.87
 H       5.942497    -3.000627    -1.787197      24.34
 O       6.016017    -0.860668    -1.461120     236.80
 H       5.765323    -0.212876    -0.694924      24.00
 C       3.860292    -2.258115    -1.360135      75.71
 H       3.435527    -3.141438    -1.007623      21.50
 C       3.582346    -2.184032    -2.886077      85.38
 O       3.549214    -3.547501    -3.487607     254.79
 H       4.503025    -3.717651    -3.800069      26.05
 H       4.313082    -1.616383    -3.482853      23.86
 H       2.488850    -1.740398    -3.158624      23.94
 C      -0.468504    -1.761209     0.331631      38.89
 H      -1.188703    -2.538275     0.423201      20.85
 C       0.038800     0.552573     0.540182      58.28
 H      -0.080510     1.564280     1.078813      17.88
 C       1.352031     0.337340    -0.098037      12.40
 O       2.095796     1.462185    -0.258618     201.85
 C       1.598410     2.852121    -0.449446      99.41
 H       2.547175     3.374623    -0.762463      24.09
 H       0.948214     2.991404    -1.145364      29.16
 H       1.167744     3.016122     0.730387      20.43
 C       1.857551    -0.989067    -0.346486      24.09
 O       3.239073    -1.101168    -0.578208     176.34
 C       0.896200    -2.009618    -0.220051      56.94
 H       1.145566    -2.983759    -0.469289      23.16
 C      -0.831616    -0.460192     0.749313      56.23
 C      -2.269617    -0.158527     0.988511      93.39
 H      -2.896027    -1.032832     1.365328      22.74
 O      -2.489312     0.977253     1.943488     304.52
 H      -2.053263     0.568218     2.702627      26.44
 C      -3.140443     0.243652    -0.274630      69.77
 H      -2.535192     1.205753    -0.636195      22.72
 O      -3.109689    -0.931818    -1.190780     223.34
 H      -3.092949    -0.647435    -2.081529      27.40
 C      -4.562893     0.730183    -0.076929      97.36
 O      -4.972771     1.835195    -0.825185     274.63
 H      -5.278595     2.543986    -0.232184      27.63
 H      -4.650907     0.994718     1.007515      25.96
 H      -5.488410    -0.211767    -0.211037      23.91
55
name = lig-etoh-Waterframe_464
 C       6.450295    -1.637478     1.285079      56.13
 H       6.842906    -0.759821     0.790192      23.94
 C       5.544592    -3.843067     0.918081      25.51
 H       5.048564    -4.688230     0.354954      11.95
 C       5.850292    -4.169873     2.191567      48.72
 O       5.542912    -5.468801     2.666602     258.62
 C       5.170120    -6.462883     1.773803     118.01
 H       6.014658    -6.611960     0.915234      31.49
 H       4.250346    -6.168299     1.157871      27.46
 H       4.986899    -7.351160     2.328457      25.80
 C       6.380078    -3.313716     3.203688      18.20
 O       6.615437    -3.590608     4.528610     170.94
 H       6.636886    -4.567659     4.720076      28.50
 C       6.703200    -2.043817     2.630399      63.46
 H       7.173380    -1.264290     3.225565      25.33
 C       5.755972    -2.488310     0.461392      36.09
 C       5.476875    -2.170620    -1.087322      83.05
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 H       5.965698    -2.818710    -1.612213      27.03
 O       6.018291    -0.850439    -1.429559     292.16
 H       5.587269    -0.134825    -0.858095      25.37
 C       3.887000    -2.204913    -1.394090      74.68
 H       3.513326    -3.152942    -1.031882      22.85
 C       3.589539    -2.157693    -2.851701      99.33
 O       3.546615    -3.510961    -3.478304     263.36
 H       4.477183    -3.720583    -3.814270      25.65
 H       4.402060    -1.558321    -3.298616      23.67
 H       2.601429    -1.761611    -2.909545      26.76
 C      -0.416094    -1.792490     0.324925      36.01
 H      -1.228823    -2.490870     0.383809      19.26
 C       0.106708     0.522737     0.587991      68.66
 H      -0.453780     1.527363     0.615506      18.09
 C       1.248452     0.364367    -0.052464      21.17
 O       2.184930     1.455164    -0.239828     161.94
 C       1.634152     2.834005    -0.388901     101.46
 H       2.503442     3.456294    -0.617134      25.09
 H       0.869253     2.674032    -1.209471      24.92
 H       1.025394     3.508467     0.534554      22.56
 C       1.839858    -0.931872    -0.366369      11.24
 O       3.215107    -1.090695    -0.576983     161.66
 C       0.824520    -1.987126    -0.183440      55.42
 H       1.070896    -2.948080    -0.590695      22.10
 C      -0.839558    -0.521155     0.650336      58.03
 C      -2.349538    -0.191857     1.018108      80.06
 H      -2.717552    -1.151900     1.471035      24.04
 O      -2.524526     0.961704     1.974335     267.55
 H      -1.982559     0.676628     2.832357      27.59
 C      -3.081338     0.238415    -0.333431      72.94
 H      -2.622809     0.988091    -1.072709      22.45
 O      -3.092575    -0.898592    -1.205071     234.11
 H      -2.989576    -0.502111    -2.065929      27.32
 C      -4.675792     0.701156    -0.001323      74.49
 O      -5.031508     1.852452    -0.871115     277.92
 H      -5.048722     2.717772    -0.411797      27.51
 H      -4.663015     0.828551     1.096215      26.19
 H      -5.298924    -0.202507    -0.498130      25.03
55
name = lig-etoh-Waterframe_465
 C       6.443598    -1.656005     1.319868      41.26
 H       6.774714    -0.659030     1.053820      25.18
 C       5.548670    -3.854545     0.885451      42.03
 H       5.044348    -4.607958     0.234201      16.61
 C       5.854994    -4.249147     2.245339      26.27
 O       5.548099    -5.460733     2.667430     231.54
 C       5.127767    -6.483132     1.712278     113.54
 H       6.061477    -6.663137     1.045942      30.86
 H       4.284902    -6.208989     1.156227      30.90
 H       5.047569    -7.291573     2.280637      29.33
 C       6.423416    -3.310399     3.137415       3.42
 O       6.644885    -3.595560     4.573989     129.31
 H       6.371361    -4.563818     4.648602      28.41
 C       6.682738    -2.041125     2.644160      61.61
 H       7.244257    -1.322524     3.340910      22.02
 C       5.722759    -2.561008     0.390030      24.24
 C       5.440637    -2.161070    -1.021012      80.22
 H       5.921531    -2.867636    -1.750450      25.89
 O       6.019551    -0.866781    -1.409099     284.80
 H       5.541485    -0.070969    -1.104733      27.33
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 C       3.921216    -2.193952    -1.320176      70.09
 H       3.560663    -3.192678    -0.878382      21.80
 C       3.587118    -2.127914    -2.866802     103.89
 O       3.553246    -3.461896    -3.448057     269.09
 H       4.374867    -3.611860    -3.985876      26.91
 H       4.191426    -1.387242    -3.442603      25.29
 H       2.674924    -1.756198    -2.960791      28.69
 C      -0.458859    -1.836598     0.318908      32.61
 H      -0.914909    -2.843630     0.284060      18.03
 C       0.001040     0.564899     0.599800      51.70
 H      -0.356672     1.627221     0.506783      17.39
 C       1.400395     0.422890    -0.028359      -0.78
 O       2.267649     1.470824    -0.201132     185.93
 C       1.658837     2.782829    -0.360858     107.55
 H       2.389802     3.471561    -0.684557      25.92
 H       0.848512     2.835970    -1.400678      22.97
 H       1.175557     3.203666     0.524014      24.80
 C       1.731751    -0.922496    -0.348764      16.44
 O       3.209000    -1.072661    -0.612021     147.54
 C       0.907631    -1.998594    -0.215059      50.28
 H       1.139336    -3.053637    -0.539966      20.92
 C      -0.916331    -0.524112     0.629426      50.79
 C      -2.371612    -0.173501     1.020542      94.48
 H      -2.863521    -1.066642     1.414948      25.38
 O      -2.535335     0.897262     1.977137     255.28
 H      -1.920163     0.667799     2.861085      26.79
 C      -3.130928     0.240700    -0.338472      76.54
 H      -2.612699     1.155494    -0.642024      23.70
 O      -3.080217    -0.909375    -1.265774     257.56
 H      -2.951759    -0.508576    -2.160810      25.01
 C      -4.668702     0.674266    -0.006269      99.88
 O      -5.090486     1.861686    -0.892863     281.84
 H      -4.813828     2.710203    -0.555794      29.84
 H      -5.110107     0.880780     0.978735      27.37
 H      -5.202307    -0.113301    -0.296968      28.93
55
name = lig-etoh-Waterframe_466
 C       6.389905    -1.683028     1.310357      47.91
 H       6.513734    -0.624586     1.109069      22.28
 C       5.527366    -3.875795     0.868826      60.91
 H       5.137561    -4.508942     0.092491      23.50
 C       5.845740    -4.250211     2.206158      17.25
 O       5.531200    -5.532396     2.726513     215.59
 C       5.143043    -6.499766     1.674306     114.69
 H       5.895097    -6.726905     0.921385      29.70
 H       4.255526    -6.240439     1.191551      30.65
 H       4.875485    -7.356810     2.252079      27.72
 C       6.448692    -3.331898     3.159816      -6.35
 O       6.657648    -3.612806     4.519888      97.20
 H       6.197707    -4.446152     4.866703      25.40
 C       6.717277    -2.019510     2.673797      16.66
 H       7.206175    -1.311664     3.462779      18.66
 C       5.821136    -2.567435     0.428010      21.53
 C       5.376354    -2.063544    -0.968680      78.23
 H       5.733168    -3.022299    -1.880364      22.31
 O       6.035097    -0.904093    -1.409619     293.77
 H       5.549686    -0.176611    -0.992841      27.50
 C       3.871741    -2.177268    -1.265917      72.38
 H       3.430952    -3.191119    -0.907645      21.65
 C       3.551090    -2.091760    -2.847647      92.53
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 O       3.569762    -3.421322    -3.437536     247.84
 H       4.423199    -3.540329    -3.931548      26.85
 H       4.264004    -1.480544    -3.458430      24.61
 H       2.475987    -1.797085    -2.926906      25.35
 C      -0.412410    -1.882420     0.259225      49.75
 H      -1.116546    -2.777971     0.499684      23.02
 C       0.003232     0.609109     0.463168      71.10
 H      -0.358967     1.541188     0.902879      18.81
 C       1.384703     0.429413     0.077167       4.72
 O       2.344316     1.496246    -0.169099     170.47
 C       1.692583     2.757994    -0.374790     111.89
 H       2.522565     3.381655    -0.618473      26.19
 H       0.774784     2.738722    -1.224703      23.28
 H       1.299072     2.871909     0.489314      27.46
 C       1.829709    -0.904468    -0.345149       9.71
 O       3.192691    -1.035012    -0.653149     156.38
 C       0.880236    -2.028322    -0.213878      51.43
 H       1.464207    -3.025973    -0.380591      21.03
 C      -0.955501    -0.509380     0.652194      33.64
 C      -2.417133    -0.202764     0.981348      97.33
 H      -2.959636    -1.071175     1.311798      22.61
 O      -2.529302     0.845990     1.969027     255.68
 H      -1.878997     0.343461     2.781282      21.33
 C      -3.225117     0.269395    -0.234578      74.95
 H      -2.682728     1.135786    -0.527760      25.06
 O      -3.072450    -0.877009    -1.323986     201.14
 H      -3.022356    -0.475672    -2.275420      22.89
 C      -4.669883     0.698132    -0.101376     111.79
 O      -5.126457     1.810795    -0.900924     289.67
 H      -4.823377     2.597360    -0.473843      31.28
 H      -4.849846     0.973452     0.979229      27.19
 H      -5.307309    -0.080976    -0.368029      28.13
55
name = lig-etoh-Waterframe_467
 C       6.377466    -1.626036     1.400165      52.92
 H       6.364427    -0.639483     0.932943      21.03
 C       5.538370    -3.893844     0.866620      61.66
 H       5.185206    -4.663810     0.242533      21.69
 C       5.825828    -4.265886     2.183311      15.88
 O       5.523542    -5.607985     2.736856     260.68
 C       5.127896    -6.524746     1.694325     113.37
 H       5.853240    -6.638844     0.962139      29.84
 H       4.260041    -6.012135     1.170108      25.17
 H       4.840871    -7.569880     2.197981      23.05
 C       6.424063    -3.352862     3.151794      29.10
 O       6.669106    -3.628083     4.450112     232.62
 H       6.246880    -4.503859     4.764302      24.45
 C       6.750316    -2.056973     2.696416      60.18
 H       7.055238    -1.178811     3.332127      23.70
 C       5.887602    -2.551919     0.452651       5.57
 C       5.327609    -2.085107    -0.954289      81.72
 H       5.834069    -2.984224    -1.624249      21.34
 O       6.030122    -0.911071    -1.411876     336.81
 H       5.844096    -0.124462    -0.913100      27.47
 C       3.759045    -2.116778    -1.283392      80.58
 H       3.387312    -3.082829    -0.858698      21.42
 C       3.503776    -2.092804    -2.787368      89.53
 O       3.587188    -3.403088    -3.448481     259.75
 H       4.533825    -3.561366    -3.715170      26.18
 H       4.245596    -1.351737    -3.172337      22.57
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 H       2.376498    -1.599383    -2.931818      23.18
 C      -0.430076    -1.794532     0.261005      38.31
 H      -1.179260    -2.649749     0.492353      20.59
 C      -0.006538     0.590153     0.381480     118.24
 H      -0.269375     1.429051     0.948553      19.78
 C       1.364626     0.374314     0.114253       4.48
 O       2.377221     1.446824    -0.147335     158.04
 C       1.735619     2.738880    -0.363349      99.28
 H       2.458859     3.581804    -0.559478      24.59
 H       1.015428     2.621477    -1.064303      26.44
 H       1.165995     3.266478     0.657287      22.26
 C       1.872984    -0.894105    -0.290563      19.48
 O       3.177573    -0.964115    -0.676246     198.14
 C       0.951888    -1.998181    -0.197237      52.88
 H       1.281813    -3.117346    -0.262749      19.66
 C      -0.845507    -0.549254     0.568806      25.29
 C      -2.488065    -0.283344     0.951412      73.26
 H      -2.799121    -1.261637     1.350846      21.72
 O      -2.495067     0.776376     1.976548     268.83
 H      -2.073515     0.404517     2.962200      22.17
 C      -3.242828     0.278568    -0.290727      79.85
 H      -2.737119     1.101886    -0.787021      23.09
 O      -3.085250    -0.796095    -1.334038     230.43
 H      -3.060122    -0.152259    -2.168343      21.61
 C      -4.721589     0.703853    -0.119808      90.39
 O      -5.131320     1.771303    -0.920301     294.33
 H      -5.129498     2.620510    -0.494015      29.67
 H      -4.656096     0.941957     0.960446      26.39
 H      -5.480673    -0.272626    -0.377545      25.55
55
name = lig-etoh-Waterframe_468
 C       6.360853    -1.599286     1.423409      43.38
 H       6.606238    -0.501048     1.322041      19.86
 C       5.603737    -3.888812     0.886788      48.80
 H       5.169017    -4.543758     0.168776      18.61
 C       5.809917    -4.346413     2.245890      18.33
 O       5.547912    -5.613869     2.716872     264.47
 C       5.089309    -6.526982     1.709604     122.63
 H       5.923173    -6.638160     1.048469      30.96
 H       4.102161    -6.183546     1.124905      26.13
 H       4.885741    -7.645293     2.215212      22.69
 C       6.379675    -3.360691     3.079787      35.60
 O       6.678201    -3.673380     4.426313     221.29
 H       6.497908    -4.672238     4.529840      24.17
 C       6.739339    -2.045468     2.693105      44.28
 H       7.077458    -1.440980     3.522348      22.11
 C       5.816586    -2.554158     0.466493      26.34
 C       5.356460    -2.152276    -0.934248     121.94
 H       5.653099    -2.771558    -1.575915      28.23
 O       6.011216    -0.904165    -1.429667     348.44
 H       5.926449    -0.171014    -0.857604      27.57
 C       3.709342    -2.104152    -1.246555      85.90
 H       3.260671    -2.917468    -0.743160      22.28
 C       3.466184    -2.065704    -2.746528      86.12
 O       3.599214    -3.375144    -3.444276     258.33
 H       4.549118    -3.441175    -3.741364      26.80
 H       4.140398    -1.340961    -3.188390      22.92
 H       2.347451    -1.725697    -3.095075      23.41
 C      -0.353021    -1.777582     0.247014      51.13
 H      -0.933815    -2.710596     0.226697      15.87
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 C       0.030239     0.567440     0.407173      70.87
 H      -0.329826     1.559220     0.553182      16.90
 C       1.406400     0.383664     0.054630      10.44
 O       2.340507     1.390099    -0.091398     208.92
 C       1.771100     2.743136    -0.303762      94.92
 H       2.610154     3.393658    -0.820475      22.43
 H       1.130586     2.694798    -1.096509      26.43
 H       1.087919     3.325754     0.685036      20.73
 C       1.830112    -0.938224    -0.213629      25.26
 O       3.188489    -0.864760    -0.686428     189.11
 C       0.980261    -1.983213    -0.126081      64.66
 H       1.215972    -3.020026    -0.422868      20.74
 C      -0.894323    -0.488636     0.466455      80.71
 C      -2.389567    -0.308359     0.943124      67.96
 H      -2.890094    -1.304920     1.259887      25.83
 O      -2.494853     0.700815     1.976823     247.24
 H      -2.013942     0.208007     2.821024      26.34
 C      -3.226057     0.242910    -0.413760      83.70
 H      -2.687344     1.251529    -0.569644      22.55
 O      -3.124921    -0.703182    -1.341650     263.21
 H      -2.980824    -0.410667    -2.387979      20.52
 C      -4.736020     0.662629    -0.029470      86.38
 O      -5.143497     1.778410    -0.971909     218.23
 H      -5.353685     2.522247    -0.429579      28.60
 H      -5.084883     0.987994     0.952014      28.16
 H      -5.508387    -0.375523    -0.193677      26.01
55
name = lig-etoh-Waterframe_469
 C       6.351556    -1.590082     1.412658      57.14
 H       6.600344    -0.505817     1.182059      22.84
 C       5.643756    -3.896334     0.920813      65.16
 H       5.217196    -4.467892     0.104854      10.17
 C       5.807745    -4.343681     2.211297      30.17
 O       5.560910    -5.603241     2.711795     245.14
 C       5.085928    -6.565060     1.708267      98.83
 H       5.821596    -6.754895     0.854825      31.46
 H       4.113861    -6.221117     1.187843      29.93
 H       4.944578    -7.464872     2.427360      26.03
 C       6.376120    -3.403488     3.109689       4.02
 O       6.685144    -3.739125     4.391115     136.41
 H       6.626639    -4.719210     4.675585      23.36
 C       6.670401    -2.087046     2.713044      73.17
 H       7.203976    -1.585588     3.451991      24.50
 C       5.734570    -2.495659     0.530493      37.46
 C       5.356624    -2.139318    -0.951317     117.29
 H       5.653645    -2.952452    -1.717879      27.06
 O       5.975778    -0.925181    -1.438664     326.67
 H       5.729683    -0.293239    -0.808247      29.79
 C       3.748750    -2.086933    -1.152638      79.79
 H       3.245013    -2.911444    -0.732834      21.50
 C       3.421961    -2.050288    -2.777469      94.21
 O       3.622923    -3.345335    -3.417446     259.22
 H       4.462566    -3.339725    -3.946621      28.12
 H       4.061047    -1.360094    -3.266783      23.59
 H       2.361780    -1.832329    -2.809016      25.12
 C      -0.341987    -1.804284     0.216918      35.90
 H      -0.944064    -2.654890     0.207607      19.79
 C       0.065965     0.616663     0.431949      71.77
 H      -0.365920     1.609590     0.222600      18.92
 C       1.361430     0.395280     0.019788      18.96
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 O       2.286378     1.395868    -0.022949     195.84
 C       1.809290     2.734946    -0.310706     103.71
 H       2.826104     3.189299    -0.525300      23.10
 H       0.922809     2.768667    -1.163101      23.07
 H       1.516375     3.110974     0.725510      23.67
 C       1.917791    -0.881010    -0.181295       7.45
 O       3.187116    -0.810709    -0.680761     177.33
 C       1.010050    -2.042513    -0.073437      58.33
 H       1.358695    -2.907937    -0.498241      19.65
 C      -0.939994    -0.476351     0.424187      53.90
 C      -2.309812    -0.270486     0.842548      95.05
 H      -2.756462    -1.297808     1.101679      24.30
 O      -2.498141     0.597610     1.974041     275.02
 H      -1.863167     0.324213     2.646874      28.88
 C      -3.222189     0.312900    -0.298876      69.98
 H      -2.732715     1.320080    -0.668481      22.53
 O      -3.172440    -0.715627    -1.430392     216.69
 H      -2.962564    -0.189965    -2.389789      20.23
 C      -4.757980     0.630081     0.012794      99.17
 O      -5.150532     1.750635    -0.988045     204.95
 H      -5.346591     2.491459    -0.439136      28.69
 H      -4.880166     0.989725     1.042186      27.96
 H      -5.335505    -0.214742    -0.297094      28.39
55
name = lig-etoh-Waterframe_470
 C       6.326251    -1.599271     1.432852      66.23
 H       6.464146    -0.625595     0.959004      23.78
 C       5.600420    -3.844307     0.861014      74.84
 H       5.319778    -4.702023     0.199022      15.40
 C       5.829806    -4.305207     2.176644      28.88
 O       5.574442    -5.601200     2.670391     271.89
 C       5.091043    -6.604967     1.747942     122.00
 H       5.806997    -6.846278     0.855544      29.67
 H       4.201340    -6.195790     1.379931      28.79
 H       4.896700    -7.481813     2.242948      27.61
 C       6.376424    -3.454885     3.154277      17.68
 O       6.724595    -3.802143     4.412801     169.49
 H       6.280012    -4.709501     4.697079      23.87
 C       6.621849    -2.128451     2.738968      66.11
 H       7.221183    -1.442793     3.276229      25.13
 C       5.699898    -2.473467     0.548853      39.56
 C       5.295145    -2.108765    -0.946419      81.51
 H       5.823265    -3.194020    -1.534273      20.63
 O       5.930622    -0.952541    -1.427772     328.92
 H       5.601902    -0.178886    -1.027887      30.05
 C       3.830389    -2.049153    -1.182120      81.85
 H       3.437584    -2.950088    -0.672513      18.48
 C       3.393934    -2.059697    -2.728245     104.25
 O       3.630063    -3.329938    -3.397328     268.90
 H       4.494060    -3.298287    -3.898178      27.05
 H       3.877735    -1.215584    -3.200069      24.48
 H       2.426060    -1.839577    -2.751683      27.38
 C      -0.405130    -1.799883     0.203049      47.64
 H      -1.102221    -2.552996     0.358292      24.83
 C      -0.038737     0.629202     0.375093      62.30
 H      -0.352835     1.728072     0.486126      17.50
 C       1.321828     0.401651     0.059664      13.46
 O       2.260574     1.427366     0.002643     218.47
 C       1.897555     2.723332    -0.259254     124.36
 H       2.627615     3.452056    -0.660280      24.74
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 H       0.921041     2.949715    -1.078782      23.13
 H       1.575249     3.228109     0.507625      28.14
 C       1.923683    -0.881090    -0.167175      18.25
 O       3.232302    -0.817723    -0.659635     194.90
 C       1.127334    -2.006145    -0.075680      68.32
 H       1.381787    -2.962727    -0.280856      18.16
 C      -0.775133    -0.505800     0.400873      27.78
 C      -2.358064    -0.262024     0.746879      83.01
 H      -2.653598    -1.282854     0.893728      23.51
 O      -2.492370     0.523185     1.971782     310.48
 H      -1.898551     0.293163     2.596541      30.36
 C      -3.244174     0.367530    -0.248170      80.19
 H      -2.851633     1.260167    -0.758669      22.76
 O      -3.226951    -0.713442    -1.467314     184.67
 H      -3.070177    -0.092703    -2.287573      21.15
 C      -4.713036     0.656510    -0.022242     115.42
 O      -5.140211     1.684986    -0.930813     281.88
 H      -5.163185     2.570136    -0.594705      29.32
 H      -4.768667     0.911613     1.061943      27.17
 H      -5.248739    -0.131733    -0.176896      30.41
55
name = lig-etoh-Waterframe_471
 C       6.252057    -1.651344     1.453557      50.75
 H       6.524929    -0.623958     1.362979      18.52
 C       5.522361    -3.853323     0.848590      48.11
 H       5.265245    -4.553875    -0.020424      20.46
 C       5.839526    -4.309272     2.156252      20.68
 O       5.616541    -5.607115     2.624367     241.19
 C       5.082313    -6.613643     1.766929     137.23
 H       5.878152    -6.772437     0.961727      27.09
 H       4.242436    -6.303056     1.243341      27.96
 H       4.943304    -7.465341     2.288792      26.72
 C       6.378785    -3.426739     3.162500     -10.39
 O       6.767401    -3.858514     4.460118     270.27
 H       6.242277    -4.656593     4.828992      25.32
 C       6.637986    -2.085303     2.731864      27.61
 H       7.084038    -1.427668     3.542668      21.57
 C       5.668222    -2.501037     0.477414      32.01
 C       5.302634    -2.094411    -0.864893      77.66
 H       5.684224    -2.922244    -1.711364      22.56
 O       5.933154    -0.940721    -1.441487     290.03
 H       5.494166    -0.148534    -1.255925      29.82
 C       3.821923    -2.070553    -1.256969      82.87
 H       3.380445    -2.964542    -0.686358      20.25
 C       3.380706    -2.061767    -2.645469     101.32
 O       3.625022    -3.310086    -3.389233     244.65
 H       4.594272    -3.386538    -3.664187      26.25
 H       3.893782    -1.221744    -3.202251      24.30
 H       2.292130    -1.977632    -2.738766      25.55
 C      -0.264517    -1.814740     0.180234      54.45
 H      -0.946755    -2.636181     0.415432      26.32
 C      -0.011793     0.675936     0.283168      82.42
 H      -0.547122     1.507294     0.872637      18.31
 C       1.326792     0.460793     0.119472      12.03
 O       2.293363     1.440865     0.006115     159.59
 C       1.904120     2.856858    -0.232884     102.97
 H       2.742525     3.187076    -0.786662      25.81
 H       1.086972     2.637586    -0.990839      24.62
 H       1.438580     3.472895     0.709330      23.39
 C       1.907998    -0.870864    -0.188488       7.90
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 O       3.294868    -0.841081    -0.610101     154.31
 C       1.049636    -1.998695    -0.059090      65.08
 H       1.533531    -2.966793    -0.013831      20.38
 C      -0.865072    -0.507521     0.400865      25.76
 C      -2.337725    -0.325798     0.750733      87.14
 H      -2.859260    -1.261577     0.849592      23.72
 O      -2.506251     0.477819     1.941056     261.88
 H      -1.977867     0.011866     2.689166      25.48
 C      -3.237591     0.344875    -0.425085      87.95
 H      -2.750656     1.253542    -0.636616      25.44
 O      -3.287754    -0.665168    -1.420041     267.83
 H      -3.120581    -0.406567    -2.328773      25.62
 C      -4.654186     0.700169     0.020570     101.86
 O      -5.144155     1.647823    -0.886989     275.60
 H      -4.912956     2.495601    -0.517267      30.24
 H      -4.930146     1.077443     1.040310      26.04
 H      -5.310439    -0.293858    -0.072135      26.20
55
name = lig-etoh-Waterframe_472
 C       6.201260    -1.647696     1.489699      43.58
 H       6.310527    -0.590231     1.271380      19.98
 C       5.457525    -3.892359     0.858867      59.34
 H       5.057778    -4.570911     0.048537      21.40
 C       5.829363    -4.325336     2.148723      16.56
 O       5.661457    -5.604153     2.615568     246.31
 C       5.125497    -6.596595     1.721292     124.80
 H       5.861697    -6.905160     0.984459      27.34
 H       4.210264    -6.270773     1.128006      25.48
 H       4.990746    -7.433291     2.501990      23.57
 C       6.392484    -3.413640     3.168093      16.77
 O       6.808996    -3.823970     4.436644     275.95
 H       6.568049    -4.743833     4.831780      21.46
 C       6.639996    -2.113323     2.778913      45.27
 H       6.920103    -1.310346     3.588612      21.10
 C       5.684896    -2.521053     0.510095      18.68
 C       5.314560    -2.080810    -0.972804      96.88
 H       5.662797    -2.821325    -1.469674      28.27
 O       5.976399    -0.891969    -1.458937     294.15
 H       5.475175    -0.166275    -1.182526      29.03
 C       3.761768    -2.112680    -1.158736      79.32
 H       3.240426    -3.068899    -0.811183      20.91
 C       3.368016    -2.069658    -2.692277      94.60
 O       3.623165    -3.309129    -3.372010     250.43
 H       4.593128    -3.399485    -3.653599      26.20
 H       3.842954    -1.172473    -3.244010      24.31
 H       2.156250    -1.935523    -2.609485      22.92
 C      -0.289973    -1.775390     0.222959      40.74
 H      -0.714530    -2.848801     0.349796      21.05
 C      -0.064416     0.632810     0.299617      90.15
 H      -0.366283     1.636233     0.740641      18.71
 C       1.427234     0.481242     0.101563       8.52
 O       2.364225     1.495506     0.044681     170.14
 C       1.857477     2.908901    -0.277745      93.29
 H       2.760236     3.338872    -0.623292      25.18
 H       1.055395     2.965914    -0.876124      26.43
 H       1.732702     3.535579     0.882630      21.56
 C       1.902834    -0.796022    -0.220615      20.93
 O       3.287667    -0.871471    -0.533314     177.92
 C       1.108952    -1.978768    -0.054599      44.03
 H       1.562516    -3.047738     0.045037      18.47
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 C      -0.923371    -0.533434     0.351647      28.18
 C      -2.368284    -0.394666     0.748437      74.32
 H      -2.831260    -1.418425     0.953288      22.89
 O      -2.527512     0.443829     1.905216     214.69
 H      -2.019147     0.005449     2.812641      22.51
 C      -3.147596     0.321491    -0.476494      84.15
 H      -2.615780     1.187399    -0.882691      23.65
 O      -3.351648    -0.667316    -1.419789     282.49
 H      -3.135969    -0.277890    -2.239027      27.11
 C      -4.633451     0.695409     0.104875      66.09
 O      -5.177369     1.670834    -0.883439     258.39
 H      -4.962423     2.558881    -0.573138      29.29
 H      -4.518338     1.113651     1.140377      24.50
 H      -5.339265    -0.382383    -0.079259      24.67
55
name = lig-etoh-Waterframe_473
 C       6.177839    -1.623605     1.519554      62.46
 H       6.132699    -0.610905     1.112182      26.05
 C       5.433687    -3.885760     0.893957      50.60
 H       4.948525    -4.697941     0.343280      18.08
 C       5.825318    -4.308220     2.175994      39.33
 O       5.704034    -5.613145     2.618378     268.74
 C       5.202932    -6.594026     1.690745     122.16
 H       5.861477    -6.940378     0.948450      32.61
 H       4.204132    -6.121170     1.256199      24.42
 H       4.761032    -7.555564     2.361305      24.32
 C       6.408786    -3.472396     3.147438      24.88
 O       6.870835    -3.740927     4.388227     220.53
 H       6.542971    -4.701180     4.615366      24.57
 C       6.570924    -2.096777     2.800233      49.48
 H       7.007391    -1.321932     3.544963      23.97
 C       5.695549    -2.525438     0.551017      27.59
 C       5.320239    -2.115387    -1.018452      71.54
 H       5.759599    -2.940217    -1.604328      22.18
 O       5.999630    -0.851169    -1.469211     251.93
 H       5.686081    -0.101047    -1.006866      30.53
 C       3.737756    -2.107086    -1.128690      78.02
 H       3.446810    -3.027005    -0.585914      20.75
 C       3.332236    -2.060787    -2.703364      90.84
 O       3.619609    -3.333388    -3.359260     249.97
 H       4.500645    -3.238319    -3.856007      25.36
 H       3.823730    -1.180752    -3.204208      23.93
 H       2.132383    -1.876203    -2.890789      22.81
 C      -0.283535    -1.815983     0.252574      30.67
 H      -1.087202    -2.694662     0.398209      15.12
 C       0.006824     0.571769     0.359153      71.62
 H      -0.396383     1.568010     0.299187      18.70
 C       1.374628     0.501104     0.050035       6.62
 O       2.396365     1.602668     0.067498     195.28
 C       1.884153     2.929784    -0.258507     112.85
 H       2.522326     3.638743    -0.839578      24.43
 H       0.989287     3.155408    -0.768198      26.39
 H       1.617117     3.442605     0.799765      23.57
 C       1.950199    -0.793573    -0.232885      26.81
 O       3.262327    -0.914624    -0.453754     199.24
 C       1.145961    -1.871919    -0.029125      58.74
 H       1.517741    -2.987373    -0.156395      19.83
 C      -0.879561    -0.543231     0.324294      43.87
 C      -2.400251    -0.418248     0.718098      69.56
 H      -2.762943    -1.514538     0.852915      22.52
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 O      -2.571847     0.424954     1.887479     196.20
 H      -1.735267     0.125286     2.662679      23.28
 C      -3.155703     0.287349    -0.338185      90.70
 H      -2.607772     1.096769    -0.878133      21.88
 O      -3.400258    -0.731041    -1.510182     224.56
 H      -3.310146    -0.272631    -2.318918      26.93
 C      -4.530630     0.741073     0.088776      95.13
 O      -5.209243     1.695076    -0.845540     269.74
 H      -5.184000     2.631642    -0.560619      28.48
 H      -4.445903     1.080456     1.118395      27.00
 H      -5.271473    -0.185727     0.267236      26.92
55
name = lig-etoh-Waterframe_474
 C       6.146555    -1.611297     1.488211      53.26
 H       6.353949    -0.507693     1.435144      22.93
 C       5.444288    -3.854675     0.967391      72.08
 H       4.998458    -4.459527     0.209956      22.60
 C       5.829424    -4.326553     2.226024      14.25
 O       5.757532    -5.664968     2.635398     260.56
 C       5.210952    -6.583142     1.687985      99.35
 H       5.928535    -6.748260     0.906242      29.55
 H       4.327101    -6.177473     1.056607      28.13
 H       5.004673    -7.607472     2.309089      25.71
 C       6.445326    -3.384747     3.093891      10.38
 O       6.936562    -3.713502     4.358931     156.91
 H       6.508913    -4.527406     4.869120      24.96
 C       6.481233    -2.046879     2.769619      52.67
 H       7.031264    -1.519156     3.542612      20.73
 C       5.656015    -2.541834     0.493112      48.31
 C       5.343853    -2.109994    -0.929091      83.86
 H       5.718949    -2.868409    -1.917041      21.90
 O       5.998935    -0.862662    -1.466483     211.44
 H       5.870177    -0.149549    -0.863614      28.66
 C       3.780416    -2.089280    -1.190887      86.58
 H       3.440689    -2.947535    -0.667025      21.31
 C       3.283166    -2.055852    -2.668909     103.16
 O       3.616765    -3.344472    -3.363849     242.29
 H       4.440569    -3.246054    -3.944952      27.16
 H       3.928162    -1.334994    -3.084552      24.35
 H       2.214560    -1.885737    -2.853399      24.88
 C      -0.260238    -1.816196     0.258047      30.27
 H      -0.881262    -2.777864     0.367530      18.36
 C       0.054812     0.596608     0.360778      56.39
 H      -0.508345     1.450409     0.257698      18.13
 C       1.417219     0.539469    -0.008596      11.44
 O       2.348007     1.669647     0.040279     187.58
 C       1.859063     3.017234    -0.186168      99.63
 H       2.697007     3.459269    -0.888661      22.25
 H       0.822320     2.650154    -0.761789      21.55
 H       1.711628     3.534683     0.623177      27.49
 C       1.939369    -0.755346    -0.176563      15.24
 O       3.316164    -0.941277    -0.402359     182.74
 C       1.048335    -1.892651    -0.005586      48.01
 H       1.645603    -2.809016    -0.300550      18.98
 C      -0.823884    -0.561077     0.377296      65.20
 C      -2.329000    -0.431548     0.706846      82.87
 H      -2.811402    -1.427928     0.849573      24.76
 O      -2.594154     0.396646     1.876565     220.62
 H      -1.836537     0.159874     2.678673      24.17
 C      -3.245623     0.207453    -0.392006      75.09
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 H      -2.578454     1.137116    -0.550975      22.00
 O      -3.429698    -0.785714    -1.545764     252.09
 H      -3.415406    -0.312062    -2.379409      25.47
 C      -4.510700     0.841118     0.113663     126.37
 O      -5.216839     1.701697    -0.782104     279.88
 H      -5.165906     2.553282    -0.295022      28.36
 H      -4.450244     1.443449     0.980308      27.20
 H      -5.079340     0.049270     0.235425      29.59
55
name = lig-etoh-Waterframe_475
 C       6.125945    -1.565985     1.425862      53.87
 H       6.401535    -0.494643     1.158025      23.14
 C       5.445873    -3.834602     0.959977      73.72
 H       5.133606    -4.517208     0.217644      23.85
 C       5.851976    -4.350911     2.261026      31.49
 O       5.793660    -5.684564     2.666058     255.92
 C       5.247421    -6.584829     1.639688     126.80
 H       6.066574    -6.710806     0.892172      29.21
 H       4.289029    -6.319951     1.266822      27.25
 H       5.171897    -7.512879     2.162219      27.72
 C       6.438799    -3.371850     3.125393      25.98
 O       7.010971    -3.692506     4.352623     193.98
 H       6.492408    -4.527749     4.718580      28.94
 C       6.447097    -2.008545     2.737461      54.60
 H       6.830940    -1.286361     3.373129      21.51
 C       5.653267    -2.473975     0.506344      37.32
 C       5.335016    -2.061291    -0.946676     101.58
 H       5.833891    -3.095421    -1.527055      22.44
 O       5.994547    -0.907802    -1.423034     238.95
 H       5.846795    -0.188744    -0.825784      28.86
 C       3.808116    -2.093165    -1.190335      85.76
 H       3.382534    -3.042475    -0.922341      21.94
 C       3.330313    -2.057395    -2.660078     108.05
 O       3.587301    -3.345242    -3.365997     256.80
 H       4.486976    -3.234935    -3.817465      26.49
 H       3.760860    -1.258457    -3.219505      25.68
 H       2.358607    -1.859629    -2.600422      27.76
 C      -0.291169    -1.848655     0.266017      43.98
 H      -0.727687    -2.796258     0.359728      22.89
 C       0.002589     0.640681     0.301484      55.42
 H      -0.398012     1.600471     0.599878      19.56
 C       1.493648     0.605918    -0.002896       6.59
 O       2.304895     1.657223     0.023313     211.19
 C       1.791477     3.024498    -0.178934      98.74
 H       2.602950     3.540415    -0.870087      24.29
 H       0.681446     3.173282    -0.885003      21.81
 H       1.727457     3.696597     0.652875      25.68
 C       1.927515    -0.770020    -0.108474      19.57
 O       3.361389    -0.932949    -0.374260     159.04
 C       1.133675    -1.914526    -0.053797      52.00
 H       1.437742    -2.951005    -0.125337      21.59
 C      -0.795542    -0.519730     0.471349      24.47
 C      -2.307478    -0.456940     0.721646      80.77
 H      -2.544254    -1.468952     0.955819      24.43
 O      -2.595328     0.374501     1.874352     291.39
 H      -2.138329     0.024748     2.631400      28.81
 C      -3.215239     0.184882    -0.515041      60.69
 H      -2.655296     0.994040    -1.120008      21.37
 O      -3.454221    -0.792841    -1.508060     253.95
 H      -3.311378    -0.272661    -2.339475      25.36
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 C      -4.578603     0.873825     0.185794      99.00
 O      -5.222505     1.745073    -0.743911     291.41
 H      -5.146383     2.730172    -0.499710      27.81
 H      -4.098425     1.386591     1.030825      23.10
 H      -5.288504     0.100203     0.520815      26.77
55
name = lig-etoh-Waterframe_476
 C       6.141679    -1.499820     1.406724      78.05
 H       6.237184    -0.513702     0.926859      24.32
 C       5.474498    -3.835488     0.945209      52.04
 H       5.181191    -4.623099     0.301367      21.73
 C       5.875466    -4.292202     2.220783      28.78
 O       5.800222    -5.669802     2.669262     226.01
 C       5.329498    -6.607087     1.636740     140.34
 H       5.928838    -6.651170     0.620846      29.46
 H       4.393227    -6.281812     1.356646      26.39
 H       5.263008    -7.488032     2.060140      29.66
 C       6.405963    -3.356330     3.175787       3.15
 O       7.059616    -3.687774     4.355857     289.39
 H       6.747486    -4.614409     4.668153      27.88
 C       6.461414    -1.957396     2.708511      50.30
 H       6.704660    -1.188022     3.375342      25.80
 C       5.626895    -2.461064     0.542018      33.05
 C       5.331022    -2.132319    -0.943492     102.62
 H       5.776757    -2.862792    -1.532885      24.80
 O       6.008832    -0.938361    -1.378998     280.65
 H       5.636131    -0.159906    -0.963990      29.40
 C       3.839911    -2.093707    -1.177098      73.16
 H       3.485255    -3.052962    -0.686813      20.75
 C       3.389603    -2.025156    -2.682460     100.33
 O       3.558808    -3.317202    -3.350771     257.66
 H       4.460668    -3.319120    -3.800350      26.36
 H       3.673992    -1.175504    -3.352934      24.33
 H       2.300461    -2.007640    -2.577495      25.66
 C      -0.206813    -1.813488     0.255626      49.73
 H      -0.869969    -2.547957     0.441120      27.35
 C       0.039927     0.696382     0.264043      80.11
 H      -0.322805     1.641294     0.796223      20.24
 C       1.346174     0.531164     0.073460       7.30
 O       2.288089     1.684411    -0.003141     137.36
 C       1.735080     3.064200    -0.245518      95.86
 H       2.502206     3.612499    -0.815164      25.20
 H       0.698165     3.263915    -0.684544      24.10
 H       1.650760     3.490838     0.973488      23.13
 C       2.036948    -0.787492    -0.105025       9.63
 O       3.357202    -0.921042    -0.365114     164.67
 C       1.136420    -1.942676    -0.060995      55.56
 H       1.621324    -2.866264    -0.049976      22.74
 C      -0.797532    -0.512223     0.498993      32.98
 C      -2.306790    -0.431525     0.718196      78.49
 H      -2.671518    -1.462491     0.802928      23.41
 O      -2.605513     0.357805     1.887119     299.41
 H      -2.156479     0.001450     2.557322      31.10
 C      -3.197252     0.195691    -0.529277      65.29
 H      -2.744665     1.027622    -1.065603      22.48
 O      -3.491426    -0.825065    -1.487112     234.10
 H      -3.273791    -0.559023    -2.448014      25.10
 C      -4.542595     0.866424     0.209857      76.88
 O      -5.248874     1.803165    -0.730435     272.30
 H      -4.931807     2.778020    -0.510769      26.99
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 H      -4.076813     1.431655     1.099409      20.80
 H      -5.425863     0.189434     0.828634      23.56
55
name = lig-etoh-Waterframe_477
 C       6.136725    -1.500261     1.408434      39.20
 H       6.214914    -0.433281     1.295725      21.18
 C       5.518730    -3.842752     0.946404      46.68
 H       5.129612    -4.470705     0.150679      19.36
 C       5.902657    -4.248139     2.228400      16.73
 O       5.819294    -5.618167     2.617357     230.51
 C       5.380156    -6.584120     1.643809     115.76
 H       6.035001    -6.541119     0.673866      28.05
 H       4.343052    -6.334186     1.334694      27.14
 H       5.415630    -7.576313     2.103715      26.89
 C       6.395751    -3.262094     3.150629      -3.26
 O       7.079283    -3.688462     4.355802     278.33
 H       6.796579    -4.580572     4.703689      27.72
 C       6.497619    -1.919919     2.736537      43.00
 H       6.892820    -1.301030     3.571096      22.21
 C       5.604742    -2.526208     0.529778      25.39
 C       5.364707    -2.188118    -0.916614     118.41
 H       5.648161    -2.872085    -1.602854      28.03
 O       6.029481    -0.941188    -1.343507     270.84
 H       5.435012    -0.193081    -1.208332      28.47
 C       3.864985    -2.082322    -1.176879      76.25
 H       3.367594    -2.983401    -0.659799      19.45
 C       3.353321    -2.021766    -2.670943      86.64
 O       3.568135    -3.286704    -3.344306     259.30
 H       4.389094    -3.303977    -3.912536      27.23
 H       3.944793    -1.137594    -3.168185      22.55
 H       2.140921    -1.889939    -2.745562      22.54
 C      -0.185270    -1.701495     0.272475      55.38
 H      -0.805711    -2.597929     0.458707      24.65
 C      -0.032756     0.660374     0.357124      76.42
 H      -0.439773     1.769471     0.475054      17.64
 C       1.409003     0.469994     0.097115      -0.89
 O       2.226762     1.685080    -0.069285     177.27
 C       1.699054     3.064554    -0.223711     103.11
 H       2.401031     3.622147    -0.707173      25.82
 H       0.864358     2.938753    -0.638431      28.36
 H       1.558570     3.599819     0.953653      22.99
 C       1.991970    -0.809228    -0.123264      22.04
 O       3.379463    -0.890955    -0.386318     181.26
 C       1.217537    -1.929474    -0.026743      47.35
 H       1.650359    -2.875212    -0.141789      18.54
 C      -0.778511    -0.486784     0.420566      41.47
 C      -2.323521    -0.389576     0.666289      72.49
 H      -2.859284    -1.393116     0.729857      22.52
 O      -2.615382     0.340724     1.911728     244.93
 H      -1.980991     0.061630     2.634814      26.88
 C      -3.244452     0.243358    -0.433724      78.91
 H      -2.702749     1.073414    -0.760907      23.07
 O      -3.532354    -0.894054    -1.472447     188.19
 H      -3.251604    -0.442332    -2.395258      22.86
 C      -4.466553     0.910140     0.184040      84.56
 O      -5.249054     1.820737    -0.703918     250.74
 H      -4.943795     2.736745    -0.289739      25.53
 H      -4.222328     1.666685     0.992462      21.26
 H      -5.225597    -0.037996     0.474101      23.26
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name = lig-etoh-Waterframe_478
 C       6.112857    -1.552491     1.490444      63.76
 H       6.140986    -0.520408     1.195817      27.06
 C       5.544038    -3.854422     0.930816      49.23
 H       5.176458    -4.654066     0.227821      17.75
 C       5.906946    -4.243366     2.237243      24.69
 O       5.858703    -5.539339     2.587013     216.18
 C       5.414200    -6.519039     1.629640     121.61
 H       6.141632    -6.558282     0.816110      30.71
 H       4.300887    -6.488856     1.278768      25.54
 H       5.586877    -7.536201     2.296480      25.57
 C       6.447130    -3.269208     3.151084     -11.38
 O       7.062109    -3.660209     4.327209     195.74
 H       6.537885    -4.417234     4.591028      34.40
 C       6.532298    -1.917678     2.779343      52.10
 H       7.137205    -1.152448     3.416241      20.78
 C       5.679056    -2.482265     0.542597      15.55
 C       5.362392    -2.156862    -0.939810      61.52
 H       5.775943    -3.198064    -1.599889      20.71
 O       6.045475    -0.956099    -1.316529     264.37
 H       5.413205    -0.223570    -1.252052      29.13
 C       3.791562    -2.068463    -1.155829      80.90
 H       3.365419    -3.043066    -0.797611      20.56
 C       3.342820    -2.005522    -2.635617      96.22
 O       3.579613    -3.272098    -3.359866     260.28
 H       4.419192    -3.121407    -3.854975      25.69
 H       4.026836    -1.228256    -3.124863      23.95
 H       2.247093    -1.493262    -2.744019      23.67
 C      -0.146328    -1.727666     0.282265      30.37
 H      -0.702888    -2.787268     0.396236      19.61
 C       0.040493     0.650881     0.430783      60.67
 H      -0.546745     1.614201     0.195248      18.62
 C       1.425904     0.572833     0.104371      12.71
 O       2.204529     1.635294    -0.134998     197.71
 C       1.652833     2.991862    -0.149075     117.96
 H       2.317391     3.552042    -0.741940      26.26
 H       0.707726     2.985619    -0.863101      24.44
 H       1.384249     3.554733     0.715727      26.82
 C       2.014185    -0.757854    -0.151550      12.14
 O       3.400245    -0.846748    -0.439646     174.81
 C       1.195394    -1.915998     0.043162      54.63
 H       1.420373    -2.947784    -0.175894      20.51
 C      -0.884784    -0.450374     0.339525      33.85
 C      -2.380318    -0.382436     0.670557      83.26
 H      -2.544888    -1.502660     0.847539      23.71
 O      -2.613528     0.334371     1.920673     199.80
 H      -1.862778    -0.035669     2.734271      23.26
 C      -3.230624     0.301896    -0.377546      85.47
 H      -2.634390     0.898791    -1.093539      23.96
 O      -3.543347    -0.865217    -1.418774     156.37
 H      -3.393990    -0.300524    -2.322025      24.12
 C      -4.483190     0.946407     0.134081     121.99
 O      -5.214980     1.813493    -0.683245     295.08
 H      -5.324035     2.775466    -0.348906      27.81
 H      -4.168643     1.238268     1.150569      25.16
 H      -5.078279     0.119110     0.384211      28.40
55
name = lig-etoh-Waterframe_480
 C       6.110918    -1.513770     1.480301      35.46
 H       6.276001    -0.429670     1.383617      16.54
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 C       5.605347    -3.807441     0.884583      67.09
 H       5.337012    -4.476557     0.022016      19.57
 C       5.957260    -4.178673     2.211692      18.63
 O       5.919126    -5.481306     2.643878     257.06
 C       5.530182    -6.486521     1.679851     106.42
 H       6.227909    -6.574149     0.888787      29.39
 H       4.537962    -6.189636     1.352818      31.53
 H       5.371714    -7.486652     2.159982      25.66
 C       6.542677    -3.278670     3.111382       6.80
 O       6.997802    -3.677170     4.407400     200.16
 H       6.708072    -4.641976     4.567842      25.11
 C       6.625902    -1.923056     2.756123      11.13
 H       6.985135    -1.306592     3.618444      21.21
 C       5.696682    -2.478680     0.524483      18.44
 C       5.317597    -2.110591    -0.848642      85.41
 H       5.483131    -2.859292    -1.575996      27.38
 O       6.047334    -0.948376    -1.377341     134.40
 H       5.896510    -0.151561    -0.786302      27.33
 C       3.812639    -2.039779    -1.134689      86.59
 H       3.296229    -2.857562    -0.702545      24.45
 C       3.452365    -1.927128    -2.677822     112.53
 O       3.523798    -3.197475    -3.339405     274.27
 H       4.382319    -3.259398    -3.877149      25.75
 H       3.983108    -1.101475    -3.023473      28.03
 H       2.467652    -1.723954    -2.715243      28.78
 C      -0.284152    -1.782849     0.274053      50.81
 H      -0.947971    -2.659689     0.504728      28.44
 C      -0.016388     0.658123     0.324885      70.30
 H      -0.364959     1.486156     0.820058      21.13
 C       1.423266     0.528553     0.045847       2.18
 O       2.251762     1.644060    -0.245334     139.66
 C       1.565805     2.920023    -0.192682      97.67
 H       2.275648     3.886268    -0.292917      24.04
 H       0.601171     2.793910    -0.947697      22.71
 H       1.221151     2.967163     0.940182      24.69
 C       1.982368    -0.743212    -0.075922      32.29
 O       3.324295    -0.748773    -0.563336     164.73
 C       1.171045    -1.783288     0.090784      60.72
 H       1.730966    -2.786165     0.181239      21.64
 C      -0.808331    -0.500501     0.438921      25.51
 C      -2.336244    -0.393923     0.710555      77.68
 H      -2.868412    -1.311455     0.804189      23.21
 O      -2.582499     0.337498     1.940419     254.92
 H      -1.979497    -0.009772     2.733876      24.29
 C      -3.200047     0.313104    -0.453455      73.75
 H      -2.653566     1.279133    -0.795118      21.31
 O      -3.559619    -0.723551    -1.328494     225.50
 H      -3.558519    -0.337648    -2.340093      22.13
 C      -4.542126     0.846421     0.204426      77.85
 O      -5.187723     1.875033    -0.738689     230.85
 H      -4.972224     2.830668    -0.391960      27.39
 H      -4.415773     1.470845     1.046785      24.03
 H      -5.295902    -0.108480     0.351162      24.67
55
name = lig-etoh-Waterframe_481
 C       6.202096    -1.452211     1.482082      69.35
 H       6.066015    -0.353405     1.225486      25.52
 C       5.651900    -3.809934     0.880608      45.94
 H       5.328524    -4.571057     0.161535      15.66
 C       6.022184    -4.244404     2.179150      43.60
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 O       5.954400    -5.508206     2.691839     221.12
 C       5.515225    -6.468609     1.710553     143.16
 H       6.363712    -6.539442     0.956759      30.19
 H       4.658915    -6.227903     1.164603      30.61
 H       5.448997    -7.296186     2.267088      26.98
 C       6.563954    -3.271877     3.154506       4.56
 O       6.979339    -3.677231     4.429489     222.12
 H       6.557758    -4.634425     4.600382      28.71
 C       6.635013    -1.936852     2.724660      73.37
 H       6.886319    -1.200990     3.442459      22.94
 C       5.678148    -2.385840     0.558995      19.69
 C       5.315197    -2.068033    -0.885776      82.79
 H       5.599142    -2.904895    -1.409486      26.56
 O       6.036641    -0.918106    -1.417641     107.04
 H       6.078494    -0.246613    -0.674920      28.72
 C       3.829194    -1.925580    -1.139808      91.15
 H       3.399856    -2.880734    -0.834584      22.97
 C       3.449967    -1.912859    -2.647128     100.05
 O       3.529989    -3.184798    -3.350188     259.20
 H       4.280541    -3.026491    -4.017769      24.34
 H       4.102814    -1.191268    -3.226331      23.84
 H       2.459487    -1.482722    -2.646332      25.81
 C      -0.224485    -1.776878     0.279485      54.94
 H      -0.657790    -2.680640     0.484791      28.29
 C       0.001157     0.657326     0.304250      70.91
 H      -0.538470     1.468076     0.705553      19.24
 C       1.364406     0.600520    -0.013919      12.78
 O       2.269779     1.627287    -0.305545     187.03
 C       1.527715     2.906787    -0.137329     113.86
 H       2.154872     3.805526    -0.479757      24.65
 H       0.905428     2.938420    -0.862932      29.25
 H       0.748853     3.172666     0.791547      23.11
 C       1.978939    -0.724235    -0.097399      10.28
 O       3.250694    -0.718394    -0.583896     163.97
 C       1.107526    -1.914122     0.130484      55.57
 H       1.550925    -2.956323     0.214320      19.26
 C      -0.855870    -0.503722     0.515628      50.13
 C      -2.331606    -0.353655     0.696003      90.06
 H      -2.530405    -1.414551     0.791389      21.69
 O      -2.569628     0.372299     1.953577     300.64
 H      -2.015439    -0.010124     2.550338      29.33
 C      -3.237471     0.381156    -0.276697      89.39
 H      -2.749112     1.074483    -0.901897      22.41
 O      -3.551511    -0.692329    -1.388544     166.63
 H      -3.474096    -0.169392    -2.331150      22.73
 C      -4.562206     0.885804     0.170319      86.22
 O      -5.163266     1.869894    -0.757253     285.12
 H      -4.863531     2.785906    -0.401559      27.51
 H      -4.347013     1.139028     1.220297      23.47
 H      -5.382730    -0.071987     0.391866      24.58
55
name = lig-etoh-Waterframe_482
 C       6.242879    -1.437758     1.453567      45.99
 H       6.127905    -0.319203     1.267906      24.65
 C       5.706490    -3.766614     0.930497      55.91
 H       5.324581    -4.469145     0.237008      16.02
 C       6.120664    -4.212125     2.192607      24.80
 O       5.962513    -5.533231     2.705462     263.49
 C       5.526291    -6.495043     1.743826     119.79
 H       6.365891    -6.731156     0.901732      27.72
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 H       4.614322    -6.209133     1.196781      28.59
 H       5.361246    -7.369703     2.271355      25.72
 C       6.556783    -3.296869     3.150168      21.21
 O       6.954181    -3.645724     4.405134     239.44
 H       6.582939    -4.460443     4.906897      24.80
 C       6.649270    -1.908053     2.767097      54.64
 H       7.011517    -1.160727     3.377690      24.15
 C       5.693502    -2.370818     0.597086      36.78
 C       5.321912    -1.988322    -0.919794      78.45
 H       5.845951    -2.978604    -1.476582      24.88
 O       6.047301    -0.894992    -1.456626     122.87
 H       6.066052    -0.113357    -0.809845      28.27
 C       3.797765    -1.883430    -1.194767      89.74
 H       3.357947    -2.732706    -0.586440      20.95
 C       3.445050    -1.824330    -2.649089      86.97
 O       3.523478    -3.174817    -3.358937     234.01
 H       4.333669    -3.142747    -3.998743      25.19
 H       4.217465    -1.208665    -3.274715      22.62
 H       2.316568    -1.464603    -2.830766      24.12
 C      -0.250655    -1.769859     0.368277      46.08
 H      -0.831000    -2.606255     0.465372      21.34
 C      -0.037805     0.665726     0.354062      74.09
 H      -0.437495     1.712863     0.143240      17.15
 C       1.338033     0.553595    -0.065409       3.17
 O       2.215973     1.664881    -0.304628     178.17
 C       1.486480     2.940023    -0.195814     102.97
 H       2.348955     3.562433    -0.187373      24.99
 H       0.791840     3.072004    -1.038572      25.40
 H       1.074991     2.938327     0.944104      23.41
 C       1.876738    -0.744855    -0.147716      18.04
 O       3.221019    -0.698743    -0.573723     171.43
 C       1.207335    -1.968524     0.133855      56.03
 H       1.506640    -3.002923     0.023527      17.78
 C      -0.805002    -0.490284     0.452435      38.53
 C      -2.344382    -0.339289     0.780760      76.77
 H      -2.852716    -1.408671     0.801219      22.48
 O      -2.558442     0.410902     1.970744     256.73
 H      -2.082021    -0.029611     2.713896      27.60
 C      -3.265642     0.340868    -0.311254      80.98
 H      -2.711636     1.162845    -0.680654      23.66
 O      -3.515489    -0.633720    -1.423268     226.70
 H      -3.399740    -0.113083    -2.356255      22.62
 C      -4.619618     0.930863     0.211684     102.39
 O      -5.108363     1.849987    -0.728623     274.33
 H      -4.988480     2.732950    -0.280801      27.72
 H      -4.659376     1.450875     1.232400      25.83
 H      -5.350513     0.080282     0.018847      25.58
55
name = lig-etoh-Waterframe_483
 C       6.258902    -1.449152     1.514825      46.51
 H       6.446933    -0.381361     1.317282      22.12
 C       5.736114    -3.712087     0.962601      49.16
 H       5.373624    -4.358611     0.223004      18.54
 C       6.164704    -4.218399     2.221249      25.67
 O       5.978192    -5.522548     2.675009     282.32
 C       5.524344    -6.564651     1.754988      99.17
 H       6.316496    -6.802736     0.898317      25.29
 H       4.529343    -6.145323     1.352772      25.52
 H       5.223979    -7.534438     2.305003      21.55
 C       6.568128    -3.229333     3.155192       9.12
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 O       6.955913    -3.578512     4.430293     215.90
 H       6.587894    -4.542280     4.511518      34.02
 C       6.666762    -1.868020     2.784164      57.60
 H       7.165313    -1.335536     3.571664      21.83
 C       5.726642    -2.380059     0.535351      40.34
 C       5.351814    -1.959940    -0.877415      64.28
 H       5.499606    -2.839500    -1.818063      22.43
 O       6.086768    -0.844901    -1.497283     162.72
 H       5.742122     0.046612    -1.068008      25.75
 C       3.762483    -1.881048    -1.189010      71.64
 H       3.286537    -2.857885    -0.782082      20.89
 C       3.443932    -1.796046    -2.764135      86.76
 O       3.503676    -3.151625    -3.347149     252.75
 H       4.433470    -3.172293    -3.768385      24.28
 H       4.101870    -0.899994    -3.044689      22.91
 H       2.301746    -1.411546    -2.943958      23.99
 C      -0.203054    -1.796963     0.461642      48.14
 H      -1.033394    -2.521221     0.578184      14.50
 C      -0.010024     0.718864     0.311936      75.64
 H      -0.635128     1.689727    -0.021116      15.68
 C       1.278193     0.509506    -0.065251       6.93
 O       2.094171     1.650644    -0.307036     189.16
 C       1.557716     2.961384    -0.213140     107.99
 H       2.249894     3.721688    -0.140646      25.69
 H       0.554930     3.345432    -1.008915      21.72
 H       1.032446     3.025390     0.724121      26.43
 C       1.880544    -0.805935    -0.224598      16.47
 O       3.227609    -0.668386    -0.553842     180.93
 C       1.157961    -1.943419     0.119700      63.90
 H       1.710927    -2.793724    -0.117895      21.31
 C      -0.845729    -0.485548     0.410821      49.73
 C      -2.395107    -0.370098     0.824889      72.29
 H      -2.907503    -1.386704     1.112499      22.23
 O      -2.562524     0.467830     1.994765     206.16
 H      -1.993466    -0.012285     2.836503      23.83
 C      -3.233292     0.323055    -0.366233      79.91
 H      -2.736573     1.280892    -0.593901      23.10
 O      -3.462624    -0.551010    -1.432140     268.44
 H      -3.351727    -0.057833    -2.358741      23.14
 C      -4.693064     0.877113     0.234884     105.92
 O      -5.070314     1.913319    -0.726488     284.80
 H      -5.086691     2.821849    -0.378203      29.20
 H      -4.727662     1.343601     1.282958      27.86
 H      -5.310783     0.111017     0.290590      30.14
55
name = lig-etoh-Waterframe_484
 C       6.280418    -1.419699     1.535359      58.39
 H       6.540370    -0.463356     1.169134      21.44
 C       5.731744    -3.730073     0.931174      55.15
 H       5.457730    -4.522488     0.250187      23.93
 C       6.129429    -4.186675     2.204333      20.78
 O       6.022294    -5.526237     2.647533     256.94
 C       5.474255    -6.584855     1.755216     117.25
 H       6.180215    -6.798739     0.960018      26.65
 H       4.518418    -6.298198     1.154829      25.22
 H       5.418542    -7.466850     2.570845      21.43
 C       6.598086    -3.188324     3.181021      39.66
 O       6.948642    -3.532158     4.460506     202.60
 H       6.874141    -4.542049     4.633474      24.71
 C       6.699706    -1.872516     2.809436      55.26
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 H       7.160243    -1.109264     3.532568      22.47
 C       5.826679    -2.321580     0.535714      10.30
 C       5.294205    -1.954621    -0.936471      76.97
 H       5.718297    -2.870448    -1.432179      20.01
 O       6.098577    -0.788602    -1.503250     209.13
 H       5.530268     0.060371    -1.295722      24.42
 C       3.774898    -1.854038    -1.202252      77.56
 H       3.350728    -2.850082    -0.935919      20.83
 C       3.420864    -1.762099    -2.781249      95.96
 O       3.516909    -3.085857    -3.340362     257.59
 H       4.367660    -3.178116    -3.878477      25.04
 H       4.087659    -1.180179    -3.419352      24.14
 H       2.349268    -1.439189    -2.866581      23.96
 C      -0.250033    -1.742083     0.516160      44.08
 H      -0.648579    -2.854271     0.856103      13.37
 C      -0.134083     0.653582     0.193413      68.69
 H      -0.578010     1.751907     0.394550      15.98
 C       1.259980     0.535442    -0.069475      15.75
 O       2.024548     1.609559    -0.353804     201.06
 C       1.547476     3.019804    -0.148914     106.28
 H       2.365730     3.691428    -0.415849      24.37
 H       0.841610     3.210362    -1.246494      21.33
 H       0.998128     3.180667     0.639822      28.02
 C       1.890653    -0.722207    -0.249655      14.78
 O       3.242889    -0.698598    -0.546370     175.72
 C       1.104942    -1.917008     0.064943      55.50
 H       1.505015    -2.913863     0.104522      23.69
 C      -0.898800    -0.511373     0.466187      50.60
 C      -2.423789    -0.375437     0.815079      84.60
 H      -2.636631    -1.406704     1.040571      25.67
 O      -2.578803     0.542915     2.011227     222.47
 H      -1.774618     0.038348     2.626528      23.27
 C      -3.263212     0.363972    -0.256617      75.88
 H      -2.683013     1.248429    -0.738490      20.75
 O      -3.400879    -0.492014    -1.472923     237.64
 H      -3.292136     0.074171    -2.335169      24.21
 C      -4.684875     0.830085     0.223272      97.26
 O      -5.078288     1.972670    -0.741623     273.51
 H      -4.877736     2.727918    -0.167337      28.92
 H      -4.377243     1.126872     1.236569      26.21
 H      -5.496529     0.066457     0.312307      27.11
55
name = lig-etoh-Waterframe_485
 C       6.331440    -1.379621     1.479112      74.22
 H       6.382818    -0.345923     1.249045      25.74
 C       5.743032    -3.728741     0.884788      38.42
 H       5.440818    -4.485422     0.108897      14.67
 C       6.070551    -4.128948     2.198772      31.09
 O       6.058455    -5.503043     2.603045     259.51
 C       5.472577    -6.553417     1.762927     139.14
 H       6.125914    -6.873118     1.091297      32.16
 H       4.446072    -6.402719     1.399602      29.73
 H       5.334220    -7.477836     2.500377      26.28
 C       6.601647    -3.247595     3.193178     -18.51
 O       6.964334    -3.502918     4.511659     191.07
 H       6.752456    -4.440109     4.859327      22.50
 C       6.735805    -1.828765     2.800616       7.88
 H       7.100601    -0.948013     3.495542      22.28
 C       5.852910    -2.319782     0.558701      10.96
 C       5.354089    -1.941868    -0.959444      89.19
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 H       5.681374    -2.689824    -1.476664      25.30
 O       6.051569    -0.775528    -1.496869     228.97
 H       5.575503     0.120519    -1.228365      26.76
 C       3.825822    -1.838861    -1.292703      88.73
 H       3.350369    -2.663121    -0.836049      22.52
 C       3.423113    -1.735399    -2.764818     111.79
 O       3.514123    -3.068687    -3.353061     277.10
 H       4.299777    -3.025373    -3.964759      25.46
 H       3.994115    -1.088176    -3.368574      26.31
 H       2.471722    -1.409737    -2.799220      26.83
 C      -0.254170    -1.745261     0.512791      36.63
 H      -0.725274    -2.680466     1.161899      25.67
 C      -0.234086     0.573788     0.113788      68.46
 H      -0.606440     1.526190     0.519611      20.15
 C       1.175205     0.567906    -0.104237       9.49
 O       2.026552     1.649495    -0.385429     181.65
 C       1.528348     3.022585    -0.223875     115.83
 H       2.606051     3.500705    -0.219617      23.66
 H       0.874974     3.231151    -0.983194      27.45
 H       1.150460     3.288701     0.797439      26.05
 C       1.840663    -0.705609    -0.224008      12.03
 O       3.252129    -0.730357    -0.531138     163.41
 C       1.073233    -1.821004     0.031459      58.57
 H       1.405372    -2.835123     0.253926      21.30
 C      -0.991249    -0.518846     0.539670      38.89
 C      -2.413740    -0.335468     0.830190      97.67
 H      -2.926321    -1.250272     0.962813      22.76
 O      -2.561903     0.573165     1.984376     229.59
 H      -2.133848     0.294195     2.922307      23.63
 C      -3.321500     0.347469    -0.253379      77.45
 H      -2.726793     1.380398    -0.279093      20.74
 O      -3.339648    -0.458810    -1.501043     242.69
 H      -3.233229     0.187813    -2.278720      22.68
 C      -4.608983     0.844066     0.185324      95.99
 O      -5.084279     1.981361    -0.665466     256.32
 H      -4.788779     2.809628    -0.258825      29.24
 H      -4.628979     1.311904     1.156613      25.21
 H      -5.525488     0.027030    -0.035677      23.68
55
name = lig-etoh-Waterframe_486
 C       6.392812    -1.369973     1.468122      41.27
 H       6.211434    -0.300355     1.337024      19.43
 C       5.769441    -3.662367     0.868369      61.81
 H       5.397180    -4.376635     0.056129      15.57
 C       6.038812    -4.156562     2.202658      18.89
 O       6.073550    -5.456221     2.562174     267.34
 C       5.473820    -6.525020     1.810872     109.18
 H       6.055402    -6.807233     0.917407      30.22
 H       4.562843    -6.119518     1.458246      34.74
 H       5.336900    -7.348731     2.512806      26.25
 C       6.597342    -3.170382     3.180193       0.78
 O       6.977369    -3.501957     4.558494     191.36
 H       6.437449    -4.309359     4.736927      26.54
 C       6.735237    -1.836674     2.735966      49.10
 H       7.109531    -1.217079     3.622592      20.71
 C       5.799174    -2.340101     0.491169       9.64
 C       5.446530    -1.909862    -0.948787      93.49
 H       5.695381    -2.684577    -1.768967      25.07
 O       5.998390    -0.753742    -1.493370     266.46
 H       5.700697     0.039818    -0.841084      25.59
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 C       3.852440    -1.859932    -1.278859      71.47
 H       3.465801    -2.821659    -0.993491      22.27
 C       3.435372    -1.707537    -2.761105     105.77
 O       3.494856    -3.065674    -3.391104     250.70
 H       4.352780    -3.132897    -3.911143      25.82
 H       4.001478    -0.842887    -3.085606      25.65
 H       2.408613    -1.429433    -2.783641      26.61
 C      -0.320745    -1.742061     0.530183      78.19
 H      -0.843099    -2.607203     0.990295      21.93
 C      -0.258476     0.616773     0.119293      68.10
 H      -0.771947     1.479799     0.122750      22.30
 C       1.114713     0.563202    -0.191980       6.15
 O       2.004361     1.682981    -0.393990     188.47
 C       1.577739     3.003641    -0.276057     107.27
 H       2.449932     3.860523    -0.389376      22.49
 H       0.842449     3.447905    -0.846433      26.50
 H       1.093011     3.125973     0.918874      23.01
 C       1.836024    -0.683226    -0.236793       6.31
 O       3.217402    -0.704930    -0.500931     148.63
 C       1.025949    -1.807895     0.088416      53.85
 H       1.764727    -2.650339     0.028605      22.91
 C      -0.998366    -0.579101     0.522532      29.66
 C      -2.509017    -0.327950     0.922048      81.45
 H      -3.069681    -1.262708     1.241672      22.54
 O      -2.575461     0.634686     1.960576     242.68
 H      -2.235562    -0.042724     2.679167      23.18
 C      -3.222781     0.374182    -0.292476      76.87
 H      -2.725141     1.325547    -0.542790      23.89
 O      -3.281090    -0.402642    -1.483732     258.17
 H      -3.219413     0.102749    -2.329969      24.36
 C      -4.683605     0.916477     0.151044      96.44
 O      -5.085368     1.986654    -0.606002     321.31
 H      -4.837131     2.848413    -0.279524      29.80
 H      -4.850237     0.984152     1.230856      26.17
 H      -5.387305    -0.089963    -0.056982      24.67
55
name = lig-etoh-Waterframe_487
 C       6.359074    -1.406206     1.402837      55.38
 H       6.391378    -0.276558     1.251363      22.50
 C       5.760633    -3.662313     0.885564      46.03
 H       5.445814    -4.476715     0.168417      17.16
 C       6.082542    -4.091250     2.191276      24.02
 O       6.108256    -5.427417     2.579113     222.81
 C       5.437626    -6.446981     1.822780     128.69
 H       6.085551    -6.739473     0.805367      26.98
 H       4.483802    -6.099768     1.435938      28.80
 H       5.355965    -7.232585     2.473930      25.86
 C       6.561439    -3.163247     3.157872      15.49
 O       6.944923    -3.496617     4.508017     197.07
 H       6.545504    -4.345753     4.817280      26.83
 C       6.740987    -1.869236     2.729597      60.30
 H       7.150307    -1.131478     3.407044      24.58
 C       5.826940    -2.241615     0.466196     -27.16
 C       5.401494    -1.908385    -0.993004      80.17
 H       5.971051    -2.911070    -1.648000      23.48
 O       5.979878    -0.662745    -1.460933     232.65
 H       5.919324     0.052656    -0.674847      27.71
 C       3.842077    -1.902827    -1.186294      68.96
 H       3.465795    -2.919468    -0.893638      22.06
 C       3.442672    -1.696412    -2.714872      85.97
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 O       3.489142    -3.024104    -3.437348     235.78
 H       4.392523    -3.112008    -3.865727      26.12
 H       4.131493    -1.015180    -3.367256      23.84
 H       2.282685    -1.467253    -2.783731      24.97
 C      -0.356057    -1.833046     0.546636      40.12
 H      -0.780509    -2.707241     0.696008      16.76
 C      -0.275760     0.668072     0.143084      68.21
 H      -0.741631     1.512906    -0.225216      21.49
 C       1.121876     0.604799    -0.275829       6.15
 O       1.980520     1.672291    -0.445124     153.77
 C       1.579158     3.060391    -0.230831      87.13
 H       2.460237     3.696748    -0.577408      23.39
 H       0.539999     3.341076    -1.082847      21.19
 H       1.134588     3.154439     0.891546      23.01
 C       1.775139    -0.669498    -0.251696      19.06
 O       3.176913    -0.692595    -0.479424     134.37
 C       1.082390    -1.823493     0.148499      40.14
 H       1.472549    -2.913595     0.058191      21.51
 C      -1.025296    -0.511638     0.466008       6.11
 C      -2.579279    -0.311204     0.904965      84.83
 H      -2.947065    -1.350750     1.281118      24.30
 O      -2.597546     0.671965     1.983543     242.86
 H      -2.002122     0.387319     2.754147      27.72
 C      -3.178982     0.482126    -0.304754      85.77
 H      -2.541725     1.218621    -0.595527      26.09
 O      -3.237113    -0.398401    -1.462787     259.93
 H      -3.189058     0.075637    -2.294613      27.22
 C      -4.735617     0.840267     0.152821      96.24
 O      -5.125818     2.047652    -0.600538     304.39
 H      -4.926160     2.756597     0.009886      29.27
 H      -4.713569     0.940538     1.252117      26.96
 H      -5.377218     0.134277    -0.295272      27.20
55
name = lig-etoh-Waterframe_488
 C       6.340034    -1.382619     1.414400      44.26
 H       6.708532    -0.347458     1.088978      22.19
 C       5.736124    -3.632118     0.884222      63.56
 H       5.479136    -4.426525     0.184119      23.88
 C       6.138218    -4.056265     2.151725      12.16
 O       6.137572    -5.388455     2.623773     267.55
 C       5.401409    -6.350718     1.790568     124.62
 H       6.146722    -6.752184     0.909687      23.53
 H       4.328576    -6.141872     1.522625      27.17
 H       5.324122    -7.213470     2.375121      25.06
 C       6.541685    -3.183771     3.186506      30.01
 O       6.892494    -3.488487     4.418399     229.18
 H       6.839029    -4.434978     4.654671      23.27
 C       6.740454    -1.821411     2.695369      42.90
 H       7.185576    -1.067552     3.243114      26.24
 C       5.839028    -2.290876     0.441506      16.35
 C       5.351843    -1.860628    -0.962283      81.94
 H       5.768499    -2.704084    -1.754873      21.04
 O       5.976227    -0.591431    -1.428576     283.04
 H       5.802383     0.161006    -0.688341      21.67
 C       3.795428    -1.897363    -1.167705      71.55
 H       3.295866    -2.754368    -0.602758      19.93
 C       3.442234    -1.777730    -2.677644      86.30
 O       3.482512    -2.983895    -3.454721     254.54
 H       4.351002    -2.894232    -3.951170      24.88
 H       4.132479    -0.968946    -3.227278      21.49
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 H       2.363290    -1.202697    -2.735651      22.74
 C      -0.315005    -1.783900     0.492534      52.73
 H      -0.829987    -2.691298     0.678599      21.68
 C      -0.233090     0.678068     0.097071      57.97
 H      -0.775199     1.706611    -0.040232      16.67
 C       1.104340     0.608094    -0.270240       7.59
 O       1.979612     1.676921    -0.520890     187.40
 C       1.509544     3.072628    -0.220864     107.53
 H       2.344589     3.596943    -0.478601      25.79
 H       0.540021     3.239532    -1.080273      21.14
 H       1.360545     3.394718     0.720198      27.84
 C       1.757185    -0.713890    -0.247140       8.95
 O       3.162218    -0.714777    -0.470694     143.27
 C       1.020182    -1.875833     0.205232      50.59
 H       1.495235    -2.916475     0.228699      18.27
 C      -1.048694    -0.499391     0.457738      60.37
 C      -2.472421    -0.238870     0.837223      88.12
 H      -3.104834    -1.184067     0.944589      22.54
 O      -2.636025     0.711033     2.018917     242.54
 H      -1.865333     0.527678     2.562988      29.54
 C      -3.283312     0.505018    -0.282272      91.19
 H      -2.745773     1.465433    -0.277556      23.08
 O      -3.206394    -0.430180    -1.443088     251.36
 H      -3.181242     0.055620    -2.243901      25.52
 C      -4.686333     0.797229     0.064366     108.58
 O      -5.176416     2.118532    -0.561389     281.04
 H      -5.080226     2.915287     0.006049      29.57
 H      -4.867188     1.011118     1.138960      26.54
 H      -5.288679     0.044788    -0.210488      28.47
55
name = lig-etoh-Waterframe_489
 C       6.369303    -1.364739     1.401208      37.79
 H       6.678773    -0.358496     1.040677      23.85
 C       5.717818    -3.646336     0.843479      76.30
 H       5.366157    -4.316442     0.104901      23.49
 C       6.168888    -4.076933     2.161264       8.18
 O       6.118684    -5.357490     2.628919     262.58
 C       5.416579    -6.323210     1.797909     101.36
 H       5.885191    -6.443744     0.818269      26.89
 H       4.475444    -5.755351     1.426883      28.08
 H       5.301693    -7.220799     2.455170      23.00
 C       6.542539    -3.067607     3.084357      22.86
 O       6.868236    -3.503781     4.406479     198.92
 H       6.840702    -4.470784     4.373092      25.15
 C       6.728436    -1.767138     2.691021      66.25
 H       7.211847    -1.175692     3.412810      22.69
 C       5.826015    -2.320425     0.436788       5.60
 C       5.328092    -1.787588    -0.927279     112.65
 H       5.545555    -2.350550    -1.664555      26.31
 O       5.951820    -0.561438    -1.373638     314.86
 H       5.410264     0.222864    -0.925217      21.54
 C       3.727632    -1.849904    -1.132922      76.71
 H       3.442144    -2.886920    -0.728948      19.43
 C       3.417631    -1.769718    -2.641082      99.22
 O       3.476170    -2.961838    -3.459370     268.37
 H       4.287853    -2.947485    -4.052781      26.11
 H       4.190063    -1.017840    -2.825304      21.01
 H       2.352659    -1.406945    -2.774051      24.11
 C      -0.393483    -1.668713     0.449410      48.38
 H      -1.003858    -2.542865     0.999508      26.96
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 C      -0.238921     0.657084     0.047270      60.62
 H      -0.683940     1.710094     0.489646      15.58
 C       1.146524     0.528899    -0.225220      -0.19
 O       1.961242     1.698999    -0.565740     180.89
 C       1.475836     3.040777    -0.297954     132.29
 H       2.164730     3.696828    -0.651078      27.40
 H       0.608253     3.463067    -0.719759      26.90
 H       1.303713     3.161108     0.727828      28.61
 C       1.770113    -0.763459    -0.213160      13.34
 O       3.139706    -0.733281    -0.472714     204.56
 C       1.023666    -1.870979     0.194873      50.93
 H       1.608815    -2.756088     0.422278      18.00
 C      -0.955855    -0.457625     0.431815      46.87
 C      -2.447646    -0.139032     0.796158      84.02
 H      -2.889452    -1.108462     1.048116      20.70
 O      -2.647290     0.719782     2.004062     304.02
 H      -2.072094     0.298487     2.608899      24.94
 C      -3.297465     0.494153    -0.280210      72.66
 H      -2.999498     1.630430    -0.640976      18.45
 O      -3.177376    -0.426308    -1.416866     259.78
 H      -3.212264    -0.038965    -2.247111      25.70
 C      -4.749238     0.877223     0.017443      99.08
 O      -5.229423     2.127054    -0.546035     290.95
 H      -4.954536     2.876974     0.094575      27.98
 H      -4.823909     0.834773     1.146856      25.59
 H      -5.414354     0.005592    -0.275932      25.45
55
name = lig-etoh-Waterframe_490
 C       6.410966    -1.346488     1.325556      63.54
 H       6.390574    -0.314925     1.053236      19.47
 C       5.718108    -3.710502     0.822542      51.77
 H       5.277206    -4.386510     0.153304      16.80
 C       6.132811    -4.044007     2.092310       7.33
 O       6.105351    -5.349729     2.635563     274.82
 C       5.424374    -6.244772     1.777121     119.42
 H       5.946720    -6.476807     0.952703      31.30
 H       4.380072    -5.822685     1.589524      28.49
 H       5.176158    -7.266858     2.322876      23.99
 C       6.571028    -3.059633     3.040823      -6.27
 O       6.853492    -3.488230     4.360753     178.03
 H       6.634773    -4.437718     4.515668      27.91
 C       6.728792    -1.687207     2.702100      51.79
 H       7.161519    -1.009243     3.475642      22.21
 C       5.826336    -2.233203     0.479238       6.12
 C       5.284771    -1.753814    -0.915685      88.05
 H       5.686140    -2.565178    -1.648508      24.50
 O       5.890334    -0.520902    -1.296256     274.91
 H       5.377085     0.325261    -1.057283      23.73
 C       3.734772    -1.875080    -1.083281      82.75
 H       3.440025    -2.861540    -0.721960      21.52
 C       3.380234    -1.694599    -2.615946     104.66
 O       3.479279    -2.962346    -3.446164     245.18
 H       4.393901    -2.900489    -3.886658      25.77
 H       3.956775    -1.034121    -3.162557      25.70
 H       2.416517    -1.415723    -2.752815      27.05
 C      -0.404295    -1.679301     0.463144      45.60
 H      -1.103129    -2.520804     1.080712      23.34
 C      -0.140294     0.712353     0.064193      42.41
 H      -0.556734     1.786087     0.369651      16.02
 C       1.182001     0.547178    -0.210147      15.74
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 O       1.930813     1.664933    -0.620344     202.28
 C       1.439427     3.019303    -0.343523      97.47
 H       2.242480     3.758467    -0.748058      22.75
 H       0.507616     3.179186    -0.688735      25.80
 H       1.364955     2.950546     0.920200      23.10
 C       1.784434    -0.736696    -0.185597      24.21
 O       3.113206    -0.748465    -0.459013     202.18
 C       0.997005    -1.849196     0.191733      65.18
 H       1.389466    -2.752707     0.494933      20.16
 C      -0.990410    -0.326939     0.392785      58.61
 C      -2.467232    -0.085669     0.833066      82.22
 H      -2.774168    -1.069884     1.059330      22.89
 O      -2.604979     0.705596     1.980731     320.18
 H      -2.430740     0.261320     2.742195      28.51
 C      -3.291132     0.558368    -0.402970      65.60
 H      -2.557586     1.383271    -0.858611      18.62
 O      -3.157507    -0.444055    -1.404445     274.89
 H      -3.257844    -0.030288    -2.205727      27.23
 C      -4.875385     0.895315     0.052903      76.26
 O      -5.270852     2.125298    -0.524301     284.94
 H      -4.863785     2.889530     0.054391      26.06
 H      -4.926082     0.935739     1.173138      25.99
 H      -5.591687     0.173866    -0.625460      22.80
55
name = lig-etoh-Waterframe_491
 C       6.434546    -1.271007     1.346873      58.09
 H       6.316328    -0.271525     1.076402      21.39
 C       5.717760    -3.622655     0.767816      76.12
 H       5.308353    -4.396428     0.140956      17.41
 C       6.103949    -4.024359     2.077779       9.95
 O       6.095352    -5.315634     2.636911     243.97
 C       5.382503    -6.232908     1.758383     122.67
 H       6.032030    -6.481922     0.907248      29.08
 H       4.394299    -5.954587     1.369921      28.87
 H       5.344364    -7.215689     2.413284      25.24
 C       6.613780    -3.063518     3.054884      20.25
 O       6.847764    -3.444212     4.303748     192.82
 H       6.475072    -4.286205     4.632864      24.69
 C       6.732969    -1.684496     2.667693      42.17
 H       7.021668    -0.773945     3.329106      22.30
 C       5.786273    -2.264600     0.473650       7.20
 C       5.271955    -1.771358    -0.872982      64.19
 H       5.872363    -2.659967    -1.671649      20.55
 O       5.829081    -0.485222    -1.261289     254.84
 H       5.396082     0.226277    -0.697929      24.95
 C       3.776742    -1.887424    -1.127010      83.03
 H       3.319499    -2.721589    -0.703322      23.68
 C       3.328524    -1.676083    -2.650767     103.01
 O       3.497262    -2.952549    -3.386132     246.83
 H       4.418440    -2.939125    -3.833549      24.45
 H       3.829050    -0.864086    -3.155750      25.47
 H       2.315356    -1.392774    -2.557199      26.05
 C      -0.421429    -1.585187     0.504459      43.27
 H      -0.955118    -2.604727     0.738547      14.94
 C      -0.117860     0.826253     0.147751      60.31
 H      -0.470468     1.802726    -0.099019      16.28
 C       1.231697     0.615167    -0.234487      11.60
 O       1.967527     1.623921    -0.703858     200.13
 C       1.409718     2.934212    -0.321480      79.41
 H       2.219746     3.748529    -0.852547      21.68
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 H       0.370509     2.977664    -0.872599      20.70
 H       1.416830     3.433616     0.876870      21.46
 C       1.756603    -0.705380    -0.161107      15.54
 O       3.138759    -0.753417    -0.414128     162.51
 C       0.913155    -1.831816     0.227923      54.96
 H       1.323112    -2.796336     0.311894      24.78
 C      -1.028889    -0.320594     0.392212      50.39
 C      -2.471317    -0.088929     0.814620      91.04
 H      -3.063987    -1.034934     0.862572      24.81
 O      -2.582929     0.750046     1.984788     270.99
 H      -2.356094     0.196208     2.679268      29.81
 C      -3.279204     0.583655    -0.428046      75.96
 H      -2.848671     1.546650    -0.597203      24.11
 O      -3.168557    -0.492492    -1.437654     262.40
 H      -3.276598    -0.174951    -2.292905      27.28
 C      -4.884073     0.904827     0.004856      86.55
 O      -5.323945     2.183393    -0.499534     285.12
 H      -4.913482     3.028864    -0.046713      27.89
 H      -5.152346     0.796573     1.050156      27.69
 H      -5.532926    -0.048657    -0.370988      24.82
55
name = lig-etoh-Waterframe_492
 C       6.349828    -1.284974     1.357551      51.19
 H       6.539108    -0.252797     1.159489      21.92
 C       5.719155    -3.565542     0.796049      62.59
 H       5.369017    -4.202030    -0.065773      19.91
 C       6.125183    -3.973196     2.119878      22.19
 O       6.034147    -5.260984     2.587074     221.75
 C       5.392211    -6.298487     1.751787      96.09
 H       6.058252    -6.434919     0.747711      25.91
 H       4.491269    -5.920827     1.392754      32.38
 H       5.309326    -7.183874     2.421795      25.58
 C       6.601243    -3.022856     2.982001      11.47
 O       6.873937    -3.384684     4.337073     201.17
 H       6.521723    -4.304965     4.420127      28.14
 C       6.745411    -1.699065     2.609994      36.24
 H       7.058002    -0.998358     3.484949      22.30
 C       5.791386    -2.199932     0.467652      -2.40
 C       5.331833    -1.806005    -0.877549      32.96
 H       5.669476    -2.379226    -1.850773      24.58
 O       5.762217    -0.480902    -1.237387     242.86
 H       5.523724     0.147759    -0.558867      26.13
 C       3.744211    -1.844533    -1.196628      67.98
 H       3.424341    -2.856694    -0.899335      23.94
 C       3.291346    -1.704555    -2.647139      98.88
 O       3.517821    -2.931233    -3.320353     250.94
 H       4.298701    -2.895585    -3.974589      25.04
 H       3.894402    -0.756902    -2.932749      23.80
 H       2.111891    -1.622931    -2.612249      25.10
 C      -0.465051    -1.536280     0.530666      46.16
 H      -1.153474    -2.293105     0.631857      16.67
 C      -0.186448     0.842192     0.189738      74.34
 H      -0.711582     1.637018    -0.087214      20.49
 C       1.175224     0.592245    -0.212357     -11.15
 O       2.058474     1.657585    -0.748419     150.59
 C       1.451183     2.924956    -0.390885      94.59
 H       2.044990     3.690604    -1.058365      23.82
 H       0.303642     3.289970    -0.866836      22.14
 H       1.335716     2.987825     0.706747      25.64
 C       1.751376    -0.720177    -0.130404      20.13
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 O       3.179397    -0.749233    -0.354620     153.79
 C       0.927685    -1.743222     0.233479      57.90
 H       1.294492    -2.784528     0.104711      23.93
 C      -0.996917    -0.257730     0.446402      38.53
 C      -2.527364    -0.062070     0.714563      83.97
 H      -3.036175    -1.094595     1.018308      24.10
 O      -2.584774     0.787375     1.984812     212.42
 H      -1.897354     0.399108     2.614554      28.38
 C      -3.345231     0.583644    -0.348169      93.47
 H      -3.083050     1.501508    -0.728322      25.11
 O      -3.186841    -0.498835    -1.476552     208.10
 H      -3.264405    -0.161414    -2.353101      26.13
 C      -4.813404     0.881952    -0.043350     101.59
 O      -5.394250     2.230331    -0.503005     250.50
 H      -4.916130     2.851768     0.170689      27.79
 H      -4.855262     0.848397     1.026516      28.01
 H      -5.439223     0.219081    -0.614849      26.40
55
name = lig-etoh-Waterframe_493
 C       6.278877    -1.235503     1.366019      51.31
 H       6.587300    -0.221614     1.016687      23.09
 C       5.725809    -3.522110     0.849421      66.15
 H       5.419216    -4.319933     0.075918      21.93
 C       6.098674    -3.974583     2.045006      25.14
 O       5.964116    -5.245545     2.549127     265.15
 C       5.426500    -6.299851     1.730580     121.44
 H       6.126036    -6.689765     0.809552      23.95
 H       4.415147    -6.037743     1.494770      28.19
 H       5.307639    -7.165002     2.283807      25.48
 C       6.596620    -3.001953     3.036849      25.26
 O       6.896265    -3.322532     4.342440     180.18
 H       6.855077    -4.314569     4.505897      24.30
 C       6.761175    -1.705490     2.621431      49.37
 H       7.286242    -1.064311     3.382712      23.89
 C       5.805276    -2.164842     0.436146      21.00
 C       5.309457    -1.751065    -1.018475      94.16
 H       5.753471    -2.422266    -1.581479      26.03
 O       5.744437    -0.479367    -1.245967     348.95
 H       5.435783     0.242011    -0.735854      24.86
 C       3.708439    -1.839703    -1.149717      77.91
 H       3.395627    -2.901236    -0.803530      22.76
 C       3.266411    -1.688800    -2.588046      97.06
 O       3.558377    -2.942882    -3.309532     257.74
 H       4.289026    -2.773359    -3.979750      24.69
 H       3.679939    -0.848587    -3.291964      23.37
 H       2.089594    -1.468900    -2.793402      24.06
 C      -0.476055    -1.524583     0.528207      38.98
 H      -1.112792    -2.243079     0.764566      26.44
 C      -0.207621     0.854696     0.140176      74.82
 H      -0.677620     1.791265     0.150226      21.74
 C       1.147389     0.619658    -0.199042       1.81
 O       2.054499     1.650890    -0.742720     182.79
 C       1.510778     2.987542    -0.527230     121.92
 H       2.191867     3.739766    -0.693718      26.11
 H       0.399786     2.890957    -0.819669      23.48
 H       1.486052     2.985966     0.451828      30.86
 C       1.812249    -0.642924    -0.109950      16.69
 O       3.171110    -0.777731    -0.304125     172.46
 C       0.904293    -1.735694     0.231709      51.39
 H       1.292536    -2.833801     0.194859      20.27
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 C      -1.043987    -0.214493     0.523280      39.33
 C      -2.515278    -0.007673     0.764660      81.27
 H      -2.839478    -1.099860     0.982052      24.10
 O      -2.595746     0.800402     1.960018     253.30
 H      -1.672602     0.772815     2.381333      26.48
 C      -3.396921     0.577393    -0.428163      84.64
 H      -2.733106     1.390746    -0.873539      22.89
 O      -3.218078    -0.465976    -1.489443     221.27
 H      -3.221131     0.085321    -2.278085      25.58
 C      -4.823353     0.894574    -0.080752     110.69
 O      -5.396831     2.213936    -0.471718     273.08
 H      -5.132738     3.055737     0.075778      26.73
 H      -4.945038     0.813624     1.019118      26.36
 H      -5.407225     0.229540    -0.561666      28.02
55
name = lig-etoh-Waterframe_494
 C       6.284461    -1.184058     1.370497      30.55
 H       6.361356    -0.097420     1.000125      23.15
 C       5.701065    -3.495915     0.767090      56.32
 H       5.323811    -4.357036     0.153973      19.46
 C       6.093019    -3.953838     2.114655      30.18
 O       5.915823    -5.270031     2.535290     245.67
 C       5.433317    -6.324130     1.711691     126.44
 H       6.111149    -6.461409     0.823692      25.71
 H       4.418708    -6.157626     1.163560      25.53
 H       5.472880    -7.090788     2.413594      24.60
 C       6.568260    -3.050161     3.066070      26.01
 O       6.934634    -3.283604     4.362066     191.07
 H       7.008281    -4.245217     4.640999      22.92
 C       6.773954    -1.651496     2.643277      40.70
 H       7.352129    -0.935083     3.142168      26.73
 C       5.768051    -2.149151     0.392569      -0.86
 C       5.238938    -1.722400    -1.013489      86.27
 H       5.730854    -2.456914    -1.712121      23.13
 O       5.790858    -0.423808    -1.350109     310.59
 H       5.203262     0.206272    -0.977057      27.75
 C       3.706647    -1.853615    -1.094093      71.55
 H       3.282406    -2.803497    -0.606328      23.15
 C       3.213540    -1.680075    -2.632320      98.61
 O       3.588728    -2.954773    -3.313524     254.70
 H       4.452726    -2.875121    -3.822654      24.86
 H       3.878288    -0.802313    -2.999530      23.31
 H       2.117587    -1.502511    -2.490893      25.02
 C      -0.465175    -1.497910     0.522647      43.85
 H      -0.900865    -2.443779     0.935934      23.62
 C      -0.202051     0.882425     0.088929      70.23
 H      -0.383956     1.990433     0.329673      21.00
 C       1.215073     0.695380    -0.223054       4.98
 O       2.020286     1.621183    -0.728069     215.38
 C       1.567959     3.007113    -0.583996     112.41
 H       2.238486     3.678289    -0.985885      27.14
 H       0.763150     3.230680    -1.212372      27.87
 H       1.381630     3.381416     0.653156      25.22
 C       1.756095    -0.633640    -0.073426      15.48
 O       3.154473    -0.789719    -0.253084     171.54
 C       0.896756    -1.715007     0.219927      60.24
 H       1.329100    -2.766443     0.448222      23.56
 C      -1.046880    -0.218779     0.518819      37.29
 C      -2.494234    -0.003452     0.853029      87.92
 H      -3.045970    -0.890639     0.997817      25.30
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 O      -2.639457     0.856074     1.936895     272.70
 H      -1.738056     0.866246     2.427645      25.28
 C      -3.291357     0.557599    -0.521719      55.83
 H      -2.757155     1.655867    -0.736488      22.20
 O      -3.270934    -0.411372    -1.508815     241.65
 H      -3.183021    -0.071448    -2.456598      23.93
 C      -4.895667     0.956836    -0.068032      94.26
 O      -5.387882     2.182293    -0.467242     288.78
 H      -4.958001     2.955149     0.074082      27.27
 H      -5.128537     0.689219     1.031702      26.04
 H      -5.513025     0.145083    -0.492045      26.37
55
name = lig-etoh-Waterframe_495
 C       6.294541    -1.219456     1.339617      56.78
 H       6.269569    -0.090046     1.236432      21.53
 C       5.694367    -3.523122     0.769946      50.90
 H       5.239011    -4.095273    -0.017929      18.99
 C       6.031274    -3.936621     2.109610      17.96
 O       5.874616    -5.261656     2.559744     221.70
 C       5.466665    -6.346728     1.647402     110.98
 H       6.187243    -6.439158     0.954564      30.38
 H       4.363234    -6.171125     1.221619      27.72
 H       5.449843    -7.290682     2.282664      25.22
 C       6.583214    -2.965215     3.057140      -2.21
 O       6.991574    -3.267383     4.417440     135.78
 H       6.812883    -4.260849     4.559305      26.45
 C       6.742847    -1.620248     2.594847      55.35
 H       7.219434    -1.006087     3.280337      23.98
 C       5.736534    -2.111048     0.409069       2.41
 C       5.231363    -1.721986    -0.935477      68.72
 H       5.459226    -2.374021    -1.966546      21.26
 O       5.814341    -0.389427    -1.489515     266.71
 H       5.334112     0.390417    -1.139680      24.05
 C       3.661587    -1.837194    -1.081761      66.61
 H       3.477963    -2.876853    -0.748735      23.66
 C       3.248528    -1.722745    -2.575716     111.71
 O       3.584483    -2.935510    -3.317767     249.57
 H       4.472524    -2.908323    -3.758499      25.83
 H       3.693892    -0.799944    -2.901773      24.95
 H       2.232901    -1.667996    -2.762774      27.45
 C      -0.430954    -1.502814     0.531808      39.16
 H      -1.159880    -2.405960     0.993463      19.99
 C      -0.129504     0.889200     0.093993      76.49
 H      -0.673890     1.984003     0.193070      17.84
 C       1.168946     0.649329    -0.212328      15.47
 O       2.030621     1.677200    -0.707833     202.27
 C       1.645599     3.072035    -0.673442      94.31
 H       2.599145     3.403285    -1.180256      21.85
 H       0.887121     3.376826    -1.311627      26.27
 H       1.188036     3.538607     0.524097      21.50
 C       1.717672    -0.642907    -0.084625      24.26
 O       3.127867    -0.759467    -0.201296     160.12
 C       0.911395    -1.682774     0.247994      65.08
 H       1.408238    -2.634190     0.506905      23.93
 C      -0.987888    -0.212041     0.456527      77.28
 C      -2.525900    -0.020082     0.811092      77.71
 H      -3.003864    -0.910341     1.143118      25.65
 O      -2.697478     0.976241     1.944440     234.47
 H      -2.004419     0.682598     2.715588      25.10
 C      -3.259300     0.636236    -0.434732      64.08
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 H      -2.895561     1.637891    -0.939768      22.03
 O      -3.306525    -0.391058    -1.562790     206.13
 H      -3.190435    -0.044017    -2.552699      22.82
 C      -4.894648     0.885528    -0.036384      72.98
 O      -5.379696     2.203834    -0.483952     256.27
 H      -4.826684     2.876857     0.040307      27.40
 H      -4.904772     0.896436     1.100102      25.51
 H      -5.567437     0.207954    -0.757769      23.81
55
name = lig-etoh-Waterframe_496
 C       6.288781    -1.207428     1.312513      63.82
 H       6.310204    -0.139464     1.033593      21.52
 C       5.674465    -3.486390     0.802042      76.77
 H       5.329345    -4.229615     0.124395      19.71
 C       5.964385    -3.943664     2.074870      16.49
 O       5.833530    -5.240338     2.603028     215.26
 C       5.514749    -6.337708     1.609919     102.66
 H       6.205230    -6.445798     0.818489      29.69
 H       4.493999    -6.077631     1.178309      27.33
 H       5.392203    -7.373965     2.184854      24.39
 C       6.604198    -2.916264     3.059620       6.97
 O       7.020034    -3.257744     4.392949     140.96
 H       6.726328    -4.210100     4.582921      25.61
 C       6.716124    -1.647229     2.608218      67.97
 H       6.997273    -0.906771     3.353122      24.07
 C       5.750939    -2.130837     0.452950      21.08
 C       5.212690    -1.619304    -0.983286      94.99
 H       5.774635    -2.588605    -1.481286      23.35
 O       5.797990    -0.422492    -1.600538     302.02
 H       5.627660     0.395444    -1.018784      24.96
 C       3.657103    -1.797427    -1.043798      82.39
 H       3.381131    -2.759287    -0.686530      24.52
 C       3.260392    -1.740162    -2.527022     114.15
 O       3.595020    -2.919042    -3.323309     276.98
 H       4.400209    -2.779930    -3.879470      27.00
 H       3.661357    -0.949547    -3.021787      25.03
 H       2.213856    -1.670970    -2.660755      26.71
 C      -0.452660    -1.485631     0.561213      37.69
 H      -1.257849    -2.403505     0.823674      16.03
 C      -0.190980     0.873399     0.146418      65.15
 H      -0.680321     1.905257    -0.224002      15.56
 C       1.170732     0.682011    -0.238421      21.51
 O       2.039143     1.697180    -0.659523     219.78
 C       1.732924     3.139140    -0.813030      90.27
 H       2.756053     3.769618    -0.825916      20.77
 H       0.821489     3.229038    -1.480956      23.07
 H       1.609362     3.494531     0.231236      24.83
 C       1.753819    -0.617877    -0.127664      20.64
 O       3.094731    -0.751236    -0.185684     207.91
 C       0.935999    -1.740292     0.327266      32.41
 H       1.409506    -2.672491     0.423364      20.39
 C      -0.984050    -0.204898     0.419931      60.42
 C      -2.493766     0.065134     0.743333      70.49
 H      -2.836243    -0.991459     1.024258      25.05
 O      -2.727698     1.071271     1.934479     169.02
 H      -2.463359     0.421023     2.752518      24.55
 C      -3.389020     0.649312    -0.387123      96.01
 H      -2.814259     1.481694    -0.672285      24.39
 O      -3.319498    -0.379350    -1.583996     174.26
 H      -3.207554     0.330326    -2.363260      21.67
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 C      -4.797362     0.881468    -0.044452      92.00
 O      -5.343617     2.220293    -0.495600     276.46
 H      -4.992656     3.046578    -0.055154      28.39
 H      -5.027075     0.718902     1.020344      27.23
 H      -5.464389    -0.053264    -0.456620      24.78
55
name = lig-etoh-Waterframe_497
 C       6.297627    -1.173947     1.341936      52.08
 H       6.442964    -0.197829     0.957443      23.96
 C       5.621231    -3.494734     0.823654      55.38
 H       5.355674    -4.280300     0.143531      17.94
 C       5.992053    -3.899099     2.173256      20.81
 O       5.802117    -5.238589     2.607447     259.24
 C       5.526255    -6.274756     1.595735      91.25
 H       6.363550    -6.297419     0.769715      27.26
 H       4.640364    -6.105401     1.075197      30.85
 H       5.498359    -7.207226     2.311129      23.50
 C       6.561187    -3.030661     3.041063      13.01
 O       7.018202    -3.243119     4.308945     221.73
 H       6.898575    -4.201627     4.649143      22.52
 C       6.692477    -1.590670     2.639308      62.16
 H       7.049832    -0.751917     3.328258      24.32
 C       5.751388    -2.073515     0.415425      31.64
 C       5.271351    -1.631612    -0.974795     114.34
 H       5.593177    -2.380407    -1.720948      22.96
 O       5.764620    -0.490140    -1.659279     334.66
 H       5.626981     0.281861    -0.986113      23.97
 C       3.724892    -1.767393    -1.029698      73.10
 H       3.407050    -2.667792    -0.522608      20.22
 C       3.211088    -1.711751    -2.548671      93.75
 O       3.611179    -2.920772    -3.317734     270.45
 H       4.360300    -2.697178    -3.917259      26.56
 H       3.745071    -0.843337    -2.924809      19.94
 H       2.093281    -1.583986    -2.338273      22.33
 C      -0.453620    -1.502523     0.577132      49.35
 H      -1.068647    -2.417485     0.769785      18.28
 C      -0.191634     0.914872     0.082508      50.47
 H      -0.648857     1.892056    -0.129407      15.06
 C       1.168441     0.755125    -0.249338      13.35
 O       2.097825     1.706578    -0.631751     236.73
 C       1.803565     3.158958    -0.826044     107.32
 H       2.671993     3.720765    -1.447061      20.79
 H       1.032768     3.435132    -1.748295      22.48
 H       1.393315     3.533098    -0.042003      29.03
 C       1.698077    -0.638512    -0.102189      33.29
 O       3.121171    -0.735244    -0.215636     200.83
 C       0.933617    -1.721971     0.373600      20.45
 H       1.265307    -2.704122     0.422509      16.42
 C      -1.071217    -0.183351     0.439052      63.86
 C      -2.479263     0.140078     0.744953      88.77
 H      -3.017573    -0.873594     1.067492      22.09
 O      -2.730501     1.079851     1.867317     204.38
 H      -2.654346     0.525434     2.782885      24.92
 C      -3.385688     0.583392    -0.419628     105.10
 H      -3.052939     1.544707    -0.625379      24.03
 O      -3.323078    -0.302515    -1.536947     241.54
 H      -3.276014     0.143560    -2.539441      19.58
 C      -4.813585     0.947812     0.009120     103.32
 O      -5.312959     2.183010    -0.525441     294.41
 H      -4.974570     2.853181     0.090856      30.41
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 H      -4.940309     0.859453     1.056662      28.94
 H      -5.442900     0.224622    -0.572027      25.89
55
name = lig-etoh-Waterframe_498
 C       6.318460    -1.145805     1.374198      51.05
 H       6.569594    -0.144976     1.209397      23.68
 C       5.597272    -3.431049     0.868434      53.84
 H       5.230570    -4.103797     0.083546      19.91
 C       5.969492    -3.927897     2.145963      21.80
 O       5.778569    -5.216213     2.605363     258.70
 C       5.552203    -6.185474     1.603216     109.90
 H       6.571890    -6.285551     0.959333      25.85
 H       4.653048    -6.153705     1.090587      29.55
 H       5.509553    -7.173200     2.091368      25.05
 C       6.547021    -2.924278     3.043117      13.50
 O       7.025018    -3.259369     4.273656     129.59
 H       7.014554    -4.251452     4.507221      27.97
 C       6.646454    -1.599572     2.646806      52.48
 H       7.314938    -1.018171     3.405727      22.71
 C       5.773002    -2.104087     0.405305      28.29
 C       5.306015    -1.759320    -1.018671     111.54
 H       5.433495    -2.453652    -1.705778      26.46
 O       5.752820    -0.520721    -1.653305     328.25
 H       5.413336     0.410361    -1.287614      21.69
 C       3.759542    -1.777366    -1.048925      67.60
 H       3.603392    -2.847574    -0.671279      18.31
 C       3.207841    -1.680601    -2.499640      88.68
 O       3.588593    -2.888985    -3.292067     256.04
 H       4.387152    -2.736934    -3.861341      26.33
 H       3.509096    -0.645551    -2.993672      20.22
 H       2.011142    -1.684625    -2.734306      21.40
 C      -0.503490    -1.464417     0.586178      36.57
 H      -1.010814    -2.236972     0.888158      26.80
 C      -0.209069     0.968647    -0.019688      93.25
 H      -0.586939     1.870464     0.120271      19.03
 C       1.169295     0.721125    -0.222660      -1.77
 O       2.170699     1.742959    -0.621429     150.57
 C       1.819975     3.145684    -0.920910      81.71
 H       2.890903     3.355265    -1.195035      20.47
 H       0.964304     3.012680    -1.731154      22.87
 H       1.305397     3.869145    -0.044642      22.91
 C       1.708276    -0.593410    -0.055362      17.39
 O       3.136133    -0.674225    -0.259911     175.79
 C       0.883461    -1.653445     0.369349      48.04
 H       1.332676    -2.633136     0.504283      17.17
 C      -1.029990    -0.172512     0.463104      34.95
 C      -2.574967     0.104170     0.801787      71.23
 H      -3.016173    -0.863733     1.190805      20.11
 O      -2.718846     1.091095     1.776283     247.38
 H      -2.432869     0.637778     2.717269      22.12
 C      -3.313854     0.663134    -0.473016      67.27
 H      -3.049864     1.664821    -0.932623      20.82
 O      -3.325528    -0.277825    -1.494813     252.10
 H      -3.241446     0.137760    -2.507375      20.62
 C      -4.916772     0.938513     0.036523     100.78
 O      -5.275460     2.181636    -0.536285     292.50
 H      -4.987856     2.958316    -0.043749      29.32
 H      -4.928096     1.060935     1.098111      27.99
 H      -5.560155     0.250189    -0.354115      28.15
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name = lig-etoh-Waterframe_499
 C       6.324773    -1.141217     1.345833      55.80
 H       6.480926    -0.102254     1.089606      24.00
 C       5.577376    -3.396409     0.872585      59.44
 H       5.061878    -4.111506     0.184867      18.30
 C       5.936785    -3.864822     2.105736      28.31
 O       5.755322    -5.161133     2.629257     269.33
 C       5.610653    -6.195036     1.602586     104.16
 H       6.435407    -6.122503     0.782441      27.49
 H       4.712040    -5.893537     0.941379      26.19
 H       5.482657    -7.084641     2.077097      25.12
 C       6.496178    -2.922105     3.034276       4.22
 O       7.052108    -3.287259     4.286829     141.11
 H       6.847364    -4.280408     4.308672      30.53
 C       6.661284    -1.601215     2.666655      44.11
 H       7.313284    -0.957645     3.340038      22.46
 C       5.846486    -2.069282     0.458641      17.43
 C       5.279078    -1.788368    -1.062968      80.00
 H       5.757307    -2.720623    -1.604715      21.25
 O       5.785435    -0.550331    -1.637965     274.03
 H       5.054906     0.106900    -1.209976      21.38
 C       3.699662    -1.810313    -1.087615      68.54
 H       3.232082    -2.786251    -0.670865      20.48
 C       3.189818    -1.671510    -2.506968      96.44
 O       3.570007    -2.833423    -3.270616     246.64
 H       4.461598    -2.750994    -3.696262      26.66
 H       3.612551    -0.687262    -3.036462      21.27
 H       2.020755    -1.776925    -2.405651      23.03
 C      -0.525198    -1.403100     0.599903      42.46
 H      -1.159574    -2.090080     1.052850      26.31
 C      -0.233960     0.947786    -0.041945      81.00
 H      -0.538665     1.934146     0.108561      20.09
 C       1.207291     0.755664    -0.221706       4.85
 O       2.169335     1.717389    -0.555419     181.11
 C       1.808849     3.052949    -1.025232     106.85
 H       2.632547     3.609689    -1.288486      25.10
 H       1.136806     3.083198    -1.868156      25.79
 H       1.677035     3.810336     0.057233      21.84
 C       1.782451    -0.541511    -0.035390      16.90
 O       3.141984    -0.639454    -0.295342     183.75
 C       0.875044    -1.591173     0.340410      57.25
 H       1.405756    -2.563325     0.606854      20.25
 C      -1.030513    -0.094039     0.455955      31.27
 C      -2.578903     0.058250     0.764858      74.33
 H      -3.030827    -0.855985     0.980500      22.81
 O      -2.702777     1.136465     1.751546     231.88
 H      -1.978365     0.890172     2.539180      22.42
 C      -3.400065     0.750119    -0.440910      64.53
 H      -2.662563     1.669472    -0.727729      18.63
 O      -3.318074    -0.332659    -1.502722     226.45
 H      -3.202745     0.248576    -2.404202      21.56
 C      -4.902787     0.944624     0.042360      94.45
 O      -5.293398     2.244360    -0.579929     287.79
 H      -4.932643     2.983830    -0.073948      29.73
 H      -4.989845     0.991738     1.192615      26.79
 H      -5.549884     0.087729    -0.101376      27.20
55
name = lig-etoh-Waterframe_500
 C       6.359523    -1.113367     1.355059      53.56
 H       6.402694    -0.087939     0.892657      25.12
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 C       5.552658    -3.393549     0.831077      27.49
 H       5.005177    -4.100222     0.143655      14.42
 C       5.904662    -3.803044     2.159840      21.45
 O       5.745682    -5.105776     2.629741     266.63
 C       5.635149    -6.162839     1.558920     106.86
 H       6.502538    -6.191617     0.951509      29.70
 H       4.585269    -5.945501     0.976095      26.29
 H       5.524025    -7.056476     2.070725      25.06
 C       6.495430    -2.944607     3.079963       4.20
 O       7.044013    -3.341624     4.262083     260.56
 H       6.788505    -4.254409     4.642279      27.57
 C       6.714282    -1.539467     2.643421      63.83
 H       7.075754    -0.793195     3.326496      23.36
 C       5.815449    -2.045126     0.401218       1.35
 C       5.283077    -1.791801    -0.983586      67.18
 H       5.822364    -2.694641    -1.755985      19.48
 O       5.779885    -0.608842    -1.600664     295.11
 H       5.253253     0.264449    -1.194633      20.91
 C       3.633879    -1.835302    -1.101908      67.01
 H       3.149115    -2.676349    -0.558598      20.33
 C       3.144211    -1.676633    -2.525287     114.67
 O       3.555109    -2.808765    -3.281425     262.07
 H       4.479910    -2.649909    -3.598611      26.39
 H       3.529901    -0.711031    -2.932943      23.20
 H       2.123038    -1.523560    -2.434091      26.18
 C      -0.464532    -1.312252     0.609211      34.14
 H      -1.130220    -2.194437     1.099117      17.76
 C      -0.160609     0.967893    -0.006875      76.05
 H      -0.623664     2.033555    -0.277542      19.14
 C       1.189984     0.785233    -0.218219      21.22
 O       2.138153     1.705953    -0.510355     264.67
 C       1.837695     3.011208    -1.062253     120.65
 H       2.617085     3.390208    -1.624045      23.50
 H       1.041498     3.036189    -1.697840      28.07
 H       1.187050     3.495073    -0.263585      23.87
 C       1.776979    -0.513755    -0.051242      12.17
 O       3.180575    -0.639814    -0.325497     168.23
 C       0.913410    -1.546830     0.344081      71.98
 H       1.252532    -2.616412     0.607647      21.45
 C      -1.112566    -0.061247     0.404607      75.04
 C      -2.534229     0.137408     0.676136     101.40
 H      -2.938578    -0.809649     1.001252      26.55
 O      -2.669514     1.157140     1.783628     180.26
 H      -1.726238     1.142839     2.317730      27.18
 C      -3.446103     0.644529    -0.360715      87.52
 H      -3.051753     1.753208    -0.625108      21.38
 O      -3.320330    -0.335830    -1.504133     198.96
 H      -3.284939    -0.013795    -2.508679      21.45
 C      -4.814949     1.043236     0.038773      91.87
 O      -5.354144     2.275239    -0.616703     231.21
 H      -4.995339     2.934951    -0.023351      29.60
 H      -4.826034     1.180654     1.207595      25.65
 H      -5.484144     0.204656    -0.496296      24.40
55
name = lig-etoh-Waterframe_501
 C       6.363199    -1.122662     1.293265      39.29
 H       6.572061     0.011303     1.160870      17.62
 C       5.549133    -3.371043     0.846446      63.89
 H       5.155903    -4.107725     0.111807      18.64
 C       5.853991    -3.788484     2.159086      12.80
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 O       5.734276    -5.091928     2.591319     247.78
 C       5.623632    -6.098067     1.573353     113.41
 H       6.466192    -6.129891     1.005752      29.65
 H       4.690306    -6.142343     0.867376      29.22
 H       5.592574    -7.067633     2.165543      25.07
 C       6.542477    -2.834619     3.088685      -2.65
 O       7.037459    -3.383125     4.277403     221.03
 H       6.638012    -4.277242     4.553500      26.69
 C       6.741719    -1.529939     2.641076      51.15
 H       7.066209    -0.849407     3.354564      22.90
 C       5.743908    -2.092873     0.410413      31.69
 C       5.252247    -1.768640    -0.945091      80.51
 H       5.405046    -2.639491    -1.704891      23.40
 O       5.764073    -0.626202    -1.572021     279.18
 H       5.659413     0.312250    -1.062868      22.55
 C       3.625170    -1.822170    -1.037873      76.11
 H       3.396392    -2.799078    -0.673305      22.11
 C       3.098804    -1.636628    -2.522293     110.13
 O       3.526147    -2.809001    -3.324430     263.94
 H       4.412914    -2.674784    -3.777998      26.43
 H       3.551208    -0.782869    -2.874923      24.97
 H       2.098646    -1.601753    -2.774848      26.21
 C      -0.418583    -1.229642     0.623267      44.18
 H      -0.967034    -2.306759     0.958703      14.46
 C      -0.183156     1.039520     0.014392      78.32
 H      -0.638193     2.020881    -0.585735      17.32
 C       1.193222     0.750403    -0.191542       6.38
 O       2.134059     1.734565    -0.503416     191.80
 C       1.719794     2.971827    -1.092328     105.51
 H       2.790759     3.267429    -1.441985      21.56
 H       0.986940     2.556039    -1.861587      23.63
 H       1.523642     3.751160    -0.473129      26.68
 C       1.780906    -0.531719    -0.088234      10.42
 O       3.178964    -0.640278    -0.343774     192.34
 C       0.934784    -1.523797     0.382216      45.51
 H       1.322321    -2.580696     0.475926      19.65
 C      -1.027973    -0.049227     0.303415      55.36
 C      -2.511535     0.217975     0.730663      86.41
 H      -2.821471    -0.788192     1.226538      24.70
 O      -2.627594     1.169651     1.810095     214.44
 H      -1.643384     1.129460     2.253722      28.06
 C      -3.411970     0.632514    -0.454742     102.29
 H      -3.066725     1.498972    -0.929581      25.98
 O      -3.349854    -0.352037    -1.479255     237.16
 H      -3.381601     0.222227    -2.328172      24.04
 C      -4.831946     1.113813    -0.007898     100.75
 O      -5.380108     2.290796    -0.614358     293.67
 H      -5.221446     3.158330    -0.240388      29.73
 H      -4.955840     1.194653     1.109744      26.68
 H      -5.676610     0.267208    -0.299943      24.83
55
name = lig-etoh-Waterframe_502
 C       6.363590    -1.169052     1.299908      59.79
 H       6.530901    -0.083278     0.950756      21.09
 C       5.536249    -3.418695     0.902662      50.03
 H       5.258635    -4.186007     0.191878      17.04
 C       5.870350    -3.732366     2.172873       8.41
 O       5.704426    -5.062433     2.563544     295.12
 C       5.620774    -6.104736     1.587679      66.02
 H       6.456394    -6.008939     0.881456      27.39
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 H       4.758269    -5.958454     0.997984      34.36
 H       5.608040    -7.107328     2.249262      22.93
 C       6.532432    -2.865156     3.046129     -10.80
 O       7.018375    -3.366419     4.291909     187.82
 H       6.642001    -4.271208     4.247289      26.89
 C       6.748638    -1.523337     2.622442      65.12
 H       7.327994    -0.865518     3.210363      26.01
 C       5.723398    -2.029384     0.470157      13.40
 C       5.122967    -1.746913    -0.992429      98.95
 H       5.442210    -2.513125    -1.499056      27.07
 O       5.791407    -0.596758    -1.572805     258.79
 H       5.626334     0.060308    -0.769559      26.38
 C       3.630270    -1.781176    -1.020265      87.79
 H       3.306814    -2.712217    -0.586310      22.33
 C       3.131692    -1.635822    -2.540444      94.84
 O       3.499297    -2.818178    -3.373199     264.53
 H       4.310133    -2.707195    -3.979951      25.74
 H       3.585166    -0.756577    -2.899655      23.35
 H       1.943678    -1.650312    -2.575069      23.09
 C      -0.368063    -1.279888     0.616994      36.62
 H      -1.249538    -1.986804     0.976432      15.93
 C      -0.172592     1.083039    -0.067282      74.61
 H      -0.605392     2.178348    -0.259236      16.26
 C       1.219955     0.781744    -0.172110      10.96
 O       2.125039     1.746485    -0.456962     204.89
 C       1.640379     2.921700    -1.147735     101.03
 H       2.637916     3.382020    -1.789791      22.69
 H       0.978298     2.909098    -2.198904      22.06
 H       1.442773     3.795125    -0.519614      24.30
 C       1.798343    -0.533141    -0.102134      25.06
 O       3.118966    -0.646009    -0.323766     220.52
 C       0.976474    -1.542260     0.401482      39.41
 H       1.382638    -2.539360     0.520825      18.50
 C      -0.985596     0.012689     0.289054      55.81
 C      -2.461719     0.229731     0.790550      64.98
 H      -2.974823    -0.806739     1.083103      23.23
 O      -2.563284     1.209819     1.825193     211.84
 H      -1.747421     1.040146     2.522444      25.87
 C      -3.372167     0.739902    -0.538944      81.62
 H      -2.775280     1.475694    -0.955392      24.61
 O      -3.406372    -0.398877    -1.470982     230.69
 H      -3.460438     0.028778    -2.396102      24.63
 C      -4.927859     1.127108    -0.011310      97.49
 O      -5.413322     2.323631    -0.658869     312.99
 H      -4.992298     3.051519    -0.081564      27.35
 H      -4.825815     1.251188     1.025268      27.22
 H      -5.604665     0.270179    -0.152148      26.41
55
name = lig-etoh-Waterframe_503
 C       6.360873    -1.140907     1.333528      49.09
 H       6.556806    -0.198456     0.848555      25.75
 C       5.520693    -3.355697     0.869623      66.55
 H       5.120870    -4.123190     0.260276      16.92
 C       5.896061    -3.779197     2.179775      20.69
 O       5.688621    -5.030894     2.616468     245.25
 C       5.603238    -6.096134     1.574125      78.31
 H       6.531734    -6.141345     0.843303      26.79
 H       4.673516    -6.038395     1.161028      31.86
 H       5.587110    -7.173471     2.105058      24.22
 C       6.549869    -2.872320     3.069568      10.18
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 O       6.963510    -3.316908     4.249085     148.83
 H       6.886590    -4.233284     4.537860      24.53
 C       6.785131    -1.552175     2.610227      66.74
 H       7.539250    -0.910654     3.111241      21.92
 C       5.635230    -2.070805     0.447033       0.65
 C       5.140521    -1.752375    -0.965199      81.40
 H       5.511520    -2.589372    -1.587466      24.34
 O       5.794324    -0.560145    -1.544338     246.46
 H       5.531580     0.337805    -1.062461      24.91
 C       3.588531    -1.753833    -1.097342      75.69
 H       3.145263    -2.625877    -0.566829      22.02
 C       3.185032    -1.689961    -2.562304     101.11
 O       3.462005    -2.819440    -3.405726     267.76
 H       4.326995    -2.610330    -3.907281      24.83
 H       3.466441    -0.699257    -3.031941      23.13
 H       1.983096    -1.483982    -2.324359      22.37
 C      -0.434156    -1.268877     0.577104      47.41
 H      -0.972739    -2.038076     1.065154      25.77
 C      -0.125477     1.090477    -0.140563     106.48
 H      -0.399450     2.063996     0.107743      20.57
 C       1.211261     0.818118    -0.189246       5.51
 O       2.121319     1.814137    -0.447722     169.84
 C       1.653127     2.985456    -1.270838      60.84
 H       2.625262     3.353149    -1.834362      22.75
 H       0.610573     2.610330    -1.776554      21.33
 H       0.993335     3.527298    -0.446677      21.79
 C       1.724012    -0.494665    -0.066145      16.27
 O       3.102488    -0.623779    -0.290404     197.60
 C       0.990944    -1.609931     0.404556      37.83
 H       1.392017    -2.531697     0.701828      18.15
 C      -0.979367     0.001487     0.387177      45.74
 C      -2.437093     0.241178     0.701550      82.90
 H      -2.893442    -0.720736     1.042325      23.33
 O      -2.486944     1.260995     1.846369     208.05
 H      -2.088530     0.728668     2.694737      23.10
 C      -3.368302     0.798824    -0.493584      57.47
 H      -2.869527     1.786746    -0.946443      20.73
 O      -3.465600    -0.434017    -1.469526     209.45
 H      -3.479942    -0.303110    -2.433499      25.55
 C      -4.893584     1.131502    -0.028623     100.25
 O      -5.442002     2.353793    -0.683563     264.28
 H      -4.895793     3.133778    -0.239959      26.38
 H      -4.781300     1.394193     0.982217      26.58
 H      -5.468569     0.355961    -0.288065      28.04
55
name = lig-etoh-Waterframe_504
 C       6.307954    -1.143167     1.288437      45.46
 H       6.660969    -0.203598     1.092326      22.35
 C       5.475520    -3.382953     0.877818      52.13
 H       4.897439    -3.975506     0.222376      15.45
 C       5.914228    -3.774325     2.128376      13.23
 O       5.688188    -5.093981     2.679818     243.92
 C       5.555242    -6.102445     1.599855      97.01
 H       6.435945    -5.982840     0.789463      27.97
 H       4.612807    -6.087471     0.987447      29.85
 H       5.636144    -7.016906     2.216856      22.53
 C       6.531733    -2.892143     3.019158      13.57
 O       6.957536    -3.245542     4.304081     155.02
 H       6.735945    -4.175668     4.510160      26.61
 C       6.854360    -1.582130     2.574093      18.96
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 H       7.513415    -0.938451     3.281943      21.65
 C       5.615646    -2.020934     0.459061      25.22
 C       5.218691    -1.714987    -0.929398      75.35
 H       5.462217    -2.586170    -1.798007      22.26
 O       5.784533    -0.525019    -1.512868     295.79
 H       5.171258     0.253495    -1.288255      22.32
 C       3.595750    -1.742617    -1.120423      67.04
 H       3.258774    -2.807907    -0.834811      19.95
 C       3.128186    -1.655732    -2.573204      98.92
 O       3.436486    -2.811128    -3.418560     234.08
 H       4.359859    -2.761035    -3.848650      26.37
 H       3.660029    -0.740770    -3.106588      21.92
 H       2.023548    -1.728988    -2.836726      23.14
 C      -0.452402    -1.326552     0.576121      49.38
 H      -0.961334    -2.042907     1.009307      27.66
 C      -0.171947     1.040744    -0.077097      69.79
 H      -0.476490     1.966232     0.074225      20.37
 C       1.227783     0.848679    -0.248164      -3.17
 O       2.138145     1.899317    -0.476747     190.69
 C       1.555295     2.976107    -1.286123     108.88
 H       2.261152     3.488945    -1.793650      26.76
 H       1.015519     2.435436    -2.000377      26.69
 H       1.347059     4.033779    -0.670883      21.27
 C       1.719865    -0.526734    -0.029556      15.38
 O       3.105955    -0.588122    -0.285396     197.33
 C       0.892141    -1.566025     0.394312      58.65
 H       1.348121    -2.448341     0.729363      19.79
 C      -0.960804     0.006877     0.408692      48.78
 C      -2.443111     0.309106     0.639331      91.72
 H      -2.851662    -0.564949     1.005425      24.54
 O      -2.424456     1.270805     1.844839     208.52
 H      -2.361107     0.538420     2.574859      22.83
 C      -3.395890     0.779993    -0.460416      75.51
 H      -3.084510     1.748666    -1.173648      20.57
 O      -3.503406    -0.431012    -1.422677     200.42
 H      -3.442128     0.076336    -2.227877      25.82
 C      -4.772049     1.200989    -0.056621     102.13
 O      -5.436985     2.352180    -0.697347     247.75
 H      -5.109335     3.310070    -0.507958      26.52
 H      -5.001940     1.228711     1.080108      25.93
 H      -5.452239     0.413431    -0.336460      26.74
55
name = lig-etoh-Waterframe_505
 C       6.351266    -1.121121     1.332602      74.08
 H       6.448730    -0.139187     0.959937      21.55
 C       5.395989    -3.386401     0.877591      55.45
 H       4.832021    -4.096324     0.273705      17.39
 C       5.888869    -3.846014     2.134921      -2.31
 O       5.686600    -5.128859     2.673644     239.51
 C       5.518464    -6.123481     1.656164     119.92
 H       6.364804    -5.942165     0.951791      29.21
 H       4.471269    -5.971559     1.089037      26.19
 H       5.578501    -7.056490     2.050993      24.84
 C       6.566394    -2.871368     2.992854      11.86
 O       6.947273    -3.186020     4.362821     177.13
 H       6.571954    -4.071169     4.455477      25.29
 C       6.861469    -1.633886     2.501200      61.23
 H       7.296214    -0.880805     3.252359      25.71
 C       5.648118    -2.005891     0.484755      -3.89
 C       5.178463    -1.652648    -1.013151      86.86
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 H       5.798319    -2.590662    -1.493800      20.81
 O       5.760583    -0.477721    -1.490366     315.14
 H       5.137763     0.201379    -1.137389      25.17
 C       3.643372    -1.744022    -1.109106      71.70
 H       3.293884    -2.707712    -0.617568      20.73
 C       3.068757    -1.590522    -2.677636      97.82
 O       3.464282    -2.834571    -3.417803     245.60
 H       4.393337    -2.779195    -3.814615      26.54
 H       3.612470    -0.639247    -3.043683      23.63
 H       2.044929    -1.394194    -2.693204      27.15
 C      -0.529961    -1.348711     0.609561      31.61
 H      -1.268793    -2.068239     0.892251      16.33
 C      -0.152741     1.041409     0.033316      51.63
 H      -0.697958     1.960414    -0.269364      20.79
 C       1.227421     0.817455    -0.267500      -0.13
 O       2.115354     1.956310    -0.505629     205.50
 C       1.526995     2.999329    -1.325626     112.72
 H       2.354413     3.319896    -1.907893      24.39
 H       0.813804     2.834793    -2.038815      28.13
 H       0.864158     3.804228    -0.716119      23.72
 C       1.767121    -0.445128    -0.068600      25.10
 O       3.107372    -0.631982    -0.305463     200.51
 C       0.868677    -1.510868     0.380360      54.13
 H       1.280558    -2.509330     0.570643      24.38
 C      -1.015802    -0.045655     0.346368      30.50
 C      -2.442047     0.374884     0.693193     101.21
 H      -2.971604    -0.530273     0.944914      26.87
 O      -2.399379     1.248920     1.805118     219.15
 H      -2.280196     0.705930     2.667619      27.74
 C      -3.388087     0.771824    -0.503291      92.03
 H      -2.759193     1.484328    -1.127339      24.85
 O      -3.517891    -0.354616    -1.368395     221.15
 H      -3.499977     0.025681    -2.238594      28.09
 C      -4.792749     1.263856    -0.035559      83.81
 O      -5.411404     2.346945    -0.738580     269.04
 H      -4.973139     3.123196    -0.187811      25.56
 H      -4.820626     1.292859     1.184834      24.64
 H      -5.437168     0.349958    -0.461141      24.46
55
name = lig-etoh-Waterframe_506
 C       6.371312    -1.118106     1.273088      56.98
 H       6.381075    -0.059788     0.964473      21.19
 C       5.356740    -3.352146     0.923422      65.29
 H       4.888420    -4.082122     0.212394      21.33
 C       5.862895    -3.854060     2.180949      20.15
 O       5.685595    -5.129433     2.674682     249.71
 C       5.482972    -6.155242     1.668073     128.47
 H       6.176021    -6.162442     0.904842      31.22
 H       4.397249    -5.988172     1.243148      26.67
 H       5.423128    -7.086698     2.066479      26.63
 C       6.601194    -2.946549     3.022449      10.03
 O       6.901929    -3.141448     4.344652      92.58
 H       6.714175    -4.007118     4.743509      25.22
 C       6.864348    -1.601275     2.521863      24.89
 H       7.359321    -0.892635     3.220227      24.58
 C       5.636990    -2.057781     0.467197      11.71
 C       5.188301    -1.668994    -0.992167      95.26
 H       5.565912    -2.386466    -1.728308      25.24
 O       5.711798    -0.385273    -1.482877     300.72
 H       5.540342     0.346370    -0.934141      27.80
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 C       3.621661    -1.746675    -1.174107      81.34
 H       3.290240    -2.667022    -0.696523      22.03
 C       3.111298    -1.559504    -2.687182     109.17
 O       3.491090    -2.815788    -3.399148     248.96
 H       4.363103    -2.561639    -3.788688      27.71
 H       3.552598    -0.716642    -3.196732      25.92
 H       2.102979    -1.397731    -2.591440      27.70
 C      -0.571651    -1.301831     0.596671      32.36
 H      -1.225161    -2.292525     0.814724      16.08
 C      -0.132016     1.018859     0.074266      62.66
 H      -0.600709     2.029942    -0.435566      20.25
 C       1.201107     0.891025    -0.229684       2.82
 O       2.018452     1.938357    -0.551249     203.58
 C       1.474202     3.060007    -1.380851      88.19
 H       2.520177     3.621828    -1.799430      21.37
 H       0.631010     2.595788    -2.004227      24.05
 H       1.116873     3.649574    -0.611935      25.01
 C       1.753840    -0.457011    -0.112307       3.37
 O       3.135245    -0.670451    -0.330121     179.12
 C       0.882912    -1.481960     0.358245      41.71
 H       1.332377    -2.529024     0.359271      22.35
 C      -1.085971    -0.053057     0.299190      33.98
 C      -2.488228     0.298695     0.742518      88.39
 H      -3.020521    -0.679769     1.153981      25.85
 O      -2.412160     1.277291     1.788356     213.62
 H      -1.896991     0.827592     2.534798      28.77
 C      -3.304937     0.871404    -0.515195      88.71
 H      -2.828837     1.653458    -0.948770      27.24
 O      -3.518335    -0.305178    -1.360956     252.58
 H      -3.558438    -0.234707    -2.273462      30.19
 C      -4.837789     1.232182    -0.041104      83.02
 O      -5.343024     2.376516    -0.741318     272.11
 H      -5.118766     3.317646    -0.329685      25.77
 H      -4.754187     1.631888     1.013044      24.74
 H      -5.529949     0.230452    -0.086451      24.83
55
name = lig-etoh-Waterframe_507
 C       6.362896    -1.191939     1.223141      35.32
 H       6.650508    -0.104207     1.048293      22.94
 C       5.371256    -3.361016     0.988980      56.99
 H       4.871700    -4.044958     0.242222      19.80
 C       5.847707    -3.797040     2.205749      27.30
 O       5.695124    -5.143972     2.677259     243.49
 C       5.387138    -6.195825     1.658000      99.74
 H       6.088692    -6.263923     0.862273      29.35
 H       4.432722    -6.029907     1.151933      30.65
 H       5.374997    -7.047620     2.395702      25.60
 C       6.598474    -2.942212     3.011917      -4.97
 O       6.875377    -3.117243     4.356625     111.91
 H       6.739770    -4.057124     4.622919      28.36
 C       6.838785    -1.586640     2.560480      37.73
 H       7.460422    -0.995489     3.172215      19.88
 C       5.630521    -2.062123     0.414863      36.39
 C       5.185995    -1.655246    -0.989353     120.63
 H       5.499723    -2.233083    -1.724439      27.56
 O       5.677517    -0.321202    -1.474680     299.26
 H       5.545034     0.237270    -0.752801      30.79
 C       3.606829    -1.727687    -1.230127      88.64
 H       3.251241    -2.725200    -1.123668      22.87
 C       3.186507    -1.574622    -2.625721     107.50
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 O       3.515166    -2.749996    -3.384355     239.88
 H       4.372216    -2.706617    -3.885443      28.05
 H       3.609302    -0.752552    -3.101160      25.61
 H       2.055752    -1.674886    -2.786830      24.09
 C      -0.466259    -1.290561     0.505395      44.86
 H      -1.115608    -2.264997     0.941963      23.79
 C      -0.217736     1.014260     0.003338      57.24
 H      -0.594759     2.194088     0.102090      17.60
 C       1.184678     0.878411    -0.164388       9.30
 O       1.972801     1.913890    -0.625877     184.13
 C       1.426775     3.089393    -1.324377     100.21
 H       2.269940     3.801636    -2.038339      23.06
 H       0.851684     2.640795    -2.287247      22.80
 H       1.072713     3.845193    -0.743158      26.45
 C       1.725534    -0.489870    -0.131224       7.74
 O       3.114603    -0.665932    -0.349466     184.65
 C       0.857040    -1.475927     0.303003      51.02
 H       1.309258    -2.524702     0.404739      18.74
 C      -1.100508    -0.031285     0.335472      32.06
 C      -2.549809     0.230828     0.717881      78.25
 H      -3.093335    -0.725361     1.189253      21.19
 O      -2.432134     1.318439     1.802254     216.29
 H      -1.649474     1.009421     2.255059      26.88
 C      -3.358730     0.913234    -0.442587      84.32
 H      -2.979508     1.812457    -0.862363      22.89
 O      -3.481418    -0.293796    -1.388291     242.72
 H      -3.440958     0.134851    -2.197211      27.78
 C      -4.769339     1.289117     0.011766     106.73
 O      -5.321212     2.396614    -0.801665     292.44
 H      -4.986116     3.233546    -0.281636      26.14
 H      -4.733232     1.538144     1.009952      26.91
 H      -5.532196     0.497247     0.016296      25.52
55
name = lig-etoh-Waterframe_508
 C       6.417290    -1.241564     1.282140      62.07
 H       6.772198    -0.313637     0.710476      23.88
 C       5.377365    -3.357438     0.936865      44.20
 H       4.779753    -4.183916     0.487841      13.66
 C       5.834709    -3.820553     2.218490      25.74
 O       5.701162    -5.128638     2.640525     246.38
 C       5.288345    -6.200968     1.689123      94.76
 H       6.209664    -6.340364     1.019699      30.35
 H       4.361430    -6.076056     1.245087      32.14
 H       5.220392    -7.249264     2.348899      25.25
 C       6.566703    -2.822508     3.048421      16.88
 O       6.871217    -3.143066     4.384321     149.87
 H       6.524744    -4.071142     4.474851      29.58
 C       6.793772    -1.618086     2.517346      91.61
 H       7.385200    -0.964341     3.060646      22.41
 C       5.638586    -2.062437     0.405033       9.10
 C       5.158807    -1.605052    -1.059792      97.03
 H       5.754181    -2.416684    -1.644796      21.06
 O       5.650434    -0.319722    -1.428723     319.93
 H       5.184069     0.384077    -0.877061      22.72
 C       3.632821    -1.726332    -1.186762      77.83
 H       3.284320    -2.697571    -0.736868      19.99
 C       3.221984    -1.542825    -2.677695      98.73
 O       3.572999    -2.740191    -3.412296     260.67
 H       4.499678    -2.676911    -3.780894      26.31
 H       3.581984    -0.581505    -2.978883      23.41
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 H       1.984356    -1.362307    -2.661202      22.52
 C      -0.469201    -1.290144     0.431671      36.95
 H      -1.086881    -2.127615     0.977896      25.90
 C      -0.294682     1.073675    -0.035903      79.63
 H      -0.709856     2.040393     0.340856      17.57
 C       1.109643     0.807341    -0.173529       2.35
 O       1.991142     1.922987    -0.691581     132.38
 C       1.396569     3.094831    -1.334527     101.16
 H       2.397902     3.408183    -1.662438      23.38
 H       0.533949     2.907414    -2.109330      23.28
 H       0.634875     3.729338    -0.717641      23.57
 C       1.725000    -0.439788    -0.154339      20.16
 O       3.041924    -0.661123    -0.366710     206.76
 C       0.914805    -1.545382     0.222115      47.01
 H       1.282080    -2.555739     0.552289      16.89
 C      -1.077011    -0.046528     0.382211      33.84
 C      -2.556239     0.296220     0.727390      90.31
 H      -3.107346    -0.629311     1.019087      21.45
 O      -2.461803     1.318470     1.800357     268.24
 H      -1.659001     1.197843     2.257031      27.62
 C      -3.460868     0.806504    -0.347095      77.77
 H      -2.776348     1.652318    -0.855096      20.03
 O      -3.420270    -0.211798    -1.448622     246.81
 H      -3.375860     0.251712    -2.224233      26.76
 C      -4.756222     1.394017     0.092588     119.29
 O      -5.289807     2.397905    -0.841849     292.11
 H      -4.983588     3.298397    -0.509154      27.23
 H      -4.690672     1.679153     1.099105      27.37
 H      -5.340703     0.592449    -0.126384      27.27
55
name = lig-etoh-Waterframe_509
 C       6.439320    -1.245887     1.152523      47.00
 H       6.877808    -0.275521     0.771947      20.56
 C       5.366271    -3.400247     0.906349      55.13
 H       4.732644    -4.017813     0.266892      17.89
 C       5.852346    -3.776527     2.176473       4.09
 O       5.687279    -5.117969     2.623950     273.48
 C       5.248709    -6.189582     1.755578      72.86
 H       6.018136    -6.376663     0.846853      25.49
 H       4.359618    -5.916374     1.221165      33.32
 H       5.002737    -7.183821     2.428554      21.71
 C       6.434097    -2.888749     3.114094      -4.76
 O       6.864607    -3.198337     4.388019     271.31
 H       6.367945    -4.014296     4.742268      25.84
 C       6.834356    -1.558359     2.535221      22.69
 H       7.349522    -0.801574     3.129464      23.72
 C       5.639084    -2.080556     0.430850      35.55
 C       5.183808    -1.590630    -1.012256      87.26
 H       5.650716    -2.404498    -1.928000      21.26
 O       5.632171    -0.321666    -1.385435     316.04
 H       4.959225     0.391576    -1.119057      23.28
 C       3.632103    -1.739352    -1.145207      68.01
 H       3.372858    -2.685340    -0.547764      17.97
 C       3.215221    -1.497252    -2.677370      91.02
 O       3.631540    -2.720743    -3.453375     237.91
 H       4.541614    -2.541950    -3.781670      26.26
 H       3.814949    -0.647072    -3.133226      22.32
 H       2.025394    -1.363429    -2.794024      23.11
 C      -0.504742    -1.355320     0.417353      47.75
 H      -1.095810    -2.118260     0.769813      21.11
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 C      -0.300322     1.083096     0.015862      56.48
 H      -0.654067     2.014342    -0.026537      20.51
 C       1.054023     0.906021    -0.311349      -3.71
 O       1.957801     1.858345    -0.709827     214.40
 C       1.336565     3.072112    -1.325872     105.48
 H       2.013651     3.734746    -1.564895      26.37
 H       0.779533     2.682777    -2.145301      25.37
 H       1.016523     3.638580    -0.271588      21.94
 C       1.673180    -0.496880    -0.177548       8.13
 O       3.039370    -0.595103    -0.391018     175.30
 C       0.902331    -1.586877     0.169463      55.82
 H       1.433753    -2.499631     0.406365      22.31
 C      -1.087719    -0.018058     0.356624      32.66
 C      -2.509676     0.287669     0.833260     101.93
 H      -2.846733    -0.564844     1.287105      26.65
 O      -2.517866     1.320111     1.792836     302.64
 H      -1.854266     1.050958     2.381045      32.57
 C      -3.379615     0.782804    -0.377844      65.08
 H      -2.787643     1.809697    -0.756202      21.62
 O      -3.393100    -0.125309    -1.490108     281.25
 H      -3.430331     0.242120    -2.310597      27.80
 C      -4.826932     1.439246     0.109239     101.41
 O      -5.244033     2.407846    -0.865644     289.23
 H      -4.968106     3.293487    -0.609067      30.43
 H      -4.802928     1.965647     1.150283      25.93
 H      -5.585118     0.622616     0.184584      26.50
55
name = lig-etoh-Waterframe_510
 C       6.531519    -1.215617     1.157553      68.02
 H       6.690328    -0.212438     0.741317      23.79
 C       5.352395    -3.385764     0.869616      73.40
 H       4.902838    -4.086325     0.192776      22.35
 C       5.820543    -3.828174     2.128883     -16.60
 O       5.686472    -5.094703     2.640545     210.73
 C       5.191192    -6.139038     1.765689     107.20
 H       5.938236    -6.502979     0.987649      25.19
 H       4.235204    -5.776513     1.285616      28.61
 H       5.034931    -6.926252     2.518639      22.60
 C       6.367128    -2.835332     3.089047     -18.11
 O       6.834803    -3.267943     4.394674     178.53
 H       6.355568    -4.085807     4.795509      21.24
 C       6.812049    -1.591624     2.539440      32.01
 H       7.354142    -0.851958     3.232213      22.14
 C       5.646326    -2.108977     0.378635      20.78
 C       5.172330    -1.639827    -0.933197      89.70
 H       5.536300    -2.309588    -1.828175      24.53
 O       5.643485    -0.322235    -1.390692     253.23
 H       5.104863     0.378288    -0.757894      22.50
 C       3.615202    -1.683481    -1.137513      79.89
 H       3.170979    -2.719413    -0.991314      23.23
 C       3.249531    -1.548068    -2.647392     104.07
 O       3.657064    -2.674015    -3.472331     257.05
 H       4.493086    -2.640799    -3.992673      26.97
 H       3.837948    -0.611682    -3.020395      23.23
 H       2.251947    -1.417230    -2.925893      26.82
 C      -0.555335    -1.382540     0.413609      50.41
 H      -1.127238    -2.161185     0.603225      20.46
 C      -0.242751     1.112234     0.031521      73.08
 H      -0.716919     1.945983    -0.314837      20.58
 C       1.056583     0.839487    -0.429887       9.18
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 O       1.958239     1.819146    -0.752251     195.90
 C       1.337805     3.038989    -1.223469     111.73
 H       1.924980     3.893294    -1.778637      23.92
 H       0.646985     2.829526    -1.978694      27.20
 H       0.546307     3.574843    -0.473690      23.46
 C       1.598485    -0.455377    -0.243683       9.88
 O       3.058138    -0.512215    -0.420961     161.07
 C       0.814023    -1.592426     0.142847      52.53
 H       1.270094    -2.533495     0.153202      24.09
 C      -1.074151    -0.075067     0.347440      36.44
 C      -2.474910     0.197868     0.878545      90.31
 H      -2.838509    -0.688778     1.400037      26.18
 O      -2.553513     1.347929     1.832630     257.66
 H      -2.232879     0.970326     2.588007      31.42
 C      -3.325117     0.880794    -0.382621      63.07
 H      -2.874515     1.864125    -0.623562      23.52
 O      -3.388251    -0.075517    -1.503004     267.61
 H      -3.512038     0.412097    -2.259948      27.72
 C      -4.853458     1.419644     0.091231      86.34
 O      -5.219054     2.422209    -0.917793     294.70
 H      -4.875899     3.148435    -0.449843      30.64
 H      -4.544478     2.054785     1.098417      24.30
 H      -5.811794     0.789852     0.407330      25.62
55
name = lig-etoh-Waterframe_511
 C       6.532585    -1.252945     1.215541     120.01
 H       6.718612    -0.267684     0.892343      24.04
 C       5.362479    -3.402326     0.838897      55.71
 H       5.013924    -4.181075     0.212253      23.93
 C       5.779026    -3.804537     2.141250       2.35
 O       5.697820    -5.069042     2.653897     225.62
 C       5.131132    -6.102634     1.797764     144.13
 H       5.883474    -6.374223     1.129746      28.08
 H       4.121286    -5.852958     1.275840      25.55
 H       4.916307    -6.888518     2.349012      25.61
 C       6.365993    -2.853323     3.033746      -4.60
 O       6.779126    -3.295678     4.355342     185.38
 H       6.352304    -4.224736     4.409164      25.12
 C       6.762485    -1.634452     2.523364      36.84
 H       7.391914    -0.993789     3.258646      23.07
 C       5.758861    -2.059332     0.405787      -0.98
 C       5.120861    -1.656610    -0.968245      91.49
 H       5.516934    -2.353934    -1.513439      26.31
 O       5.648473    -0.343563    -1.372312     251.29
 H       5.647324     0.362585    -0.599314      25.65
 C       3.570890    -1.636763    -1.179893      85.25
 H       3.092995    -2.501937    -0.666220      21.51
 C       3.341580    -1.527744    -2.680269     112.98
 O       3.661999    -2.670881    -3.487794     281.72
 H       4.535626    -2.521953    -3.940007      26.50
 H       3.724329    -0.506444    -2.973731      23.73
 H       2.333664    -1.424069    -2.687982      28.10
 C      -0.592915    -1.389089     0.394201      32.23
 H      -1.277591    -2.245479     0.631033      22.00
 C      -0.251072     1.014276    -0.025149      64.10
 H      -0.834943     1.993659    -0.164026      17.69
 C       1.051465     0.763885    -0.459568       6.96
 O       1.990776     1.839868    -0.824242     187.37
 C       1.237416     3.049585    -1.176178      89.06
 H       2.400891     3.559327    -1.519878      19.05
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 H       0.510900     2.797175    -1.982885      24.50
 H       0.721798     3.521512    -0.353107      24.32
 C       1.625868    -0.492614    -0.318135      24.81
 O       3.001947    -0.490028    -0.456670     182.65
 C       0.767921    -1.552571     0.075726      64.36
 H       1.052058    -2.562095     0.051497      20.56
 C      -1.044853    -0.058083     0.402289      79.07
 C      -2.498972     0.219142     0.825268      74.09
 H      -3.118640    -0.757078     1.101504      23.68
 O      -2.556268     1.330164     1.895718     242.81
 H      -2.510004     1.017744     2.726732      31.22
 C      -3.397597     0.886258    -0.307182      95.59
 H      -2.846043     1.672116    -0.565643      27.11
 O      -3.382157    -0.001997    -1.474490     273.21
 H      -3.513432     0.423021    -2.293054      25.72
 C      -4.764094     1.432500     0.076531      92.07
 O      -5.196954     2.436415    -0.949779     288.36
 H      -4.991400     3.329151    -0.692052      31.51
 H      -4.518183     1.952406     1.082082      25.19
 H      -5.558564     0.561299     0.128025      26.13
55
name = lig-etoh-Waterframe_512
 C       6.488066    -1.237153     1.258089      44.76
 H       6.933363    -0.321211     1.037569      22.69
 C       5.443982    -3.396294     0.847901      84.64
 H       4.961602    -3.994692     0.114487      20.08
 C       5.727375    -3.748340     2.133000      46.83
 O       5.671566    -5.074270     2.670837     238.90
 C       5.095303    -6.098435     1.822236     118.09
 H       5.750709    -6.270065     1.020022      30.97
 H       4.220955    -5.626295     1.228395      29.70
 H       4.906108    -6.944223     2.388325      26.75
 C       6.413939    -2.938359     3.032504      18.81
 O       6.700285    -3.294977     4.247069     104.98
 H       6.419596    -4.232492     4.575352      27.26
 C       6.773531    -1.658802     2.590376      31.48
 H       7.403232    -0.958247     3.215929      19.33
 C       5.747423    -2.100842     0.399089     -33.36
 C       5.140921    -1.598109    -0.949596      75.36
 H       5.460316    -2.380270    -1.735373      25.61
 O       5.688112    -0.400620    -1.387732     281.85
 H       5.548766     0.272631    -0.585090      25.19
 C       3.602201    -1.640482    -1.140909      83.37
 H       3.246062    -2.535873    -0.671459      22.34
 C       3.322244    -1.453516    -2.712658      94.25
 O       3.682432    -2.661190    -3.496118     264.70
 H       4.595303    -2.577485    -3.913807      26.51
 H       3.884368    -0.646717    -3.165402      23.58
 H       2.160682    -1.400014    -2.782676      23.64
 C      -0.598203    -1.345564     0.365634      49.44
 H      -1.283513    -2.286530     0.786020      24.60
 C      -0.293176     0.921041    -0.113393      75.50
 H      -0.556296     2.083773     0.176780      17.91
 C       1.083814     0.807912    -0.454752       3.58
 O       1.929334     1.797076    -0.868969     217.83
 C       1.249102     3.047230    -1.142003     106.37
 H       1.971750     4.048192    -1.469889      23.07
 H       0.605187     2.963620    -2.095412      24.32
 H       1.018036     3.485637    -0.290785      27.68
 C       1.627872    -0.560621    -0.368760      19.51
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 O       2.963503    -0.508670    -0.522368     195.60
 C       0.749365    -1.594420    -0.015216      63.05
 H       1.190703    -2.600289     0.067042      20.25
 C      -1.129204    -0.051828     0.472774      48.69
 C      -2.584453     0.313742     0.794990      78.64
 H      -3.034576    -0.745612     1.164155      21.45
 O      -2.561400     1.268922     1.931804     286.48
 H      -2.482783     0.733976     2.650211      27.99
 C      -3.372812     0.901487    -0.306964      96.33
 H      -2.765293     1.828451    -0.582454      22.93
 O      -3.398585     0.033030    -1.410523     281.72
 H      -3.397426     0.467582    -2.274531      23.92
 C      -4.681149     1.487101     0.052873     114.84
 O      -5.177774     2.422604    -0.967185     290.56
 H      -4.972775     3.325617    -0.646965      29.74
 H      -4.900098     1.790703     0.984293      28.96
 H      -5.354923     0.639238    -0.089811      27.95
55
name = lig-etoh-Waterframe_513
 C       6.453488    -1.218417     1.324832      35.81
 H       6.839420    -0.322223     0.870526      24.08
 C       5.483258    -3.384624     0.801979      70.90
 H       4.894424    -4.076507     0.189696      12.79
 C       5.716856    -3.834075     2.152607      41.73
 O       5.616380    -5.080753     2.685344     252.61
 C       5.075325    -6.059302     1.776962     115.11
 H       5.786480    -6.393904     0.938555      31.61
 H       4.055436    -5.723023     1.505033      30.08
 H       4.863909    -6.989479     2.468499      25.82
 C       6.435636    -2.936014     2.973612      12.28
 O       6.679215    -3.317823     4.274266     162.71
 H       6.137539    -4.114126     4.662793      24.74
 C       6.816863    -1.645893     2.617951      75.16
 H       7.350197    -1.040082     3.321056      21.28
 C       5.705476    -2.070979     0.381879     -12.57
 C       5.206367    -1.619216    -0.933339      73.62
 H       5.438521    -2.370562    -1.938112      21.75
 O       5.761159    -0.399152    -1.399282     307.75
 H       5.253907     0.401555    -0.932573      22.34
 C       3.660461    -1.654607    -1.148968      79.13
 H       3.321340    -2.647344    -1.026735      23.94
 C       3.291477    -1.463019    -2.725517      92.84
 O       3.695583    -2.654136    -3.478315     259.61
 H       4.535621    -2.601733    -4.050681      24.99
 H       3.874767    -0.616791    -2.995890      24.37
 H       2.174353    -1.140511    -3.170381      22.28
 C      -0.609511    -1.336483     0.372226      56.34
 H      -1.170833    -2.343662     0.813986      20.31
 C      -0.280146     0.967797    -0.121787      92.73
 H      -0.641893     2.102819     0.064094      17.77
 C       1.026773     0.741497    -0.428466      15.90
 O       1.877307     1.777175    -0.922780     221.63
 C       1.315333     3.126248    -1.130284     101.99
 H       2.025376     3.723722    -1.502100      25.10
 H       0.309002     3.059706    -1.735364      23.89
 H       0.638985     3.406801    -0.192000      23.00
 C       1.541534    -0.514742    -0.413628      19.43
 O       2.984718    -0.551249    -0.579882     172.13
 C       0.745494    -1.654233    -0.089271      65.00
 H       1.204956    -2.688709     0.101406      21.57
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 C      -1.187565    -0.071555     0.422214      65.09
 C      -2.598758     0.329899     0.875425      77.06
 H      -3.197554    -0.567849     1.175442      22.81
 O      -2.583210     1.190044     1.974669     299.68
 H      -2.137497     0.637896     2.587300      25.64
 C      -3.238356     1.050499    -0.357411      63.49
 H      -2.592283     2.043986    -0.710312      20.62
 O      -3.433945     0.013631    -1.364191     253.56
 H      -3.274318     0.441820    -2.251097      23.65
 C      -4.764773     1.483920     0.000497     103.75
 O      -5.145872     2.440900    -0.971397     301.14
 H      -4.852596     3.310223    -0.588650      29.46
 H      -4.910854     1.848775     0.989714      27.77
 H      -5.383370     0.663010    -0.146012      28.74
55
name = lig-etoh-Waterframe_514
 C       6.416408    -1.196350     1.297384      62.86
 H       6.561822    -0.134010     0.944921      20.94
 C       5.442995    -3.447707     0.810279      44.93
 H       4.971394    -4.177519     0.091934      19.72
 C       5.791944    -3.846157     2.095383      -0.86
 O       5.548573    -5.110528     2.682698     227.86
 C       5.019460    -6.077994     1.768360     113.80
 H       5.749313    -6.220830     0.820326      26.91
 H       4.059855    -5.895335     1.326810      28.81
 H       4.959231    -7.129543     2.444803      22.41
 C       6.416968    -2.941678     2.993550     -38.77
 O       6.695785    -3.326190     4.364685     253.67
 H       6.027387    -4.050252     4.561696      22.32
 C       6.844138    -1.629820     2.586049      57.76
 H       7.314271    -1.083674     3.320458      30.52
 C       5.723133    -2.026841     0.470194     -39.57
 C       5.225806    -1.632965    -1.028672      66.02
 H       5.829048    -2.522662    -1.511129      23.17
 O       5.841733    -0.341140    -1.409330     268.43
 H       5.182607     0.411768    -1.174158      23.74
 C       3.632637    -1.692662    -1.297523      78.14
 H       3.239555    -2.635719    -0.795292      23.17
 C       3.368627    -1.458826    -2.765817     109.81
 O       3.687238    -2.669744    -3.467049     273.31
 H       4.464633    -2.446608    -4.061894      25.85
 H       3.949086    -0.588182    -2.992771      25.72
 H       2.192650    -1.254226    -2.774189      24.40
 C      -0.588320    -1.416627     0.375634      37.39
 H      -1.275757    -2.211434     0.762450      16.75
 C      -0.376804     1.028386    -0.021524      56.85
 H      -0.806790     2.003937    -0.289577      17.14
 C       0.962476     0.781009    -0.467321      -5.51
 O       1.838871     1.772616    -0.966609     172.37
 C       1.277994     3.126233    -1.086792      96.75
 H       2.092902     3.571518    -1.395072      26.00
 H       0.513499     3.061799    -1.911131      24.68
 H       1.041318     3.735707     0.089897      22.18
 C       1.569460    -0.600869    -0.452126      19.50
 O       2.963030    -0.584319    -0.581663     178.46
 C       0.702464    -1.621053    -0.106687      63.64
 H       1.104937    -2.704228    -0.028177      24.64
 C      -1.137520    -0.065650     0.307403      40.36
 C      -2.577867     0.305890     0.860295      77.42
 H      -3.251068    -0.445864     0.846096      24.53
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 O      -2.580873     1.127487     2.084387     276.85
 H      -1.789576     0.989577     2.619718      30.43
 C      -3.252269     1.142771    -0.334545      72.73
 H      -2.567733     1.940508    -0.865788      21.62
 O      -3.435437     0.008831    -1.342156     215.90
 H      -3.270635     0.162538    -2.369330      23.57
 C      -4.783481     1.470532    -0.048988      89.25
 O      -5.136701     2.519561    -0.988399     279.33
 H      -4.858503     3.466675    -0.778604      28.75
 H      -4.733009     1.940448     1.048035      25.64
 H      -5.357448     0.546363    -0.123340      28.45
55
name = lig-etoh-Waterframe_515
 C       6.402043    -1.139523     1.290638      33.88
 H       6.416686     0.002337     1.134292      20.46
 C       5.422104    -3.419129     0.826110      78.99
 H       5.082253    -4.096902    -0.014217      21.87
 C       5.867771    -3.870702     2.087142      -7.26
 O       5.472502    -5.118308     2.651832     220.58
 C       4.987467    -6.148903     1.733460     109.23
 H       5.743414    -6.145579     0.885798      26.01
 H       4.079251    -5.878461     1.312655      28.81
 H       5.067501    -7.218045     2.248132      23.41
 C       6.448930    -2.916724     3.095791      18.53
 O       6.704997    -3.295508     4.378266     234.41
 H       6.337931    -4.128883     4.791225      19.22
 C       6.823160    -1.678180     2.566938      53.09
 H       7.317163    -0.956929     3.171122      27.70
 C       5.648620    -2.088538     0.464839       4.08
 C       5.283313    -1.611836    -1.017611      83.35
 H       5.694626    -2.247742    -1.740968      26.04
 O       5.889322    -0.327196    -1.445670     273.82
 H       5.306017     0.354814    -0.963771      25.71
 C       3.670472    -1.714210    -1.355179      69.69
 H       3.234829    -2.718793    -0.917062      22.63
 C       3.400901    -1.467903    -2.772103     116.62
 O       3.672813    -2.679823    -3.499557     258.35
 H       4.549188    -2.720713    -4.010398      25.61
 H       3.942066    -0.661422    -3.275211      25.47
 H       2.375889    -1.314655    -2.886676      27.35
 C      -0.644240    -1.395933     0.348032      44.10
 H      -1.201497    -2.176675     0.623812      18.61
 C      -0.363154     1.070181    -0.019828      64.04
 H      -0.877513     1.911457    -0.225403      19.16
 C       0.949373     0.778539    -0.517913       4.43
 O       1.780185     1.763080    -0.969460     195.76
 C       1.299468     3.100017    -1.055579     102.05
 H       2.278496     3.852332    -1.527778      22.15
 H       0.549127     3.370295    -1.755928      25.48
 H       1.193594     3.682262    -0.020820      23.52
 C       1.556734    -0.541902    -0.472672      11.98
 O       2.947197    -0.621282    -0.580119     153.82
 C       0.699684    -1.654969    -0.086445      45.82
 H       1.078267    -2.705648    -0.185679      23.06
 C      -1.160846    -0.118402     0.315066      48.79
 C      -2.537322     0.329028     0.763028      80.62
 H      -3.068296    -0.645943     0.949533      24.66
 O      -2.565456     1.074725     2.156756     197.06
 H      -1.643070     0.890245     2.484339      29.54
 C      -3.345152     1.069923    -0.345726     106.61
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 H      -2.898174     1.966862    -0.718003      24.79
 O      -3.412335    -0.013328    -1.335093     210.54
 H      -3.250463     0.414647    -2.339648      21.48
 C      -4.663339     1.587022    -0.054919      98.47
 O      -5.177104     2.590267    -1.032078     258.63
 H      -4.789282     3.445483    -0.617263      28.59
 H      -4.988844     1.867324     1.096998      25.36
 H      -5.401170     0.723624    -0.241977      26.39
55
name = lig-etoh-Waterframe_516
 C       6.323521    -1.218279     1.321596      54.94
 H       6.548329    -0.132703     1.049028      22.40
 C       5.457178    -3.374843     0.847272      43.44
 H       5.016391    -4.151141     0.173635      21.37
 C       5.876440    -3.886272     2.174155       6.36
 O       5.416024    -5.119230     2.623710     236.40
 C       5.031530    -6.181169     1.651053     124.37
 H       5.666304    -6.317852     0.839066      30.17
 H       4.011124    -6.006702     1.350778      28.56
 H       4.950544    -7.063858     2.216240      26.47
 C       6.448748    -2.992553     3.073369       7.85
 O       6.750694    -3.237840     4.415419     287.68
 H       6.327519    -4.109142     4.651316      21.56
 C       6.790545    -1.651460     2.558756      40.20
 H       7.346416    -0.935631     3.246843      24.82
 C       5.629037    -2.020671     0.385359      20.67
 C       5.296602    -1.582796    -1.010099     113.85
 H       5.578631    -2.204457    -1.777867      25.68
 O       5.872901    -0.337025    -1.440534     334.74
 H       5.754527     0.385439    -0.789248      25.22
 C       3.760419    -1.661127    -1.272533      67.03
 H       3.469642    -2.758318    -1.287871      23.36
 C       3.392479    -1.484550    -2.873274     100.83
 O       3.665052    -2.737673    -3.566886     244.33
 H       4.626485    -2.744550    -3.884911      25.67
 H       4.020038    -0.578043    -3.207989      24.31
 H       2.437852    -1.248657    -3.106573      28.52
 C      -0.672454    -1.399679     0.286724      52.02
 H      -1.239721    -2.203297     0.528269      28.38
 C      -0.322281     0.977597    -0.084641      66.99
 H      -0.642040     1.940463     0.013337      21.89
 C       0.936263     0.772857    -0.531127      15.89
 O       1.765057     1.778546    -0.988920     230.22
 C       1.373906     3.162898    -1.036784     105.84
 H       2.437597     3.715397    -1.663947      20.42
 H       0.412315     3.241657    -1.425672      26.56
 H       1.170473     3.390318    -0.129995      29.19
 C       1.490695    -0.532627    -0.451814      10.97
 O       2.951411    -0.646206    -0.587942     142.10
 C       0.718276    -1.624252    -0.084984      50.36
 H       1.091359    -2.622868    -0.093537      21.21
 C      -1.170991    -0.015569     0.363149      52.41
 C      -2.565204     0.311325     0.778979      74.86
 H      -3.080841    -0.703512     1.176557      22.22
 O      -2.523482     1.023079     2.101263     214.90
 H      -1.750139     0.505534     2.641797      21.19
 C      -3.340815     0.977729    -0.362201      92.60
 H      -2.739620     1.747226    -0.690727      26.15
 O      -3.382105    -0.015486    -1.366359     239.69
 H      -3.381514     0.491754    -2.359981      20.31
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 C      -4.754781     1.672061    -0.046561      91.02
 O      -5.171977     2.658782    -1.015513     277.40
 H      -4.883754     3.666143    -0.884778      27.11
 H      -4.732468     2.098953     1.027831      25.47
 H      -5.502536     0.815673    -0.266126      25.99
55
name = lig-etoh-Waterframe_517
 C       6.280528    -1.245370     1.333943      60.37
 H       6.690475    -0.298383     0.981274      24.33
 C       5.502129    -3.363692     0.887377      56.70
 H       4.909623    -4.068040     0.327255      17.90
 C       5.781561    -3.857272     2.146842      23.09
 O       5.391745    -5.152448     2.595174     229.64
 C       5.062845    -6.187054     1.603309     121.85
 H       5.744522    -6.325282     0.816805      31.94
 H       4.041412    -5.977339     1.041710      25.98
 H       5.032570    -6.961933     2.223143      28.90
 C       6.498695    -2.969955     3.043297      12.67
 O       6.797091    -3.202084     4.430263     193.15
 H       6.210562    -3.919272     4.809637      26.96
 C       6.723228    -1.692340     2.597767      47.80
 H       7.313637    -1.008525     3.346675      19.03
 C       5.670392    -2.039666     0.388770       5.74
 C       5.241437    -1.521847    -1.040614     116.98
 H       5.786433    -2.465782    -1.576323      22.37
 O       5.863188    -0.328675    -1.422527     341.95
 H       5.873098     0.285640    -0.673426      26.21
 C       3.722006    -1.600453    -1.333778      83.21
 H       3.522337    -2.544325    -0.816656      22.99
 C       3.440329    -1.476078    -2.923477      93.96
 O       3.681901    -2.777257    -3.619592     244.00
 H       4.579353    -2.657237    -4.072023      25.55
 H       4.193138    -0.703120    -3.356961      23.53
 H       2.330664    -1.213668    -2.989858      24.68
 C      -0.671905    -1.349914     0.225004      54.42
 H      -1.382043    -2.196083     0.512151      26.00
 C      -0.339003     0.983403    -0.120724      74.40
 H      -0.474184     2.045260     0.182284      19.80
 C       1.013104     0.755923    -0.556714      -1.13
 O       1.822970     1.769053    -1.032476     203.58
 C       1.404599     3.178216    -0.994236     110.58
 H       2.179327     3.821946    -1.572069      24.18
 H       0.491053     3.249868    -1.592382      25.44
 H       1.485558     3.613037     0.054357      25.91
 C       1.562057    -0.575702    -0.459761      17.95
 O       2.943588    -0.649017    -0.568055     188.14
 C       0.652194    -1.591797    -0.069489      61.09
 H       1.129448    -2.491566     0.092546      21.68
 C      -1.158989    -0.066717     0.379266      23.40
 C      -2.621711     0.218591     0.911375      63.66
 H      -3.266007    -0.772228     0.844063      21.75
 O      -2.461300     1.000929     2.007904     256.55
 H      -2.265278     0.322464     2.841625      22.65
 C      -3.329135     0.998061    -0.353955      52.69
 H      -2.527121     1.723293    -0.704980      21.16
 O      -3.369938    -0.031568    -1.415663     224.93
 H      -3.540220     0.197356    -2.494895      19.81
 C      -4.822264     1.713462    -0.046011     103.24
 O      -5.158709     2.731988    -1.018858     301.48
 H      -4.679623     3.665171    -0.746721      26.30
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 H      -4.649597     2.156499     0.833632      27.79
 H      -5.664873     1.017482     0.137631      27.48
55
name = lig-etoh-Waterframe_518
 C       6.345569    -1.185011     1.338264      60.00
 H       6.592592    -0.176907     1.144566      23.17
 C       5.441673    -3.406756     0.839153      61.73
 H       4.900198    -3.992212     0.151572      19.26
 C       5.717726    -3.838244     2.164770      24.67
 O       5.397656    -5.151060     2.556777     188.92
 C       5.091941    -6.173876     1.561397      94.76
 H       6.045182    -6.199571     0.939047      27.51
 H       4.090708    -5.896985     0.936912      26.06
 H       4.957933    -7.163799     2.057917      26.18
 C       6.484108    -2.998216     3.101128      20.49
 O       6.831426    -3.189594     4.404342     186.22
 H       6.311366    -3.864567     4.914152      25.93
 C       6.681246    -1.689316     2.625250      45.07
 H       7.212673    -0.933229     3.319155      20.27
 C       5.685435    -2.079159     0.441632      18.40
 C       5.223316    -1.540160    -1.004484     101.83
 H       5.669315    -2.319930    -1.919998      22.53
 O       5.875062    -0.301080    -1.410903     294.75
 H       5.571042     0.331862    -0.735797      27.48
 C       3.664620    -1.613136    -1.400485      78.88
 H       3.260665    -2.536986    -1.040236      23.95
 C       3.497751    -1.510790    -2.901874      97.97
 O       3.693286    -2.761412    -3.640228     256.30
 H       4.509444    -2.740652    -4.215001      26.34
 H       4.101944    -0.723740    -3.417865      24.47
 H       2.335434    -1.144566    -3.147290      23.71
 C      -0.703135    -1.361779     0.205387      38.07
 H      -1.361152    -2.350064     0.536254      24.49
 C      -0.280372     1.027026    -0.097666      69.71
 H      -0.769237     2.109473     0.085289      18.20
 C       1.028017     0.738055    -0.564959       2.71
 O       1.926489     1.776458    -1.068787     169.00
 C       1.434935     3.153868    -0.969128     112.60
 H       2.061224     3.606691    -1.505968      27.36
 H       0.431716     3.499196    -1.449021      23.67
 H       1.555474     3.846350     0.130888      22.96
 C       1.598294    -0.569531    -0.488071      17.34
 O       2.973173    -0.609664    -0.543573     173.54
 C       0.697668    -1.605511    -0.071438      50.20
 H       0.976712    -2.599922     0.182481      20.69
 C      -1.206689    -0.095675     0.334853      52.54
 C      -2.636255     0.118175     0.816896      75.57
 H      -3.182253    -0.765201     1.161531      23.41
 O      -2.465120     1.016104     1.992692     218.58
 H      -2.322472     0.457617     2.924039      24.12
 C      -3.377967     1.016724    -0.367077      55.42
 H      -2.790480     2.059829    -0.619406      20.74
 O      -3.376516    -0.070445    -1.413432     213.66
 H      -3.412176     0.390191    -2.384349      20.17
 C      -4.752179     1.746574    -0.021357     104.33
 O      -5.137801     2.792795    -1.031199     285.73
 H      -4.620804     3.594868    -0.574736      26.45
 H      -4.604208     2.274660     0.905643      26.75
 H      -5.598500     1.122766     0.129054      27.82
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name = lig-etoh-Waterframe_519
 C       6.406476    -1.168726     1.351307      74.08
 H       6.392600    -0.139995     1.163621      25.00
 C       5.351798    -3.414512     0.802163      49.11
 H       4.999295    -4.115967     0.073671      22.70
 C       5.702825    -3.866104     2.184003      21.68
 O       5.402697    -5.155389     2.570517     184.63
 C       5.159618    -6.125342     1.507049     100.58
 H       6.064421    -6.261049     0.726733      25.53
 H       4.294498    -5.840822     0.840727      26.13
 H       4.845090    -7.160181     2.035624      24.55
 C       6.365730    -3.006659     3.089079      12.76
 O       6.867490    -3.214882     4.408386     159.24
 H       6.482279    -4.080368     4.731345      25.37
 C       6.681600    -1.628501     2.634164      11.72
 H       7.114440    -0.982415     3.393239      20.29
 C       5.680319    -2.038396     0.431292     -47.32
 C       5.232816    -1.608454    -1.003241      83.36
 H       5.662143    -2.279565    -1.802766      24.45
 O       5.844712    -0.273545    -1.355824     258.82
 H       5.292765     0.451479    -1.119410      27.06
 C       3.670747    -1.652616    -1.359238      69.17
 H       3.295156    -2.623360    -1.351619      27.51
 C       3.500716    -1.477838    -2.945790     100.39
 O       3.689043    -2.735324    -3.630030     268.29
 H       4.608613    -2.727869    -4.010887      25.57
 H       4.197980    -0.712507    -3.170299      27.10
 H       2.381859    -1.198777    -3.215933      26.30
 C      -0.644298    -1.432218     0.199056      42.37
 H      -1.322693    -2.381031     0.535293      20.23
 C      -0.291930     0.979604    -0.030033      65.94
 H      -0.700519     2.095076    -0.271978      19.01
 C       1.015270     0.798553    -0.559298     -11.13
 O       1.960607     1.773273    -1.050699     166.66
 C       1.506537     3.186354    -0.973170      90.87
 H       2.275499     3.688513    -1.693709      23.32
 H       0.354566     3.118180    -1.189066      22.43
 H       1.529514     3.294980     0.244903      23.98
 C       1.551397    -0.562712    -0.481633       3.30
 O       3.026272    -0.575615    -0.562687     130.88
 C       0.744220    -1.632997    -0.077436      53.26
 H       1.133241    -2.684213     0.019041      23.31
 C      -1.190966    -0.052813     0.215066      41.84
 C      -2.618367     0.191147     0.719128      87.14
 H      -3.041603    -0.696426     1.025897      27.61
 O      -2.529939     1.058552     1.982290     173.86
 H      -1.862201     0.465288     2.689055      24.65
 C      -3.452461     0.970963    -0.346694      87.81
 H      -2.632963     1.718550    -0.734302      23.40
 O      -3.398763    -0.022036    -1.373000     262.65
 H      -3.272806     0.291819    -2.333571      23.87
 C      -4.682414     1.760610    -0.002718     100.59
 O      -5.073869     2.819458    -1.002434     269.61
 H      -4.896757     3.835316    -0.899375      27.33
 H      -4.477235     2.272193     1.088383      25.47
 H      -5.487602     1.050905    -0.066078      27.60
55
name = lig-etoh-Waterframe_520
 C       6.361428    -1.186674     1.326144      47.67
 H       6.512182    -0.160613     0.998534      23.47
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 C       5.345047    -3.340592     0.866214      85.93
 H       5.025718    -4.086787     0.124244      24.15
 C       5.679503    -3.856545     2.104761     -53.38
 O       5.421233    -5.193422     2.594970     160.86
 C       5.196076    -6.084680     1.428118     114.84
 H       6.151980    -6.284869     0.813625      27.54
 H       4.399167    -5.765583     0.906938      26.80
 H       4.992831    -7.059903     2.089253      24.28
 C       6.298247    -2.897212     3.064828     -26.66
 O       6.866468    -3.281500     4.364263     136.87
 H       6.564623    -4.139029     4.819096      11.43
 C       6.668701    -1.652357     2.668567      66.91
 H       7.152774    -1.090073     3.389820      28.57
 C       5.655698    -2.049052     0.416912     -30.11
 C       5.255725    -1.602973    -1.012028      78.32
 H       5.743075    -2.291979    -1.505268      29.55
 O       5.780681    -0.289653    -1.307596     305.36
 H       5.094430     0.323527    -1.165199      29.62
 C       3.712812    -1.662797    -1.342058      82.67
 H       3.409445    -2.590267    -0.792232      27.26
 C       3.493070    -1.391959    -2.939915     107.60
 O       3.714208    -2.693069    -3.598173     282.74
 H       4.606333    -2.827509    -4.007658      25.98
 H       4.216376    -0.736190    -3.295994      29.19
 H       2.523194    -1.020993    -3.103429      28.31
 C      -0.581024    -1.407645     0.201295      63.36
 H      -1.254639    -2.234697     0.471159      19.54
 C      -0.277131     0.995642    -0.080883      70.72
 H      -0.791007     2.022581    -0.098134      20.63
 C       1.055936     0.795239    -0.526051      11.22
 O       1.949828     1.731201    -1.014026     210.09
 C       1.558474     3.100506    -0.917348     111.87
 H       2.143249     4.140354    -1.532428      23.38
 H       0.534286     3.301941    -1.391838      24.88
 H       1.711548     3.550220     0.003679      28.12
 C       1.585375    -0.496936    -0.460285       3.93
 O       3.020611    -0.597148    -0.614591     142.52
 C       0.760393    -1.657898    -0.096051      54.62
 H       1.403519    -2.596569    -0.139428      26.75
 C      -1.124550    -0.143462     0.135851      29.75
 C      -2.591302     0.326339     0.731870      83.53
 H      -3.067557    -0.666164     0.718320      26.85
 O      -2.580627     1.062765     1.945236     251.46
 H      -1.594206     0.776820     2.309242      28.59
 C      -3.344594     0.980737    -0.371056      98.44
 H      -2.705779     1.756359    -0.711616      27.79
 O      -3.479111    -0.006451    -1.371783     279.12
 H      -3.375091     0.323647    -2.258111      27.31
 C      -4.663216     1.800462    -0.011862      99.68
 O      -5.006730     2.809379    -0.991942     291.21
 H      -4.706597     3.695099    -0.546174      27.43
 H      -4.572633     2.130447     1.194072      25.50
 H      -5.554889     1.130704     0.033855      27.70
55
name = lig-etoh-Waterframe_521
 C       6.283076    -1.199614     1.321666      38.75
 H       6.804688    -0.275827     0.965628      18.52
 C       5.344260    -3.330780     0.882678      75.75
 H       4.826586    -3.948467     0.107196      24.70
 C       5.682924    -3.799081     2.166760     -16.08
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 O       5.468929    -5.164567     2.552345     192.77
 C       5.226644    -6.095867     1.433328     122.93
 H       6.101348    -6.036855     0.844442      30.12
 H       4.407717    -5.829285     0.851234      27.98
 H       4.957908    -7.133441     1.730249      26.80
 C       6.275292    -2.948492     3.108861     -14.44
 O       6.843865    -3.331127     4.257190     133.07
 H       6.194244    -3.965203     4.749950      18.17
 C       6.640273    -1.617949     2.626084      19.71
 H       7.280012    -1.050408     3.215303      27.33
 C       5.632174    -2.009783     0.461930     -11.17
 C       5.269184    -1.560961    -0.977770      60.00
 H       5.735614    -2.323745    -1.798238      25.40
 O       5.720451    -0.316907    -1.290267     319.81
 H       5.161649     0.310074    -0.840302      29.26
 C       3.749319    -1.645866    -1.338136      75.68
 H       3.332283    -2.666378    -0.937316      27.33
 C       3.532165    -1.395082    -2.855362     121.36
 O       3.719810    -2.647432    -3.565532     273.52
 H       4.508881    -2.613885    -4.157713      26.49
 H       4.215802    -0.632948    -3.236197      29.48
 H       2.607718    -1.038523    -3.052617      29.22
 C      -0.547359    -1.438867     0.197725      67.97
 H      -1.127682    -2.196382     0.466075      26.93
 C      -0.263428     1.003598    -0.191092      77.74
 H      -0.619698     1.924018     0.086666      23.11
 C       1.085765     0.784746    -0.474219      -2.66
 O       1.972713     1.728396    -0.983148     187.62
 C       1.558400     3.142769    -0.869971     111.90
 H       2.557544     3.383251    -1.615391      22.25
 H       0.590853     3.352555    -1.252766      28.45
 H       1.571819     3.577233     0.057796      30.63
 C       1.668234    -0.544580    -0.430068      33.17
 O       3.000675    -0.584338    -0.657287     168.79
 C       0.864172    -1.573222    -0.157515      50.55
 H       1.152873    -2.676288     0.004959      27.21
 C      -1.091291    -0.089080     0.172563      18.67
 C      -2.523647     0.296152     0.700166      72.91
 H      -3.234195    -0.640342     1.022297      22.12
 O      -2.580010     1.062932     1.894064     242.42
 H      -1.749057     1.106229     2.552352      27.56
 C      -3.244244     1.147524    -0.438176      83.07
 H      -2.779486     1.963081    -0.865019      26.93
 O      -3.581806    -0.008522    -1.402431     230.60
 H      -3.605426     0.316951    -2.254928      27.33
 C      -4.657994     1.753460     0.006733      98.73
 O      -4.922290     2.805144    -0.954031     293.25
 H      -4.469107     3.667539    -0.636767      28.12
 H      -4.565272     2.382035     0.915434      25.88
 H      -5.509379     1.004268     0.049387      27.60
55
name = lig-etoh-Waterframe_522
 C       6.298093    -1.139426     1.369628      29.66
 H       6.762658    -0.171073     0.970584      26.09
 C       5.308305    -3.327786     0.871310      63.00
 H       4.704400    -4.040108     0.253473      23.63
 C       5.639709    -3.801812     2.196560      15.39
 O       5.501004    -5.122470     2.508267     235.60
 C       5.246795    -6.084174     1.407542     105.17
 H       6.007768    -6.048163     0.704224      24.80
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 H       4.311735    -5.749076     0.756835      20.94
 H       5.193725    -7.019438     1.864204      24.30
 C       6.302893    -2.907164     3.064219      22.38
 O       6.818707    -3.394214     4.216650     181.16
 H       6.246102    -3.961480     4.882149      21.43
 C       6.602159    -1.629725     2.604298      80.25
 H       7.335837    -1.008670     3.131257      22.71
 C       5.562396    -2.026873     0.451428     -55.30
 C       5.228156    -1.595978    -0.931969      38.30
 H       5.731372    -2.267089    -1.915609      21.10
 O       5.695514    -0.250683    -1.285755     254.65
 H       5.572629     0.394383    -0.582844      30.63
 C       3.734274    -1.636277    -1.320292      80.91
 H       3.293299    -2.704356    -1.335433      28.14
 C       3.573658    -1.410494    -2.779661     112.65
 O       3.723110    -2.610865    -3.556930     252.97
 H       4.489568    -2.533588    -4.166886      25.59
 H       4.344506    -0.565067    -2.986885      26.87
 H       2.488038    -1.136039    -2.932625      27.74
 C      -0.508741    -1.366912     0.166226      65.13
 H      -0.969329    -2.232109     0.504125      29.99
 C      -0.241785     0.995802    -0.235928      79.10
 H      -0.445809     1.961861    -0.109009      23.53
 C       1.136893     0.752042    -0.463171      11.70
 O       1.974248     1.739117    -0.903529     197.56
 C       1.627477     3.166171    -0.894077     114.37
 H       2.392305     3.665836    -1.377130      27.54
 H       0.725988     3.307970    -1.351577      29.49
 H       1.633759     3.418718     0.293269      27.16
 C       1.729122    -0.529406    -0.432984      24.84
 O       3.072581    -0.542934    -0.680870     162.42
 C       0.825897    -1.617848    -0.146171      51.09
 H       1.285128    -2.650159     0.017881      25.88
 C      -1.074163    -0.071054     0.263963      36.06
 C      -2.448925     0.261542     0.633778      70.58
 H      -3.098575    -0.737791     0.803488      22.33
 O      -2.565336     1.137231     1.879645     195.34
 H      -1.880578     0.709224     2.580723      23.76
 C      -3.274458     1.171520    -0.475250      70.14
 H      -2.565429     1.849385    -1.052528      23.32
 O      -3.660447     0.059481    -1.422564     222.57
 H      -3.710399     0.223793    -2.312464      28.19
 C      -4.559210     1.770446     0.035927     106.20
 O      -4.876874     2.801428    -0.962960     305.15
 H      -4.467396     3.696069    -0.907433      28.77
 H      -4.509388     2.054389     1.001998      28.85
 H      -5.305379     0.936051    -0.059662      28.32
55
name = lig-etoh-Waterframe_523
 C       6.268859    -1.134983     1.297983      28.09
 H       6.485035    -0.032734     1.112199      25.03
 C       5.227121    -3.338770     0.900716      89.47
 H       4.756268    -4.025933     0.168190      26.54
 C       5.587752    -3.765237     2.101595      38.97
 O       5.506830    -5.107204     2.481774     137.71
 C       5.258472    -6.038835     1.364561     109.73
 H       6.067345    -6.110267     0.598794      26.31
 H       4.048603    -5.944226     1.032313      23.40
 H       5.250284    -6.868541     1.980556      24.61
 C       6.296150    -2.925343     3.010836     -11.24
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 O       6.845669    -3.423775     4.243415     160.19
 H       6.315015    -4.165882     4.754832      21.08
 C       6.638646    -1.599342     2.642973      -4.71
 H       7.262555    -1.037121     3.458323      18.32
 C       5.555536    -1.996686     0.483641     -14.14
 C       5.179001    -1.567697    -0.952141      45.65
 H       5.824407    -2.338472    -1.446775      27.06
 O       5.708156    -0.193559    -1.280482     220.41
 H       5.630901     0.386088    -0.514444      31.59
 C       3.713652    -1.678659    -1.305504      99.51
 H       3.245313    -2.529915    -0.741224      25.97
 C       3.575200    -1.364951    -2.778978      98.00
 O       3.745790    -2.592128    -3.569052     264.02
 H       4.629510    -2.700311    -4.030684      25.85
 H       4.286286    -0.535647    -3.202671      26.18
 H       2.452213    -0.906418    -2.942308      26.22
 C      -0.498187    -1.328528     0.181505      53.38
 H      -1.192829    -2.195767     0.586047      30.88
 C      -0.175706     0.979871    -0.191459      67.73
 H      -0.612756     1.969712    -0.446668      21.66
 C       1.146782     0.755700    -0.493353      17.16
 O       2.031262     1.770340    -0.837956     203.43
 C       1.683365     3.155479    -0.875212     111.05
 H       2.333241     3.916332    -1.184516      26.32
 H       0.797400     3.411246    -1.469542      27.16
 H       1.547034     3.706507     0.313905      24.84
 C       1.713083    -0.549594    -0.438750       9.49
 O       3.158833    -0.511901    -0.658959     130.13
 C       0.871931    -1.636200    -0.128268      63.13
 H       1.276183    -2.639064    -0.122112      24.36
 C      -0.998337    -0.026960     0.270255      36.18
 C      -2.490242     0.316995     0.600885      83.72
 H      -2.911454    -0.653804     0.626241      25.97
 O      -2.507966     1.160407     1.859032     237.49
 H      -2.198391     0.469902     2.472663      26.30
 C      -3.247906     1.005933    -0.507332      86.50
 H      -2.466254     1.818481    -0.980400      22.50
 O      -3.737182     0.125725    -1.446083     272.71
 H      -3.555632     0.451660    -2.332512      27.03
 C      -4.428385     1.838658     0.033630     104.78
 O      -4.889359     2.791387    -0.997781     288.74
 H      -4.476477     3.615560    -0.759490      29.33
 H      -4.444186     1.980106     1.096685      26.94
 H      -5.255071     1.126074    -0.132768      27.76
55
name = lig-etoh-Waterframe_524
 C       6.262876    -1.135825     1.372508      99.41
 H       6.282757    -0.088174     1.033916      25.66
 C       5.129205    -3.256703     0.814772      61.78
 H       4.783523    -3.948551     0.045196      23.75
 C       5.600373    -3.769095     2.102514     -17.91
 O       5.490492    -5.079323     2.438201     196.73
 C       5.213527    -6.053718     1.417738     103.96
 H       5.921444    -5.869275     0.484681      26.64
 H       4.147883    -5.938299     0.911731      24.85
 H       5.297977    -7.106161     1.773691      23.70
 C       6.329979    -2.949478     3.044145     -18.88
 O       6.873139    -3.409402     4.214644     201.57
 H       6.325229    -4.149981     4.611452      18.98
 C       6.655975    -1.605577     2.645805      14.76
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 H       7.073380    -0.893997     3.483439      24.75
 C       5.518907    -1.951431     0.492049       4.76
 C       5.247685    -1.504213    -0.923340      88.11
 H       5.669157    -2.115937    -1.596380      29.81
 O       5.728668    -0.221087    -1.280442     292.70
 H       5.267224     0.462936    -0.709482      26.66
 C       3.721201    -1.646768    -1.256230      79.99
 H       3.330339    -2.559407    -0.839036      27.08
 C       3.533196    -1.370451    -2.850287      99.14
 O       3.764363    -2.592030    -3.592261     279.47
 H       4.710414    -2.639628    -3.914341      26.65
 H       4.364787    -0.607738    -2.977903      25.89
 H       2.470514    -0.972313    -3.188592      25.93
 C      -0.476954    -1.349848     0.254379      40.34
 H      -1.342922    -2.201473     0.501354      18.09
 C      -0.120483     1.048769    -0.153065      67.46
 H      -0.713176     2.040624    -0.525807      19.51
 C       1.198453     0.802350    -0.524401       7.00
 O       2.141833     1.819776    -0.795649     180.19
 C       1.670656     3.214653    -0.806287      71.45
 H       2.843861     3.601686    -1.268056      20.40
 H       0.739467     3.306158    -1.550387      23.51
 H       1.218536     3.518163     0.196861      25.08
 C       1.764447    -0.536115    -0.451168      22.43
 O       3.140128    -0.478265    -0.587995     170.16
 C       0.904547    -1.609865    -0.113794      64.51
 H       1.099887    -2.633045    -0.123300      27.78
 C      -0.979709    -0.006375     0.225630      41.69
 C      -2.467049     0.312918     0.628228      96.38
 H      -3.015954    -0.512278     0.937304      26.61
 O      -2.455235     1.111453     1.808357     263.18
 H      -2.230282     0.668074     2.585010      31.08
 C      -3.188919     0.989510    -0.495803      88.76
 H      -2.524632     1.741292    -1.088200      23.77
 O      -3.805174     0.131448    -1.532302     263.30
 H      -3.524141     0.482015    -2.419949      27.14
 C      -4.407135     1.830926    -0.021169      94.23
 O      -4.882370     2.803837    -1.002042     305.44
 H      -4.617104     3.708823    -0.896024      30.14
 H      -4.176874     2.622031     0.915374      23.74
 H      -5.232726     1.130730     0.220375      27.72
55
name = lig-etoh-Waterframe_525
 C       6.223967    -1.113770     1.451533      86.90
 H       6.549869    -0.128484     1.195781      16.97
 C       5.121206    -3.204397     0.830963      74.50
 H       4.632917    -3.837682     0.112802      24.61
 C       5.616829    -3.732457     2.052348     -54.68
 O       5.449363    -5.097000     2.435160     178.33
 C       5.134615    -6.049529     1.392192     111.81
 H       5.900324    -5.798088     0.543870      29.36
 H       4.194232    -5.904660     1.081488      27.75
 H       5.371644    -7.096785     1.829187      23.95
 C       6.362549    -2.931089     3.014437      30.13
 O       6.899530    -3.394652     4.185331     211.87
 H       6.443298    -4.068696     4.727965      18.85
 C       6.623132    -1.637297     2.665309      53.67
 H       7.143612    -0.875057     3.306362      29.33
 C       5.504704    -1.906059     0.484574     -23.39
 C       5.273352    -1.469699    -0.937657      94.77
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 H       5.730721    -2.126909    -1.741420      25.94
 O       5.758469    -0.213262    -1.261368     302.03
 H       5.070026     0.509246    -1.191817      26.44
 C       3.731523    -1.550105    -1.273515      89.21
 H       3.370625    -2.511747    -1.167807      28.44
 C       3.525509    -1.404630    -2.850401     113.38
 O       3.788040    -2.608341    -3.616848     271.52
 H       4.643766    -2.580705    -4.162029      25.53
 H       4.201672    -0.651976    -3.155902      28.53
 H       2.550249    -1.083149    -3.131843      27.81
 C      -0.442517    -1.305359     0.294218      44.96
 H      -0.993850    -2.324062     0.466403      17.12
 C      -0.113100     1.106509    -0.169321      60.08
 H      -0.421269     2.299353    -0.120230      18.64
 C       1.274874     0.860187    -0.510877       9.17
 O       2.209735     1.839016    -0.749509     198.65
 C       1.658086     3.204304    -0.778900      89.86
 H       2.743627     4.040086    -1.025739      21.91
 H       1.009942     3.367085    -1.756249      23.69
 H       1.365372     3.508404     0.077127      28.72
 C       1.753455    -0.449459    -0.433892      19.22
 O       3.111192    -0.496443    -0.517430     189.94
 C       0.868092    -1.577680    -0.085557      57.41
 H       1.282772    -2.517450    -0.054309      28.55
 C      -0.990131    -0.052779     0.193859      45.84
 C      -2.375511     0.209134     0.681106      76.86
 H      -3.006935    -0.757450     0.903053      24.71
 O      -2.414331     1.127263     1.790265     267.17
 H      -1.929180     0.679697     2.416139      32.59
 C      -3.237267     1.092002    -0.560831      62.40
 H      -2.491081     1.657735    -1.042213      24.61
 O      -3.833641     0.104992    -1.590522     228.89
 H      -3.666194     0.310144    -2.630986      25.04
 C      -4.397909     1.918449    -0.024227     101.16
 O      -4.901838     2.781068    -1.066124     322.13
 H      -4.610708     3.666779    -0.781822      29.07
 H      -3.741144     2.587818     0.819157      23.50
 H      -5.093352     1.351791     0.590875      28.17
55
name = lig-etoh-Waterframe_526
 C       6.183135    -1.063570     1.419090      51.55
 H       6.642716    -0.153689     1.233917      23.46
 C       5.160311    -3.186016     0.895238      74.12
 H       4.479867    -3.750800     0.310868      25.29
 C       5.631491    -3.748085     2.047698      26.38
 O       5.404802    -5.084742     2.459293     158.66
 C       5.085521    -6.001284     1.348415     126.43
 H       5.741297    -6.047629     0.476316      30.34
 H       4.081494    -6.002436     1.093769      28.95
 H       5.138990    -7.002720     1.958218      26.02
 C       6.347746    -2.978929     2.971883      -2.37
 O       6.942837    -3.390736     4.188966     206.60
 H       6.432188    -4.125541     4.594601      25.93
 C       6.603119    -1.597797     2.696908       5.03
 H       7.306440    -1.182718     3.368714      19.91
 C       5.529896    -1.837774     0.501862      13.05
 C       5.211642    -1.461694    -0.996592      86.54
 H       5.902993    -2.377246    -1.438116      23.06
 O       5.825167    -0.144409    -1.267069     259.26
 H       5.075272     0.524094    -1.249722      25.16
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 C       3.761562    -1.511500    -1.374815      92.44
 H       3.327972    -2.443607    -0.969620      25.54
 C       3.538819    -1.363751    -2.867243     120.53
 O       3.803718    -2.651211    -3.625090     260.45
 H       4.531995    -2.566690    -4.320786      25.38
 H       4.011695    -0.623245    -3.375721      29.46
 H       2.533460    -1.198831    -2.897271      28.60
 C      -0.400361    -1.335701     0.273142      37.22
 H      -1.023222    -2.082451     0.697238      21.41
 C      -0.092710     1.087850    -0.167903      73.11
 H      -0.468652     2.072516     0.250466      18.97
 C       1.221375     0.925767    -0.442315       5.81
 O       2.238444     1.889995    -0.713639     228.49
 C       1.733785     3.225572    -0.809742     117.68
 H       2.479602     4.006934    -0.734947      25.95
 H       0.983279     3.362721    -1.615197      27.42
 H       1.178969     3.550126     0.139154      28.04
 C       1.675662    -0.421239    -0.393840      23.50
 O       3.127562    -0.551948    -0.469978     156.47
 C       0.950808    -1.477380    -0.078344      61.86
 H       1.461617    -2.394411     0.054831      24.80
 C      -0.948809     0.020672     0.174120      63.26
 C      -2.407533     0.197036     0.603391      52.44
 H      -2.782136    -0.958208     0.733197      21.78
 O      -2.351739     1.130221     1.809300     263.39
 H      -1.700344     0.808644     2.357219      30.63
 C      -3.296315     1.050472    -0.648352      76.49
 H      -2.604116     1.690318    -1.055499      25.59
 O      -3.835124     0.077154    -1.587165     240.24
 H      -3.661758     0.516939    -2.599862      22.39
 C      -4.284839     2.034491     0.019932     107.28
 O      -4.939567     2.753563    -1.128133     301.55
 H      -4.743828     3.726562    -0.905470      27.82
 H      -3.777024     2.665348     0.744830      25.81
 H      -5.142019     1.575854     0.542305      27.20
55
name = lig-etoh-Waterframe_527
 C       6.251638    -0.976590     1.439366      57.74
 H       6.400622    -0.003089     1.008983      24.65
 C       5.177684    -3.134503     0.905945      61.58
 H       4.512327    -3.715040     0.313024      20.74
 C       5.646823    -3.792806     2.118961      16.75
 O       5.360788    -5.073291     2.438043     203.41
 C       5.009609    -6.014279     1.382831     113.59
 H       5.694940    -5.977020     0.599489      29.74
 H       3.909857    -5.762223     0.841066      23.45
 H       5.025308    -7.052024     1.812684      25.79
 C       6.383404    -2.951673     3.010722      22.73
 O       6.959303    -3.408881     4.172772     185.02
 H       6.541760    -4.233256     4.558179      23.71
 C       6.584827    -1.614792     2.678035      67.35
 H       7.238180    -1.157172     3.333012      19.33
 C       5.479143    -1.834906     0.500913       5.43
 C       5.264065    -1.423675    -0.948916      90.61
 H       5.772051    -2.142255    -1.794972      22.86
 O       5.878324    -0.128482    -1.306529     255.26
 H       5.301525     0.628116    -0.875237      23.70
 C       3.798683    -1.538887    -1.411489      63.80
 H       3.429153    -2.647900    -1.179079      23.19
 C       3.483962    -1.351938    -2.943802     103.01
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 O       3.788827    -2.671946    -3.601570     241.30
 H       4.650551    -2.576021    -4.134173      24.98
 H       4.052874    -0.474388    -3.250314      26.28
 H       2.369874    -1.282956    -3.043464      25.74
 C      -0.415563    -1.284626     0.234400      25.95
 H      -0.960371    -1.962384     0.715410      23.93
 C      -0.151893     1.139797    -0.089393      72.82
 H      -0.627630     2.026410     0.055683      18.81
 C       1.254425     0.959635    -0.397498       8.55
 O       2.215876     1.929816    -0.675568     204.75
 C       1.751573     3.299788    -0.783804     108.64
 H       2.561806     3.744424    -0.832987      26.73
 H       1.205382     3.354120    -1.675681      27.55
 H       0.861977     3.369730     0.145430      23.04
 C       1.796144    -0.331052    -0.415108      15.96
 O       3.127982    -0.559929    -0.457034     151.57
 C       0.983593    -1.490528    -0.021136      50.97
 H       1.525824    -2.461082     0.163921      19.06
 C      -0.917769    -0.018622     0.162719      46.71
 C      -2.413376     0.296503     0.462652      76.58
 H      -2.998741    -0.594344     0.874441      22.40
 O      -2.313638     1.093688     1.784742     235.09
 H      -1.710684     0.674410     2.403708      27.06
 C      -3.279747     0.961588    -0.608034      87.91
 H      -2.619529     1.593495    -1.283692      22.05
 O      -3.832363     0.073091    -1.547484     233.57
 H      -3.773922     0.488307    -2.590154      21.89
 C      -4.244247     2.114244    -0.000565     106.80
 O      -4.951045     2.741741    -1.151737     295.15
 H      -4.843496     3.722018    -1.245992      30.44
 H      -3.793453     2.797886     0.508245      28.07
 H      -5.058530     1.565592     0.561679      26.77
55
name = lig-etoh-Waterframe_528
 C       6.250609    -1.008262     1.394279      75.71
 H       6.431472     0.124560     1.316170      24.33
 C       5.174085    -3.152828     0.938746      67.41
 H       4.723621    -3.756657     0.154522      25.06
 C       5.632512    -3.711241     2.113700      -3.90
 O       5.320894    -5.115633     2.447862     131.79
 C       4.931477    -6.016202     1.378523     119.29
 H       5.738290    -5.922380     0.716338      31.01
 H       3.866847    -5.534398     0.860018      23.35
 H       4.780601    -6.982035     1.801978      26.64
 C       6.394648    -2.962305     3.039772      10.15
 O       6.984861    -3.431697     4.174073     234.72
 H       6.494918    -4.207951     4.654874      22.69
 C       6.632942    -1.558208     2.638917       4.55
 H       7.069579    -0.865115     3.339264      21.06
 C       5.511520    -1.798795     0.547236     -28.07
 C       5.332346    -1.359961    -0.980362      90.58
 H       5.907599    -2.015996    -1.591771      28.09
 O       5.888091    -0.120533    -1.326934     248.16
 H       5.804165     0.542034    -0.537645      27.28
 C       3.788435    -1.551331    -1.389861      73.23
 H       3.452137    -2.666219    -1.216916      25.19
 C       3.421079    -1.384136    -2.952263      96.50
 O       3.781072    -2.642491    -3.581692     243.47
 H       4.735287    -2.700753    -3.894937      25.97
 H       4.120175    -0.541304    -3.373092      27.11
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 H       2.318038    -1.056641    -3.342615      25.30
 C      -0.364542    -1.298414     0.217763      41.88
 H      -0.934532    -2.172475     0.463438      21.66
 C      -0.138677     1.193461    -0.041443      59.78
 H      -0.569535     2.067450    -0.307561      20.05
 C       1.263774     0.986586    -0.362898      -0.99
 O       2.174787     1.956601    -0.629251     191.11
 C       1.697167     3.318419    -0.780675     107.22
 H       2.730487     3.961604    -0.711208      23.57
 H       1.406557     3.546300    -1.765766      26.16
 H       1.174908     3.958562     0.194883      23.76
 C       1.825367    -0.393172    -0.386103      18.06
 O       3.204393    -0.546917    -0.501410     160.51
 C       0.993605    -1.438051     0.026186      41.76
 H       1.425698    -2.511302     0.177115      22.74
 C      -0.990813     0.011095     0.123111      35.62
 C      -2.391894     0.345768     0.480123      97.56
 H      -2.994510    -0.489642     0.596271      25.69
 O      -2.305999     1.084898     1.714706     212.86
 H      -1.988590     0.296157     2.287070      26.45
 C      -3.195227     1.076154    -0.579795      72.58
 H      -2.415659     1.661349    -1.279770      22.13
 O      -3.878284     0.015474    -1.477966     186.00
 H      -3.793841     0.369087    -2.534078      23.07
 C      -4.257696     2.114573    -0.097505     104.22
 O      -4.962297     2.698572    -1.188456     318.35
 H      -4.528185     3.604572    -1.012062      27.81
 H      -3.612310     2.842545     0.452830      26.36
 H      -4.889431     1.733906     0.768458      27.72
55
name = lig-etoh-Waterframe_529
 C       6.239281    -1.038621     1.436877      37.15
 H       6.551235     0.084179     1.320743      19.10
 C       5.190380    -3.120563     0.890227      65.91
 H       4.845974    -3.867603     0.125594      24.95
 C       5.583874    -3.728315     2.128870     -29.24
 O       5.312888    -5.100793     2.500119     173.69
 C       4.866203    -5.945143     1.357579     123.15
 H       5.604076    -6.264279     0.544336      27.01
 H       3.905714    -5.656835     0.833968      24.39
 H       4.610991    -6.817434     1.848109      26.67
 C       6.408214    -2.886974     3.024098     -14.00
 O       7.006081    -3.451249     4.199887     172.40
 H       6.356710    -4.124993     4.655357      18.64
 C       6.677847    -1.559141     2.666086      56.52
 H       7.087316    -0.831899     3.447003      26.31
 C       5.544552    -1.806862     0.482732     -21.91
 C       5.363165    -1.390015    -1.010931      85.01
 H       5.943239    -2.128667    -1.379816      28.10
 O       5.898158    -0.081945    -1.331818     250.56
 H       5.931126     0.528188    -0.501404      26.48
 C       3.765411    -1.522487    -1.389444      89.54
 H       3.423387    -2.409703    -0.880972      27.28
 C       3.462873    -1.374746    -2.923087      97.84
 O       3.755701    -2.633035    -3.579377     254.73
 H       4.702159    -2.548008    -3.897227      25.72
 H       4.141056    -0.606073    -3.477826      26.76
 H       2.293886    -1.133062    -3.056914      25.98
 C      -0.397630    -1.258467     0.213745      54.44
 H      -1.027633    -2.248272     0.166487      17.41
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 C      -0.072471     1.149167    -0.082241      65.48
 H      -0.419078     2.187020    -0.380245      19.95
 C       1.234744     0.909723    -0.316168      10.87
 O       2.123472     2.018594    -0.577616     186.17
 C       1.750540     3.413584    -0.781320      87.00
 H       2.905433     4.117592    -0.628801      20.76
 H       1.101669     3.584618    -1.697890      25.34
 H       1.052169     3.736213    -0.047099      27.31
 C       1.810547    -0.382815    -0.312123      20.01
 O       3.270952    -0.510145    -0.563188     157.91
 C       1.017686    -1.433951     0.048963      57.00
 H       1.452312    -2.502613     0.077913      24.68
 C      -0.955849     0.054960     0.085107      36.09
 C      -2.429415     0.318792     0.501671      79.39
 H      -2.861618    -0.640797     0.516683      27.90
 O      -2.324740     1.070491     1.677471     228.26
 H      -2.155325     0.548471     2.611507      26.07
 C      -3.163521     1.200658    -0.652603      80.65
 H      -2.466841     1.857914    -1.317298      23.45
 O      -3.897152    -0.003832    -1.365520     179.12
 H      -3.788391     0.193663    -2.431710      24.13
 C      -4.198726     2.055441    -0.121899      99.43
 O      -4.947742     2.690967    -1.207014     251.07
 H      -4.697627     3.689203    -1.260102      30.55
 H      -3.520824     3.009601     0.395687      23.62
 H      -4.930558     1.675490     0.619363      28.23
55
name = lig-etoh-Waterframe_530
 C       6.245420    -1.021197     1.486326      45.51
 H       6.492210    -0.038352     1.030727      25.12
 C       5.242017    -3.150433     0.844303      59.86
 H       4.715801    -3.798777     0.072255      25.04
 C       5.578733    -3.694349     2.151727      18.85
 O       5.324446    -5.030815     2.484939     161.90
 C       4.772672    -5.925049     1.387019     105.02
 H       5.682067    -6.174644     0.612295      23.26
 H       4.050243    -5.453578     0.930293      26.81
 H       4.507416    -6.788968     1.971999      24.71
 C       6.391132    -2.926921     3.043508      15.36
 O       6.984772    -3.424498     4.188939     119.87
 H       6.504513    -4.233103     4.653805      23.61
 C       6.674948    -1.577810     2.725686      33.58
 H       7.409954    -1.024153     3.473038      19.34
 C       5.584552    -1.827902     0.446006     -70.15
 C       5.352814    -1.430523    -0.997052      77.36
 H       5.870602    -2.152794    -1.834603      22.53
 O       5.910519    -0.082486    -1.348578     253.51
 H       5.531592     0.573045    -0.599207      24.26
 C       3.837035    -1.499497    -1.364432      84.34
 H       3.453222    -2.451594    -1.165297      28.60
 C       3.514569    -1.370766    -2.848606     113.46
 O       3.730341    -2.634752    -3.590024     248.45
 H       4.543236    -2.614131    -4.189250      25.30
 H       3.978440    -0.434867    -3.190298      27.79
 H       2.454534    -1.238705    -2.862422      28.09
 C      -0.407388    -1.206527     0.162475      52.53
 H      -1.249060    -2.073439     0.395903      25.80
 C      -0.078125     1.095621    -0.178155      59.24
 H      -0.481081     2.241852     0.025945      19.11
 C       1.323514     0.950985    -0.308033      14.15
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 O       2.109821     2.039841    -0.530580     194.68
 C       1.727027     3.473373    -0.741357      89.47
 H       2.865557     3.954085    -0.968951      22.98
 H       1.257161     3.507864    -1.809136      25.30
 H       1.138311     3.683976     0.003061      29.46
 C       1.919471    -0.349760    -0.255549      13.15
 O       3.227805    -0.377874    -0.590619     152.94
 C       0.982642    -1.495359     0.051806      52.83
 H       1.444646    -2.488058     0.032718      22.61
 C      -0.921958     0.044765     0.099474      34.10
 C      -2.387906     0.311038     0.427949      64.23
 H      -3.036804    -0.639472     0.706300      22.53
 O      -2.398239     1.107908     1.707119     182.93
 H      -1.908535     0.490645     2.543004      22.84
 C      -3.159356     1.109040    -0.695085      98.34
 H      -2.582023     1.558531    -1.464166      25.62
 O      -3.866636     0.048014    -1.278141     245.36
 H      -3.923729     0.121108    -2.309712      26.50
 C      -4.173139     2.129744    -0.116730      93.07
 O      -4.940714     2.694455    -1.240178     256.19
 H      -4.825805     3.719310    -1.267853      28.68
 H      -3.714680     2.958992     0.694001      23.52
 H      -4.822887     1.438071     0.383240      28.18
55
name = lig-etoh-Waterframe_531
 C       6.252480    -1.033412     1.443326      35.91
 H       6.585208    -0.028786     1.325690      24.68
 C       5.306508    -3.191876     0.842907     102.13
 H       4.679111    -3.788052     0.143024      24.34
 C       5.586769    -3.656412     2.092635      34.78
 O       5.330982    -4.975139     2.453876     186.07
 C       4.734419    -5.872412     1.481201     111.11
 H       5.638558    -6.062528     0.725893      24.85
 H       3.957866    -5.379543     0.957589      26.69
 H       4.342665    -6.839979     1.957826      25.65
 C       6.352480    -2.970606     3.069737       7.36
 O       6.954405    -3.402118     4.193024     129.55
 H       6.665711    -4.313930     4.524359      23.23
 C       6.649384    -1.591768     2.731016     -24.87
 H       7.478587    -1.098651     3.358396      17.23
 C       5.672384    -1.880122     0.519180      22.52
 C       5.351308    -1.398393    -1.013741      70.86
 H       5.877718    -2.119788    -1.929222      22.75
 O       5.884224    -0.118175    -1.334488     280.21
 H       5.178763     0.597730    -1.052263      24.50
 C       3.910995    -1.494313    -1.302470      84.77
 H       3.474179    -2.454117    -1.004083      27.98
 C       3.519255    -1.334841    -2.788577     112.05
 O       3.717117    -2.613821    -3.595638     243.19
 H       4.492047    -2.566179    -4.225285      26.47
 H       3.989580    -0.541899    -3.290937      29.70
 H       2.532253    -1.208872    -2.852871      29.95
 C      -0.381930    -1.275788     0.133597      44.50
 H      -1.030511    -2.088548     0.671905      27.69
 C      -0.053905     1.127648    -0.223344      54.51
 H      -0.602498     2.166326     0.079437      19.17
 C       1.320471     1.014192    -0.307259       8.20
 O       2.195199     2.066765    -0.490259     177.08
 C       1.703246     3.415610    -0.757547     117.08
 H       2.537308     3.980366    -0.752395      27.02
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 H       1.085444     3.564102    -1.729006      26.03
 H       1.325215     4.177367     0.160831      24.60
 C       1.876799    -0.379484    -0.209604      17.18
 O       3.226545    -0.282452    -0.627392     118.99
 C       1.027981    -1.456605    -0.004868      69.30
 H       1.259467    -2.464384     0.085479      24.79
 C      -0.941314     0.048220     0.105964      18.23
 C      -2.332340     0.377762     0.434761      69.74
 H      -2.986084    -0.655606     0.581050      21.98
 O      -2.466690     1.144402     1.738201     174.59
 H      -1.709923     0.474384     2.213202      22.88
 C      -3.114314     1.040323    -0.675307      93.88
 H      -2.444390     1.415977    -1.366386      26.30
 O      -3.900012     0.035394    -1.271526     254.70
 H      -4.039228     0.408048    -2.186404      26.74
 C      -4.192229     2.154624    -0.121177      98.99
 O      -4.923168     2.723163    -1.257016     290.62
 H      -4.676636     3.704643    -1.044987      26.29
 H      -3.907002     2.842798     0.631655      26.55
 H      -4.897845     1.541128     0.412555      27.91
55
name = lig-etoh-Waterframe_532
 C       6.325437    -1.059121     1.482644      84.79
 H       6.513268    -0.041282     1.281102      23.15
 C       5.348717    -3.192033     0.815930      88.93
 H       4.867960    -3.863534     0.107761      25.03
 C       5.622162    -3.716602     2.095087       5.54
 O       5.314273    -4.969872     2.480590     230.17
 C       4.740501    -5.796906     1.530374     123.86
 H       5.309819    -6.219983     0.742601      27.54
 H       3.716375    -5.467011     0.951097      23.20
 H       4.477874    -6.760687     2.188732      23.85
 C       6.331711    -2.882712     3.037501      13.26
 O       6.930019    -3.412850     4.228613     115.08
 H       6.517540    -4.275921     4.509716      20.18
 C       6.617665    -1.632522     2.683359      82.45
 H       7.127016    -0.992698     3.378122      27.24
 C       5.729314    -1.869616     0.458569     -75.07
 C       5.416486    -1.378706    -0.969321      92.49
 H       5.948025    -2.213885    -1.448135      24.03
 O       5.854526    -0.131362    -1.334801     311.50
 H       5.153314     0.606783    -1.161604      22.75
 C       3.862517    -1.467528    -1.257778      79.55
 H       3.494197    -2.294210    -0.575024      24.05
 C       3.503132    -1.336818    -2.797246     104.54
 O       3.700948    -2.571211    -3.571915     262.59
 H       4.619849    -2.443573    -3.918078      26.70
 H       4.146487    -0.627255    -3.274606      27.34
 H       2.436069    -1.046641    -2.839654      26.53
 C      -0.368967    -1.279755     0.175672      65.21
 H      -0.761262    -2.177825     0.508886      22.79
 C      -0.084362     1.193157    -0.178225      66.00
 H      -0.418147     2.227528    -0.373970      20.74
 C       1.279815     0.992957    -0.292004      -4.13
 O       2.274925     2.099776    -0.447917     159.19
 C       1.722566     3.416723    -0.752582      92.74
 H       2.540198     3.950517    -1.004504      24.76
 H       0.909207     3.345253    -1.497947      26.18
 H       0.980224     3.813914     0.338932      22.82
 C       1.840876    -0.274705    -0.264765       2.85
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 O       3.249320    -0.275445    -0.655577     128.03
 C       1.048389    -1.450351    -0.062532      47.41
 H       1.538848    -2.376918     0.045306      28.32
 C      -0.865335     0.019479     0.077516      17.79
 C      -2.365926     0.403154     0.528879      87.99
 H      -2.718758    -0.646908     0.620223      25.91
 O      -2.476485     1.135703     1.722496     252.63
 H      -1.972083     0.916718     2.646523      26.12
 C      -3.109818     1.113579    -0.605081      81.62
 H      -2.418766     1.644090    -1.302022      24.76
 O      -3.966369    -0.003159    -1.335068     219.09
 H      -4.247580     0.384118    -2.160919      28.07
 C      -4.215128     2.071415    -0.140198     107.29
 O      -4.863191     2.791453    -1.237526     284.68
 H      -4.726014     3.803707    -1.335951      28.09
 H      -3.764837     2.811880     0.357555      27.89
 H      -5.006060     1.603149     0.483726      27.55
55
name = lig-etoh-Waterframe_533
 C       6.356711    -1.056837     1.398624      64.27
 H       6.495939    -0.024883     1.161919      24.48
 C       5.400750    -3.194116     0.783051      62.67
 H       5.113034    -3.839505    -0.000969      24.36
 C       5.692432    -3.706541     2.094639       8.77
 O       5.311090    -4.975563     2.542407     189.91
 C       4.681936    -5.872816     1.544307     111.41
 H       5.331431    -6.073250     0.785682      26.17
 H       3.642472    -5.252829     1.268728      23.04
 H       4.471156    -6.735060     2.254325      24.06
 C       6.328767    -2.947551     3.060361     -14.53
 O       6.871776    -3.394182     4.232391     282.40
 H       6.393262    -4.172912     4.601047      19.20
 C       6.644622    -1.547239     2.720936      11.21
 H       6.860607    -0.962632     3.530774      29.02
 C       5.763131    -1.827832     0.452802      27.88
 C       5.408825    -1.419014    -0.902496      94.67
 H       5.799023    -1.991300    -1.634646      27.33
 O       5.878661    -0.098849    -1.372721     292.96
 H       5.287648     0.537840    -0.790163      25.91
 C       3.798014    -1.442330    -1.208023      72.16
 H       3.351731    -2.475363    -0.870608      25.79
 C       3.491617    -1.370747    -2.771128     101.35
 O       3.692369    -2.523681    -3.533627     271.12
 H       4.617611    -2.705832    -3.826277      27.18
 H       4.168985    -0.494132    -2.994588      26.52
 H       2.377007    -0.920413    -2.991935      26.14
 C      -0.264173    -1.267608     0.218603      58.09
 H      -0.969554    -1.977705     0.376298      20.45
 C      -0.087061     1.222390    -0.144567      64.07
 H      -0.565611     2.032787    -0.486809      23.20
 C       1.336581     1.088181    -0.290312       7.30
 O       2.274379     2.076323    -0.415615     184.46
 C       1.678116     3.369274    -0.699589     106.39
 H       2.437080     4.152416    -1.289136      24.79
 H       1.027739     3.206073    -1.499745      27.49
 H       1.280428     3.742655     0.272674      26.78
 C       1.898966    -0.240745    -0.393907      19.23
 O       3.234807    -0.265814    -0.648751     162.32
 C       1.089824    -1.396678    -0.109309      66.07
 H       1.674182    -2.309266    -0.102756      27.20
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 C      -0.895025     0.082118     0.106945      16.46
 C      -2.338070     0.291572     0.601200      88.46
 H      -2.936247    -0.510810     0.798260      26.48
 O      -2.490786     1.193595     1.734353     202.14
 H      -2.109110     0.560364     2.526132      26.42
 C      -3.244049     1.114300    -0.588577      67.02
 H      -2.575344     1.688037    -1.382628      23.39
 O      -3.970216     0.006004    -1.375891     238.81
 H      -4.204242     0.311886    -2.217841      29.01
 C      -4.219906     2.103672    -0.141042      91.99
 O      -4.821660     2.820609    -1.267182     282.80
 H      -4.492782     3.794626    -1.082694      26.00
 H      -3.506125     2.829301     0.548522      24.27
 H      -5.002562     1.560186     0.516402      26.74
55
name = lig-etoh-Waterframe_534
 C       6.399482    -0.983772     1.401559      44.78
 H       6.614837     0.073536     1.206206      21.08
 C       5.497381    -3.205749     0.785758     128.36
 H       5.140003    -3.827166     0.013514      23.91
 C       5.716181    -3.735683     2.044888       8.54
 O       5.330378    -4.984104     2.582272     228.40
 C       4.621880    -5.917585     1.637457     115.96
 H       5.269984    -6.000659     0.752203      27.90
 H       3.672510    -5.436974     1.162958      25.97
 H       4.423402    -6.901114     1.948492      26.41
 C       6.396842    -2.870606     3.054280       9.09
 O       6.793831    -3.362905     4.265200     170.67
 H       6.418467    -4.278674     4.532862      24.58
 C       6.623854    -1.521221     2.760137      43.87
 H       6.942927    -0.870058     3.535057      22.30
 C       5.768938    -1.899742     0.468830      -3.60
 C       5.316356    -1.394253    -0.992837      96.72
 H       5.692272    -2.048225    -1.841154      24.32
 O       5.874810    -0.068028    -1.359723     261.53
 H       5.857057     0.611222    -0.583423      26.61
 C       3.776056    -1.489091    -1.228277      82.43
 H       3.273553    -2.438132    -0.860248      23.45
 C       3.525821    -1.287438    -2.693832      90.13
 O       3.682189    -2.536575    -3.505637     241.23
 H       4.600173    -2.550922    -3.900082      25.86
 H       4.168635    -0.471356    -3.198983      25.19
 H       2.342230    -1.160420    -2.913903      24.95
 C      -0.233989    -1.137100     0.228818      49.29
 H      -0.909374    -2.020424     0.456981      24.59
 C      -0.063006     1.227646    -0.143381      74.34
 H      -0.611557     2.096893    -0.180782      21.50
 C       1.345938     1.090785    -0.299980      21.73
 O       2.275957     2.092788    -0.408705     188.08
 C       1.634732     3.332826    -0.699646     113.03
 H       2.635033     4.196660    -0.931423      22.37
 H       0.802743     3.276422    -1.366221      27.20
 H       1.344214     3.875297     0.074741      28.63
 C       1.879388    -0.204023    -0.469925      16.91
 O       3.240896    -0.261996    -0.622703     144.18
 C       1.166199    -1.323126    -0.154817      66.13
 H       1.413513    -2.410030    -0.235503      21.16
 C      -0.889738     0.071694     0.209635      23.48
 C      -2.411173     0.279525     0.542621      72.45
 H      -2.900092    -0.665750     0.809401      23.83
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 O      -2.470450     1.214608     1.777212     206.82
 H      -2.109215     0.589567     2.507491      24.95
 C      -3.323237     0.972371    -0.641191      76.74
 H      -2.530595     1.470181    -1.339458      21.96
 O      -3.950782     0.034819    -1.381661     306.44
 H      -3.863951     0.302649    -2.236162      29.97
 C      -4.231900     2.171183    -0.088631      87.83
 O      -4.757789     2.854607    -1.274371     266.68
 H      -4.605459     3.880143    -1.125087      25.72
 H      -3.745776     2.934469     0.821913      22.23
 H      -5.138027     1.759582     0.479919      25.77
55
name = lig-etoh-Waterframe_535
 C       6.391128    -1.000417     1.465900      58.67
 H       6.628054     0.068685     1.250148      23.35
 C       5.563264    -3.289122     0.771295      62.79
 H       4.984839    -3.891942     0.070468      21.00
 C       5.774230    -3.750547     2.109941       8.47
 O       5.331979    -5.015836     2.579065     223.61
 C       4.618679    -5.902708     1.670355     111.01
 H       5.280735    -6.128627     0.685493      25.84
 H       3.705235    -5.581938     1.370391      31.71
 H       4.582603    -6.786043     2.221509      26.88
 C       6.412960    -2.842086     2.998769      -0.60
 O       6.719235    -3.316374     4.324042     124.83
 H       6.352457    -4.269285     4.342618      24.64
 C       6.604373    -1.465771     2.720154      59.71
 H       7.222378    -0.864006     3.454748      20.60
 C       5.808958    -1.827652     0.418921     -52.59
 C       5.292660    -1.354768    -1.046655      99.19
 H       5.876246    -2.230612    -1.642198      22.70
 O       5.852379    -0.071680    -1.341169     292.84
 H       5.995564     0.445429    -0.472354      27.87
 C       3.807398    -1.452304    -1.249197      93.58
 H       3.449006    -2.312999    -0.749382      24.73
 C       3.491972    -1.267691    -2.729815     102.99
 O       3.689567    -2.550636    -3.464490     263.36
 H       4.531183    -2.458898    -3.980708      26.29
 H       4.071334    -0.393836    -3.158259      25.84
 H       2.451385    -0.927612    -2.658719      26.30
 C      -0.220409    -1.102301     0.217862      59.36
 H      -0.508853    -2.152728     0.668377      24.05
 C      -0.078796     1.228858    -0.105771      85.94
 H      -0.288066     2.292838     0.264106      18.49
 C       1.273861     1.051029    -0.324803       4.82
 O       2.246903     2.134523    -0.417879     152.81
 C       1.647103     3.406966    -0.684239      85.68
 H       2.595429     3.916375    -1.201042      22.70
 H       0.866137     3.382762    -1.502727      24.73
 H       1.065706     3.893769     0.441728      22.02
 C       1.901623    -0.198649    -0.475640      18.24
 O       3.271964    -0.264968    -0.601247     153.33
 C       1.063486    -1.290325    -0.176784      55.23
 H       1.500187    -2.346600    -0.330358      21.01
 C      -0.883415     0.149963     0.272421      32.30
 C      -2.482640     0.334089     0.525782      77.10
 H      -2.718224    -0.781630     0.725549      22.23
 O      -2.450286     1.174874     1.787246     276.58
 H      -1.975442     0.828025     2.530234      27.35
 C      -3.246609     0.959487    -0.572288      80.13
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 H      -2.536052     1.477076    -1.184269      23.42
 O      -3.984335     0.001342    -1.437819     297.54
 H      -3.720050     0.099960    -2.296520      31.26
 C      -4.295163     2.179755    -0.043398      92.37
 O      -4.679480     2.910869    -1.274553     262.60
 H      -4.697386     3.928755    -1.198287      28.01
 H      -3.675365     2.935304     0.555521      22.78
 H      -5.180521     1.768350     0.373370      26.15
55
name = lig-etoh-Waterframe_536
 C       6.320163    -1.010737     1.385706      45.40
 H       6.547369     0.076765     1.246536      23.47
 C       5.606777    -3.247925     0.766412      81.84
 H       5.027819    -3.943580     0.093663      21.50
 C       5.806433    -3.743137     2.094304      12.05
 O       5.360755    -4.993285     2.565596     225.54
 C       4.687912    -5.925604     1.706030     113.98
 H       5.313098    -6.224000     0.712560      26.12
 H       3.778233    -5.606586     1.460188      31.09
 H       4.584864    -6.714573     2.447498      27.21
 C       6.405080    -2.870807     3.067361       1.96
 O       6.636928    -3.237904     4.327634      91.19
 H       6.322537    -4.177430     4.642161      23.33
 C       6.654467    -1.494682     2.718948      24.46
 H       7.287850    -0.856182     3.490039      19.21
 C       5.813113    -1.849340     0.413427       8.84
 C       5.432862    -1.373133    -0.952365      90.72
 H       5.782474    -2.032490    -1.888697      24.23
 O       5.843922    -0.086789    -1.354523     321.32
 H       5.640621     0.470978    -0.510011      26.66
 C       3.867442    -1.370592    -1.251904      85.94
 H       3.527840    -2.311007    -0.938360      27.43
 C       3.419083    -1.286506    -2.775972     113.19
 O       3.668571    -2.521702    -3.419911     276.00
 H       4.535368    -2.606662    -3.898580      27.75
 H       4.086827    -0.514979    -3.118640      26.79
 H       2.469702    -1.016330    -2.975171      28.64
 C      -0.290236    -1.154436     0.248913      32.22
 H      -1.013100    -1.952430     0.720662      18.83
 C      -0.074432     1.291154     0.006001      46.29
 H      -0.420955     2.426520     0.347855      17.59
 C       1.312288     1.078156    -0.374367      11.64
 O       2.148885     2.133577    -0.430174     193.47
 C       1.675274     3.503654    -0.701167      98.93
 H       2.319664     4.164536    -0.946396      27.24
 H       0.908129     3.405163    -1.544384      25.01
 H       1.232236     4.057539     0.449355      22.10
 C       1.903218    -0.216729    -0.441359      26.65
 O       3.290736    -0.253857    -0.578535     166.58
 C       1.053643    -1.277650    -0.241381      63.32
 H       1.509490    -2.332944    -0.165760      24.87
 C      -0.948768     0.201123     0.261693      30.42
 C      -2.356971     0.316438     0.659851      78.56
 H      -3.066330    -0.641253     0.776873      20.14
 O      -2.475353     1.139732     1.775966     299.31
 H      -1.898469     0.679252     2.281760      32.04
 C      -3.245413     1.085790    -0.530153      53.17
 H      -2.626106     1.619890    -1.153133      24.43
 O      -4.004735    -0.038292    -1.454636     221.90
 H      -3.747951     0.124933    -2.403458      26.29
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 C      -4.286256     2.154847    -0.105933     113.55
 O      -4.619970     2.948058    -1.294906     325.00
 H      -4.417021     3.810258    -0.852491      27.12
 H      -3.799201     2.658710     0.600670      28.81
 H      -5.084507     1.757317     0.452556      28.20
55
name = lig-etoh-Waterframe_537
 C       6.306058    -1.011470     1.398822      26.04
 H       6.402200     0.041448     1.055713      19.21
 C       5.604820    -3.217531     0.789413     102.16
 H       5.293517    -3.897940    -0.073885      22.73
 C       5.814492    -3.704796     2.037028      20.04
 O       5.432488    -4.922197     2.555707     222.71
 C       4.770035    -5.966664     1.763357     114.53
 H       5.406727    -6.312830     0.917318      25.28
 H       3.903816    -5.575046     1.295371      28.50
 H       4.528891    -6.979228     2.275308      25.14
 C       6.364621    -2.849507     3.077256      10.95
 O       6.573533    -3.172690     4.412977     139.44
 H       6.337545    -4.171910     4.599530      18.71
 C       6.706804    -1.580854     2.660585      36.63
 H       7.030042    -0.805126     3.463265      25.67
 C       5.812640    -1.930436     0.424952      40.02
 C       5.476002    -1.393119    -0.987020      89.50
 H       5.949056    -2.072696    -1.699817      26.23
 O       5.882632    -0.046652    -1.325449     300.86
 H       5.312942     0.703758    -1.031822      25.27
 C       3.875520    -1.373300    -1.266756      74.15
 H       3.385821    -2.309888    -0.898042      26.78
 C       3.449876    -1.253500    -2.785562     103.76
 O       3.632908    -2.553328    -3.408440     265.00
 H       4.588547    -2.527210    -3.703313      25.69
 H       4.011536    -0.571169    -3.359987      27.88
 H       2.379742    -1.113160    -2.972228      26.84
 C      -0.425398    -1.095883     0.244682      48.38
 H      -1.090719    -1.982946     0.354741      20.99
 C      -0.038312     1.316197     0.121900      59.98
 H      -0.633062     2.364419     0.013684      20.40
 C       1.250965     1.137392    -0.360945      12.96
 O       2.134699     2.209976    -0.464669     187.81
 C       1.659761     3.569088    -0.690143     126.38
 H       2.548813     4.196506    -0.800181      25.89
 H       0.782445     3.667732    -1.378852      26.02
 H       1.215423     3.947699     0.115240      29.52
 C       1.870411    -0.181233    -0.415104       5.46
 O       3.283461    -0.231872    -0.539383     121.88
 C       1.011128    -1.357813    -0.219653      42.78
 H       1.466109    -2.359569    -0.103912      25.22
 C      -0.890985     0.120672     0.226222      33.62
 C      -2.381181     0.346920     0.655807      71.06
 H      -2.794860    -0.705986     0.869969      24.31
 O      -2.487897     1.126255     1.849169     278.74
 H      -2.018754     0.789645     2.609821      30.56
 C      -3.272308     1.106765    -0.575056      73.46
 H      -2.581213     1.578458    -1.272318      24.07
 O      -3.967670    -0.015968    -1.387747     211.37
 H      -3.859623     0.358784    -2.369508      24.97
 C      -4.247294     2.088878    -0.148356     110.69
 O      -4.563933     2.983644    -1.269613     309.07
 H      -4.405005     3.953781    -1.148494      28.83
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 H      -3.859110     2.686768     0.663483      26.64
 H      -5.224921     1.633218     0.226924      26.83
55
name = lig-etoh-Waterframe_538
 C       6.326005    -1.060938     1.406131      57.67
 H       6.443736     0.009534     1.222778      19.27
 C       5.571466    -3.285477     0.714247      34.88
 H       5.383237    -4.072015    -0.071849      19.00
 C       5.818398    -3.691348     2.094989      10.06
 O       5.488875    -4.932406     2.572255     191.24
 C       4.878675    -5.979426     1.743185     101.56
 H       5.610050    -6.294973     1.126570      25.47
 H       3.930583    -5.542358     1.165203      25.53
 H       4.620474    -6.769641     2.616197      23.27
 C       6.329577    -2.824181     3.046200      -3.45
 O       6.506761    -3.136259     4.494147     144.59
 H       6.424523    -4.157307     4.500520      19.11
 C       6.716318    -1.541122     2.612264      40.13
 H       6.988895    -0.889735     3.440435      27.13
 C       5.828649    -1.851287     0.419605      14.93
 C       5.399806    -1.363443    -1.045969      87.49
 H       5.889544    -1.979619    -1.667404      28.17
 O       5.961056    -0.010448    -1.305056     295.88
 H       5.126734     0.477553    -1.226984      26.92
 C       3.856481    -1.397457    -1.299622      66.41
 H       3.396089    -2.344150    -0.792059      26.73
 C       3.488230    -1.254978    -2.780336      99.42
 O       3.619540    -2.604095    -3.409096     249.62
 H       4.538873    -2.676754    -3.861490      25.22
 H       3.992607    -0.451709    -3.299295      27.24
 H       2.351279    -0.898293    -2.552141      25.80
 C      -0.372973    -1.189681     0.124410      55.66
 H      -1.019576    -2.020270     0.173112      23.40
 C      -0.088999     1.274462     0.142430      60.68
 H      -0.536467     2.273133     0.012647      21.76
 C       1.234023     1.192926    -0.283065     -19.90
 O       2.156291     2.291408    -0.527847     162.81
 C       1.609968     3.633047    -0.640581      97.89
 H       2.765318     4.104834    -1.045757      21.52
 H       1.078344     3.788119    -1.596265      25.64
 H       1.216604     3.914873     0.294149      27.02
 C       1.782239    -0.209637    -0.375022      -0.77
 O       3.248562    -0.207797    -0.505170      78.05
 C       0.942290    -1.330208    -0.118942      65.90
 H       1.305386    -2.312997    -0.194893      26.38
 C      -0.917631     0.214431     0.258664      28.63
 C      -2.431618     0.376000     0.592082      78.44
 H      -2.729363    -0.605296     0.704350      27.42
 O      -2.507748     1.156198     1.937808     218.71
 H      -2.128180     0.621672     2.722699      27.14
 C      -3.214593     0.970916    -0.618763      79.70
 H      -2.415763     1.499918    -1.305146      23.37
 O      -3.905112     0.045562    -1.281721     235.42
 H      -3.948131     0.218993    -2.360231      23.75
 C      -4.278061     2.129389    -0.145305      75.43
 O      -4.525510     2.995956    -1.286557     283.20
 H      -4.447692     3.931591    -0.951929      27.19
 H      -3.889601     2.760237     0.845263      22.95
 H      -5.247115     1.449981    -0.068280      26.35
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name = lig-etoh-Waterframe_539
 C       6.374900    -1.010577     1.351191      10.49
 H       6.540602     0.046533     1.242636      23.85
 C       5.601243    -3.283514     0.700322     119.82
 H       5.244769    -4.039948     0.016640      25.50
 C       5.775871    -3.710584     2.063781      -4.89
 O       5.530925    -4.968574     2.616129     196.22
 C       5.013896    -5.958646     1.750511     114.63
 H       5.700525    -6.486075     1.140863      26.03
 H       4.003820    -5.662870     1.103459      24.99
 H       4.573718    -6.698471     2.526670      24.75
 C       6.347381    -2.780427     3.121990       7.43
 O       6.430078    -3.113593     4.458581      59.73
 H       6.461934    -4.078801     4.745227      23.41
 C       6.693921    -1.501324     2.714264      59.66
 H       7.199532    -0.843357     3.331495      22.57
 C       5.761212    -1.900028     0.323421     -61.66
 C       5.368067    -1.305702    -1.028763      78.30
 H       5.647358    -1.987079    -1.894648      24.05
 O       5.983703    -0.030144    -1.303591     291.71
 H       5.382600     0.730215    -1.119596      25.83
 C       3.859683    -1.371957    -1.263516      70.54
 H       3.522046    -2.439080    -0.943825      25.24
 C       3.481049    -1.302749    -2.720603      90.59
 O       3.592563    -2.603872    -3.413922     245.79
 H       4.415138    -2.574973    -4.020667      25.09
 H       4.182081    -0.539323    -3.153552      25.48
 H       2.320819    -1.027092    -3.035587      24.38
 C      -0.446674    -1.140343     0.035668      50.09
 H      -1.007200    -1.986743     0.250429      25.73
 C      -0.128803     1.347667     0.089779      46.24
 H      -0.506234     2.236227     0.335769      21.27
 C       1.321184     1.163806    -0.205643      12.98
 O       2.131159     2.268413    -0.581527     156.37
 C       1.655833     3.662735    -0.665358      82.94
 H       2.564612     4.613361    -0.695107      22.30
 H       0.874959     3.749249    -1.461124      25.08
 H       1.208287     4.209002     0.480307      22.68
 C       1.775493    -0.124405    -0.315280      21.04
 O       3.176859    -0.235228    -0.503712     118.12
 C       1.001654    -1.296739    -0.066039      55.43
 H       1.362762    -2.244525    -0.268835      24.69
 C      -0.993391     0.140637     0.315737       8.72
 C      -2.417974     0.381808     0.609504      86.88
 H      -2.998202    -0.485123     0.746498      24.00
 O      -2.555378     1.168101     1.957743     218.06
 H      -2.069945     0.369741     2.383809      24.49
 C      -3.130315     1.051248    -0.543357      65.01
 H      -2.374974     1.517508    -1.326145      22.15
 O      -3.906958    -0.017407    -1.234425     206.12
 H      -3.671646     0.147059    -2.338057      22.72
 C      -4.268423     2.114801    -0.190336      89.35
 O      -4.496439     3.009658    -1.305339     297.81
 H      -4.427913     3.901350    -0.912363      26.89
 H      -4.130259     2.674585     0.920564      23.57
 H      -5.193056     1.535916     0.143780      26.89
55
name = lig-etoh-Waterframe_540
 C       6.396782    -1.039461     1.317452      47.07
 H       6.604293    -0.069017     0.927630      25.26
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 C       5.617266    -3.270288     0.742183     103.72
 H       5.117038    -3.874771     0.046898      23.60
 C       5.793486    -3.651402     2.096561      12.35
 O       5.576330    -4.959059     2.629637     198.18
 C       5.063917    -6.027766     1.774810     100.84
 H       5.906646    -6.490248     1.073969      24.51
 H       4.373123    -5.480348     1.050673      26.95
 H       4.632930    -6.828327     2.259442      27.24
 C       6.312845    -2.804149     3.107047       1.48
 O       6.370853    -3.093677     4.439401     138.42
 H       6.261566    -4.085844     4.567932      23.84
 C       6.653305    -1.423454     2.717880      36.32
 H       7.259117    -0.826059     3.331651      21.35
 C       5.778627    -1.896662     0.354446     -34.36
 C       5.345674    -1.267719    -1.014518      74.00
 H       5.755460    -2.038220    -1.902390      22.15
 O       5.979494    -0.051138    -1.322352     310.26
 H       5.817372     0.668829    -0.669148      27.01
 C       3.766780    -1.340990    -1.181944      85.69
 H       3.523570    -2.307202    -0.739716      26.07
 C       3.456144    -1.330642    -2.751268      94.48
 O       3.567638    -2.589323    -3.422642     266.57
 H       4.467278    -2.560814    -3.904843      24.54
 H       4.222571    -0.678334    -3.257892      24.46
 H       2.442963    -0.878451    -2.966490      25.34
 C      -0.472024    -1.093162     0.040036      55.57
 H      -1.060384    -1.959355     0.230323      24.94
 C      -0.117499     1.333506     0.075693      86.36
 H      -0.459650     2.210520     0.488541      20.95
 C       1.225081     1.260655    -0.148574      -4.65
 O       2.134580     2.241168    -0.611596     159.86
 C       1.662260     3.709998    -0.628256      87.73
 H       2.587028     4.234468    -0.903073      24.17
 H       0.816814     3.809838    -1.275478      26.58
 H       1.014587     3.843701     0.494679      23.22
 C       1.860364    -0.136764    -0.248834      12.88
 O       3.153524    -0.280884    -0.520778     185.21
 C       0.998864    -1.221067    -0.092300      58.79
 H       1.522572    -2.152208    -0.158121      22.97
 C      -0.962742     0.152400     0.309480      19.05
 C      -2.461803     0.410866     0.710816      69.42
 H      -3.078909    -0.565953     0.856830      19.24
 O      -2.584341     1.119039     1.899936     269.04
 H      -2.058371     0.829213     2.833060      24.04
 C      -3.151818     1.194707    -0.487292      61.90
 H      -2.448630     1.646994    -1.216377      21.55
 O      -3.881267    -0.098610    -1.217082     151.38
 H      -3.613564    -0.043869    -2.307405      21.79
 C      -4.247191     2.083454    -0.172922     112.45
 O      -4.480938     3.013563    -1.314124     293.50
 H      -4.340499     3.940704    -1.114798      29.49
 H      -3.895486     2.790123     0.575107      25.04
 H      -5.120156     1.525066    -0.068988      27.76
55
name = lig-etoh-Waterframe_541
 C       6.423703    -1.065746     1.341240      74.03
 H       6.820693    -0.116597     1.022663      24.45
 C       5.579814    -3.223917     0.781759      72.59
 H       5.141604    -3.927088     0.107374      24.52
 C       5.823584    -3.668319     2.131797      -0.51
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 O       5.614441    -4.950963     2.640159     237.05
 C       5.112253    -6.049500     1.715728     115.15
 H       6.123632    -6.333497     1.135980      25.75
 H       4.414636    -5.694808     1.046858      28.07
 H       4.698412    -6.746634     2.325268      28.76
 C       6.276015    -2.679281     3.050348      -0.65
 O       6.326138    -3.109186     4.434772     110.49
 H       5.993042    -4.032541     4.473441      22.88
 C       6.604669    -1.420621     2.621261      70.52
 H       7.035099    -0.777205     3.413156      23.98
 C       5.831837    -1.879064     0.435575      12.22
 C       5.324119    -1.314759    -0.973511      88.09
 H       5.817566    -2.050640    -1.758052      23.37
 O       5.972426    -0.041755    -1.330500     299.03
 H       5.984476     0.338910    -0.463474      29.03
 C       3.712909    -1.385764    -1.176806      86.42
 H       3.333520    -2.218048    -0.688560      26.74
 C       3.430214    -1.292914    -2.766982     100.59
 O       3.542769    -2.602637    -3.431336     282.32
 H       4.465391    -2.737362    -3.796520      26.48
 H       4.154706    -0.549779    -3.180399      25.18
 H       2.542048    -0.882924    -2.789907      29.04
 C      -0.384776    -1.094233     0.103866      38.87
 H      -1.076130    -1.968990     0.103335      17.98
 C      -0.150456     1.328236     0.162252      43.51
 H      -0.654786     2.385247     0.265221      18.87
 C       1.255158     1.246625    -0.191365       2.16
 O       2.110298     2.253945    -0.611548     216.52
 C       1.626387     3.618025    -0.566567     136.31
 H       2.401326     4.067995    -0.839073      28.40
 H       1.006014     3.864948    -1.393493      26.56
 H       1.558327     3.910790     0.437086      27.68
 C       1.792508    -0.087212    -0.189142      20.24
 O       3.208727    -0.231789    -0.510301     154.14
 C       0.942457    -1.179229    -0.144313      75.50
 H       1.327428    -2.230084    -0.030433      23.89
 C      -0.972074     0.244116     0.283161      33.63
 C      -2.462743     0.410094     0.758395      56.98
 H      -2.840828    -0.728044     0.711191      21.33
 O      -2.634502     1.165360     1.907698     241.57
 H      -1.882766     0.692261     2.681426      22.27
 C      -3.193227     1.116116    -0.489972      70.11
 H      -2.498551     1.634454    -1.055817      25.44
 O      -3.794566    -0.117919    -1.185037     239.66
 H      -3.737766     0.044798    -2.213343      25.02
 C      -4.261830     2.193396    -0.164991     113.38
 O      -4.484947     2.996415    -1.366192     344.80
 H      -4.265321     3.853893    -0.966292      28.60
 H      -3.977392     2.647097     0.684944      29.64
 H      -5.135229     1.647681     0.082031      28.64
55
name = lig-etoh-Waterframe_542
 C       6.491754    -0.968548     1.313005      34.24
 H       6.900225     0.055243     1.192411      18.88
 C       5.520141    -3.224446     0.851939      75.36
 H       5.197700    -3.923013     0.049389      23.38
 C       5.839034    -3.673383     2.096962      21.39
 O       5.622474    -4.951695     2.624050     208.51
 C       5.189590    -5.990114     1.665381     120.26
 H       5.971897    -6.538195     0.999823      24.88
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 H       4.361254    -5.849313     1.077463      29.76
 H       4.903493    -6.766737     2.434192      26.05
 C       6.203753    -2.699069     3.113073      17.53
 O       6.290679    -3.090803     4.385644     190.81
 H       5.905405    -3.967711     4.527960      21.42
 C       6.607591    -1.419663     2.676886      38.21
 H       6.832715    -0.540870     3.406965      25.79
 C       5.811603    -1.887476     0.394418       9.67
 C       5.351731    -1.428088    -0.935957      90.93
 H       5.603115    -2.104208    -1.679670      26.47
 O       5.926190    -0.081694    -1.298120     276.23
 H       5.949640     0.607103    -0.640399      27.15
 C       3.755645    -1.421575    -1.213615      65.64
 H       3.274217    -2.320777    -0.908852      26.42
 C       3.419202    -1.267147    -2.706811     101.87
 O       3.507594    -2.600533    -3.424892     249.76
 H       4.408863    -2.590123    -3.839698      25.92
 H       4.085490    -0.504213    -3.136619      26.73
 H       2.367676    -1.067608    -2.942193      26.79
 C      -0.427896    -0.995636     0.183557      42.60
 H      -0.995181    -2.001584     0.212803      20.32
 C      -0.120503     1.417759     0.229411      48.51
 H      -0.688202     2.470139    -0.078332      18.80
 C       1.244853     1.203671    -0.233785      11.52
 O       2.075902     2.236405    -0.593617     205.65
 C       1.667762     3.552536    -0.527539     116.17
 H       2.625452     4.261564    -0.854468      22.94
 H       0.663895     3.766027    -1.088290      23.96
 H       1.468691     3.999225     0.378558      27.66
 C       1.809430    -0.053619    -0.219224      21.25
 O       3.223150    -0.115956    -0.465273      63.71
 C       0.939334    -1.222208    -0.149782      48.59
 H       1.340146    -2.308080    -0.251561      23.97
 C      -0.990821     0.231693     0.307997      37.56
 C      -2.427707     0.393133     0.646301      82.71
 H      -2.884006    -0.585497     1.010328      24.69
 O      -2.656127     1.223203     1.972459     159.80
 H      -2.082037     0.515575     2.603868      23.27
 C      -3.244601     0.962850    -0.476826      80.99
 H      -2.520140     1.405709    -1.124163      24.90
 O      -3.695570    -0.089982    -1.163328     298.90
 H      -3.779143     0.180194    -2.077159      28.12
 C      -4.303232     2.216769    -0.158702      94.08
 O      -4.485378     2.997633    -1.386552     293.31
 H      -4.405695     4.003760    -1.263911      26.92
 H      -3.987098     2.849501     0.717702      26.40
 H      -5.336573     1.832143     0.237541      26.84
55
name = lig-etoh-Waterframe_543
 C       6.503587    -0.964816     1.317131      57.75
 H       6.661830     0.083318     0.916612      21.90
 C       5.485194    -3.197075     0.817272      49.31
 H       5.102228    -3.958935     0.056560      20.31
 C       5.833418    -3.653627     2.126134      17.80
 O       5.627546    -4.952522     2.545895     251.65
 C       5.233504    -5.995372     1.671105     101.85
 H       5.977956    -6.167032     0.915604      24.91
 H       4.255820    -5.611449     1.173926      26.88
 H       5.032487    -6.980647     2.360469      22.49
 C       6.157558    -2.740606     3.096957      14.43
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 O       6.257582    -3.075906     4.419637     195.30
 H       6.011692    -3.998606     4.567504      23.47
 C       6.593579    -1.376653     2.722111      -0.00
 H       6.912583    -0.654004     3.596385      25.86
 C       5.829463    -1.849535     0.441842      17.14
 C       5.342347    -1.442819    -0.967676     104.70
 H       5.758217    -2.064819    -1.697056      25.70
 O       5.878989    -0.180265    -1.287946     300.82
 H       5.419313     0.502128    -0.795904      27.35
 C       3.813134    -1.351720    -1.197205      67.11
 H       3.368427    -2.287141    -0.691286      22.84
 C       3.389781    -1.275050    -2.675989      89.06
 O       3.509589    -2.560811    -3.402124     246.75
 H       4.375231    -2.597543    -3.884323      26.50
 H       3.979036    -0.547184    -3.223238      26.34
 H       2.185511    -0.918337    -2.783241      24.37
 C      -0.425876    -1.002238     0.222929      44.28
 H      -1.191291    -1.819062     0.522468      22.14
 C      -0.110021     1.431939     0.180853      73.02
 H      -0.517227     2.554389     0.122314      20.57
 C       1.143078     1.253140    -0.210531     -14.37
 O       2.096696     2.183244    -0.570031     178.27
 C       1.676859     3.607221    -0.480038      71.07
 H       2.570032     4.257953    -1.285972      20.32
 H       0.648065     3.632845    -1.065445      23.33
 H       1.349657     3.775483     0.734912      23.19
 C       1.862605    -0.184064    -0.299589       5.93
 O       3.218509    -0.077950    -0.448735     108.73
 C       0.979949    -1.190606    -0.119971      66.64
 H       1.337343    -2.239727    -0.404739      23.46
 C      -0.952962     0.320704     0.387133      38.53
 C      -2.454737     0.424428     0.704557      81.00
 H      -2.902409    -0.545219     0.904458      24.64
 O      -2.635902     1.232311     1.984075     250.47
 H      -2.319502     0.818763     2.823931      28.72
 C      -3.261871     1.041184    -0.446050      67.19
 H      -2.567431     1.649867    -1.149277      22.21
 O      -3.690362    -0.164558    -1.210022     273.55
 H      -3.742328     0.045138    -2.098906      29.01
 C      -4.319505     2.191264    -0.132771      84.82
 O      -4.496336     2.977018    -1.425347     207.96
 H      -4.407091     3.984183    -1.135200      26.29
 H      -3.699371     2.997778     0.468914      23.27
 H      -5.421082     1.824309     0.129951      25.64
55
name = lig-etoh-Waterframe_544
 C       6.441085    -1.006183     1.394137      74.97
 H       6.647971     0.012729     0.963988      26.52
 C       5.512367    -3.162777     0.796635      86.17
 H       4.980665    -3.818800     0.040612      20.44
 C       5.751920    -3.663855     2.063545       8.74
 O       5.660332    -4.949543     2.533807     226.97
 C       5.232307    -5.979102     1.622264     118.42
 H       5.880031    -5.956940     0.842913      30.25
 H       4.100256    -5.735554     1.192585      25.98
 H       5.175760    -7.038370     2.190850      24.26
 C       6.201623    -2.646727     3.084877     -15.53
 O       6.226554    -3.077999     4.500888     115.70
 H       6.141100    -4.039151     4.544897      27.00
 C       6.547295    -1.388271     2.710501      66.38
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 H       7.091302    -0.860794     3.532120      20.90
 C       5.812210    -1.868438     0.481165      16.62
 C       5.345886    -1.416159    -0.987310      93.95
 H       5.809067    -2.249219    -1.694200      23.17
 O       5.857149    -0.193907    -1.308591     294.29
 H       5.145354     0.372257    -1.048220      26.97
 C       3.827247    -1.303453    -1.134074      75.77
 H       3.324795    -2.165676    -0.496226      22.65
 C       3.360742    -1.277326    -2.683671      91.68
 O       3.503542    -2.521862    -3.367063     256.37
 H       4.435525    -2.517118    -3.731400      26.05
 H       3.911283    -0.484740    -3.168776      26.30
 H       2.193991    -0.908920    -2.508542      24.28
 C      -0.396632    -0.945288     0.276181      63.20
 H      -1.001658    -1.860539     0.518809      25.08
 C      -0.172172     1.471753     0.119379      81.05
 H      -0.536173     2.431753     0.473854      21.31
 C       1.267747     1.160002    -0.213738      12.76
 O       2.134084     2.188145    -0.545032     157.21
 C       1.621611     3.565874    -0.472849     103.99
 H       2.488255     4.331749    -0.885803      23.91
 H       0.703745     3.820076    -1.035983      26.15
 H       1.899927     4.039984     0.664858      24.64
 C       1.786328    -0.079520    -0.337742      18.47
 O       3.248217    -0.137389    -0.487682     127.16
 C       0.955351    -1.240047    -0.094260      51.75
 H       1.237409    -2.320079    -0.158080      22.22
 C      -0.939726     0.317435     0.467726      23.68
 C      -2.457849     0.492422     0.868245      80.76
 H      -2.800854    -0.464635     0.750612      25.79
 O      -2.640060     1.271335     1.964829     327.36
 H      -2.183107     0.715673     2.578919      28.08
 C      -3.270319     1.161200    -0.465983      41.37
 H      -2.477544     1.782298    -1.094887      22.61
 O      -3.719431    -0.220325    -1.234016     211.21
 H      -3.581837    -0.119713    -2.157195      27.37
 C      -4.294565     2.173501    -0.203125     105.50
 O      -4.520500     2.937360    -1.452153     252.63
 H      -4.352529     3.929922    -1.110940      24.52
 H      -3.866421     2.707500     0.794856      24.80
 H      -5.171012     1.800198     0.422536      27.64
55
name = lig-etoh-Waterframe_545
 C       6.339647    -0.988374     1.391413      41.79
 H       6.787284     0.003446     1.279818      25.11
 C       5.508175    -3.220276     0.775860      62.59
 H       5.040049    -3.793176    -0.033448      21.06
 C       5.711670    -3.601568     2.115123      16.36
 O       5.678051    -4.952633     2.553208     185.70
 C       5.201687    -5.944752     1.529584     114.02
 H       5.772325    -6.064413     0.599546      28.20
 H       4.053845    -5.929456     1.307361      27.52
 H       5.435454    -6.870325     2.076479      27.34
 C       6.194347    -2.749546     3.144576       1.44
 O       6.212647    -3.054550     4.498228      41.24
 H       6.116833    -4.025801     4.583656      23.47
 C       6.562410    -1.403103     2.764734      31.32
 H       7.099478    -0.693399     3.328777      23.77
 C       5.772475    -1.832100     0.430772       8.06
 C       5.359298    -1.438794    -0.909441      85.72
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 H       5.519533    -2.304973    -1.767581      22.71
 O       5.879993    -0.113157    -1.367400     288.14
 H       5.381649     0.671180    -1.253126      26.60
 C       3.749880    -1.362706    -1.105770      75.30
 H       3.320470    -2.374763    -0.781331      22.85
 C       3.332890    -1.247326    -2.590154     101.22
 O       3.500204    -2.495926    -3.336007     250.99
 H       4.419605    -2.513835    -3.729471      27.21
 H       3.821605    -0.417972    -3.092117      26.46
 H       2.268960    -1.195185    -2.808903      26.00
 C      -0.360525    -0.963713     0.343753      56.34
 H      -0.946095    -1.836740     0.474641      22.77
 C      -0.115669     1.409214     0.113317      93.13
 H      -0.417383     2.317591     0.383850      23.55
 C       1.257498     1.244562    -0.217122      -3.73
 O       2.175601     2.246651    -0.526609     225.48
 C       1.695133     3.573190    -0.439642     138.02
 H       2.342618     3.963273    -0.963413      28.74
 H       0.717648     3.659121    -0.726689      30.90
 H       1.459498     3.924608     0.585317      29.12
 C       1.787806    -0.127030    -0.351550       1.59
 O       3.254953    -0.170556    -0.525963     130.45
 C       0.912001    -1.223590    -0.064474      60.64
 H       1.290797    -2.207303     0.061059      24.10
 C      -0.959663     0.354550     0.497803      45.89
 C      -2.452372     0.541540     0.787904      79.29
 H      -2.947990    -0.393983     1.116534      22.40
 O      -2.642837     1.320384     2.032127     300.95
 H      -2.115497     0.928995     2.654485      28.09
 C      -3.182360     1.095160    -0.494724      61.87
 H      -2.423857     1.414748    -1.255155      23.35
 O      -3.729098    -0.170417    -1.182092     232.02
 H      -3.486594    -0.060279    -2.188947      25.21
 C      -4.302802     2.152665    -0.206128     107.77
 O      -4.558495     2.911634    -1.415945     249.70
 H      -4.392554     3.935085    -1.427070      27.11
 H      -3.911475     2.918112     0.476767      25.40
 H      -5.208194     1.650294    -0.008894      28.33
55
name = lig-etoh-Waterframe_546
 C       6.282355    -0.960262     1.454189      50.44
 H       6.557210     0.017354     1.066610      20.67
 C       5.505759    -3.197200     0.778348      68.55
 H       5.276176    -4.016888     0.152739      21.46
 C       5.704776    -3.621481     2.175967       6.03
 O       5.655210    -4.969463     2.508381     197.02
 C       5.188354    -5.944563     1.503136     129.11
 H       5.704315    -5.750184     0.434421      24.49
 H       4.161160    -5.806350     1.463493      26.54
 H       5.403778    -6.848915     1.891305      27.77
 C       6.177761    -2.748803     3.199124      24.22
 O       6.215265    -3.064728     4.485575     141.68
 H       6.015958    -3.965651     4.847541      20.47
 C       6.566182    -1.457647     2.754610      52.91
 H       6.922894    -0.778257     3.452371      28.24
 C       5.740711    -1.843943     0.433601       6.30
 C       5.244902    -1.339482    -0.943125      93.84
 H       5.817433    -2.014819    -1.661481      23.89
 O       5.946626    -0.087997    -1.443499     289.89
 H       5.467165     0.590062    -0.974659      27.57
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 C       3.700168    -1.458652    -1.138371      81.68
 H       3.286237    -2.332207    -0.681462      26.33
 C       3.279994    -1.254724    -2.560905     112.64
 O       3.533057    -2.494444    -3.317121     251.59
 H       4.413086    -2.482607    -3.797793      27.27
 H       3.834299    -0.379115    -2.975411      25.87
 H       2.303027    -1.026641    -2.553536      28.33
 C      -0.458627    -0.982001     0.427636       9.82
 H      -1.090026    -1.765531     0.646873      16.77
 C      -0.033687     1.399986     0.171612      60.50
 H      -0.409447     2.346017     0.071397      19.12
 C       1.264987     1.251773    -0.251644       2.87
 O       2.206009     2.250305    -0.482948     226.36
 C       1.713518     3.610319    -0.387038     104.65
 H       2.332497     4.295214    -1.138860      23.60
 H       0.799390     3.531415    -0.981086      26.22
 H       1.673690     3.860049     0.580329      29.36
 C       1.837706    -0.137979    -0.329607      23.93
 O       3.172884    -0.194020    -0.515182     158.54
 C       0.983984    -1.164575    -0.026541      72.77
 H       1.362918    -2.126067     0.018189      25.23
 C      -0.941209     0.294767     0.458456      75.75
 C      -2.428344     0.549179     0.735325      63.91
 H      -2.932861    -0.467628     1.063092      22.99
 O      -2.645769     1.423389     2.089356     219.81
 H      -2.079505     0.991088     2.712963      27.96
 C      -3.110025     0.966462    -0.534890      92.98
 H      -2.436617     1.459986    -1.176528      25.08
 O      -3.728665    -0.085258    -1.095491     243.83
 H      -3.768179     0.098773    -2.183144      23.12
 C      -4.275570     2.149040    -0.252021      95.31
 O      -4.622788     2.893801    -1.449024     288.97
 H      -4.233875     3.810267    -1.106737      26.20
 H      -4.093267     2.763874     0.576478      28.07
 H      -5.120797     1.538286    -0.083691      29.16
55
name = lig-etoh-Waterframe_548
 C       6.191675    -0.932890     1.478868      43.97
 H       6.306179     0.127435     1.484212      23.53
 C       5.531460    -3.157158     0.834969      60.59
 H       5.170724    -3.756726    -0.001372      24.11
 C       5.764036    -3.711891     2.161067      11.98
 O       5.637733    -5.063058     2.501954     201.08
 C       5.092719    -5.890983     1.417225     124.60
 H       5.600120    -5.716909     0.423189      26.26
 H       3.961943    -5.876859     1.311685      26.53
 H       5.474500    -6.928080     1.730698      26.11
 C       6.112013    -2.786752     3.186111       8.54
 O       6.261073    -3.048746     4.551885     120.70
 H       6.191495    -4.080412     4.837554      15.08
 C       6.469216    -1.462356     2.796750      23.43
 H       6.930339    -0.675655     3.501841      24.84
 C       5.631561    -1.771172     0.485463       2.60
 C       5.331232    -1.338336    -0.992757      88.04
 H       5.527100    -2.090996    -1.707564      26.97
 O       5.880009    -0.085561    -1.455057     282.01
 H       6.088975     0.570253    -0.799400      28.71
 C       3.707803    -1.327989    -1.124612      87.62
 H       3.511471    -2.361795    -0.777771      25.52
 C       3.214982    -1.321544    -2.603898      96.30
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 O       3.524626    -2.516579    -3.345023     243.11
 H       4.465434    -2.582706    -3.727141      27.18
 H       3.654970    -0.445725    -3.160905      26.05
 H       2.059870    -1.291919    -2.935097      24.83
 C      -0.355181    -1.032610     0.468427      54.26
 H      -0.922283    -1.948404     0.775291      24.12
 C      -0.042792     1.396299     0.154624      57.51
 H      -0.492679     2.539877     0.268060      19.07
 C       1.295634     1.299875    -0.184035      -9.83
 O       2.282457     2.255104    -0.435405     198.05
 C       1.791031     3.675373    -0.385095      70.33
 H       2.812324     3.970770    -0.990310      19.80
 H       0.805103     3.791770    -1.090692      24.09
 H       1.383105     3.820958     0.745646      24.95
 C       1.757806    -0.163488    -0.173318       6.21
 O       3.164004    -0.262710    -0.450079     164.67
 C       0.932692    -1.214460     0.143349      63.08
 H       1.336470    -2.234768     0.049088      24.00
 C      -0.870037     0.346309     0.495944      39.66
 C      -2.358463     0.598587     0.859436      79.77
 H      -2.866232    -0.292010     1.248607      22.10
 O      -2.568636     1.483734     1.933406     265.39
 H      -2.347469     1.193409     2.908214      27.35
 C      -3.097423     1.200787    -0.461904      69.12
 H      -2.384703     1.509136    -1.238897      21.98
 O      -3.785795    -0.141253    -1.085584     120.52
 H      -3.772298     0.051541    -2.210698      21.75
 C      -4.281174     2.033621    -0.246278      91.22
 O      -4.656132     2.894052    -1.447684     229.02
 H      -4.366969     3.867151    -1.205403      27.85
 H      -3.949803     2.864050     0.444265      23.00
 H      -5.248434     1.347925    -0.207979      24.67
55
name = lig-etoh-Waterframe_549
 C       6.153038    -0.880018     1.570052      64.17
 H       6.405545     0.150828     1.296298      23.85
 C       5.511650    -3.140000     0.771544      44.11
 H       5.053371    -3.905586     0.127414      19.38
 C       5.784450    -3.703772     2.155517      -2.25
 O       5.626987    -5.087478     2.502769     189.38
 C       5.070518    -5.933178     1.348581     112.03
 H       5.500351    -5.703801     0.447774      28.03
 H       3.881271    -5.753944     1.402886      24.59
 H       5.282242    -7.050987     1.778286      24.30
 C       6.149316    -2.804622     3.236180      14.83
 O       6.292190    -3.028470     4.526650      98.96
 H       6.168750    -3.962272     4.977470      18.67
 C       6.359137    -1.445542     2.798163      43.09
 H       6.911226    -0.744549     3.577697      23.15
 C       5.642843    -1.748378     0.476027       9.72
 C       5.299676    -1.364986    -0.921939      77.64
 H       5.872284    -2.118339    -1.657388      22.34
 O       5.850898    -0.101953    -1.457043     268.58
 H       5.909223     0.404241    -0.652742      29.28
 C       3.737221    -1.310790    -1.181009      63.82
 H       3.247132    -2.323282    -0.764612      23.12
 C       3.209569    -1.313145    -2.690957      92.70
 O       3.515631    -2.593132    -3.377445     247.93
 H       4.464572    -2.573830    -3.781448      25.40
 H       3.480132    -0.395900    -3.211011      25.72
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 H       1.989475    -1.318262    -2.425085      23.43
 C      -0.418787    -0.946915     0.523478      51.40
 H      -1.141037    -1.828226     0.743476      23.39
 C      -0.056954     1.462988     0.113286      91.78
 H      -0.487036     2.541478     0.481154      19.10
 C       1.315002     1.225224    -0.080843       2.64
 O       2.236942     2.242568    -0.416985     185.40
 C       1.892926     3.621534    -0.408512     120.85
 H       2.569544     4.291895    -0.578720      28.40
 H       1.208732     3.785196    -1.228083      27.81
 H       1.759141     4.091798     0.693002      26.75
 C       1.804154    -0.126081    -0.136935      17.90
 O       3.163008    -0.225664    -0.352554     151.14
 C       1.040565    -1.289110     0.160612      46.89
 H       1.413151    -2.368049     0.286567      21.43
 C      -0.878567     0.282977     0.579690      33.80
 C      -2.361578     0.628636     0.840009      84.07
 H      -2.830940    -0.298179     1.021553      23.50
 O      -2.516786     1.567561     1.856782     254.32
 H      -2.192077     0.961265     2.721748      22.55
 C      -3.124797     1.058811    -0.443896      61.04
 H      -2.453759     1.696929    -1.143409      22.19
 O      -3.742551    -0.128667    -1.079615     247.64
 H      -3.446838    -0.170687    -2.117291      23.27
 C      -4.358423     2.173101    -0.241569      90.31
 O      -4.639776     2.864990    -1.434626     305.44
 H      -4.460687     3.793599    -1.034645      25.28
 H      -4.319321     2.770284     0.813755      23.60
 H      -5.217146     1.478198     0.156812      25.97
55
name = lig-etoh-Waterframe_550
 C       6.076775    -0.892516     1.526877      48.05
 H       6.470650     0.145076     1.317680      20.20
 C       5.502982    -3.157032     0.863779      69.77
 H       5.093648    -3.732928    -0.006597      22.80
 C       5.769726    -3.669504     2.103400      19.14
 O       5.613135    -5.082218     2.436981     240.67
 C       5.057582    -5.959886     1.402318     108.02
 H       5.456362    -5.828502     0.484323      29.64
 H       3.899995    -5.693411     1.329840      27.31
 H       5.151453    -7.148228     1.521683      25.02
 C       6.162396    -2.783699     3.128956      -3.02
 O       6.342312    -3.011772     4.573646      69.38
 H       6.086667    -3.951881     4.691981      22.18
 C       6.300853    -1.418538     2.863860      16.94
 H       6.674095    -0.892221     3.804098      20.68
 C       5.695715    -1.768189     0.562164      -7.31
 C       5.242617    -1.332039    -0.947678      72.72
 H       5.699922    -2.324547    -1.528441      23.23
 O       5.835759    -0.123436    -1.407375     291.19
 H       5.625624     0.652404    -0.847610      24.97
 C       3.750538    -1.380596    -1.242342      60.21
 H       3.242234    -2.283324    -0.689656      22.66
 C       3.195637    -1.320285    -2.699872     104.36
 O       3.491249    -2.628916    -3.386724     252.26
 H       4.363427    -2.506052    -3.889672      25.93
 H       3.442401    -0.522020    -3.336158      26.66
 H       2.074983    -1.318883    -2.511203      25.51
 C      -0.336364    -1.022524     0.544746      44.65
 H      -1.174321    -1.735917     0.841645      23.56
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 C      -0.066840     1.434107     0.206097      56.36
 H      -0.480275     2.509201     0.163863      19.14
 C       1.294373     1.188962    -0.023745       5.09
 O       2.241249     2.175305    -0.380774     211.21
 C       1.980884     3.622578    -0.432135     114.89
 H       2.958447     4.246582    -0.530124      23.87
 H       1.223555     3.925407    -1.000399      29.78
 H       1.487814     3.890290     0.494826      29.04
 C       1.865698    -0.144844    -0.094277      22.39
 O       3.228546    -0.172755    -0.288132     108.96
 C       0.984863    -1.240709     0.221789      50.02
 H       1.516620    -2.264516     0.305191      22.20
 C      -0.903590     0.411813     0.559350      51.28
 C      -2.390656     0.563462     0.743320      74.95
 H      -2.830364    -0.398878     1.060843      22.99
 O      -2.471535     1.674853     1.860705     162.66
 H      -1.843964     1.088637     2.592083      21.37
 C      -3.227297     1.029120    -0.447686      68.95
 H      -2.449909     1.510946    -1.170456      22.06
 O      -3.655871    -0.115356    -1.062924     286.35
 H      -3.474288    -0.093239    -2.041542      25.94
 C      -4.418804     2.129578    -0.126550      97.19
 O      -4.614693     2.885516    -1.398948     258.46
 H      -4.554920     3.862256    -1.324025      28.92
 H      -4.172993     2.974781     0.668265      23.76
 H      -5.311175     1.595824     0.032851      27.76
55
name = lig-etoh-Waterframe_551
 C       6.081276    -0.886428     1.579271      49.57
 H       6.163627     0.231481     1.328741      23.79
 C       5.479721    -3.130351     0.875468      85.04
 H       5.215889    -3.827781     0.028918      23.05
 C       5.738311    -3.748901     2.110951      20.76
 O       5.622706    -5.057946     2.372325     278.89
 C       5.019729    -5.954663     1.428711     126.22
 H       5.537478    -5.828746     0.434184      27.25
 H       3.928949    -5.813547     1.317450      27.45
 H       5.259298    -6.903920     1.940861      24.83
 C       6.163278    -2.740276     3.148803       5.73
 O       6.382712    -3.008425     4.508271      49.60
 H       6.196005    -3.939506     4.907750      22.20
 C       6.264139    -1.375659     2.868872      67.36
 H       6.440678    -0.684308     3.659352      23.00
 C       5.659835    -1.803522     0.545338       8.13
 C       5.245278    -1.355100    -0.926820      85.94
 H       5.586104    -2.017282    -1.761917      24.60
 O       5.844614    -0.130889    -1.360813     287.52
 H       5.250741     0.608810    -1.140867      26.54
 C       3.725298    -1.392501    -1.186401      74.16
 H       3.443622    -2.404927    -0.856819      24.65
 C       3.160640    -1.384162    -2.682612     114.05
 O       3.450612    -2.616672    -3.376808     269.34
 H       4.269846    -2.698656    -3.943069      27.21
 H       3.621037    -0.571035    -3.213308      27.19
 H       2.193237    -1.290835    -2.836444      28.63
 C      -0.365280    -0.946878     0.578967      45.50
 H      -0.752139    -1.940997     0.891485      20.04
 C      -0.035028     1.458089     0.303727      88.63
 H      -0.395036     2.311619    -0.101395      21.40
 C       1.325054     1.184411    -0.025192       6.33
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 O       2.274128     2.105638    -0.357002     163.83
 C       2.002274     3.633579    -0.383736      76.97
 H       3.233229     3.670388    -0.772808      19.40
 H       1.396085     3.931225    -1.285977      24.13
 H       1.700376     3.769242     0.593385      26.73
 C       1.853921    -0.122664    -0.012567      19.12
 O       3.309622    -0.187448    -0.299024     125.82
 C       1.001902    -1.167756     0.287549      51.95
 H       1.316876    -2.250084     0.245907      21.93
 C      -0.917517     0.321774     0.472177      50.47
 C      -2.416638     0.579861     0.760898      86.22
 H      -2.847570    -0.265486     1.376418      25.52
 O      -2.422764     1.699480     1.850719     151.33
 H      -1.774861     1.608079     2.713864      28.43
 C      -3.284901     1.142594    -0.423749      80.75
 H      -2.677491     1.728862    -1.138395      23.81
 O      -3.616939    -0.181676    -1.095933     259.38
 H      -3.722466     0.020402    -1.977220      28.39
 C      -4.420652     2.067750    -0.092460     112.30
 O      -4.610214     2.891657    -1.389244     244.43
 H      -4.380639     3.787529    -1.022416      27.75
 H      -3.971146     2.657591     0.711553      27.53
 H      -5.307234     1.613202     0.102507      30.31
55
name = lig-etoh-Waterframe_552
 C       6.052817    -0.880333     1.538278      56.35
 H       5.925079     0.220872     1.376918      22.81
 C       5.458090    -3.177226     0.823535      61.07
 H       5.191399    -3.940904     0.079211      22.13
 C       5.738133    -3.652194     2.171119      28.89
 O       5.647426    -5.042549     2.374599     208.07
 C       5.004261    -5.965340     1.461711     124.95
 H       5.556801    -6.054930     0.361737      24.92
 H       3.994538    -5.849619     1.389819      30.12
 H       5.160777    -6.832182     1.965109      26.46
 C       6.116048    -2.792410     3.189899      18.04
 O       6.441008    -3.009812     4.447855     189.48
 H       6.115801    -3.963404     4.774546      23.95
 C       6.237091    -1.347864     2.832677      27.57
 H       6.543146    -0.660962     3.555401      23.70
 C       5.610978    -1.765080     0.495243     -14.35
 C       5.288576    -1.399382    -0.950211      93.59
 H       5.738496    -2.087061    -1.543088      27.28
 O       5.857159    -0.106084    -1.324580     303.81
 H       5.130638     0.517019    -1.198652      27.64
 C       3.669805    -1.401984    -1.075918      83.76
 H       3.334594    -2.257915    -0.616841      25.34
 C       3.194102    -1.387779    -2.669727     100.71
 O       3.408551    -2.644874    -3.369747     280.01
 H       4.315277    -2.586274    -3.766557      27.68
 H       3.834256    -0.562747    -3.070099      25.75
 H       2.142388    -1.126350    -2.705772      27.08
 C      -0.359386    -0.947442     0.618380      32.36
 H      -1.005917    -1.786206     0.880833      19.35
 C       0.007588     1.447864     0.291847      73.61
 H      -0.396815     2.320904     0.027491      22.79
 C       1.346476     1.205401    -0.007487      13.46
 O       2.310331     2.091596    -0.356748     197.65
 C       2.094503     3.495062    -0.366012     110.86
 H       3.129064     4.275667    -0.515663      21.84
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 H       1.398303     3.880024    -1.315936      23.18
 H       1.979555     4.178594     0.500722      24.54
 C       1.924161    -0.102999     0.051168      17.89
 O       3.285900    -0.278499    -0.350316     197.76
 C       1.056347    -1.140176     0.341291      62.78
 H       1.326126    -2.172402     0.281018      22.82
 C      -0.993292     0.273999     0.422879      39.98
 C      -2.388038     0.699946     0.909558      90.01
 H      -3.003630    -0.253667     1.189580      24.45
 O      -2.404180     1.749551     1.808644     221.47
 H      -1.707276     1.279707     2.516688      26.77
 C      -3.261828     1.127504    -0.404563      79.22
 H      -2.687869     1.791673    -0.963990      26.05
 O      -3.605723    -0.207488    -1.117071     248.79
 H      -3.763446    -0.071622    -1.995017      27.75
 C      -4.421452     2.028144    -0.128196     113.94
 O      -4.615139     2.905414    -1.314014     277.57
 H      -4.211002     3.717126    -0.989645      29.59
 H      -4.183287     2.529392     0.711092      30.19
 H      -5.304611     1.523735     0.357964      28.68
55
name = lig-etoh-Waterframe_553
 C       5.951873    -0.887315     1.444454      52.49
 H       6.147204     0.169591     1.274336      22.65
 C       5.476141    -3.162982     0.822756      84.52
 H       5.147525    -3.844839     0.077322      22.39
 C       5.692115    -3.589797     2.089745       7.85
 O       5.690753    -5.021733     2.431335     211.13
 C       5.009444    -6.002170     1.517470     126.94
 H       5.503766    -6.099103     0.403583      26.38
 H       4.012743    -5.681265     1.405064      25.95
 H       5.008159    -6.982024     1.863563      26.06
 C       6.077801    -2.676747     3.150073       8.20
 O       6.507284    -3.064304     4.469992     219.37
 H       6.104378    -3.982637     4.732477      25.02
 C       6.229140    -1.403166     2.790393      51.71
 H       6.727936    -0.891980     3.518698      25.03
 C       5.583886    -1.812161     0.484349       7.97
 C       5.296676    -1.415585    -0.951449      89.96
 H       5.722040    -2.251293    -1.511226      26.81
 O       5.851965    -0.103973    -1.310737     299.82
 H       5.307330     0.651652    -1.029423      25.85
 C       3.674047    -1.508317    -1.063242      80.93
 H       3.238985    -2.296311    -0.514575      24.23
 C       3.264155    -1.356971    -2.569745      86.97
 O       3.386739    -2.646843    -3.344900     250.47
 H       4.291587    -2.654329    -3.752685      27.48
 H       3.861609    -0.594989    -3.198941      24.17
 H       2.092075    -0.994695    -2.570541      24.40
 C      -0.345054    -0.996258     0.626136      25.32
 H      -1.043261    -1.724558     0.838041      18.76
 C      -0.044102     1.372211     0.198768      68.50
 H      -0.342175     2.458149     0.413794      20.75
 C       1.382021     1.201089     0.038831      -0.90
 O       2.405084     2.148903    -0.350036     177.98
 C       2.207725     3.525030    -0.384024     107.37
 H       3.141237     3.849863    -0.751661      23.81
 H       1.241164     3.653400    -1.078943      23.89
 H       1.554119     3.809251     0.652990      24.48
 C       1.959413    -0.132563     0.072593      18.02
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 O       3.208702    -0.298159    -0.379697     184.25
 C       1.048940    -1.180495     0.401609      56.10
 H       1.525914    -2.091357     0.433323      23.19
 C      -0.937545     0.396145     0.474346      40.23
 C      -2.441125     0.724857     0.861683      80.13
 H      -2.878929    -0.179932     1.401149      22.91
 O      -2.352556     1.797245     1.827639     234.97
 H      -1.915073     1.359550     2.687425      26.49
 C      -3.183510     1.023525    -0.405754      85.03
 H      -2.443643     1.467225    -1.061798      24.60
 O      -3.590169    -0.166343    -1.067285     267.06
 H      -3.425945    -0.092198    -2.074815      24.46
 C      -4.446725     2.009710    -0.115247      86.68
 O      -4.647259     2.920649    -1.209175     283.93
 H      -4.207728     3.735173    -1.126598      30.59
 H      -4.259718     2.743758     0.690592      25.48
 H      -5.494019     1.329469    -0.131962      25.50
55
name = lig-etoh-Waterframe_554
 C       5.906590    -0.894627     1.453247      70.12
 H       6.313939    -0.017414     1.064164      23.76
 C       5.461523    -3.172812     0.777305      69.87
 H       5.217415    -3.851233     0.000821      23.32
 C       5.660398    -3.682949     2.099217       0.67
 O       5.726482    -5.002381     2.477737     182.82
 C       5.009359    -5.976798     1.563224     119.98
 H       5.576802    -5.935340     0.634314      27.74
 H       3.958807    -5.549347     1.379012      23.98
 H       4.993893    -6.963164     2.160421      23.97
 C       6.055806    -2.713898     3.158557      -6.00
 O       6.543825    -3.101592     4.425704     224.29
 H       6.247936    -3.964876     4.854959      21.10
 C       6.257656    -1.326812     2.711783      40.59
 H       6.764251    -0.668991     3.403491      24.41
 C       5.579959    -1.817539     0.464051      26.88
 C       5.237996    -1.414507    -0.909392      89.23
 H       5.665278    -2.009267    -1.876367      22.35
 O       5.836748    -0.151465    -1.326684     299.60
 H       5.572265     0.525150    -0.635151      25.28
 C       3.733892    -1.552360    -1.112353      75.24
 H       3.415249    -2.586360    -0.830802      22.76
 C       3.303647    -1.372827    -2.497962      94.40
 O       3.374887    -2.617074    -3.297961     243.23
 H       4.196109    -2.691711    -3.832506      28.09
 H       3.937690    -0.523793    -2.932566      23.55
 H       2.116172    -1.112008    -2.653463      23.44
 C      -0.371687    -0.935260     0.603791      53.40
 H      -0.831265    -1.842453     0.843677      22.77
 C       0.019217     1.436176     0.124864      70.13
 H      -0.405947     2.546347     0.498584      18.46
 C       1.456865     1.178532     0.044229       5.47
 O       2.494587     2.101192    -0.318957     127.67
 C       2.147061     3.571895    -0.402088     118.72
 H       2.977185     3.977336    -0.697929      29.37
 H       1.505308     3.876465    -1.195307      26.66
 H       2.097380     3.829316     0.752291      25.79
 C       1.838204    -0.147985     0.059826      15.75
 O       3.196743    -0.285229    -0.400888     113.86
 C       1.029140    -1.236231     0.455713      48.93
 H       1.393462    -2.202915     0.634588      21.60
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 C      -0.851481     0.325271     0.586489      26.24
 C      -2.368739     0.649352     0.847779      85.48
 H      -2.791724    -0.134112     1.425401      22.87
 O      -2.321444     1.865382     1.870403     207.20
 H      -2.111789     1.421942     2.769915      25.30
 C      -3.167254     1.042278    -0.418961      74.57
 H      -2.459741     1.614595    -1.146064      21.89
 O      -3.588687    -0.170054    -1.016413     258.10
 H      -3.220328    -0.154025    -2.006099      23.29
 C      -4.421266     1.999938    -0.143885      82.22
 O      -4.701982     2.947717    -1.184152     310.76
 H      -4.229191     3.681220    -0.842492      29.27
 H      -4.454401     2.289498     1.065256      24.14
 H      -5.295402     1.172009    -0.248214      25.67
55
name = lig-etoh-Waterframe_555
 C       5.955510    -0.890190     1.423026      52.87
 H       6.220827     0.106882     1.180976      21.66
 C       5.431363    -3.258066     0.771886      68.26
 H       5.317987    -3.946955    -0.054862      23.54
 C       5.679959    -3.683812     2.166449      15.76
 O       5.722965    -5.026617     2.511655     210.22
 C       5.040666    -5.883839     1.637481     126.26
 H       5.541930    -6.154456     0.811874      28.17
 H       3.886573    -5.637749     1.436727      24.63
 H       5.028547    -6.937009     2.276354      23.13
 C       6.066433    -2.781928     3.128347       6.45
 O       6.568385    -3.096363     4.349541     223.00
 H       6.269116    -3.976710     4.665706      19.82
 C       6.292482    -1.319967     2.741038      -2.18
 H       6.673553    -0.435415     3.377038      25.26
 C       5.573234    -1.864437     0.453247       2.16
 C       5.226223    -1.393576    -0.972749      89.93
 H       5.726908    -2.312631    -1.627399      22.86
 O       5.799620    -0.176263    -1.324891     287.14
 H       5.870946     0.447076    -0.551121      25.60
 C       3.740209    -1.501733    -1.110029      75.54
 H       3.431447    -2.546008    -0.657649      22.32
 C       3.296882    -1.366280    -2.561912     111.33
 O       3.387075    -2.602251    -3.275579     274.40
 H       4.215459    -2.505477    -3.783474      28.08
 H       3.873146    -0.554726    -2.962686      26.24
 H       2.233523    -1.052321    -2.437133      25.57
 C      -0.338502    -0.992452     0.632175      50.98
 H      -1.125109    -1.751511     0.952309      22.11
 C       0.132646     1.483069     0.191889      64.54
 H      -0.396278     2.564333    -0.058908      18.22
 C       1.427976     1.233164    -0.007269      11.76
 O       2.522778     2.062267    -0.300525     154.14
 C       2.148957     3.570311    -0.376156     111.05
 H       3.193008     4.229767    -0.676837      23.57
 H       1.346819     3.829072    -0.955741      27.53
 H       1.925875     4.180971     0.447392      28.18
 C       1.845404    -0.246871    -0.002009      12.31
 O       3.186775    -0.336809    -0.395902     152.15
 C       0.997664    -1.226907     0.469353      62.61
 H       1.325344    -2.248244     0.496259      23.87
 C      -0.810022     0.356378     0.611542      34.83
 C      -2.210968     0.659837     0.941963      79.19
 H      -2.788809    -0.159943     1.206962      23.50
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 O      -2.317151     1.885561     1.871462     240.44
 H      -2.061504     1.377096     2.676431      26.10
 C      -3.150068     1.151891    -0.400843      58.79
 H      -2.516822     1.841432    -1.111337      20.86
 O      -3.574199    -0.220527    -0.986692     175.23
 H      -3.547078    -0.266916    -2.111563      21.51
 C      -4.427527     1.849526    -0.163015      96.96
 O      -4.722362     3.000812    -1.136205     267.86
 H      -4.457067     3.869637    -0.782562      27.79
 H      -4.544216     2.336583     0.952800      25.04
 H      -5.191477     1.156624    -0.239089      28.48
55
name = lig-etoh-Waterframe_556
 C       6.050577    -0.956099     1.425205      44.43
 H       5.946025     0.115578     1.328058      23.43
 C       5.442951    -3.285752     0.842706      85.15
 H       5.256206    -4.093808     0.107720      23.62
 C       5.698878    -3.655220     2.104341       4.35
 O       5.715961    -5.014037     2.570088     214.97
 C       5.042819    -5.930578     1.719647     107.25
 H       5.522743    -6.156575     0.759292      27.10
 H       3.991441    -5.464282     1.493237      25.51
 H       4.934711    -6.939570     2.323206      23.68
 C       6.156144    -2.656451     3.083901      26.01
 O       6.589363    -3.105950     4.313988     181.48
 H       6.351557    -4.010966     4.606899      25.56
 C       6.275598    -1.396511     2.742369      52.45
 H       6.610598    -0.791367     3.707205      21.83
 C       5.574374    -1.919423     0.465853      -6.91
 C       5.285692    -1.474533    -0.958665      87.13
 H       5.639192    -2.229632    -1.656188      27.22
 O       5.791934    -0.175063    -1.363599     263.32
 H       5.785532     0.499474    -0.616779      28.32
 C       3.692670    -1.443614    -1.109319      86.38
 H       3.250122    -2.362305    -0.548972      23.13
 C       3.231167    -1.311276    -2.601869     114.67
 O       3.427886    -2.593954    -3.298969     269.04
 H       4.280629    -2.639726    -3.778622      28.87
 H       3.724044    -0.635670    -3.212571      27.86
 H       2.257221    -1.062768    -2.657539      28.51
 C      -0.387399    -0.945110     0.722325      48.54
 H      -1.212673    -1.758572     1.025651      19.11
 C       0.102273     1.483263     0.290175      72.96
 H      -0.200164     2.415614    -0.177621      19.06
 C       1.493556     1.134982    -0.075173       1.91
 O       2.489325     2.134011    -0.276847     159.40
 C       2.174856     3.576226    -0.340611      90.06
 H       3.225399     3.889435    -1.136611      20.49
 H       1.342237     3.477409    -1.059182      24.96
 H       1.793776     3.855285     0.592824      26.65
 C       1.901074    -0.203311    -0.062210      24.06
 O       3.187847    -0.404758    -0.363080     207.63
 C       1.027569    -1.274095     0.403620      44.87
 H       1.462096    -2.295279     0.212126      21.24
 C      -0.709236     0.435933     0.569902      31.75
 C      -2.191488     0.817076     0.931491      79.75
 H      -2.632915    -0.139119     1.363306      24.84
 O      -2.306388     1.816418     1.875527     288.88
 H      -1.856283     1.626867     2.664792      31.58
 C      -3.074161     1.143990    -0.372818      65.03
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 H      -2.489548     1.672912    -1.169403      22.63
 O      -3.513993    -0.251706    -0.969616     156.14
 H      -3.787374     0.075334    -2.007482      23.18
 C      -4.515376     1.830111    -0.155112     100.85
 O      -4.740361     2.997240    -1.082564     282.59
 H      -4.470505     3.851145    -0.584383      26.55
 H      -4.440863     2.301694     0.799037      27.28
 H      -5.246727     1.186973    -0.345593      30.05
55
name = lig-etoh-Waterframe_557
 C       6.080777    -1.037283     1.434993      72.84
 H       5.980135     0.030999     1.136271      25.44
 C       5.454013    -3.279999     0.826253      67.73
 H       5.026826    -4.026691     0.095220      18.68
 C       5.770441    -3.675102     2.158196      33.22
 O       5.714696    -4.934794     2.635976     235.30
 C       4.991624    -6.013100     1.779239      89.84
 H       5.654298    -6.039291     0.797889      26.35
 H       4.050625    -5.590285     1.548020      30.44
 H       4.896666    -6.904219     2.362400      25.47
 C       6.231170    -2.773996     3.060402      10.76
 O       6.624303    -3.102279     4.322089     218.25
 H       6.308979    -4.012432     4.560781      28.11
 C       6.288765    -1.369635     2.761702      32.39
 H       6.593594    -0.664096     3.625558      20.17
 C       5.638976    -1.917077     0.490446      27.59
 C       5.267023    -1.523808    -0.941284      87.57
 H       5.624965    -2.058030    -1.684587      28.06
 O       5.813049    -0.195635    -1.412645     253.57
 H       5.446323     0.493665    -0.759725      27.26
 C       3.656699    -1.468507    -1.165536      80.85
 H       3.285400    -2.485741    -1.036117      23.72
 C       3.183503    -1.292783    -2.662608      99.38
 O       3.460223    -2.607300    -3.336515     244.70
 H       4.368879    -2.660812    -3.713513      27.61
 H       3.773215    -0.446214    -3.077012      25.40
 H       2.135797    -1.201869    -2.840072      26.59
 C      -0.280837    -0.856073     0.756748      37.37
 H      -1.033072    -1.712322     1.055271      17.84
 C       0.226601     1.479329     0.269708      69.39
 H      -0.214428     2.374693     0.268268      21.14
 C       1.502304     1.153701    -0.076735      19.41
 O       2.481513     2.136821    -0.246568     201.49
 C       2.126995     3.464858    -0.409695     116.06
 H       3.039982     4.207953    -0.660530      23.42
 H       1.260588     3.848241    -1.200757      22.96
 H       2.125338     3.973195     0.652343      23.73
 C       1.878690    -0.221863    -0.071921      19.95
 O       3.266802    -0.382636    -0.298706     181.33
 C       0.984910    -1.247971     0.279893      63.71
 H       1.289162    -2.370807     0.312574      21.46
 C      -0.766518     0.460567     0.590085      48.22
 C      -2.212477     0.856179     0.846017      81.15
 H      -2.588699    -0.119700     1.400647      23.02
 O      -2.307187     1.835279     1.920662     274.62
 H      -1.638145     1.510419     2.471764      31.50
 C      -3.090092     1.043269    -0.370283      87.07
 H      -2.506954     1.560374    -1.074777      25.06
 O      -3.409831    -0.221594    -0.927563     201.28
 H      -3.703064    -0.038283    -1.992559      22.38
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 C      -4.518869     1.915141    -0.135979      90.06
 O      -4.765550     2.956334    -1.033473     313.86
 H      -4.193750     3.751905    -0.613028      25.80
 H      -4.669897     2.059907     0.861424      28.46
 H      -5.332057     1.086622    -0.295882      26.96
55
name = lig-etoh-Waterframe_558
 C       6.074288    -0.996695     1.441949       2.55
 H       6.426482     0.041890     1.072653      18.78
 C       5.463172    -3.284776     0.821326      80.99
 H       4.930284    -3.899163     0.047419      23.45
 C       5.817737    -3.724102     2.117340       3.08
 O       5.664470    -4.973013     2.700499     241.12
 C       4.989272    -5.990964     1.861944     125.81
 H       5.661855    -6.365329     0.913923      28.71
 H       4.009339    -5.830737     1.631843      32.57
 H       5.041513    -6.803046     2.432329      27.13
 C       6.328662    -2.777386     3.115321      15.00
 O       6.668775    -3.124477     4.378754     174.77
 H       6.305132    -4.000631     4.759137      21.83
 C       6.341701    -1.392898     2.785979      44.08
 H       6.599997    -0.518278     3.330142      21.56
 C       5.684077    -1.974915     0.433375      -6.00
 C       5.204151    -1.478194    -1.009551      87.21
 H       5.709297    -2.340139    -1.616817      24.54
 O       5.820525    -0.247274    -1.423058     277.42
 H       5.314551     0.556694    -1.048869      23.63
 C       3.673394    -1.538030    -1.251162      74.51
 H       3.280013    -2.429311    -0.850061      24.67
 C       3.204537    -1.312411    -2.726707      98.10
 O       3.487922    -2.601115    -3.377104     247.85
 H       4.413144    -2.579726    -3.722358      27.10
 H       3.733506    -0.354014    -3.144083      24.33
 H       2.024782    -1.142245    -2.687340      24.60
 C      -0.242330    -0.783709     0.726258      42.09
 H      -0.875191    -1.588400     1.115541      20.04
 C       0.183494     1.495958     0.254069      72.01
 H       0.062833     2.464908     0.640061      22.03
 C       1.528401     1.190077    -0.043592       9.28
 O       2.520121     2.081368    -0.259431     173.75
 C       2.112098     3.519805    -0.425310     109.42
 H       2.926324     3.876346    -0.713229      28.25
 H       1.098771     3.754305    -1.048264      23.23
 H       1.690675     4.034050     0.617102      24.43
 C       1.931052    -0.237015    -0.088879      15.23
 O       3.312374    -0.384180    -0.245381     145.20
 C       0.962881    -1.188158     0.177731      69.73
 H       1.212819    -2.294474     0.382073      23.73
 C      -0.762473     0.490248     0.605656      42.84
 C      -2.243608     0.750813     0.869792      71.84
 H      -2.795232    -0.190843     1.167427      22.85
 O      -2.295659     1.898984     1.949680     253.20
 H      -1.765630     1.465322     2.555267      29.55
 C      -3.167736     1.083416    -0.396363      86.31
 H      -2.642747     1.723756    -1.060647      24.37
 O      -3.312920    -0.237774    -0.897455     236.56
 H      -3.306835    -0.316390    -1.972489      22.57
 C      -4.476986     1.858058    -0.076868      75.82
 O      -4.768223     2.947674    -0.989031     279.71
 H      -4.214210     3.838369    -0.947287      26.71
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 H      -4.721255     2.211288     1.002865      25.18
 H      -5.349377     1.012986    -0.492617      23.86
55
name = lig-etoh-Waterframe_559
 C       6.101026    -1.005552     1.385803      50.42
 H       6.485971     0.052241     1.181611      20.46
 C       5.465733    -3.325070     0.828466      53.39
 H       5.052318    -4.127116     0.194128      22.87
 C       5.874108    -3.716059     2.122314     -30.64
 O       5.588717    -5.040320     2.717089     219.69
 C       5.023004    -6.035906     1.971776     133.88
 H       5.551860    -6.195087     0.957511      30.25
 H       3.976127    -5.773497     1.700539      28.24
 H       5.015364    -6.858490     2.651594      26.57
 C       6.372634    -2.736901     3.145149     -22.33
 O       6.728566    -3.153893     4.475459     210.49
 H       6.297353    -4.071051     4.772043      23.06
 C       6.416285    -1.407042     2.723341      52.00
 H       6.745093    -0.812288     3.504788      21.82
 C       5.679079    -1.902401     0.399334      -4.54
 C       5.226794    -1.507773    -1.064663      81.20
 H       5.666925    -2.403877    -1.877040      21.98
 O       5.825174    -0.307589    -1.456127     293.37
 H       5.337887     0.486898    -1.014788      23.09
 C       3.728998    -1.529272    -1.237932      84.64
 H       3.296846    -2.348694    -0.731995      24.12
 C       3.237449    -1.362028    -2.699508      93.68
 O       3.492835    -2.567558    -3.426657     256.07
 H       4.382160    -2.638781    -3.873182      27.64
 H       3.764964    -0.565282    -3.367470      23.22
 H       2.031869    -1.135877    -2.741865      24.10
 C      -0.311539    -0.798604     0.648037      29.58
 H      -0.932664    -1.486982     1.071496      18.89
 C       0.127998     1.565518     0.288858      76.31
 H      -0.003111     2.666083     0.552419      19.59
 C       1.524047     1.109879    -0.005936       4.82
 O       2.552258     2.106413    -0.289095     119.24
 C       2.056166     3.559678    -0.404199     108.87
 H       2.950015     3.976071    -1.009319      23.88
 H       1.432739     3.331622    -1.190025      25.91
 H       1.792242     3.835088     0.653292      25.74
 C       2.005449    -0.141965    -0.119240      31.13
 O       3.316162    -0.448008    -0.266676     186.01
 C       1.016583    -1.159442     0.154752      56.98
 H       1.362438    -2.212488     0.171076      23.25
 C      -0.773316     0.539506     0.609063      35.95
 C      -2.297409     0.746803     0.949818      83.66
 H      -2.685769    -0.118752     1.441808      24.05
 O      -2.280741     1.889437     1.936227     274.07
 H      -2.130488     1.601048     2.782891      30.35
 C      -3.145316     1.189814    -0.363712      68.12
 H      -2.662924     1.857309    -1.161178      21.58
 O      -3.236642    -0.307333    -0.914853     227.44
 H      -3.072857    -0.175674    -1.892880      24.20
 C      -4.494485     1.776433    -0.060545      85.29
 O      -4.778868     2.938364    -1.001959     243.75
 H      -4.228682     3.704993    -0.491739      24.72
 H      -4.391519     2.199544     1.079886      24.30
 H      -5.415582     1.023306    -0.218552      24.98
55
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name = lig-etoh-Waterframe_560
 C       6.181416    -1.013853     1.344143      51.78
 H       6.120118     0.042579     1.058502      25.44
 C       5.512994    -3.307213     0.864772      58.50
 H       5.230043    -4.096153     0.198789      26.54
 C       5.888993    -3.723250     2.219005      14.57
 O       5.595169    -4.979637     2.754641     180.68
 C       4.977044    -6.127998     2.002006     122.19
 H       5.528926    -6.292110     1.147960      31.70
 H       3.867653    -5.764614     1.774257      25.27
 H       4.911200    -7.148144     2.604767      26.29
 C       6.366927    -2.821480     3.158889       0.67
 O       6.772069    -3.137075     4.493572     177.13
 H       6.403956    -4.087589     4.692198      24.11
 C       6.514707    -1.449421     2.693050      25.96
 H       6.901665    -0.773898     3.446039      22.14
 C       5.626311    -1.943536     0.388371     -35.09
 C       5.319193    -1.601570    -1.069524      68.08
 H       5.655982    -2.313572    -1.934950      25.52
 O       5.845648    -0.327014    -1.524804     242.43
 H       5.576403     0.342106    -0.780936      28.60
 C       3.740799    -1.500247    -1.167928      87.77
 H       3.417215    -2.574316    -1.036677      25.24
 C       3.283559    -1.391762    -2.680679      99.30
 O       3.460251    -2.589625    -3.471313     253.15
 H       4.357830    -2.591438    -3.930640      26.52
 H       3.856826    -0.487595    -3.016770      25.07
 H       2.167544    -1.236991    -2.749346      26.10
 C      -0.319465    -0.849554     0.510953      40.79
 H      -0.965862    -1.616968     0.749745      22.89
 C       0.197454     1.582736     0.337786      77.39
 H      -0.382302     2.598104     0.121910      19.63
 C       1.495090     1.261959     0.011106       4.18
 O       2.569595     2.156344    -0.293716     194.35
 C       2.059892     3.450724    -0.458112     119.89
 H       2.879891     4.560205    -0.723988      22.68
 H       1.201302     3.599502    -1.074665      27.08
 H       1.777042     3.984852     0.379101      28.56
 C       1.956757    -0.180246    -0.119162       9.17
 O       3.345736    -0.478246    -0.335056     189.38
 C       1.033652    -1.125282     0.201033      52.09
 H       1.319736    -2.114142     0.046476      23.17
 C      -0.827316     0.546229     0.611260      33.01
 C      -2.260193     0.875217     1.033279      97.11
 H      -2.669419    -0.000660     1.467122      24.73
 O      -2.304727     1.894525     1.918290     305.72
 H      -2.313758     1.452593     2.721679      30.10
 C      -3.084111     1.100385    -0.289169      61.50
 H      -2.395340     1.802734    -0.962766      22.63
 O      -3.158839    -0.297471    -0.946895     254.57
 H      -3.174305    -0.223270    -1.889164      27.14
 C      -4.541862     1.761644    -0.067985     110.55
 O      -4.768562     2.887965    -0.967636     290.32
 H      -4.596984     3.807149    -0.462135      25.33
 H      -4.469704     2.126887     1.036468      26.70
 H      -5.227484     1.076854     0.081246      30.72
55
name = lig-etoh-Waterframe_561
 C       6.209156    -1.082433     1.349044      38.04
 H       6.189051    -0.015597     1.198874      26.99
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 C       5.588272    -3.316383     0.933868     106.98
 H       5.291296    -4.000566     0.179704      30.39
 C       5.815186    -3.744934     2.234267      -5.44
 O       5.621689    -4.989437     2.812926     157.92
 C       4.908544    -6.140004     1.993196     102.58
 H       5.442635    -6.439576     1.167907      28.93
 H       3.774425    -5.957034     1.684701      25.84
 H       5.023821    -7.022627     2.840749      23.80
 C       6.407175    -2.810715     3.184411      23.55
 O       6.789750    -3.103856     4.430886      87.27
 H       6.595670    -3.981767     4.865265      20.98
 C       6.590704    -1.514935     2.656595      52.61
 H       6.951579    -0.598565     3.208928      22.81
 C       5.670148    -2.044540     0.439953     -28.32
 C       5.343563    -1.637848    -1.066935      74.21
 H       5.717549    -2.412790    -1.561380      30.51
 O       5.885551    -0.342239    -1.565131     196.87
 H       5.937512     0.366869    -0.821727      29.21
 C       3.769687    -1.621289    -1.216788      75.92
 H       3.384176    -2.542303    -0.696981      27.36
 C       3.317309    -1.363945    -2.642334     111.82
 O       3.430088    -2.612550    -3.482239     267.59
 H       4.317636    -2.702933    -3.985106      26.68
 H       3.876701    -0.538519    -2.992396      27.72
 H       2.347285    -1.105773    -2.616587      29.95
 C      -0.374278    -0.810036     0.407073      59.39
 H      -0.990862    -1.724477     0.330087      23.96
 C       0.153592     1.541674     0.366266      71.09
 H      -0.175914     2.615481    -0.004241      20.33
 C       1.577353     1.301279    -0.003439       2.00
 O       2.555646     2.208651    -0.303497     176.08
 C       2.034094     3.537769    -0.497510      96.25
 H       3.161697     3.970013    -0.916240      22.44
 H       1.132205     3.712349    -1.185412      25.45
 H       1.725252     3.739338     0.539184      26.77
 C       1.920186    -0.100628    -0.080676       1.08
 O       3.316930    -0.436924    -0.377712     119.85
 C       0.998911    -1.161151     0.222650      48.86
 H       1.221254    -2.157722     0.129211      25.49
 C      -0.727266     0.465332     0.599298      30.00
 C      -2.204113     0.861069     0.993732      87.49
 H      -2.652726    -0.054926     1.445046      25.10
 O      -2.359319     1.986330     1.972626     270.60
 H      -2.111536     1.540871     2.794293      28.61
 C      -3.067155     0.978941    -0.261192      76.90
 H      -2.491533     1.747886    -0.884591      24.56
 O      -3.086100    -0.240446    -0.955229     295.58
 H      -3.314443    -0.137949    -1.814189      29.74
 C      -4.479995     1.778556    -0.013029     103.42
 O      -4.789195     2.806092    -0.940515     269.74
 H      -4.637455     3.756525    -0.571437      26.88
 H      -4.565157     2.260560     0.896919      27.94
 H      -5.288453     1.006783    -0.191835      27.82
55
name = lig-etoh-Waterframe_562
 C       6.202781    -1.154026     1.393944      81.13
 H       6.431409    -0.165842     1.159559      23.56
 C       5.604926    -3.440536     0.922651      52.47
 H       5.233105    -4.250264     0.299943      20.89
 C       5.776031    -3.739298     2.303823       3.89
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 O       5.601690    -5.079447     2.805017     207.74
 C       4.897688    -6.103564     2.043713     100.24
 H       5.474510    -6.395856     1.117971      25.41
 H       3.856973    -5.800053     1.837264      28.13
 H       4.872559    -6.922224     2.894570      22.65
 C       6.421220    -2.784151     3.116063      18.01
 O       6.832379    -3.065438     4.423135     126.73
 H       6.500851    -3.983008     4.616435      24.02
 C       6.634645    -1.513777     2.632618      62.38
 H       7.033778    -0.810833     3.464679      24.38
 C       5.778223    -2.014364     0.459974      -8.61
 C       5.330672    -1.638688    -0.984623      87.46
 H       5.751728    -2.409359    -1.608016      26.22
 O       5.942063    -0.417645    -1.582140     213.58
 H       5.915189     0.314788    -0.855275      28.07
 C       3.813025    -1.679310    -1.225597      58.06
 H       3.276175    -2.492506    -0.615838      23.28
 C       3.339355    -1.387658    -2.642352     109.81
 O       3.386471    -2.608127    -3.453643     283.28
 H       4.254519    -2.678958    -3.985966      26.65
 H       3.991346    -0.742556    -3.112727      25.01
 H       2.356376    -1.036702    -2.625269      27.65
 C      -0.363151    -0.890890     0.331997      39.30
 H      -1.350548    -1.556400     0.323934      18.35
 C       0.241605     1.520519     0.316444      70.21
 H      -0.216046     2.535202     0.536158      19.85
 C       1.557492     1.213053     0.012331      23.90
 O       2.506024     2.215255    -0.346652     167.88
 C       2.065513     3.660651    -0.509967     112.80
 H       2.779611     4.114126    -0.894596      30.34
 H       1.385159     3.551061    -1.421996      25.23
 H       1.859137     4.139305     0.545638      26.40
 C       1.981263    -0.111434    -0.037541      23.67
 O       3.267046    -0.358734    -0.408673     119.35
 C       0.970349    -1.143514     0.180144      55.53
 H       1.314508    -2.159085     0.173918      23.71
 C      -0.713688     0.526808     0.605692      44.25
 C      -2.162085     0.754645     0.977064      68.88
 H      -2.470043    -0.098969     1.673681      21.97
 O      -2.400399     2.035471     2.006053     214.64
 H      -1.724864     1.829749     2.734949      27.32
 C      -3.061236     1.074226    -0.268374      85.57
 H      -2.667038     1.743995    -0.958865      25.68
 O      -3.049737    -0.226625    -0.948172     268.25
 H      -3.279498    -0.064501    -1.820226      27.49
 C      -4.418429     1.724366     0.057936      86.59
 O      -4.813427     2.760851    -0.977388     253.93
 H      -4.277251     3.528437    -0.608549      28.13
 H      -4.510924     1.972407     1.062330      27.95
 H      -5.330880     0.890161    -0.292786      25.23
55
name = lig-etoh-Waterframe_563
 C       6.253072    -1.067918     1.411023      27.99
 H       6.452845    -0.138374     0.956499      21.41
 C       5.587795    -3.482627     0.901664      63.83
 H       5.227234    -4.303791     0.233460      20.50
 C       5.763636    -3.813243     2.284484      16.63
 O       5.602183    -5.094821     2.807136     252.66
 C       4.876567    -6.057078     2.122190     121.26
 H       5.455470    -6.387565     1.099263      26.99
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 H       3.981586    -5.646251     1.878047      32.22
 H       4.736812    -7.010598     2.547770      26.28
 C       6.423450    -2.821322     3.114136      22.87
 O       6.861346    -3.053998     4.405373     103.93
 H       6.604566    -3.977390     4.715074      22.11
 C       6.661551    -1.504847     2.727349      43.43
 H       7.184991    -0.811559     3.485191      24.53
 C       5.802661    -2.155531     0.432817     -29.32
 C       5.354826    -1.658591    -0.926680      84.14
 H       5.612437    -2.492097    -1.807495      22.71
 O       5.994513    -0.518515    -1.543082     220.57
 H       5.620925     0.325271    -1.062111      26.01
 C       3.790240    -1.585834    -1.134262      64.67
 H       3.336948    -2.614435    -0.883678      23.02
 C       3.384810    -1.439690    -2.677658      97.37
 O       3.336314    -2.630096    -3.412947     273.59
 H       4.194092    -2.681040    -3.945058      25.38
 H       4.064569    -0.682623    -3.074838      24.03
 H       2.289614    -0.979503    -2.709493      24.51
 C      -0.396864    -0.824101     0.333961      49.55
 H      -1.135610    -1.793643     0.497555      19.72
 C       0.239318     1.528969     0.347887      77.86
 H       0.150163     2.478958     0.792727      21.09
 C       1.561849     1.213456     0.000193      -2.82
 O       2.473307     2.233506    -0.373934     164.37
 C       2.104393     3.690181    -0.538816     111.65
 H       2.988358     4.396492    -0.942136      24.52
 H       1.161249     3.836106    -1.161986      25.66
 H       1.634493     4.450806     0.171291      26.55
 C       1.991684    -0.214979    -0.021451      21.04
 O       3.297651    -0.310499    -0.450363     161.96
 C       1.016190    -1.162682     0.097234      66.34
 H       1.396180    -2.238765     0.020571      22.23
 C      -0.711448     0.501724     0.562795      40.91
 C      -2.140193     0.806024     1.043692      67.79
 H      -2.593211    -0.159084     1.495034      22.98
 O      -2.393932     2.004935     1.975461     255.95
 H      -1.541997     1.958487     2.556999      27.46
 C      -3.017716     1.165541    -0.260188      71.33
 H      -2.431307     1.876279    -0.790238      24.93
 O      -3.060746    -0.217153    -0.930587     217.24
 H      -3.089893    -0.235448    -1.959769      23.51
 C      -4.454220     1.611100     0.032778      82.95
 O      -4.788562     2.729665    -0.956196     252.84
 H      -4.183274     3.480629    -0.887714      30.47
 H      -4.492607     1.961058     1.116869      25.93
 H      -5.169727     0.612856     0.137491      25.55
55
name = lig-etoh-Waterframe_564
 C       6.296490    -1.125082     1.370968      39.11
 H       6.381976    -0.056871     1.064357      25.92
 C       5.554362    -3.499132     0.902582      71.51
 H       5.240316    -4.167075     0.046727      23.14
 C       5.815799    -3.855863     2.222746      15.08
 O       5.647243    -5.070435     2.880984     220.23
 C       4.812715    -6.051159     2.081920     111.58
 H       5.375009    -6.226091     1.062059      26.67
 H       3.844103    -5.647685     1.803790      29.12
 H       4.740767    -6.835353     2.713247      26.77
 C       6.404809    -2.885234     3.146788     -17.79
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 O       6.885419    -3.095709     4.409216     147.74
 H       6.728656    -3.946607     4.894652      22.83
 C       6.631741    -1.461545     2.718491      -1.94
 H       7.164770    -0.783650     3.394618      21.19
 C       5.831126    -2.165098     0.517118      19.40
 C       5.326777    -1.739963    -0.972532      81.96
 H       5.538006    -2.768490    -1.626608      24.66
 O       6.051715    -0.592380    -1.454407     183.85
 H       5.496678     0.258449    -1.341989      27.37
 C       3.773635    -1.460129    -1.103403      91.39
 H       3.334605    -2.369101    -0.549010      23.64
 C       3.417845    -1.397736    -2.646099      81.14
 O       3.330275    -2.693906    -3.377279     266.17
 H       4.167884    -2.938576    -3.874827      27.39
 H       4.135286    -0.674802    -3.200945      24.58
 H       2.265573    -0.935989    -2.712998      25.43
 C      -0.292268    -0.820917     0.362760      23.65
 H      -0.982494    -1.723497     0.617496      20.88
 C       0.253198     1.535562     0.440112      66.88
 H       0.102815     2.530290     0.634486      23.53
 C       1.565364     1.219011    -0.021095       2.54
 O       2.471289     2.287094    -0.372571     163.53
 C       2.047731     3.734668    -0.592732      73.81
 H       3.359656     3.992650    -1.120222      19.10
 H       1.311930     3.782524    -1.424804      23.48
 H       2.021459     3.938559     0.506016      22.27
 C       1.988721    -0.144923    -0.090061      22.02
 O       3.374990    -0.331873    -0.486648     185.33
 C       1.000451    -1.213680     0.027067      64.51
 H       1.160138    -2.367380    -0.179108      20.92
 C      -0.760779     0.502136     0.567144      41.01
 C      -2.195503     0.909070     1.060190      92.99
 H      -2.668963    -0.012741     1.453116      26.19
 O      -2.329153     1.932543     1.904639     283.18
 H      -1.623140     1.927980     2.678313      29.61
 C      -2.955957     1.118425    -0.239663      79.00
 H      -2.373899     1.963919    -0.784676      24.51
 O      -3.075698    -0.178682    -0.907087     233.16
 H      -2.934248    -0.064763    -1.976587      23.31
 C      -4.437054     1.586157     0.023702      98.78
 O      -4.799561     2.637769    -0.924800     246.73
 H      -4.170618     3.308237    -0.665879      31.71
 H      -4.515598     2.254252     0.974861      26.00
 H      -5.147215     0.837421    -0.195246      28.73
55
name = lig-etoh-Waterframe_565
 C       6.315460    -1.210859     1.385568      80.95
 H       6.344353    -0.114478     1.039740      31.00
 C       5.553904    -3.472206     0.902901      50.24
 H       5.147534    -4.229074     0.171394      22.28
 C       5.921018    -3.843890     2.267600     -15.18
 O       5.647459    -5.084636     2.897279     197.76
 C       4.787074    -6.014125     2.051686     114.20
 H       5.305267    -6.352564     1.158630      28.66
 H       3.688901    -5.577819     1.960538      24.67
 H       4.736437    -6.823632     2.746111      26.92
 C       6.409405    -2.813986     3.120423       5.16
 O       6.918695    -3.160025     4.446072     195.38
 H       6.491840    -4.051000     4.655125      25.75
 C       6.568650    -1.554118     2.679712      91.69
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 H       6.924365    -0.825613     3.322474      23.21
 C       5.775756    -2.101617     0.493401      25.39
 C       5.294888    -1.818391    -0.926548      97.89
 H       5.537386    -2.599786    -1.636844      24.25
 O       6.127494    -0.673611    -1.388475     157.96
 H       5.502889     0.128238    -1.328774      29.61
 C       3.805180    -1.516494    -1.137464      95.19
 H       3.190261    -2.207153    -0.619587      24.44
 C       3.412829    -1.380635    -2.624274      91.94
 O       3.351520    -2.755700    -3.307501     252.61
 H       4.269500    -2.866640    -3.668726      26.40
 H       4.202793    -0.801118    -3.231863      24.66
 H       2.364436    -0.916632    -2.759353      26.03
 C      -0.253549    -0.856070     0.436015      17.69
 H      -1.008342    -1.537604     0.527485      20.47
 C       0.254075     1.523880     0.507683      66.44
 H      -0.210817     2.471442     0.396740      22.14
 C       1.554015     1.271699    -0.030220      12.58
 O       2.476537     2.259873    -0.379036     193.53
 C       2.101239     3.635980    -0.614369     111.40
 H       3.050025     4.286901    -1.164076      23.75
 H       1.289086     3.925432    -1.256149      26.71
 H       1.988694     4.253671     0.343502      26.18
 C       2.012673    -0.095067    -0.237885      17.54
 O       3.404511    -0.244727    -0.459713     155.25
 C       1.040853    -1.164027    -0.047123      59.70
 H       1.206344    -2.292465    -0.296678      21.90
 C      -0.718486     0.552736     0.645197      42.42
 C      -2.197506     0.805777     0.994072      97.65
 H      -2.584361     0.011759     1.551963      26.46
 O      -2.251340     1.979953     1.892216     232.86
 H      -1.851992     1.444108     2.802469      25.41
 C      -2.999265     1.081585    -0.231937      88.12
 H      -2.550141     1.802320    -1.053070      24.09
 O      -3.061085    -0.139979    -0.904078     230.99
 H      -2.993649     0.097365    -1.978766      22.74
 C      -4.397688     1.641252     0.009189     115.69
 O      -4.806219     2.581418    -0.933606     269.34
 H      -4.443419     3.437156    -0.710586      31.42
 H      -4.609260     1.739686     1.153054      28.56
 H      -5.021988     0.882442    -0.137169      31.32
55
name = lig-etoh-Waterframe_566
 C       6.268135    -1.199323     1.337118      34.08
 H       6.517371    -0.107395     1.032922      27.43
 C       5.589049    -3.448371     0.989692      83.28
 H       5.089991    -4.231767     0.423428      25.14
 C       5.962184    -3.812607     2.268408      18.10
 O       5.633898    -5.105713     2.831502     200.50
 C       4.796500    -5.985017     2.120312     130.23
 H       5.143940    -6.231931     1.186104      30.49
 H       3.735965    -5.428071     1.886127      25.42
 H       4.604362    -7.023980     2.616567      26.68
 C       6.471571    -2.891114     3.210867      17.50
 O       6.909009    -3.204999     4.412120     213.77
 H       6.508460    -4.096676     4.810962      22.47
 C       6.557075    -1.551428     2.690266      35.83
 H       6.777866    -0.822644     3.407617      21.57
 C       5.662533    -2.195516     0.449370      16.52
 C       5.311467    -1.810750    -0.903959     114.90
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 H       5.528597    -2.595019    -1.477113      29.64
 O       6.172288    -0.747391    -1.351536     119.72
 H       5.796710     0.182545    -1.164700      28.60
 C       3.786786    -1.577306    -1.158306      70.17
 H       3.271137    -2.437396    -0.897197      27.34
 C       3.412846    -1.442228    -2.655550     113.87
 O       3.395665    -2.775046    -3.201675     280.34
 H       4.247949    -2.924733    -3.705416      27.17
 H       4.163804    -0.781559    -3.117634      27.27
 H       2.517689    -0.981377    -2.744202      30.02
 C      -0.267679    -0.816525     0.493247      35.24
 H      -0.882102    -1.582787     0.457373      22.47
 C       0.244724     1.576455     0.484912      62.46
 H      -0.142599     2.650540     0.434393      19.81
 C       1.534219     1.290799    -0.033275       5.47
 O       2.497203     2.232362    -0.397608     195.41
 C       2.154141     3.636704    -0.614820     130.36
 H       2.817547     3.976002    -1.109501      30.22
 H       1.166878     3.531677    -1.078841      28.06
 H       1.890375     4.290143     0.181082      29.25
 C       2.004418    -0.041193    -0.338485      18.67
 O       3.417513    -0.144427    -0.447665      94.93
 C       1.092952    -1.055380    -0.101870      62.41
 H       1.460737    -2.061105    -0.323847      24.53
 C      -0.617600     0.430696     0.735543      60.78
 C      -2.107717     0.741119     0.977866      84.39
 H      -2.552100    -0.159274     1.418669      26.38
 O      -2.169042     2.004871     1.919195     194.96
 H      -2.107442     1.460627     2.906567      26.04
 C      -3.050676     1.109497    -0.281571      86.53
 H      -2.411435     1.899164    -0.772123      24.96
 O      -3.050173    -0.180333    -0.953047     198.93
 H      -3.171591    -0.160861    -2.098494      21.49
 C      -4.427530     1.584620     0.065503      89.32
 O      -4.823464     2.614462    -0.969699     235.49
 H      -4.698631     3.523770    -0.768405      31.28
 H      -4.546633     1.980660     1.105301      28.46
 H      -5.026492     0.588013    -0.138173      27.33
55
name = lig-etoh-Waterframe_567
 C       6.194245    -1.218171     1.333857      71.11
 H       6.433558    -0.200296     0.958440      28.81
 C       5.553513    -3.517580     1.035656      75.07
 H       5.093810    -4.250016     0.429713      25.42
 C       5.945493    -3.860402     2.322758      31.26
 O       5.675509    -5.119430     2.786614     238.81
 C       4.756568    -5.963423     2.107190     120.38
 H       5.164124    -6.143090     1.114074      27.67
 H       3.729805    -5.480246     2.039445      26.85
 H       4.606818    -6.884868     2.873869      25.50
 C       6.511831    -2.944187     3.183358      -6.22
 O       6.916206    -3.242298     4.459581     215.34
 H       6.662379    -4.166130     4.860465      28.28
 C       6.567774    -1.520819     2.704331      -5.57
 H       6.895250    -0.728555     3.405883      16.40
 C       5.655570    -2.179813     0.555443      20.53
 C       5.288559    -1.800702    -0.957076      90.04
 H       5.529677    -2.710144    -1.572305      26.34
 O       6.206367    -0.777681    -1.357326      90.47
 H       6.014860     0.084686    -0.846314      28.81
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 C       3.784345    -1.525204    -1.167837      76.32
 H       3.332232    -2.361334    -0.616833      26.36
 C       3.445440    -1.467683    -2.663143     115.26
 O       3.450144    -2.813227    -3.130078     292.50
 H       4.180057    -2.941748    -3.796221      28.70
 H       4.132814    -0.873781    -3.211543      27.44
 H       2.480005    -1.128013    -2.780224      29.43
 C      -0.125290    -0.893734     0.441001      49.91
 H      -0.796731    -1.779939     0.615157      22.33
 C       0.270484     1.584163     0.409849      88.65
 H      -0.033301     2.653326     0.795397      20.18
 C       1.532274     1.341799    -0.057028      18.34
 O       2.550019     2.232795    -0.379554     171.51
 C       2.086720     3.611386    -0.620514      96.03
 H       2.972849     3.952697    -1.430041      23.41
 H       1.215340     3.505243    -1.346367      25.52
 H       2.166509     4.012690     0.381318      26.70
 C       1.989834     0.054946    -0.320857      23.85
 O       3.401101    -0.174100    -0.505915     114.20
 C       1.098558    -0.996946    -0.114349      63.02
 H       1.392536    -1.964656    -0.238794      25.88
 C      -0.615455     0.477866     0.787149      57.88
 C      -2.047666     0.776903     1.036202      82.23
 H      -2.592209    -0.141378     1.491329      21.68
 O      -2.121449     1.942170     1.920400     243.00
 H      -1.934909     1.729343     2.994452      25.98
 C      -2.939914     1.100390    -0.280437      59.89
 H      -2.560086     1.946056    -0.812177      25.82
 O      -3.053821    -0.241646    -1.015775     213.02
 H      -3.067741    -0.104432    -2.122801      22.09
 C      -4.473820     1.576787     0.076653      77.42
 O      -4.877650     2.628534    -1.005684     226.55
 H      -4.589015     3.314744    -0.448779      30.11
 H      -4.478168     2.165865     0.930897      27.81
 H      -5.413638     0.736148    -0.050986      25.35
55
name = lig-etoh-Waterframe_568
 C       6.170722    -1.199838     1.472198      76.35
 H       6.190414    -0.225477     1.092890      31.44
 C       5.474022    -3.548549     1.010249      56.13
 H       5.134504    -4.252146     0.301314      23.25
 C       5.888598    -3.915687     2.327883       5.65
 O       5.756568    -5.173201     2.813349     222.80
 C       4.689840    -5.944379     2.096197     117.89
 H       5.073028    -6.475076     1.119962      25.95
 H       3.778546    -5.502877     2.091443      29.16
 H       4.718014    -6.879833     2.780048      25.10
 C       6.542982    -2.852837     3.147635       1.81
 O       6.955521    -3.251607     4.528860      76.46
 H       6.545756    -4.139732     4.640496      28.73
 C       6.592520    -1.581373     2.719038      75.00
 H       7.139059    -0.771089     3.319483      14.92
 C       5.632127    -2.207263     0.559124      -0.11
 C       5.287656    -1.822854    -0.904775      50.75
 H       5.474764    -2.703126    -1.751179      22.17
 O       6.218232    -0.765421    -1.398681      43.19
 H       6.135389    -0.047004    -0.686549      30.73
 C       3.797931    -1.405454    -1.138818     101.35
 H       3.156880    -2.172321    -0.550445      24.27
 C       3.445072    -1.476819    -2.647305      94.33
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 O       3.502173    -2.900410    -3.116033     264.24
 H       4.298520    -2.861477    -3.737691      26.14
 H       4.123667    -0.891496    -3.239234      26.06
 H       2.342664    -1.086967    -2.859992      25.50
 C      -0.114702    -0.830200     0.435631      48.47
 H      -0.652106    -1.865000     0.859341      21.48
 C       0.244157     1.551604     0.414317      60.47
 H      -0.052375     2.618576     0.808864      19.03
 C       1.618350     1.381574    -0.117495      19.69
 O       2.597257     2.274040    -0.358271     240.81
 C       2.085841     3.540774    -0.688050     102.72
 H       3.061370     4.390423    -1.311265      21.05
 H       1.049753     3.920577    -1.008468      24.95
 H       1.993815     4.261193     0.258146      25.41
 C       2.032190     0.045143    -0.273485      21.96
 O       3.368012    -0.229794    -0.601741     166.61
 C       1.173680    -1.056987    -0.125937      66.69
 H       1.469573    -2.004923    -0.319077      23.86
 C      -0.556403     0.484389     0.700061      44.39
 C      -2.054898     0.815173     1.106929      76.90
 H      -2.520254    -0.091886     1.684143      22.50
 O      -2.117599     1.921520     1.920273     266.30
 H      -1.515515     1.401497     2.709080      21.93
 C      -2.916968     1.015470    -0.252217      67.83
 H      -2.543531     1.674378    -0.982991      25.40
 O      -3.032083    -0.238620    -1.026973     260.06
 H      -2.874656    -0.041141    -2.004397      25.41
 C      -4.478865     1.626932    -0.002825      96.50
 O      -4.912078     2.621054    -0.979841     293.21
 H      -4.555338     3.471710    -0.741682      31.40
 H      -4.456157     2.004857     0.988213      28.04
 H      -5.275428     0.781727     0.292397      26.56
55
name = lig-etoh-Waterframe_569
 C       6.093463    -1.217843     1.487848      42.07
 H       6.101005    -0.177964     1.432432      17.15
 C       5.424341    -3.538376     0.988057      63.83
 H       5.132833    -4.315799     0.293010      22.86
 C       5.875895    -3.840086     2.297722       0.75
 O       5.802588    -5.253812     2.821246     200.31
 C       4.694362    -6.025263     2.165046      96.90
 H       4.976845    -6.237972     1.006795      25.50
 H       3.866503    -5.407418     2.069439      31.18
 H       4.407961    -6.876162     2.732050      26.24
 C       6.524294    -2.963109     3.232691      -4.87
 O       6.976805    -3.215529     4.469052     207.12
 H       6.603616    -4.063816     4.891548      24.05
 C       6.680444    -1.570761     2.761628     -33.41
 H       7.260633    -0.876813     3.492489      21.76
 C       5.620399    -2.206807     0.566946      29.40
 C       5.296760    -1.783482    -0.836578      89.12
 H       5.397152    -2.818988    -1.474232      25.60
 O       6.181629    -0.753562    -1.425482      58.26
 H       6.333922     0.034748    -0.803236      26.83
 C       3.778696    -1.428847    -1.140904      85.13
 H       3.260309    -2.411033    -0.817601      25.99
 C       3.431266    -1.524958    -2.652198      88.34
 O       3.539617    -2.936859    -3.116770     252.04
 H       4.364063    -2.982058    -3.733575      26.29
 H       4.148066    -0.881755    -3.205550      26.35
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 H       2.277489    -1.054655    -2.818301      25.37
 C      -0.089651    -0.803742     0.447259      31.13
 H      -0.872930    -1.699388     0.810289      18.36
 C       0.365035     1.581207     0.397500      60.31
 H      -0.179951     2.572686     0.457006      20.04
 C       1.611323     1.315035    -0.108050      -2.40
 O       2.617476     2.360035    -0.368555     176.17
 C       2.106336     3.716726    -0.675423      82.60
 H       2.947433     4.039165    -1.525590      21.99
 H       1.166851     3.317208    -1.217091      23.60
 H       2.052570     4.248616     0.343391      24.59
 C       2.091058    -0.062800    -0.265421      26.83
 O       3.379635    -0.136776    -0.669478     152.61
 C       1.197571    -1.110459    -0.084225      69.42
 H       1.509904    -2.108539    -0.365690      24.75
 C      -0.589778     0.457581     0.591361      67.48
 C      -2.075398     0.748978     1.034168      86.69
 H      -2.394709    -0.151131     1.565901      25.66
 O      -2.095486     1.936168     1.970191     272.45
 H      -1.562210     1.666735     2.804854      29.78
 C      -3.010190     0.958979    -0.261683      92.32
 H      -2.248544     1.677898    -0.738814      24.19
 O      -2.993994    -0.248725    -0.984380     302.51
 H      -2.875212    -0.113686    -1.910401      27.30
 C      -4.385562     1.666591     0.005116     104.39
 O      -4.941656     2.600184    -0.948070     291.23
 H      -4.525002     3.438951    -0.930043      33.09
 H      -4.312494     2.208394     1.017741      26.35
 H      -5.008868     0.869182    -0.191934      27.83
55
name = lig-etoh-Waterframe_570
 C       6.085644    -1.233438     1.573462      36.54
 H       6.011042    -0.173853     1.205577      20.83
 C       5.449221    -3.494600     1.017027      48.98
 H       5.067781    -4.305435     0.340906      22.59
 C       5.873242    -3.915035     2.332886       8.18
 O       5.812315    -5.280479     2.779731     245.55
 C       4.709861    -6.054092     2.221841     111.61
 H       5.087901    -6.330389     1.176716      26.74
 H       3.820591    -5.291380     2.194489      26.23
 H       4.436158    -6.886062     2.735347      27.07
 C       6.474217    -2.975024     3.210027      20.82
 O       7.004452    -3.223191     4.439699     285.16
 H       6.724553    -4.103678     4.879179      18.65
 C       6.712789    -1.664131     2.783837      53.75
 H       7.082271    -0.862829     3.464167      29.40
 C       5.594397    -2.128598     0.614822      35.78
 C       5.254495    -1.721545    -0.823084     110.14
 H       5.574549    -2.581046    -1.367673      28.11
 O       6.132857    -0.762450    -1.449200     113.74
 H       6.230969     0.046180    -0.842900      27.02
 C       3.809336    -1.550470    -1.201300      78.81
 H       3.223116    -2.198824    -0.507593      25.50
 C       3.456204    -1.568606    -2.672569      97.40
 O       3.532917    -2.928360    -3.110978     275.33
 H       4.297291    -2.900522    -3.804058      26.07
 H       4.116819    -0.914582    -3.313179      24.72
 H       2.331504    -1.320864    -2.818884      25.52
 C      -0.098812    -0.857203     0.444649      34.63
 H      -0.840356    -1.677386     0.492325      19.07
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 C       0.352479     1.568627     0.345419      55.80
 H       0.133327     2.606466     0.234158      21.88
 C       1.690360     1.287547    -0.072661       1.44
 O       2.608785     2.369620    -0.356918     163.65
 C       2.122296     3.765405    -0.705597     119.06
 H       2.686636     4.152666    -1.303095      30.51
 H       1.195915     3.747235    -1.372456      26.71
 H       2.046716     4.496292     0.098856      27.51
 C       2.095051    -0.065374    -0.261583      17.25
 O       3.435983    -0.069963    -0.726442      98.96
 C       1.192450    -1.153072    -0.009516      61.34
 H       1.362526    -2.302082    -0.169557      23.18
 C      -0.603462     0.533999     0.518613      49.22
 C      -2.064720     0.675165     0.979379      91.70
 H      -2.407775    -0.178040     1.471630      27.76
 O      -2.092959     1.945222     1.969607     219.14
 H      -1.814361     1.511009     2.783662      28.74
 C      -2.968622     1.043412    -0.248139      83.26
 H      -2.384424     1.915123    -0.851924      23.12
 O      -2.980581    -0.299326    -0.948675     262.63
 H      -3.064615    -0.191489    -1.830005      28.75
 C      -4.300035     1.650787     0.012394     104.71
 O      -4.946241     2.606010    -0.961625     261.36
 H      -4.430239     3.362838    -0.761316      32.43
 H      -4.386545     2.127749     1.110160      26.61
 H      -5.019008     0.898295    -0.006931      29.07
55
name = lig-etoh-Waterframe_571
 C       6.121180    -1.203369     1.613220      52.00
 H       6.262309    -0.079902     1.313268      20.57
 C       5.501407    -3.466420     1.090133      66.14
 H       5.027196    -4.116096     0.277573      25.32
 C       5.863462    -4.002911     2.328956      22.06
 O       5.821604    -5.276000     2.751513     243.79
 C       4.728466    -6.046136     2.233329     124.30
 H       4.869205    -6.527508     1.334609      29.30
 H       3.610583    -5.514622     2.195316      24.41
 H       4.750746    -6.845297     2.939097      26.97
 C       6.464801    -2.994223     3.185779       5.16
 O       7.038222    -3.281477     4.456785     194.28
 H       6.679973    -4.198071     4.639279      19.84
 C       6.648575    -1.685585     2.757169      79.78
 H       7.037944    -1.050939     3.519467      31.11
 C       5.542060    -2.091196     0.696655       9.34
 C       5.274260    -1.755240    -0.852570     100.35
 H       5.538230    -2.577628    -1.359142      29.30
 O       6.097219    -0.732208    -1.453295     170.92
 H       5.906603     0.159093    -0.996905      27.10
 C       3.817390    -1.516096    -1.184394      88.66
 H       3.191456    -2.131873    -0.581014      25.33
 C       3.435265    -1.615748    -2.683243     106.30
 O       3.511729    -2.945719    -3.142977     290.12
 H       4.291681    -3.084240    -3.803151      25.98
 H       4.060059    -0.882904    -3.253024      25.49
 H       2.502910    -1.236210    -2.739614      29.06
 C      -0.158212    -0.829928     0.401526      50.95
 H      -0.744318    -1.598442     0.475917      26.05
 C       0.331022     1.564763     0.247047      71.47
 H       0.073826     2.549191     0.402409      23.43
 C       1.708774     1.316602    -0.032691      22.49
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 O       2.574538     2.374010    -0.342494     149.69
 C       2.099377     3.753900    -0.766782     104.30
 H       3.126012     4.313199    -1.323192      23.38
 H       1.163434     3.985715    -1.129987      28.32
 H       2.036195     4.342901     0.118320      28.29
 C       2.154853    -0.014542    -0.265486       0.36
 O       3.472918    -0.122449    -0.784544     136.94
 C       1.191148    -1.144174     0.071014      41.95
 H       1.530889    -2.295984    -0.009874      21.67
 C      -0.568705     0.491824     0.505116      26.63
 C      -2.020634     0.775785     0.956331      93.30
 H      -2.447713    -0.116838     1.378133      25.32
 O      -2.114208     1.871397     1.920706     296.95
 H      -1.892448     1.403237     2.642042      31.11
 C      -2.853487     1.117182    -0.278344      71.90
 H      -2.444894     1.729227    -1.115660      25.59
 O      -2.986958    -0.307256    -0.915448     233.12
 H      -3.208020    -0.236512    -1.802816      29.50
 C      -4.373349     1.597741     0.044799      89.89
 O      -4.875228     2.616877    -0.957074     245.65
 H      -4.582742     3.493074    -0.749127      31.18
 H      -4.211576     2.160657     1.053081      26.16
 H      -5.064430     0.727236     0.395196      27.61
55
name = lig-etoh-Waterframe_572
 C       6.152645    -1.109398     1.537903      30.77
 H       6.471428    -0.025310     1.511144      24.21
 C       5.480470    -3.446985     1.078939      71.72
 H       5.106002    -4.199239     0.326157      26.52
 C       5.912023    -3.910302     2.322199      26.30
 O       5.818066    -5.285660     2.719167     136.61
 C       4.712722    -6.141560     2.270132     116.80
 H       4.907437    -6.498606     1.317925      28.40
 H       3.684756    -5.535801     2.363003      25.48
 H       4.686405    -6.930235     3.083742      25.98
 C       6.509793    -3.077473     3.228412      21.42
 O       7.037623    -3.371715     4.417484     166.63
 H       6.782714    -4.200552     4.994177      24.18
 C       6.588741    -1.670616     2.840630      -9.93
 H       7.151573    -1.103512     3.516406      18.82
 C       5.525617    -2.078813     0.716746      14.83
 C       5.311236    -1.823502    -0.834126      65.13
 H       5.500583    -2.799793    -1.393015      25.76
 O       6.082638    -0.675959    -1.430740     144.07
 H       5.559421     0.176124    -1.260030      26.84
 C       3.793779    -1.463810    -1.161347     101.78
 H       3.313498    -2.296105    -0.778410      27.73
 C       3.414198    -1.601614    -2.666157     103.59
 O       3.462713    -3.004539    -3.197879     269.30
 H       4.304295    -3.022436    -3.764571      25.24
 H       4.146304    -1.029724    -3.253520      26.65
 H       2.440629    -1.240198    -2.781728      28.56
 C      -0.137665    -0.844086     0.343401      58.82
 H      -0.822670    -1.571519     0.670261      24.61
 C       0.321635     1.554089     0.196122      77.67
 H      -0.167925     2.409286     0.518198      22.53
 C       1.665273     1.368082    -0.057718      16.16
 O       2.538930     2.390513    -0.357971     157.54
 C       2.117701     3.765587    -0.725984      79.00
 H       3.259908     3.970169    -1.605368      21.15
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 H       1.266728     3.616093    -1.360301      25.68
 H       2.247860     4.175186     0.245515      25.42
 C       2.169996    -0.024924    -0.232076      20.44
 O       3.462936    -0.191816    -0.805525     195.46
 C       1.269207    -1.011275     0.109701      62.12
 H       1.618641    -2.113746     0.085401      24.04
 C      -0.558877     0.489054     0.519312      13.90
 C      -1.964905     0.902256     0.878577      86.47
 H      -2.446479    -0.091003     1.251872      22.13
 O      -2.134793     1.796124     1.889776     317.25
 H      -1.730866     1.494873     2.677921      30.79
 C      -2.892434     1.067553    -0.392090      77.40
 H      -2.363621     1.723045    -1.013514      26.90
 O      -2.995266    -0.274462    -0.868608     269.28
 H      -3.117068    -0.196228    -1.873246      25.28
 C      -4.344386     1.653656     0.113210      83.05
 O      -4.810312     2.574295    -0.939700     270.60
 H      -4.577070     3.409053    -0.545024      30.75
 H      -4.240292     2.237957     0.986363      27.31
 H      -5.137841     0.723226     0.004510      25.98
55
name = lig-etoh-Waterframe_573
 C       6.219272    -1.119187     1.617888      41.85
 H       6.275623    -0.159376     1.110920      24.43
 C       5.429944    -3.419346     1.046152      52.20
 H       5.144667    -4.226612     0.383312      22.26
 C       5.914185    -3.913607     2.294314       3.58
 O       5.823038    -5.285032     2.696778     174.05
 C       4.696071    -6.199105     2.332049     102.16
 H       4.950257    -6.542364     1.288044      25.15
 H       3.808198    -5.637338     2.351600      29.28
 H       4.605976    -7.236003     2.902692      23.23
 C       6.544661    -3.014568     3.252287      12.77
 O       7.086863    -3.464468     4.430939     175.18
 H       6.558847    -4.300678     4.865155      21.58
 C       6.554442    -1.654744     2.892913      55.05
 H       7.121219    -0.970589     3.496268      20.25
 C       5.583816    -2.037606     0.623224      10.20
 C       5.276332    -1.783746    -0.815843      85.31
 H       5.723889    -2.737720    -1.484347      21.06
 O       6.078734    -0.665339    -1.387768     166.72
 H       5.409913     0.087391    -1.358090      26.57
 C       3.810531    -1.603480    -1.204395      87.09
 H       3.196276    -2.266551    -0.581570      22.61
 C       3.431908    -1.612763    -2.691392      95.14
 O       3.400642    -3.030389    -3.232765     264.72
 H       4.165105    -3.123023    -3.892061      25.44
 H       4.088853    -1.025762    -3.332697      25.36
 H       2.319683    -1.257469    -2.909262      24.16
 C      -0.065115    -0.814052     0.353552      67.57
 H      -0.679665    -1.792150     0.736524      20.82
 C       0.280119     1.570566     0.229268      48.69
 H      -0.011642     2.658115     0.286069      18.49
 C       1.652523     1.372217    -0.154921      23.78
 O       2.559566     2.367112    -0.376881     235.99
 C       2.217029     3.673155    -0.702827     128.97
 H       2.840879     4.222193    -1.454033      24.90
 H       1.207243     3.756878    -1.321000      25.71
 H       2.024925     4.649600    -0.074853      24.80
 C       2.150527     0.087748    -0.194042      25.12
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 O       3.407348    -0.190403    -0.746133     163.87
 C       1.302818    -0.986443     0.125097      60.34
 H       1.713607    -1.960778     0.116450      22.19
 C      -0.550909     0.503484     0.472829      48.15
 C      -1.986480     0.808400     0.777141      73.15
 H      -2.367993    -0.193985     1.244881      19.91
 O      -2.151537     1.840886     1.902704     208.95
 H      -1.539646     1.343256     2.647547      23.07
 C      -2.955976     1.072335    -0.390011      84.00
 H      -2.620129     1.760427    -1.144516      23.94
 O      -3.023537    -0.254440    -0.884233     257.85
 H      -2.906516    -0.272208    -1.957625      23.26
 C      -4.245990     1.700009     0.065955     107.99
 O      -4.764797     2.562916    -0.915872     330.37
 H      -4.478593     3.484309    -0.719555      30.06
 H      -4.349497     1.938631     1.047979      29.17
 H      -5.053265     0.817962     0.150004      26.42
55
name = lig-etoh-Waterframe_574
 C       6.191326    -1.233305     1.579555      59.03
 H       6.344707    -0.170452     1.398495      22.78
 C       5.417665    -3.406518     1.036784      57.95
 H       4.993095    -4.016498     0.291515      23.98
 C       5.872617    -3.930501     2.279240      -3.95
 O       5.828994    -5.286332     2.712441     249.45
 C       4.706712    -6.197690     2.301438      93.20
 H       4.780474    -6.551131     1.164933      23.88
 H       3.783345    -5.824367     2.391182      32.00
 H       4.899418    -7.057693     3.090327      21.49
 C       6.515098    -2.989840     3.228730     -33.79
 O       7.152586    -3.501005     4.421833     284.11
 H       6.746927    -4.386903     4.693841      26.04
 C       6.604390    -1.577053     2.913139      35.20
 H       6.947881    -0.863960     3.721718      22.52
 C       5.690369    -2.065476     0.652142      41.12
 C       5.290532    -1.703984    -0.866142      82.56
 H       5.670364    -2.704499    -1.413368      23.01
 O       6.054710    -0.660467    -1.343148     204.42
 H       5.627138     0.244685    -1.292235      25.08
 C       3.775572    -1.688918    -1.221116      50.35
 H       3.151634    -2.451040    -0.607868      20.83
 C       3.432693    -1.700527    -2.769439      99.08
 O       3.347438    -3.027885    -3.268689     287.37
 H       4.084346    -3.193793    -3.918123      26.16
 H       4.096169    -0.993898    -3.265332      25.32
 H       2.322022    -1.124757    -2.711375      23.34
 C       0.010107    -0.771523     0.444485      18.81
 H      -0.688551    -1.840918     0.513643      17.37
 C       0.334529     1.655837     0.234696      59.99
 H      -0.099948     2.760041     0.094004      18.88
 C       1.590442     1.404845    -0.214065      18.79
 O       2.648831     2.373854    -0.386012     186.37
 C       2.206686     3.715319    -0.787239     104.78
 H       2.924887     4.046642    -1.365097      26.66
 H       1.106662     3.612444    -1.217201      23.49
 H       2.148166     4.336339     0.312175      23.56
 C       2.149621     0.085973    -0.208443      19.08
 O       3.404604    -0.170231    -0.679559      88.31
 C       1.321085    -1.009898     0.130558      68.80
 H       1.647337    -1.944881     0.186436      23.93
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 C      -0.587842     0.516141     0.397433      57.74
 C      -2.053029     0.708128     0.808534      86.06
 H      -2.502379    -0.211064     1.232575      23.40
 O      -2.125932     1.864645     1.867929     159.85
 H      -1.742556     1.330157     2.857802      21.28
 C      -2.928116     1.121235    -0.350296      79.47
 H      -2.547399     1.716946    -1.237788      20.74
 O      -3.077865    -0.298936    -0.973715     198.48
 H      -2.974898    -0.179373    -2.097662      20.88
 C      -4.260414     1.646454     0.050428      96.06
 O      -4.751493     2.627104    -0.919495     330.66
 H      -4.301521     3.515857    -0.825304      30.10
 H      -4.095686     2.139923     1.111349      24.80
 H      -4.884321     0.826597     0.050865      28.66
55
name = lig-etoh-Waterframe_575
 C       6.222982    -1.190729     1.617429      24.24
 H       6.343177    -0.126739     1.445866      19.92
 C       5.427409    -3.453581     1.036980      59.24
 H       4.864267    -4.045566     0.355413      22.56
 C       5.842428    -3.909521     2.302069      11.77
 O       5.799803    -5.244796     2.707710     299.84
 C       4.761110    -6.161009     2.276017     111.19
 H       4.922881    -6.546135     1.176760      25.91
 H       3.745123    -5.800871     2.607056      27.90
 H       4.996686    -7.032035     2.961959      22.67
 C       6.502973    -3.011840     3.225321      19.70
 O       7.207169    -3.465931     4.317353     273.25
 H       6.803492    -4.213128     4.777301      19.47
 C       6.637889    -1.640675     2.906407      29.46
 H       6.844250    -0.819136     3.692645      26.40
 C       5.704511    -2.153843     0.627056      11.83
 C       5.306112    -1.738682    -0.844280      88.58
 H       5.616061    -2.488002    -1.466995      27.35
 O       6.066993    -0.600301    -1.353271     184.23
 H       5.752795     0.225453    -0.859223      25.46
 C       3.772247    -1.627848    -1.210121      65.07
 H       3.296949    -2.616035    -0.782983      21.93
 C       3.407439    -1.712906    -2.737015      99.34
 O       3.313866    -3.039790    -3.325223     270.07
 H       4.145150    -3.099342    -3.849372      26.31
 H       4.175826    -1.208587    -3.333958      24.38
 H       2.339793    -1.294601    -2.949440      24.51
 C      -0.022447    -0.724787     0.511543      40.98
 H      -0.845671    -1.564691     0.618073      17.61
 C       0.272112     1.688037     0.181255      57.43
 H      -0.272929     2.752353     0.317338      18.64
 C       1.681886     1.437020    -0.227667      -1.46
 O       2.692573     2.367045    -0.422613     170.02
 C       2.168965     3.744480    -0.784065      90.51
 H       3.152919     4.114133    -1.556460      21.64
 H       1.246855     3.718749    -1.427832      24.13
 H       2.338348     4.196169     0.200393      24.47
 C       2.135957     0.000025    -0.261651      14.75
 O       3.458806    -0.199359    -0.652358     129.17
 C       1.347017    -1.029262     0.154626      63.64
 H       1.655972    -2.003850     0.202718      23.55
 C      -0.576782     0.544653     0.394032      48.89
 C      -2.060403     0.726823     0.908795      88.69
 H      -2.481669    -0.146776     1.292387      26.06
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 O      -2.093901     1.824072     1.804188     236.00
 H      -1.809100     1.426695     2.861893      23.20
 C      -2.889373     1.040530    -0.397697      67.56
 H      -2.130257     1.805897    -0.891145      20.47
 O      -3.132756    -0.316019    -1.075187     204.30
 H      -3.256027    -0.104884    -2.215761      19.80
 C      -4.311358     1.651518     0.037702      90.53
 O      -4.760770     2.688420    -0.946557     316.59
 H      -4.310079     3.497725    -0.524211      26.94
 H      -4.126420     2.337806     1.041420      23.26
 H      -5.019580     0.931743     0.092644      28.08
55
name = lig-etoh-Waterframe_576
 C       6.256611    -1.168147     1.622681      69.94
 H       6.255383    -0.186318     1.232910      24.57
 C       5.428966    -3.507576     1.039656      49.68
 H       4.984980    -4.349002     0.466664      20.03
 C       5.824663    -3.895972     2.337690      21.04
 O       5.776585    -5.180045     2.710638     277.18
 C       4.840392    -6.141068     2.290381     113.72
 H       4.893280    -6.270947     1.204421      28.31
 H       3.686368    -5.682806     2.431899      24.31
 H       4.912106    -7.072811     2.733613      25.03
 C       6.508771    -3.040956     3.187950      34.26
 O       7.258875    -3.440675     4.244943     278.86
 H       6.641049    -4.067884     4.700016      28.75
 C       6.612749    -1.710473     2.843140      63.96
 H       7.128887    -1.064892     3.645448      21.19
 C       5.686299    -2.128571     0.612395     -15.97
 C       5.341064    -1.791491    -0.850094      76.84
 H       5.684396    -2.519837    -1.493193      25.92
 O       6.078069    -0.526553    -1.347674     143.02
 H       5.942108     0.093248    -0.592959      29.31
 C       3.829883    -1.533632    -1.185917      94.33
 H       3.225634    -2.232214    -0.562301      23.35
 C       3.387966    -1.664561    -2.718075      97.06
 O       3.326714    -3.074774    -3.353208     262.78
 H       4.141246    -3.201638    -3.886608      26.71
 H       4.119670    -1.102606    -3.331164      25.69
 H       2.506632    -1.199077    -2.902628      28.36
 C      -0.061696    -0.731343     0.520582      52.81
 H      -0.634229    -1.437601     0.936042      23.66
 C       0.282796     1.654275     0.085077      72.89
 H      -0.004970     2.685294     0.398852      20.85
 C       1.699839     1.372900    -0.182382      11.99
 O       2.672568     2.369514    -0.504925     154.89
 C       2.254042     3.727440    -0.778965     119.19
 H       3.029834     4.490879    -1.599748      22.82
 H       1.305304     3.838747    -1.199600      27.19
 H       2.018805     4.474683    -0.126736      27.78
 C       2.149540     0.036569    -0.317951       5.89
 O       3.504336    -0.296688    -0.656405     179.81
 C       1.244821    -1.060383     0.211175      43.49
 H       1.693294    -2.093805     0.196970      20.11
 C      -0.550829     0.586981     0.489967      13.36
 C      -2.009817     0.721595     0.907956      88.56
 H      -2.237033    -0.171185     1.469301      23.20
 O      -2.092347     1.819390     1.778065     263.62
 H      -1.571614     1.381099     2.630119      23.71
 C      -2.934439     0.923294    -0.383298      67.32
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 H      -2.402053     1.688825    -1.081080      22.59
 O      -3.172139    -0.256556    -1.124235     265.11
 H      -3.106611    -0.193970    -2.194288      22.00
 C      -4.300149     1.731212    -0.041228     101.79
 O      -4.765095     2.717454    -0.961069     301.53
 H      -4.667370     3.731014    -0.657975      25.30
 H      -4.301330     2.017423     1.076316      25.67
 H      -5.168851     0.977342     0.188412      26.59
55
name = lig-etoh-Waterframe_577
 C       6.206271    -1.237043     1.472709      48.75
 H       6.417675    -0.171421     1.426612      24.69
 C       5.440963    -3.467774     1.041060      76.70
 H       5.219045    -4.237748     0.223168      24.29
 C       5.785630    -3.897792     2.298678      18.39
 O       5.795558    -5.189745     2.793702     223.15
 C       4.837316    -6.089956     2.218711     124.11
 H       4.981155    -6.184526     1.207903      28.64
 H       3.703996    -5.717014     2.433621      25.05
 H       4.998949    -6.923955     2.749525      27.27
 C       6.538271    -3.019369     3.119837       0.65
 O       7.281963    -3.467566     4.243977     188.85
 H       6.831990    -4.246451     4.761359      27.82
 C       6.633786    -1.674290     2.798928      34.36
 H       7.364743    -1.190351     3.446548      19.37
 C       5.651131    -2.132248     0.642494      40.95
 C       5.406762    -1.740727    -0.896905      71.90
 H       5.781241    -2.713229    -1.498390      25.61
 O       6.081295    -0.517084    -1.309755     149.24
 H       6.049186     0.231448    -0.673028      26.29
 C       3.851495    -1.574326    -1.159589      86.98
 H       3.353668    -2.329671    -0.627058      27.20
 C       3.427101    -1.632086    -2.735132      96.32
 O       3.357880    -3.065367    -3.318741     259.82
 H       4.101228    -3.066022    -3.973181      26.81
 H       4.131056    -0.973430    -3.293726      26.96
 H       2.475288    -1.239117    -2.701160      28.54
 C      -0.087829    -0.776173     0.561261      49.57
 H      -0.545325    -1.470401     1.102592      25.32
 C       0.379418     1.598763     0.051340      76.84
 H       0.154479     2.600117     0.092332      23.54
 C       1.688190     1.326386    -0.189867       6.98
 O       2.643022     2.394774    -0.580555     122.48
 C       2.254599     3.778619    -0.819698     111.46
 H       3.174440     4.015589    -1.448468      24.44
 H       1.378673     3.577374    -1.377000      25.50
 H       2.142590     4.384778     0.237503      24.79
 C       2.131765    -0.052015    -0.297746      24.15
 O       3.499389    -0.268646    -0.648325     165.49
 C       1.251377    -0.987480     0.174452      54.11
 H       1.465612    -2.169680     0.335224      22.39
 C      -0.518458     0.596688     0.546688      27.15
 C      -1.964866     0.692087     0.825965      79.18
 H      -2.263192    -0.283438     1.373229      23.07
 O      -2.102102     1.858471     1.804993     265.38
 H      -1.600048     1.649629     2.582205      29.13
 C      -3.026479     0.955321    -0.382919      82.66
 H      -2.563730     1.575602    -1.100101      25.28
 O      -3.210503    -0.255395    -1.109647     292.35
 H      -2.948945    -0.095878    -1.944868      28.77
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 C      -4.314976     1.737610    -0.027243      87.57
 O      -4.787551     2.730933    -1.009520     247.27
 H      -4.403909     3.693861    -0.623232      24.37
 H      -4.137305     2.239628     0.869878      25.73
 H      -5.137141     0.863969    -0.320206      24.00
55
name = lig-etoh-Waterframe_578
 C       6.215811    -1.233067     1.488437      45.08
 H       6.439560    -0.181146     1.062736      23.15
 C       5.439169    -3.451516     0.976376      62.30
 H       5.137203    -4.112629     0.096468      21.94
 C       5.815534    -3.906521     2.301324       9.91
 O       5.804362    -5.206211     2.862369     268.36
 C       4.813424    -6.059642     2.159604     129.98
 H       5.076016    -6.269320     1.128703      28.15
 H       3.835581    -5.711007     2.387379      25.88
 H       4.967947    -7.016883     2.652991      25.84
 C       6.578801    -3.001917     3.133051       1.67
 O       7.280016    -3.500734     4.238727     209.71
 H       6.741170    -4.366172     4.583010      27.10
 C       6.708459    -1.642737     2.714811      77.41
 H       7.275116    -0.889274     3.156682      24.29
 C       5.599739    -2.124625     0.538970      23.51
 C       5.414456    -1.669181    -0.865091      76.64
 H       5.918769    -2.491895    -1.683370      22.08
 O       6.119744    -0.542164    -1.293571     204.19
 H       5.755206     0.191424    -0.748937      26.81
 C       3.894482    -1.675925    -1.201192      64.41
 H       3.475939    -2.549413    -0.799628      23.49
 C       3.469757    -1.644563    -2.687302      96.73
 O       3.422982    -2.979994    -3.257438     272.35
 H       4.060561    -3.005799    -4.020506      26.48
 H       4.083415    -1.009224    -3.382416      24.88
 H       2.320299    -1.335274    -2.757231      24.21
 C      -0.043437    -0.735816     0.626018      42.29
 H      -0.712746    -1.598305     1.045711      20.00
 C       0.404052     1.580734     0.088024      61.71
 H      -0.026238     2.457795    -0.186956      23.21
 C       1.776275     1.320548    -0.288633      13.22
 O       2.623776     2.315562    -0.618039     183.19
 C       2.228719     3.746106    -0.864887     109.81
 H       2.995643     4.115415    -1.275152      29.62
 H       1.389489     4.102847    -1.627621      24.34
 H       2.346881     4.244148     0.276698      23.78
 C       2.183172    -0.070832    -0.259461      28.33
 O       3.456228    -0.217300    -0.637543     122.99
 C       1.243674    -1.043503     0.150049      60.81
 H       1.754810    -2.142658     0.235592      22.82
 C      -0.503728     0.521291     0.506523      48.11
 C      -2.011372     0.778156     0.822141      75.70
 H      -2.483800    -0.238901     1.162550      23.62
 O      -2.135199     1.892932     1.804412     267.07
 H      -1.752626     1.568687     2.526564      30.56
 C      -2.995220     1.087135    -0.408995      79.60
 H      -2.443686     1.770741    -0.960513      25.58
 O      -3.265991    -0.300522    -1.057553     241.57
 H      -3.071125    -0.245040    -1.927948      28.27
 C      -4.369758     1.700582    -0.052577      95.03
 O      -4.781504     2.746270    -1.062032     270.93
 H      -4.125056     3.559289    -0.879767      27.37
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 H      -4.377319     2.132805     0.877563      27.84
 H      -5.240180     0.911849     0.137453      25.97
55
name = lig-etoh-Waterframe_579
 C       6.213175    -1.211821     1.427537      53.08
 H       6.452104    -0.153736     1.012162      20.08
 C       5.429438    -3.488652     0.921016      47.91
 H       4.912998    -4.314225     0.419154      19.26
 C       5.905961    -3.866174     2.290279      -5.21
 O       5.773605    -5.207608     2.839679     263.71
 C       4.836085    -6.083651     2.161810     115.76
 H       5.045507    -6.044602     0.984154      26.97
 H       3.920911    -5.672187     2.195934      30.59
 H       4.752953    -7.186247     2.601419      24.69
 C       6.618750    -2.980764     3.139683       6.43
 O       7.245115    -3.525977     4.222298     243.88
 H       6.654708    -4.359693     4.585142      20.97
 C       6.807287    -1.621487     2.656063      42.94
 H       7.205345    -0.869276     3.297138      23.96
 C       5.631394    -2.097851     0.548136      29.71
 C       5.386768    -1.696130    -0.916132      96.93
 H       5.809961    -2.542372    -1.523768      23.40
 O       6.159041    -0.502888    -1.266863     224.04
 H       5.642073     0.278726    -1.034428      26.06
 C       3.939561    -1.662150    -1.267370      80.58
 H       3.412186    -2.437352    -0.663744      23.13
 C       3.471194    -1.645744    -2.663924     102.74
 O       3.509408    -2.929571    -3.213650     287.11
 H       4.201241    -3.038516    -3.931504      26.15
 H       4.100457    -0.913052    -3.214298      25.07
 H       2.343634    -1.097410    -2.704694      23.76
 C       0.045896    -0.793829     0.672687      23.52
 H      -0.885964    -1.668640     0.820038      18.91
 C       0.387548     1.545156     0.092388      67.74
 H      -0.109073     2.495056    -0.213823      22.11
 C       1.693718     1.293586    -0.328430      26.24
 O       2.642777     2.269714    -0.712525     170.24
 C       2.270088     3.701522    -0.874855     116.54
 H       3.163148     4.292199    -1.298859      24.41
 H       1.206832     4.055067    -1.329474      23.12
 H       1.889102     4.192920     0.077004      25.23
 C       2.178317    -0.010095    -0.215050      18.96
 O       3.482799    -0.291840    -0.662759     135.80
 C       1.307618    -1.131309     0.158599      52.54
 H       1.710037    -2.182461     0.164938      22.05
 C      -0.544832     0.553911     0.445800      25.08
 C      -2.089279     0.886520     0.821654      83.57
 H      -2.466083    -0.022399     1.347786      23.41
 O      -2.174953     1.899709     1.787823     273.32
 H      -1.848308     1.470712     2.561280      28.41
 C      -2.949306     1.148313    -0.427844      67.45
 H      -2.501753     1.814574    -1.244245      23.08
 O      -3.287241    -0.283207    -0.982105     204.99
 H      -3.291898    -0.279989    -1.987656      24.60
 C      -4.433243     1.726944    -0.063401      93.59
 O      -4.767018     2.696055    -1.107910     284.43
 H      -4.290914     3.601264    -0.940218      27.47
 H      -4.398551     2.188513     0.986585      25.96
 H      -5.161048     0.980482    -0.041816      28.57
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name = lig-etoh-Waterframe_580
 C       6.279700    -1.185234     1.384403      31.75
 H       6.367566    -0.088998     1.200581      19.35
 C       5.453660    -3.505444     1.020027      70.22
 H       4.828177    -4.122182     0.411370      22.92
 C       5.947343    -3.870119     2.191963      15.93
 O       5.752705    -5.182785     2.779169     215.84
 C       4.826103    -6.066612     2.119634     109.32
 H       5.206628    -6.258034     0.975335      25.79
 H       3.790050    -5.674040     2.216162      26.39
 H       4.944578    -7.129227     2.718241      23.64
 C       6.664164    -2.950407     3.066337      -1.74
 O       7.204714    -3.530842     4.239208     234.60
 H       6.700128    -4.346140     4.655027      22.66
 C       6.854843    -1.634132     2.654298      39.15
 H       7.322207    -1.020089     3.464937      23.97
 C       5.656761    -2.169456     0.550674      19.49
 C       5.424093    -1.749866    -0.964283      85.32
 H       5.770983    -2.499773    -1.497019      27.59
 O       6.178332    -0.470984    -1.262870     204.67
 H       5.611909     0.292401    -1.160211      25.99
 C       3.881154    -1.553800    -1.210321      88.76
 H       3.392836    -2.463834    -0.628532      23.35
 C       3.485151    -1.550264    -2.701042      99.96
 O       3.583146    -2.952391    -3.209666     284.81
 H       4.339665    -2.951945    -3.866255      26.01
 H       4.193156    -0.915931    -3.195621      25.84
 H       2.367594    -1.279749    -2.702808      25.41
 C       0.016385    -0.801429     0.614741      44.98
 H      -0.612878    -1.824720     0.914997      17.82
 C       0.285356     1.563715     0.028998      62.62
 H       0.060259     2.740465     0.069390      19.12
 C       1.630340     1.281414    -0.324042      -3.36
 O       2.651796     2.267501    -0.835774     159.26
 C       2.215876     3.668091    -0.822221      99.18
 H       3.280142     4.232065    -1.395869      21.72
 H       1.573935     3.415645    -1.646337      22.96
 H       2.118082     3.941144     0.142460      27.79
 C       2.185665    -0.104420    -0.219531      13.97
 O       3.531699    -0.355252    -0.689619     192.96
 C       1.378291    -1.117907     0.212581      63.37
 H       1.583687    -2.097608     0.179312      23.38
 C      -0.563247     0.503822     0.461214      57.36
 C      -2.069006     0.895861     0.790060      81.97
 H      -2.484420    -0.001393     1.170596      26.39
 O      -2.212442     1.952672     1.796557     248.61
 H      -1.783159     1.605508     2.696005      25.00
 C      -3.041047     1.114274    -0.432745      79.42
 H      -2.556990     1.662772    -1.387004      22.20
 O      -3.272280    -0.220536    -0.899024     211.75
 H      -3.280847    -0.012452    -1.975747      21.42
 C      -4.404801     1.791910    -0.104272      99.97
 O      -4.775783     2.653035    -1.157183     291.41
 H      -4.687941     3.555604    -0.775387      28.26
 H      -4.383931     2.409370     0.938705      25.01
 H      -5.003010     1.002588    -0.297602      28.77
55
name = lig-etoh-Waterframe_581
 C       6.385170    -1.217781     1.427214      47.70
 H       6.326536    -0.233524     1.073203      23.00
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 C       5.427130    -3.443085     0.988241      60.05
 H       4.927241    -4.096811     0.308733      25.18
 C       6.000406    -3.944688     2.230306      33.68
 O       5.752159    -5.133050     2.707789     257.45
 C       4.847435    -6.064508     2.073779     118.69
 H       5.058745    -6.426027     1.062145      27.86
 H       3.675971    -5.824724     2.161329      25.15
 H       4.996012    -6.927985     2.795960      26.32
 C       6.707700    -3.047240     3.009520       6.98
 O       7.175244    -3.485543     4.254660     193.87
 H       6.590263    -4.249439     4.462991      29.60
 C       6.848573    -1.657244     2.664086      48.64
 H       7.464175    -0.898898     3.282626      20.80
 C       5.735534    -2.146560     0.524823      19.78
 C       5.450934    -1.735845    -0.930080      87.00
 H       5.814149    -2.415577    -1.730959      23.96
 O       6.178004    -0.507924    -1.286887     203.79
 H       5.590854     0.170100    -0.955768      28.15
 C       3.872058    -1.561982    -1.191607      76.36
 H       3.296911    -2.480264    -0.801937      22.23
 C       3.506686    -1.541901    -2.730468     108.65
 O       3.648574    -2.954325    -3.212318     282.94
 H       4.268502    -3.108742    -4.005591      25.77
 H       4.052832    -0.878281    -3.367569      26.14
 H       2.571133    -1.273689    -2.985505      26.55
 C      -0.028281    -0.800536     0.516301      59.02
 H      -0.571485    -1.554729     1.016021      22.83
 C       0.283686     1.582134    -0.037521      50.44
 H      -0.194220     2.651441     0.267391      17.18
 C       1.693644     1.257157    -0.341725      -0.94
 O       2.632605     2.168750    -0.893808     158.96
 C       2.197704     3.547910    -0.866930     116.89
 H       3.140822     4.353667    -1.190743      23.96
 H       1.344964     3.989799    -1.506905      24.92
 H       1.938905     3.990272     0.093442      27.76
 C       2.227821    -0.121306    -0.292044      10.71
 O       3.514564    -0.276966    -0.642418     199.58
 C       1.336653    -1.090282     0.300161      58.24
 H       1.661012    -2.041479     0.328646      22.10
 C      -0.594606     0.475583     0.490395      31.80
 C      -2.045732     0.830962     0.794487      79.09
 H      -2.497441    -0.056056     1.194725      22.27
 O      -2.231377     2.018320     1.792988     198.25
 H      -1.625618     1.552257     2.658409      21.28
 C      -3.064769     1.116216    -0.411542      85.09
 H      -2.487234     1.815992    -1.131931      22.40
 O      -3.266878    -0.184208    -0.866773     214.25
 H      -3.189849    -0.355081    -1.993668      21.35
 C      -4.353698     1.817847    -0.155903      93.81
 O      -4.810560     2.694190    -1.233941     297.61
 H      -4.910453     3.594072    -0.920079      29.06
 H      -4.525808     2.268654     0.914745      25.54
 H      -5.173101     0.932706     0.152324      25.86
55
name = lig-etoh-Waterframe_582
 C       6.447360    -1.270188     1.404376      70.95
 H       6.716290    -0.292412     1.174142      24.76
 C       5.444315    -3.397492     0.924393      72.02
 H       5.055376    -4.172890     0.294942      24.52
 C       5.979380    -3.877840     2.131183       4.14
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 O       5.747120    -5.186407     2.669171     240.12
 C       4.859342    -6.127402     2.081930     128.87
 H       5.107453    -6.289722     1.128522      31.34
 H       3.768663    -5.613654     2.080506      25.01
 H       4.865942    -6.966020     2.657312      28.14
 C       6.782576    -3.078091     3.031323       2.88
 O       7.144909    -3.441592     4.267588     248.32
 H       6.689570    -4.178189     4.679305      27.49
 C       6.859976    -1.714278     2.665287      20.57
 H       7.435278    -0.981223     3.342674      17.78
 C       5.832032    -2.107838     0.514893      43.72
 C       5.435752    -1.689981    -0.904095      87.23
 H       5.817497    -2.655824    -1.658903      22.37
 O       6.138647    -0.546511    -1.312685     194.44
 H       5.957356     0.208026    -0.752222      26.84
 C       3.923473    -1.596011    -1.274757      65.54
 H       3.332282    -2.288446    -0.721739      23.36
 C       3.554507    -1.597030    -2.799007     105.96
 O       3.693374    -2.957979    -3.206948     297.31
 H       4.190769    -3.009104    -4.100501      25.96
 H       4.286134    -0.900619    -3.293533      24.44
 H       2.537335    -1.251143    -2.866480      24.44
 C      -0.094195    -0.812718     0.500078      31.25
 H      -0.687870    -1.440404     0.904215      20.63
 C       0.339619     1.489369    -0.019433      57.43
 H      -0.055414     2.548318    -0.150361      18.05
 C       1.680864     1.229413    -0.382167      23.30
 O       2.576825     2.100600    -0.940514     174.32
 C       2.176913     3.539533    -0.917867     115.06
 H       3.093083     3.973481    -1.085812      25.83
 H       1.256628     3.886924    -1.413816      24.76
 H       1.803601     3.628919     0.278825      24.37
 C       2.122921    -0.048822    -0.294197      23.33
 O       3.510467    -0.201683    -0.581448     140.59
 C       1.318597    -1.051507     0.308932      50.39
 H       1.726527    -2.039991     0.673592      19.22
 C      -0.562154     0.574574     0.417028      37.33
 C      -2.108940     0.812338     0.871364      72.51
 H      -2.436909    -0.041685     1.533495      18.13
 O      -2.194732     2.006983     1.751530     216.11
 H      -1.676649     1.719753     2.765563      22.41
 C      -2.959555     1.177312    -0.383031      74.32
 H      -2.441370     1.784363    -1.080702      22.25
 O      -3.271657    -0.248494    -0.902783     199.36
 H      -3.066962    -0.112386    -2.041430      20.01
 C      -4.414785     1.847981    -0.111671      74.26
 O      -4.855939     2.728390    -1.306717     284.18
 H      -4.724065     3.593845    -0.943562      29.56
 H      -4.132689     2.560803     0.635893      24.56
 H      -5.341381     0.990175    -0.002148      23.81
55
name = lig-etoh-Waterframe_583
 C       6.551694    -1.255454     1.386833      47.92
 H       6.994812    -0.295935     1.177505      21.88
 C       5.520807    -3.415215     0.870722      70.74
 H       4.974532    -4.014646     0.125736      21.21
 C       5.950044    -3.876108     2.098663      15.11
 O       5.786474    -5.223613     2.656259     245.70
 C       4.832017    -6.145281     2.059041     129.07
 H       5.188539    -6.355461     1.006840      30.67
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 H       3.824695    -5.688211     2.034629      28.17
 H       4.768372    -7.047758     2.545225      27.97
 C       6.738572    -3.068138     3.015172      18.02
 O       7.153802    -3.431655     4.334376     268.89
 H       6.588784    -4.152676     4.658551      28.35
 C       6.928477    -1.772165     2.679740      23.53
 H       7.308396    -1.144044     3.499754      18.81
 C       5.832972    -2.091195     0.459960      20.48
 C       5.412291    -1.690506    -0.910429      72.73
 H       5.880098    -2.632608    -1.517148      23.76
 O       6.131694    -0.534328    -1.373069     119.37
 H       6.165810     0.079021    -0.652595      28.35
 C       3.942319    -1.526862    -1.261536      78.16
 H       3.455500    -2.322716    -0.805013      24.94
 C       3.635178    -1.617021    -2.792533      95.81
 O       3.714257    -2.991690    -3.227195     269.90
 H       4.274823    -3.028177    -4.082565      25.03
 H       4.405806    -0.963597    -3.361271      24.39
 H       2.499748    -1.210531    -2.830323      23.42
 C      -0.119840    -0.752770     0.532968      40.36
 H      -0.813300    -1.616106     0.786263      18.55
 C       0.364053     1.542634    -0.027998      87.16
 H       0.115370     2.440637    -0.424126      19.82
 C       1.607306     1.219419    -0.454379      13.06
 O       2.509554     2.102764    -1.023982     208.87
 C       2.139569     3.493137    -0.872777     115.75
 H       2.934548     4.011600    -1.155450      27.54
 H       1.507879     3.536483    -1.709914      25.09
 H       2.079933     3.713793     0.315973      23.74
 C       2.108238    -0.096370    -0.241922      18.86
 O       3.501911    -0.213394    -0.566103     146.26
 C       1.243158    -1.033899     0.295718      61.89
 H       1.785790    -1.993049     0.804735      21.57
 C      -0.605873     0.514710     0.374853      64.86
 C      -2.089538     0.893951     0.937353      69.80
 H      -2.478724    -0.132841     1.373557      23.12
 O      -2.143164     1.996982     1.718192     244.73
 H      -1.673116     1.649021     2.707452      23.06
 C      -2.982898     1.117153    -0.347271      73.83
 H      -2.408917     1.624904    -1.033786      24.42
 O      -3.234223    -0.257418    -0.979199     213.57
 H      -3.191341    -0.066371    -2.100937      21.04
 C      -4.399741     1.956416    -0.140353      96.23
 O      -4.877510     2.733804    -1.326682     327.83
 H      -4.519356     3.584001    -1.185740      32.63
 H      -4.307728     2.614308     0.648438      27.80
 H      -5.191135     1.183567     0.118449      27.01
55
name = lig-etoh-Waterframe_584
 C       6.668645    -1.261668     1.375479      69.50
 H       6.884508    -0.215286     0.999835      26.73
 C       5.589046    -3.425732     0.805945      43.93
 H       4.918002    -4.057452     0.150159      15.37
 C       5.961205    -4.004127     2.181798      11.86
 O       5.826709    -5.232702     2.631028     271.11
 C       4.811033    -6.123446     1.987123     110.79
 H       5.099045    -6.498640     0.833575      25.70
 H       3.844780    -5.780610     1.975034      31.23
 H       4.868986    -7.008450     2.728754      25.53
 C       6.631692    -3.109575     3.051594      -9.76
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 O       7.138024    -3.455938     4.347094     304.01
 H       6.539950    -4.188824     4.658191      26.19
 C       6.992107    -1.743540     2.651746      69.39
 H       7.398895    -1.131564     3.399764      23.06
 C       5.848856    -2.052861     0.506591      11.52
 C       5.457379    -1.687199    -0.966194      66.43
 H       5.632256    -2.376916    -1.685897      25.74
 O       6.165497    -0.500587    -1.450415     165.10
 H       6.103733     0.116289    -0.735661      29.50
 C       3.923039    -1.466785    -1.177694      94.31
 H       3.389399    -2.366736    -0.871016      24.36
 C       3.703490    -1.583201    -2.734470      91.93
 O       3.714942    -3.038056    -3.243019     257.88
 H       4.344926    -3.099613    -4.024780      25.21
 H       4.329072    -0.984193    -3.451245      24.56
 H       2.654414    -1.197914    -3.181170      23.68
 C      -0.130807    -0.749448     0.575867      23.27
 H      -0.883222    -1.759840     0.865468      17.26
 C       0.247624     1.615733    -0.077179      68.35
 H      -0.189035     2.521306    -0.226969      20.59
 C       1.606638     1.167375    -0.524320       3.29
 O       2.479587     2.097051    -1.096347     205.77
 C       2.159227     3.456412    -0.867337     114.39
 H       3.013858     4.212935    -1.348589      23.52
 H       1.166337     3.903861    -1.364291      23.78
 H       1.715287     3.897304    -0.035591      26.83
 C       2.158666    -0.137439    -0.217768      23.44
 O       3.472275    -0.302305    -0.581344     212.05
 C       1.220038    -1.060823     0.308792      59.60
 H       1.556071    -2.210250     0.531766      21.32
 C      -0.676336     0.541690     0.392481      47.37
 C      -2.052569     0.862607     0.819108      92.79
 H      -2.481651    -0.004058     1.427181      24.65
 O      -2.082647     2.027903     1.757329     232.55
 H      -1.600158     1.635143     2.600424      26.33
 C      -3.082047     1.061843    -0.371130      81.83
 H      -2.435430     1.683833    -1.063228      24.12
 O      -3.192527    -0.210744    -1.038773     262.69
 H      -3.282606    -0.087466    -2.065568      22.79
 C      -4.335455     2.032709    -0.175018     126.89
 O      -4.864907     2.722493    -1.320482     305.22
 H      -4.466152     3.542432    -1.414608      33.91
 H      -4.417087     2.601007     0.738734      28.43
 H      -5.049367     1.398743     0.065956      30.31
55
name = lig-etoh-Waterframe_585
 C       6.714274    -1.278519     1.327666      40.49
 H       6.897601    -0.145898     1.144747      26.58
 C       5.654483    -3.461886     0.906241      73.98
 H       5.125239    -4.117809     0.148117      21.88
 C       5.980877    -3.963682     2.128985      13.48
 O       5.815707    -5.316395     2.579054     276.23
 C       4.823904    -6.126870     1.957995     104.29
 H       5.180628    -6.412571     0.822067      24.69
 H       3.898136    -5.617809     1.984781      28.36
 H       4.827427    -7.099166     2.713770      23.26
 C       6.600516    -3.057766     3.115550       2.13
 O       7.079817    -3.497731     4.304591     253.43
 H       6.668298    -4.296422     4.839593      19.44
 C       7.005126    -1.765488     2.640724      40.80
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 H       7.632505    -1.161052     3.219822      21.41
 C       5.910666    -2.102295     0.509413       8.65
 C       5.490877    -1.630274    -0.989385      58.18
 H       5.704095    -2.420797    -1.639443      26.61
 O       6.210508    -0.466960    -1.509239     168.68
 H       5.962800     0.348774    -1.086593      27.98
 C       3.919523    -1.541873    -1.188569      81.78
 H       3.371578    -2.402411    -0.624990      25.26
 C       3.712510    -1.563217    -2.786049      96.77
 O       3.711495    -3.047718    -3.205720     272.95
 H       4.232022    -2.980048    -4.050979      26.52
 H       4.601845    -1.075914    -3.124379      26.56
 H       2.678836    -1.173323    -2.892071      26.12
 C      -0.125685    -0.760188     0.590367      45.92
 H      -0.923370    -1.576965     1.161774      22.69
 C       0.154881     1.532682    -0.158580      60.15
 H      -0.214155     2.581635    -0.011729      20.28
 C       1.523889     1.182844    -0.518834       3.01
 O       2.455423     2.092035    -1.139817     146.05
 C       2.092361     3.554123    -0.937297      80.15
 H       3.284144     4.074457    -1.275266      21.45
 H       1.114074     3.789505    -1.575704      22.58
 H       2.130510     3.534921     0.197944      25.56
 C       2.090371    -0.121773    -0.231082      16.47
 O       3.446819    -0.348308    -0.573898     166.53
 C       1.225226    -1.131953     0.314538      58.59
 H       1.407897    -2.221925     0.229703      20.76
 C      -0.629261     0.599574     0.400109      30.07
 C      -2.128288     0.826843     0.749522      82.69
 H      -2.406099     0.000644     1.351346      25.00
 O      -2.017580     2.043811     1.780528     260.51
 H      -1.617284     1.645242     2.501972      29.88
 C      -3.065505     1.156830    -0.466372      71.42
 H      -2.496817     1.879257    -1.246902      22.40
 O      -3.200835    -0.167607    -1.074077     278.99
 H      -3.137401    -0.049943    -1.957247      28.01
 C      -4.342286     1.984880    -0.142534      94.22
 O      -4.828215     2.722420    -1.342695     253.10
 H      -4.364781     3.515499    -1.329093      33.41
 H      -3.872580     2.816703     0.608427      23.73
 H      -5.234955     1.316122    -0.002159      26.81
55
name = lig-etoh-Waterframe_586
 C       6.683060    -1.321749     1.333056      46.61
 H       7.052910    -0.277159     1.059648      19.00
 C       5.673206    -3.453877     0.905866      34.80
 H       5.367087    -4.224964     0.169749      22.53
 C       6.020636    -3.928077     2.188955      11.80
 O       5.838737    -5.334958     2.534033     305.35
 C       4.842280    -6.139326     1.931628     122.03
 H       5.043217    -6.370849     0.937799      26.28
 H       3.829954    -5.591530     1.867757      25.15
 H       4.593437    -7.193957     2.385709      24.16
 C       6.601824    -3.034855     3.100678      -0.84
 O       7.051565    -3.524169     4.301016     161.10
 H       6.428814    -4.372706     4.469419      18.83
 C       7.005447    -1.791378     2.646428      39.35
 H       7.734481    -1.265627     3.279730      25.48
 C       5.999230    -2.126526     0.429491       8.41
 C       5.502737    -1.609755    -0.928877      21.03
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 H       6.041980    -2.519542    -1.560895      21.71
 O       6.240898    -0.449499    -1.551564     173.69
 H       5.747458     0.331930    -1.330322      29.15
 C       3.950852    -1.648665    -1.235903      64.83
 H       3.590907    -2.637029    -0.697630      26.61
 C       3.686838    -1.625615    -2.736265     116.79
 O       3.710978    -2.986442    -3.170931     305.71
 H       4.028665    -3.083768    -4.094953      28.20
 H       4.470877    -1.050621    -3.196076      28.65
 H       2.880302    -1.042282    -3.027363      27.77
 C      -0.122130    -0.737608     0.624082      55.80
 H      -0.749515    -1.444638     1.157363      25.95
 C       0.187405     1.491016    -0.248796      74.77
 H      -0.070519     2.673508    -0.283822      20.55
 C       1.489898     1.226455    -0.508201       6.94
 O       2.387126     2.081906    -1.169918     187.20
 C       2.108195     3.551488    -0.963339     108.54
 H       2.928011     4.246293    -1.530885      25.17
 H       1.250633     3.953679    -1.530018      26.12
 H       2.261692     3.703882     0.192385      27.60
 C       1.982390    -0.130547    -0.287164       1.14
 O       3.403784    -0.320610    -0.552467      93.59
 C       1.179817    -1.158497     0.268427      62.18
 H       1.556566    -2.090835     0.305569      24.89
 C      -0.655424     0.474983     0.418628      46.34
 C      -2.132486     0.902623     0.780271      77.88
 H      -2.672347     0.033789     1.071487      24.83
 O      -1.987209     2.008527     1.748696     291.17
 H      -1.661033     1.615325     2.467197      29.92
 C      -2.996966     1.249118    -0.547410      77.02
 H      -2.413241     1.925294    -1.287668      23.30
 O      -3.235962    -0.109272    -1.103281     263.36
 H      -3.061800    -0.116651    -2.027676      27.43
 C      -4.334259     1.928120    -0.168851      86.66
 O      -4.772858     2.732813    -1.365595     256.38
 H      -4.402906     3.561045    -1.180519      31.68
 H      -3.983312     2.744423     0.708322      24.01
 H      -5.189563     1.365775     0.596237      25.62
55
name = lig-etoh-Waterframe_587
 C       6.676117    -1.328570     1.382346      72.18
 H       7.077013    -0.435210     0.922625      17.34
 C       5.699727    -3.449090     0.825836      44.58
 H       5.353240    -4.202242     0.155176      21.90
 C       5.982774    -3.968683     2.179595      10.01
 O       5.898773    -5.295887     2.535435     244.14
 C       4.796731    -6.134090     1.829682     122.91
 H       5.062657    -6.329730     0.879888      28.50
 H       3.745814    -5.563727     1.884843      24.25
 H       4.830933    -6.947417     2.518061      25.89
 C       6.646215    -3.087941     3.087463       4.13
 O       7.030735    -3.518089     4.296217     148.68
 H       6.641236    -4.451054     4.762181      18.46
 C       7.014766    -1.772865     2.643099      40.93
 H       7.601116    -1.151471     3.419391      25.70
 C       6.037554    -2.134261     0.416860      22.56
 C       5.578769    -1.655922    -0.935311      58.84
 H       5.776732    -2.511925    -1.850217      20.07
 O       6.222950    -0.463286    -1.549051     177.12
 H       5.700625     0.301672    -1.343696      28.39
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 C       4.013285    -1.649060    -1.201544      57.00
 H       3.528588    -2.609302    -0.848426      26.68
 C       3.686272    -1.629472    -2.704300     108.47
 O       3.680878    -2.975132    -3.164907     281.80
 H       4.105054    -2.950669    -4.061496      26.37
 H       4.449733    -1.107860    -3.303331      27.37
 H       2.703347    -1.227552    -2.946675      26.17
 C      -0.156231    -0.837480     0.700277      39.82
 H      -0.660531    -1.510781     1.116891      21.13
 C       0.166454     1.465570    -0.251188      55.75
 H      -0.385795     2.436251    -0.747609      20.01
 C       1.533060     1.184859    -0.542596      14.25
 O       2.323475     2.122455    -1.194589     225.80
 C       2.167097     3.547205    -0.997330     143.15
 H       2.803500     3.898348    -1.582625      30.06
 H       1.191042     3.791136    -1.194058      28.31
 H       1.927860     4.085462    -0.062561      27.80
 C       1.981898    -0.156874    -0.376296      25.16
 O       3.350113    -0.339962    -0.558789     114.13
 C       1.163813    -1.117208     0.189247      59.92
 H       1.596997    -1.959054     0.580561      26.89
 C      -0.721742     0.492219     0.360308      22.54
 C      -2.077300     0.959261     0.759728      93.08
 H      -2.785803     0.185949     1.218957      23.37
 O      -1.997634     1.952451     1.702595     241.86
 H      -1.626000     1.559957     2.555846      27.43
 C      -2.941655     1.273429    -0.554207      93.85
 H      -2.437923     1.874744    -1.262815      26.59
 O      -3.263375    -0.029173    -1.135198     236.15
 H      -3.097761    -0.015649    -2.195062      23.72
 C      -4.251213     1.994182    -0.172299      92.75
 O      -4.736790     2.726657    -1.344512     277.83
 H      -4.666318     3.627819    -1.114290      30.95
 H      -4.173483     2.721934     0.601295      27.84
 H      -5.067414     1.095110     0.178453      26.31
55
name = lig-etoh-Waterframe_588
 C       6.701936    -1.285742     1.357973      58.61
 H       6.995454    -0.295919     1.159233      25.59
 C       5.731883    -3.512151     0.795900      84.28
 H       5.211996    -4.021882     0.041926      20.38
 C       5.963556    -3.954417     2.054365      25.89
 O       5.891613    -5.269645     2.508955     246.10
 C       4.820809    -6.082768     1.812975     117.89
 H       5.144367    -6.371162     0.729665      29.34
 H       3.800010    -5.527644     1.897332      27.66
 H       4.852371    -6.919293     2.393182      28.32
 C       6.672062    -3.146770     3.038287       3.72
 O       7.062165    -3.493563     4.351074     149.21
 H       6.566669    -4.315133     4.762324      20.66
 C       7.004266    -1.795648     2.700442      13.29
 H       7.420860    -0.974845     3.407968      20.10
 C       6.040962    -2.166781     0.453360       7.06
 C       5.590323    -1.704621    -1.041110      70.48
 H       5.834821    -2.556671    -1.683220      25.06
 O       6.192484    -0.500062    -1.515919     198.65
 H       5.800015     0.263847    -1.107342      29.73
 C       4.019208    -1.559246    -1.142705      82.23
 H       3.545369    -2.363587    -0.655788      25.08
 C       3.665281    -1.581276    -2.700063      89.68
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 O       3.653261    -3.030347    -3.202391     265.33
 H       4.292311    -3.037463    -3.966818      26.02
 H       4.404398    -0.891196    -3.241625      24.44
 H       2.582530    -1.272411    -2.576118      24.98
 C      -0.192754    -0.833908     0.677705      41.82
 H      -0.778859    -1.593502     1.195428      19.25
 C       0.117011     1.386763    -0.263309      59.68
 H      -0.398013     2.229740    -0.781416      19.54
 C       1.484748     1.154962    -0.605715      14.30
 O       2.320911     2.141379    -1.182341     194.41
 C       2.096123     3.570575    -1.040920     105.30
 H       2.896195     3.968323    -1.699232      24.69
 H       1.100460     3.731985    -1.615726      23.62
 H       2.535377     3.787678    -0.013706      25.02
 C       2.038090    -0.152635    -0.463215      23.08
 O       3.381436    -0.410855    -0.591943     189.50
 C       1.114285    -1.109570     0.200285      49.11
 H       1.650974    -2.016204     0.646429      22.76
 C      -0.683719     0.451624     0.309036      25.29
 C      -2.100452     0.894002     0.675600      78.62
 H      -2.433060    -0.077891     1.242613      22.80
 O      -2.017782     1.987667     1.704862     171.91
 H      -1.512966     1.484935     2.584273      23.19
 C      -2.903573     1.306266    -0.515665     102.55
 H      -2.369223     1.862909    -1.194546      27.04
 O      -3.278182     0.046244    -1.174389     217.87
 H      -3.185997     0.280747    -2.292524      21.18
 C      -4.193175     2.055550    -0.196462     122.10
 O      -4.728394     2.739278    -1.327185     306.67
 H      -4.870788     3.638904    -1.133612      32.33
 H      -4.112105     2.574822     0.641802      30.72
 H      -4.787829     1.288896    -0.261064      30.39
55
name = lig-etoh-Waterframe_589
 C       6.717108    -1.296936     1.377587      80.50
 H       6.762724    -0.247810     1.245300      26.79
 C       5.729570    -3.501860     0.711613      64.26
 H       5.144078    -4.142468     0.051845      18.27
 C       6.061814    -3.982886     2.058419      10.36
 O       5.821482    -5.263151     2.449758     268.55
 C       4.897348    -6.044303     1.850320     110.01
 H       5.120427    -6.214648     0.605945      25.60
 H       3.935511    -5.566360     1.810858      30.50
 H       4.674731    -7.008906     2.241319      26.12
 C       6.705796    -3.114756     3.023762      10.85
 O       7.080536    -3.478634     4.366106     218.57
 H       6.555047    -4.210019     4.636120      27.78
 C       6.940247    -1.805246     2.672758      35.32
 H       7.354536    -1.237858     3.551583      18.04
 C       6.050568    -2.128899     0.417954       3.49
 C       5.550901    -1.731438    -1.004268      85.55
 H       5.860583    -2.414699    -1.628887      27.47
 O       6.191652    -0.525600    -1.492297     200.39
 H       5.999488     0.107826    -0.808651      30.93
 C       3.984748    -1.578869    -1.168757      97.40
 H       3.662894    -2.433901    -0.658694      25.18
 C       3.600824    -1.614538    -2.631741      90.70
 O       3.643541    -3.028564    -3.240821     270.97
 H       4.339527    -3.150405    -3.944190      26.44
 H       4.101283    -0.846552    -3.306668      24.08
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 H       2.529480    -1.187647    -2.902761      24.05
 C      -0.167586    -0.811724     0.582026      38.75
 H      -0.910619    -1.545233     1.294622      20.64
 C       0.139235     1.354510    -0.368163      68.77
 H      -0.195336     2.305738    -0.457065      21.47
 C       1.461237     1.152256    -0.701207      10.91
 O       2.345272     2.089981    -1.175897     194.05
 C       2.059069     3.550193    -1.124669      85.60
 H       2.953158     4.200073    -1.872957      21.64
 H       1.020397     4.274474    -1.277461      22.31
 H       2.270644     3.856757     0.003895      24.66
 C       1.975968    -0.202893    -0.453369      13.45
 O       3.482074    -0.384855    -0.601182     162.48
 C       1.158953    -1.105537     0.248321      52.63
 H       1.569967    -2.238368     0.384047      19.69
 C      -0.695948     0.389856     0.303788      38.02
 C      -2.070650     0.790472     0.703855      67.50
 H      -2.725344    -0.107252     0.996581      22.14
 O      -2.040507     2.001859     1.690502     152.06
 H      -1.507279     1.582147     2.657730      21.22
 C      -2.882343     1.339386    -0.526969      85.70
 H      -2.148009     1.970941    -1.097937      23.50
 O      -3.285208     0.130794    -1.206034     203.33
 H      -3.224179     0.086018    -2.398890      19.41
 C      -4.184653     2.059665    -0.205197      98.38
 O      -4.733067     2.821335    -1.353906     278.67
 H      -4.733857     3.731067    -1.076746      29.87
 H      -4.178852     2.572664     0.803077      26.45
 H      -4.912086     1.241007     0.123139      28.33
55
name = lig-etoh-Waterframe_590
 C       6.653589    -1.309502     1.366412      68.07
 H       6.731011    -0.227338     1.159061      29.30
 C       5.765117    -3.453798     0.753952      68.73
 H       5.282666    -4.191956     0.051544      22.06
 C       6.163879    -3.985708     2.019497       8.29
 O       5.821376    -5.255612     2.481188     241.84
 C       4.845436    -6.047372     1.758613     109.54
 H       5.297177    -6.201906     0.683025      24.96
 H       3.946947    -5.574201     1.835298      31.01
 H       4.901627    -7.034994     2.415516      24.21
 C       6.718871    -3.141783     3.040116       0.37
 O       7.074600    -3.471076     4.312598     252.27
 H       6.646174    -4.228300     4.708725      25.72
 C       6.901949    -1.786964     2.663946      21.42
 H       7.331232    -1.173219     3.421895      15.92
 C       6.035889    -2.132224     0.369258      14.46
 C       5.516109    -1.691277    -0.946233      76.27
 H       5.750000    -2.502321    -1.725761      25.52
 O       6.204531    -0.522970    -1.455704     128.39
 H       6.303873     0.156589    -0.794686      29.84
 C       3.954651    -1.685522    -1.202735      63.22
 H       3.447432    -2.604581    -0.747726      27.27
 C       3.502365    -1.686423    -2.699369     101.19
 O       3.633580    -2.995659    -3.249312     274.74
 H       4.299962    -2.825543    -3.972728      25.54
 H       4.286185    -1.093984    -3.179096      26.10
 H       2.376206    -1.479907    -2.711333      25.71
 C      -0.126650    -0.865916     0.529362      40.63
 H      -0.758719    -1.787921     1.188449      21.98
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 C       0.123495     1.391281    -0.448070      70.33
 H      -0.093064     2.362623    -0.227220      22.53
 C       1.487105     1.069350    -0.773050       2.47
 O       2.361230     2.075229    -1.209982     156.08
 C       2.052258     3.599367    -1.116130      78.45
 H       2.916678     3.943024    -1.999973      22.27
 H       0.891487     3.610921    -1.398718      23.09
 H       2.181638     4.020490    -0.112833      26.86
 C       2.009786    -0.211449    -0.418225      15.15
 O       3.500153    -0.297423    -0.578559      88.85
 C       1.247048    -1.165425     0.250988      52.71
 H       1.537387    -2.315984     0.346444      22.37
 C      -0.699423     0.430982     0.258771      27.71
 C      -2.109702     0.802492     0.757000      83.10
 H      -2.721387     0.062981     1.223628      24.43
 O      -2.056380     1.937085     1.652324     209.57
 H      -1.605531     1.638914     2.686922      23.23
 C      -2.874513     1.354078    -0.552024      71.23
 H      -2.216018     2.127245    -1.202059      22.49
 O      -3.289437     0.171243    -1.245357     272.16
 H      -3.017932     0.229257    -2.198208      25.74
 C      -4.223779     2.063879    -0.160040      72.82
 O      -4.735736     2.913401    -1.349676     209.67
 H      -4.442910     3.786270    -1.070787      29.76
 H      -3.980856     3.069375     0.541374      22.84
 H      -5.100058     1.245809     0.296662      25.67
55
name = lig-etoh-Waterframe_591
 C       6.541635    -1.288778     1.322699     -20.02
 H       6.889238    -0.218576     1.133879      11.18
 C       5.825018    -3.471108     0.826182      67.20
 H       5.399452    -4.123039    -0.001318      27.88
 C       6.208904    -3.994541     2.018382      42.98
 O       5.861945    -5.239099     2.532035     174.42
 C       4.839589    -6.067333     1.685845     115.06
 H       5.064040    -6.339814     0.728774      31.86
 H       3.842175    -5.709984     1.770551      31.28
 H       4.881854    -7.120849     2.318637      27.60
 C       6.716987    -3.130720     3.004917      -4.82
 O       7.075480    -3.485901     4.280207     180.77
 H       6.547990    -4.321717     4.640719      15.99
 C       6.898789    -1.763196     2.666830      43.76
 H       7.262206    -0.996240     3.241177      31.03
 C       6.008024    -2.150552     0.406373      -0.91
 C       5.471478    -1.665153    -0.983666      52.64
 H       5.879852    -2.613492    -1.734395      27.61
 O       6.221600    -0.509637    -1.440117      87.70
 H       6.275292     0.198278    -0.797824      27.94
 C       3.908707    -1.676311    -1.181542      62.29
 H       3.342125    -2.491044    -0.529030      30.80
 C       3.448202    -1.725154    -2.709478     122.96
 O       3.640303    -3.007271    -3.289829     282.47
 H       4.224111    -3.000688    -4.125833      27.15
 H       3.921844    -0.904235    -3.240330      30.23
 H       2.463256    -1.329282    -2.672419      29.41
 C      -0.071653    -0.883955     0.476731      33.73
 H      -0.821265    -1.732768     0.854945      23.12
 C       0.125827     1.383970    -0.435563      62.27
 H      -0.189120     2.488859    -0.408252      21.80
 C       1.473144     1.054382    -0.782839       5.31
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 O       2.405122     2.080210    -1.230177     180.62
 C       2.000963     3.500930    -1.148934     134.01
 H       2.591428     4.086951    -1.822104      28.25
 H       1.173646     3.566113    -1.658699      29.47
 H       2.256779     3.957280    -0.283137      29.15
 C       2.165342    -0.180191    -0.400457      17.69
 O       3.450072    -0.301263    -0.580141     122.79
 C       1.259273    -1.230560     0.207184      56.60
 H       1.768328    -2.142201     0.567940      27.07
 C      -0.651917     0.394429     0.219776      22.51
 C      -2.139753     0.890477     0.731880      87.64
 H      -2.457247    -0.013663     1.170483      26.86
 O      -2.060097     1.905706     1.650243     247.60
 H      -1.642066     1.420115     2.560005      25.18
 C      -2.976536     1.349994    -0.498217      88.05
 H      -2.341985     2.058005    -1.189875      24.87
 O      -3.276546     0.189813    -1.267226     297.72
 H      -3.111794     0.215952    -2.154980      30.59
 C      -4.213670     2.207080    -0.157953      88.10
 O      -4.735212     2.965398    -1.315890     256.26
 H      -4.366347     3.865658    -1.231486      31.15
 H      -3.839135     2.868261     0.823134      24.79
 H      -5.156030     1.496806     0.152782      27.01
55
name = lig-etoh-Waterframe_592
 C       6.497974    -1.239524     1.380535      85.72
 H       6.746597    -0.188276     1.010119      24.88
 C       5.849175    -3.532060     0.766633      59.13
 H       5.378539    -4.307756     0.106003      24.99
 C       6.200798    -4.010722     2.092384     -10.08
 O       5.864720    -5.296750     2.509474     246.04
 C       4.899211    -6.106951     1.715193     119.23
 H       5.121656    -6.158470     0.715492      26.82
 H       3.838444    -5.583581     1.814375      25.47
 H       4.780581    -7.157626     2.186448      26.48
 C       6.747936    -3.036446     3.011996     -12.45
 O       7.076943    -3.519758     4.269481     192.90
 H       6.434480    -4.375798     4.555257      17.50
 C       6.885069    -1.704367     2.588510      92.61
 H       7.259327    -1.109986     3.400358      22.36
 C       5.930875    -2.137275     0.416267     -39.85
 C       5.476812    -1.711023    -0.997545      11.44
 H       5.768618    -2.487984    -1.867354      20.24
 O       6.220135    -0.500751    -1.450132     162.70
 H       5.910436     0.148203    -0.816309      32.74
 C       3.892059    -1.563712    -1.160760      85.05
 H       3.567610    -2.460350    -0.498754      28.31
 C       3.413273    -1.668518    -2.659690     103.95
 O       3.626886    -3.060107    -3.341224     232.69
 H       4.301816    -2.931541    -4.116662      23.88
 H       3.865741    -0.928276    -3.300406      28.13
 H       2.351264    -1.625225    -2.757592      27.70
 C      -0.077209    -0.900083     0.414270      40.40
 H      -0.687237    -1.594299     0.720541      23.55
 C       0.199012     1.346560    -0.380729      74.94
 H      -0.365832     2.307358    -0.880199      21.49
 C       1.525483     1.114229    -0.735712      21.99
 O       2.449669     2.065977    -1.240921     202.28
 C       1.977222     3.397011    -1.252338     130.06
 H       2.649627     3.910496    -1.730699      29.79
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 H       0.932252     3.759873    -1.507526      26.11
 H       1.805405     3.737350    -0.157660      27.14
 C       2.070484    -0.167078    -0.350446      21.04
 O       3.493507    -0.366089    -0.624244     152.11
 C       1.338061    -1.177524     0.132213      75.28
 H       1.693194    -1.977288     0.638752      28.45
 C      -0.637825     0.387117     0.176023      33.95
 C      -2.086595     0.851818     0.618997      82.20
 H      -2.633886    -0.106731     0.964158      24.91
 O      -2.040054     1.916398     1.713185     230.23
 H      -1.629414     1.545535     2.551208      27.73
 C      -3.067430     1.375649    -0.482391     100.61
 H      -2.385293     2.003008    -0.984933      27.97
 O      -3.290136     0.161208    -1.264326     298.09
 H      -3.292229     0.312215    -2.161771      29.44
 C      -4.220125     2.327632    -0.136024     128.17
 O      -4.717271     3.025611    -1.267557     298.25
 H      -4.399501     3.957189    -1.296848      30.98
 H      -4.086485     2.868436     0.737792      30.08
 H      -5.004759     1.749676     0.135247      30.42
55
name = lig-etoh-Waterframe_593
 C       6.435860    -1.192682     1.318165      49.44
 H       6.454399    -0.083908     1.141181      29.01
 C       5.852188    -3.578689     0.754126      86.60
 H       5.411228    -4.255297     0.026959      28.03
 C       6.131402    -3.963080     2.064343     -21.85
 O       5.893825    -5.384331     2.493930     204.55
 C       4.939997    -6.100058     1.762549     116.63
 H       5.337588    -6.094855     0.661208      24.48
 H       3.890456    -5.482638     1.839871      24.56
 H       4.959878    -7.071510     2.153685      27.11
 C       6.729795    -3.077899     3.018115       2.73
 O       7.087216    -3.507862     4.260558     152.29
 H       6.544779    -4.392379     4.651881      21.58
 C       6.905798    -1.667986     2.645891      -1.25
 H       7.361315    -0.973440     3.441967      15.98
 C       5.874184    -2.174007     0.414495     -78.88
 C       5.485524    -1.722483    -1.033498      40.08
 H       5.622853    -2.515754    -1.652889      27.15
 O       6.180530    -0.504726    -1.442649     161.59
 H       5.725941     0.282295    -1.132619      30.23
 C       3.948278    -1.574092    -1.191310      87.69
 H       3.505430    -2.429245    -0.759760      28.97
 C       3.372206    -1.695080    -2.655987      89.30
 O       3.615883    -3.069182    -3.350436     245.34
 H       4.373799    -2.836588    -3.986979      24.13
 H       3.942658    -0.967705    -3.245426      26.73
 H       2.246041    -1.676578    -2.587367      27.19
 C      -0.097268    -0.903223     0.353289      54.67
 H      -0.579573    -1.660732     0.776742      27.23
 C       0.261684     1.369267    -0.404952      63.52
 H      -0.307731     2.266872    -0.949941      19.85
 C       1.627414     1.154805    -0.641370      20.68
 O       2.450786     2.000769    -1.270402     179.05
 C       1.933995     3.395296    -1.276317      79.39
 H       2.875396     3.993623    -1.665310      24.62
 H       0.747860     3.363284    -2.001228      21.36
 H       1.788446     3.559259    -0.070385      25.61
 C       2.089245    -0.103135    -0.383576      15.94
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 O       3.509581    -0.336114    -0.630625     142.94
 C       1.262007    -1.146463     0.155881      62.13
 H       1.725141    -2.048787     0.372194      27.29
 C      -0.655355     0.378212     0.148014      43.85
 C      -2.061779     0.784025     0.592806      78.38
 H      -2.690568    -0.079995     1.097609      23.09
 O      -2.003596     1.890043     1.740919     208.30
 H      -1.609841     1.561569     2.454613      30.25
 C      -2.990912     1.434930    -0.520736      82.19
 H      -2.505185     2.063334    -1.208393      25.88
 O      -3.349372     0.145859    -1.220677     261.45
 H      -3.431747     0.352107    -2.183503      26.27
 C      -4.291168     2.349504    -0.062370     108.26
 O      -4.705616     3.122467    -1.261462     256.66
 H      -4.306841     4.039941    -1.088334      28.94
 H      -3.991068     3.080758     0.561483      29.11
 H      -5.065033     1.725560     0.223782      30.16
55
name = lig-etoh-Waterframe_594
 C       6.375282    -1.243733     1.344883      47.81
 H       6.245024    -0.202128     1.130145      29.64
 C       5.807970    -3.537777     0.736021      90.91
 H       5.536356    -4.215392    -0.026040      25.46
 C       6.060347    -4.012405     2.049059     -26.41
 O       5.994585    -5.349448     2.507150     263.07
 C       4.979532    -6.082677     1.754561     122.07
 H       5.168814    -6.405242     0.578234      25.71
 H       3.887298    -5.760782     1.840529      26.76
 H       4.926011    -6.982644     2.196145      27.46
 C       6.680121    -3.087818     2.999956     -13.35
 O       7.114221    -3.481777     4.273668     172.35
 H       6.601993    -4.297982     4.583157      24.41
 C       6.873111    -1.701770     2.651711      12.88
 H       7.385425    -0.855264     3.273903      18.16
 C       5.887541    -2.165999     0.408843      12.45
 C       5.447570    -1.714840    -1.018397      89.22
 H       5.814183    -2.485232    -1.641663      26.56
 O       6.144712    -0.530747    -1.454005     187.59
 H       5.582844     0.241271    -1.408261      29.36
 C       3.953050    -1.682487    -1.259980      70.40
 H       3.512385    -2.393135    -0.642781      25.31
 C       3.384863    -1.774891    -2.691729     103.11
 O       3.602196    -3.019685    -3.303140     296.27
 H       4.313409    -3.022168    -4.000348      26.92
 H       3.608838    -0.888711    -3.352646      24.88
 H       2.306808    -1.359859    -2.550554      25.64
 C      -0.149497    -0.907581     0.342732      42.99
 H      -0.819170    -1.752441     0.866168      23.17
 C       0.219931     1.382627    -0.441995      55.74
 H      -0.076682     2.443480    -0.563372      20.12
 C       1.635255     1.160250    -0.556397       2.14
 O       2.480575     2.006629    -1.321416     172.40
 C       1.924230     3.338226    -1.267894     104.01
 H       2.694715     4.295666    -1.711171      23.75
 H       1.185908     3.498527    -2.247006      24.54
 H       1.491250     3.883674    -0.323528      25.77
 C       2.200875    -0.160778    -0.381506      16.07
 O       3.501062    -0.262341    -0.613883     122.99
 C       1.247455    -1.109795     0.151755      58.34
 H       1.587464    -2.163741     0.087653      23.51
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 C      -0.633718     0.411912     0.112486      20.13
 C      -2.068051     0.847656     0.652714      72.61
 H      -2.492819    -0.152641     1.007596      22.99
 O      -1.955414     1.817577     1.703690     293.25
 H      -1.567520     1.428808     2.397512      31.81
 C      -2.937488     1.433930    -0.549974      69.56
 H      -2.451799     2.075846    -1.355644      23.07
 O      -3.444199     0.187701    -1.134348     224.00
 H      -3.350939     0.101073    -2.245961      22.74
 C      -4.277046     2.338639    -0.055192      70.33
 O      -4.703430     3.207595    -1.251291     227.79
 H      -4.335626     4.159777    -0.983078      25.95
 H      -3.796159     3.031849     0.814515      23.70
 H      -5.226361     1.693920     0.460048      26.07
55
name = lig-etoh-Waterframe_595
 C       6.318818    -1.302691     1.422279      92.57
 H       6.397144    -0.294306     1.169551      20.61
 C       5.746909    -3.524290     0.728937      56.09
 H       5.561246    -4.248158    -0.020162      24.00
 C       6.074456    -3.984784     2.068117     -16.26
 O       6.044945    -5.277655     2.456704     199.89
 C       4.988571    -6.178742     1.771628     101.25
 H       5.322079    -6.218435     0.642046      24.47
 H       4.166919    -5.571331     1.881615      27.17
 H       4.989423    -7.078398     2.390591      24.09
 C       6.631362    -3.060447     3.003430      -4.72
 O       7.132851    -3.457952     4.262268     316.77
 H       6.633686    -4.177562     4.601298      26.78
 C       6.783764    -1.758190     2.577808      53.73
 H       7.283512    -1.130289     3.383626      28.60
 C       5.890112    -2.141644     0.397919      13.48
 C       5.445596    -1.741032    -0.994535      89.67
 H       5.832506    -2.591411    -1.764943      22.01
 O       6.118317    -0.545583    -1.484667     226.84
 H       5.472339     0.159722    -1.474807      27.70
 C       3.922236    -1.711792    -1.259620      66.61
 H       3.501779    -2.468297    -0.569474      24.43
 C       3.373155    -1.718528    -2.719287      94.90
 O       3.564082    -3.025217    -3.259074     278.84
 H       4.298431    -2.872691    -3.902367      26.55
 H       3.937406    -0.983589    -3.394244      23.02
 H       2.251970    -1.846417    -2.655053      23.95
 C      -0.151574    -0.831811     0.341470      29.91
 H      -1.065083    -1.719667     0.687101      18.86
 C       0.237997     1.421337    -0.422355      82.82
 H      -0.118393     2.356958    -0.286254      20.70
 C       1.601190     1.105807    -0.571822      -6.90
 O       2.493998     2.077055    -1.294550     162.87
 C       1.930072     3.418439    -1.365564     119.52
 H       2.994919     3.971811    -1.494396      23.35
 H       1.184740     3.508262    -1.934902      30.54
 H       1.358041     3.553422    -0.512793      29.38
 C       2.147405    -0.161099    -0.309983      20.46
 O       3.559076    -0.289049    -0.644510     121.68
 C       1.275742    -1.158956     0.088923      49.19
 H       1.468244    -2.287802     0.235473      21.99
 C      -0.657927     0.448401     0.116814      38.10
 C      -2.031565     0.902325     0.625585      84.91
 H      -2.583614     0.048716     0.902980      25.22
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 O      -1.900437     1.764377     1.678137     266.73
 H      -1.529115     1.353043     2.538125      25.61
 C      -3.031702     1.401222    -0.523691      86.50
 H      -2.233448     1.992723    -1.174402      22.14
 O      -3.551467     0.213738    -1.077425     238.82
 H      -3.088083     0.184183    -2.118610      21.67
 C      -4.134067     2.359166    -0.111247      79.15
 O      -4.697299     3.238597    -1.176696     245.34
 H      -4.473121     4.288634    -0.968184      24.09
 H      -3.912537     2.959744     0.982612      23.64
 H      -5.171328     1.642648     0.183188      24.84
55
name = lig-etoh-Waterframe_596
 C       6.268950    -1.234370     1.358861      19.61
 H       6.580366    -0.226469     1.223017      16.00
 C       5.718707    -3.530308     0.771207      82.53
 H       5.409773    -4.256394     0.019494      23.53
 C       6.099775    -3.911953     2.018661      26.94
 O       6.050658    -5.285166     2.397986     144.46
 C       5.055048    -6.171554     1.827002     121.09
 H       5.323494    -6.460050     0.817545      27.40
 H       4.122610    -5.695774     1.816956      29.06
 H       5.061632    -7.240098     2.389270      23.98
 C       6.588938    -3.105781     3.038919      32.13
 O       7.137119    -3.431544     4.234340     249.29
 H       6.623486    -4.166649     4.614833      21.09
 C       6.733041    -1.789260     2.665482       5.23
 H       7.127114    -1.088210     3.397720      26.57
 C       5.830914    -2.192239     0.389391       6.65
 C       5.464157    -1.777853    -1.041873      87.19
 H       5.610488    -2.812138    -1.705812      23.22
 O       6.094512    -0.560063    -1.527684     213.71
 H       5.517719     0.180671    -1.318072      26.80
 C       3.891928    -1.623398    -1.181082      79.31
 H       3.328664    -2.571077    -0.771706      23.79
 C       3.344494    -1.698960    -2.678546      93.20
 O       3.563882    -3.090179    -3.259842     271.01
 H       4.358937    -3.079664    -3.863406      26.47
 H       3.898917    -0.909645    -3.241374      25.60
 H       2.287151    -1.301208    -2.749122      26.04
 C      -0.102000    -0.784257     0.303585      52.51
 H      -0.827982    -1.729086     0.608719      19.96
 C       0.254307     1.461547    -0.323581      62.64
 H      -0.087427     2.415531    -0.457558      22.48
 C       1.601796     1.156244    -0.700367       7.81
 O       2.462688     2.078577    -1.206363     187.13
 C       1.967713     3.469235    -1.391938     117.98
 H       2.745024     4.165860    -1.522695      26.90
 H       1.218323     3.608298    -2.233949      26.04
 H       1.700808     3.717941    -0.424486      27.19
 C       2.151586    -0.156070    -0.297836      -1.26
 O       3.550007    -0.382907    -0.672453     152.57
 C       1.171774    -1.238671     0.070210      51.45
 H       1.727558    -2.201900     0.411350      23.28
 C      -0.652800     0.481686     0.118543      28.45
 C      -2.067129     0.838044     0.566748      89.29
 H      -2.536679    -0.007880     0.980528      24.56
 O      -1.841526     1.809694     1.708796     176.82
 H      -1.480156     1.246495     2.662872      22.51
 C      -3.015745     1.433073    -0.470495      89.93
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 H      -2.509083     1.870612    -1.417046      23.14
 O      -3.645791     0.219582    -1.075361     188.31
 H      -3.295927     0.117053    -2.164780      21.94
 C      -4.106044     2.386334    -0.135657     108.62
 O      -4.674518     3.242120    -1.099479     284.39
 H      -4.417324     4.218968    -0.731697      25.01
 H      -3.783732     3.036417     0.759714      24.77
 H      -4.823932     1.618895     0.008889      27.18
55
name = lig-etoh-Waterframe_597
 C       6.300596    -1.239281     1.366228      67.17
 H       6.415484    -0.179346     0.998419      27.90
 C       5.681865    -3.519149     0.755536      64.68
 H       5.212995    -4.321289     0.116717      22.73
 C       6.097190    -4.008948     2.024530       2.85
 O       6.054896    -5.311950     2.364283     272.32
 C       5.109574    -6.173035     1.829779     139.92
 H       5.313767    -6.564745     0.927359      31.23
 H       3.998346    -5.968598     1.800859      25.66
 H       5.118194    -7.088142     2.678619      23.68
 C       6.580794    -3.071914     3.037590     -28.06
 O       7.128964    -3.453999     4.253431     331.52
 H       6.621985    -4.308777     4.632653      25.64
 C       6.638153    -1.672147     2.676222      63.38
 H       7.019019    -0.997739     3.371829      22.51
 C       5.783897    -2.143482     0.384495       9.36
 C       5.382910    -1.821983    -1.076537      73.02
 H       5.836603    -2.510708    -1.840493      22.77
 O       6.084151    -0.608925    -1.581075     184.20
 H       5.737869     0.109954    -1.028968      30.60
 C       3.846233    -1.644103    -1.204518      87.35
 H       3.424241    -2.475846    -0.473947      22.48
 C       3.385873    -1.689716    -2.653908     101.55
 O       3.534354    -3.117887    -3.229637     260.16
 H       4.260308    -2.933474    -3.917024      25.33
 H       4.039323    -1.102619    -3.278333      25.36
 H       2.397765    -1.291408    -2.735463      26.59
 C      -0.136279    -0.864315     0.282905      39.57
 H      -0.770116    -1.526064     0.713983      21.18
 C       0.280584     1.529388    -0.271138      63.95
 H      -0.064627     2.495392    -0.684222      19.64
 C       1.576405     1.134688    -0.726279       4.94
 O       2.475921     2.122090    -1.164750     154.99
 C       2.032247     3.508446    -1.321797     101.08
 H       2.793296     4.003255    -1.807954      26.45
 H       1.091016     3.711121    -2.315017      23.04
 H       1.610368     4.181243    -0.464596      24.52
 C       2.115853    -0.178397    -0.384318      32.22
 O       3.449341    -0.406087    -0.627631     196.77
 C       1.254205    -1.151658     0.052138      60.05
 H       1.463515    -2.215444     0.432181      22.17
 C      -0.618316     0.495587     0.109745      19.32
 C      -2.064924     0.811562     0.622927      68.17
 H      -2.503259    -0.170298     0.975135      22.47
 O      -1.815050     1.860751     1.710751     148.97
 H      -1.346044     1.268058     2.647799      21.26
 C      -2.939849     1.434689    -0.584741      71.38
 H      -2.364594     1.911613    -1.373998      24.04
 O      -3.736147     0.205498    -1.093052     194.95
 H      -3.618613     0.235012    -2.211820      23.41
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 C      -4.141327     2.376971    -0.034014     108.85
 O      -4.642394     3.257397    -1.077417     321.52
 H      -4.518098     4.239957    -0.821471      27.84
 H      -3.812869     2.875202     0.768805      29.34
 H      -4.887342     1.824622     0.409493      29.50
55
name = lig-etoh-Waterframe_598
 C       6.311511    -1.255983     1.324087      48.56
 H       6.273644    -0.111786     1.107649      21.68
 C       5.639517    -3.512892     0.769903      74.75
 H       5.150375    -4.188517    -0.002886      21.79
 C       6.091551    -3.977321     2.039552       5.66
 O       6.080804    -5.336878     2.371601     162.67
 C       5.080971    -6.302674     1.842136     104.14
 H       5.452272    -6.647595     0.842533      27.10
 H       4.109839    -5.595928     1.851090      22.80
 H       5.160071    -7.104179     2.635309      24.19
 C       6.582667    -3.001344     2.984343     -20.08
 O       7.106941    -3.482721     4.272946     196.35
 H       6.445593    -4.344010     4.567691      23.11
 C       6.552355    -1.595884     2.667095      46.48
 H       6.903837    -0.916142     3.373334      19.75
 C       5.766213    -2.146866     0.393906      14.71
 C       5.344814    -1.778805    -1.080855      99.05
 H       5.530418    -2.625620    -1.661866      28.81
 O       6.060250    -0.647349    -1.613846     174.70
 H       6.147524     0.060642    -0.957090      28.93
 C       3.819004    -1.749583    -1.221002      71.14
 H       3.356591    -2.567083    -0.635753      22.66
 C       3.438750    -1.738022    -2.679793     105.60
 O       3.486941    -3.094990    -3.182095     281.77
 H       4.119890    -2.992752    -3.977275      26.99
 H       4.142310    -1.102976    -3.172893      24.69
 H       2.409718    -1.579283    -2.809664      25.76
 C      -0.167497    -0.851989     0.264167      50.90
 H      -0.745109    -1.473536     0.708344      23.06
 C       0.299839     1.524960    -0.322618      57.39
 H      -0.177666     2.611694    -0.421384      16.32
 C       1.553409     1.151477    -0.650192       9.60
 O       2.505368     2.183086    -1.125754     154.97
 C       2.084638     3.588227    -1.339841      77.61
 H       3.043289     3.828399    -1.890092      21.65
 H       1.028855     3.329732    -1.893063      21.66
 H       1.741055     4.126852    -0.245422      22.75
 C       2.057990    -0.153143    -0.528623      26.75
 O       3.395628    -0.362448    -0.570142     155.89
 C       1.231284    -1.109416     0.089255      50.11
 H       1.658546    -2.121016     0.178767      19.26
 C      -0.611658     0.448775     0.147242      35.34
 C      -1.964787     0.869511     0.654669      72.50
 H      -2.643827    -0.011015     1.045356      19.91
 O      -1.830438     1.862314     1.668013     231.58
 H      -1.338200     1.486165     2.593059      23.28
 C      -3.013621     1.374003    -0.609828      68.59
 H      -2.347499     1.858749    -1.219468      23.84
 O      -3.776183     0.230131    -1.133913     242.84
 H      -3.703553     0.279847    -2.188347      23.90
 C      -4.097916     2.378115     0.073674      78.11
 O      -4.628677     3.248855    -1.081996     277.46
 H      -4.478554     4.135221    -0.719660      28.65
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 H      -3.624768     2.999475     0.784780      25.47
 H      -5.102078     1.809988     0.611208      24.63
55
name = lig-etoh-Waterframe_599
 C       6.257555    -1.200857     1.285315      36.36
 H       6.310528    -0.071754     1.126562      17.20
 C       5.603943    -3.493232     0.796518      82.47
 H       5.282036    -4.260687     0.031425      23.12
 C       6.060845    -3.911170     2.017367     -17.77
 O       6.130396    -5.340050     2.399423     180.49
 C       5.085486    -6.347209     1.875335      98.17
 H       5.323958    -6.756658     0.737044      25.63
 H       4.006583    -5.839073     1.700091      22.91
 H       4.887382    -7.161177     2.414087      25.04
 C       6.592945    -2.988660     3.012086       8.14
 O       7.040969    -3.469662     4.218854     330.78
 H       6.390134    -4.244251     4.549973      28.81
 C       6.532058    -1.627237     2.660183      28.41
 H       6.751782    -0.838777     3.377563      20.96
 C       5.766704    -2.173563     0.379424      24.02
 C       5.331484    -1.784938    -1.002721     100.46
 H       5.549268    -2.659879    -1.555445      29.16
 O       6.043571    -0.686098    -1.653446     164.20
 H       6.279951    -0.037297    -0.975695      29.69
 C       3.788730    -1.724766    -1.174193      82.80
 H       3.349124    -2.593378    -0.858021      24.81
 C       3.422273    -1.770361    -2.700016      99.60
 O       3.465407    -3.116059    -3.178787     292.21
 H       4.192431    -3.276765    -3.851209      28.24
 H       3.985540    -0.997717    -3.220699      24.92
 H       2.419948    -1.244155    -2.821010      25.10
 C      -0.156764    -0.840386     0.285246      41.15
 H      -0.847110    -1.666019     0.614560      19.94
 C       0.185433     1.448818    -0.346613      67.32
 H      -0.039929     2.586755    -0.030533      17.69
 C       1.627749     1.313512    -0.637143       3.90
 O       2.547592     2.176963    -1.053068     212.16
 C       2.092647     3.540755    -1.328336     116.54
 H       2.774758     4.395641    -1.939130      23.35
 H       1.274488     3.777989    -1.819009      28.62
 H       2.278838     4.101778    -0.354426      24.98
 C       1.986531    -0.127150    -0.575222      15.58
 O       3.414865    -0.380475    -0.579679     166.53
 C       1.164444    -1.118787     0.054317      40.40
 H       1.645076    -2.010543     0.202999      19.04
 C      -0.609393     0.496810     0.160861      30.96
 C      -1.976488     0.891014     0.623606      83.68
 H      -2.367743    -0.043563     1.183304      19.85
 O      -1.856946     1.901961     1.628223     290.41
 H      -1.515325     1.411114     2.387407      26.36
 C      -3.120821     1.335272    -0.463465      83.17
 H      -2.694134     1.859532    -1.354581      21.38
 O      -3.782184     0.276305    -1.178890     279.96
 H      -3.428742     0.249580    -2.064229      26.45
 C      -4.022097     2.406973     0.066999      81.94
 O      -4.612737     3.203201    -1.039043     278.34
 H      -4.433836     4.111263    -0.836291      28.85
 H      -3.440789     3.129430     0.775178      22.48
 H      -4.971549     1.649411     0.596172      23.58
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name = lig-etoh-Waterframe_600
 C       6.184533    -1.179799     1.345777      82.48
 H       6.281891    -0.182920     0.958086      26.28
 C       5.592836    -3.503211     0.787325      18.21
 H       5.335921    -4.341477     0.121764      21.53
 C       6.043843    -3.958042     2.062562     -20.00
 O       6.117958    -5.325316     2.394279     254.80
 C       5.083898    -6.300586     1.859017     110.68
 H       5.538047    -6.700875     0.815888      25.57
 H       4.086052    -5.877576     1.769284      25.73
 H       5.053739    -7.052033     2.587300      24.33
 C       6.538528    -3.015762     2.986743       2.54
 O       6.971031    -3.437222     4.192577     373.92
 H       6.507206    -4.233028     4.423408      29.69
 C       6.552749    -1.640416     2.603507      42.47
 H       6.741746    -0.902492     3.452645      21.26
 C       5.778405    -2.109856     0.400259      19.45
 C       5.313529    -1.855084    -0.984901      85.66
 H       5.699656    -2.651564    -1.719350      22.85
 O       6.037953    -0.736150    -1.676609     195.68
 H       6.119742     0.005750    -1.048753      28.76
 C       3.781988    -1.624645    -1.178035      91.97
 H       3.333859    -2.427265    -0.575077      23.76
 C       3.386750    -1.694176    -2.694323      82.47
 O       3.431521    -3.177350    -3.190253     255.90
 H       4.311275    -3.026119    -3.653550      25.86
 H       4.143852    -1.264469    -3.375470      21.73
 H       2.240325    -1.409844    -2.773307      24.01
 C      -0.194741    -0.836345     0.324570      43.15
 H      -1.030271    -1.771302     0.587511      16.95
 C       0.250870     1.544989    -0.350133      90.77
 H      -0.279247     2.539182    -0.154669      17.17
 C       1.572273     1.266436    -0.629321       6.86
 O       2.611304     2.220648    -1.033617     192.61
 C       2.150841     3.609971    -1.260301     105.92
 H       2.936307     3.786963    -2.181757      21.47
 H       1.103640     3.785066    -1.557795      26.16
 H       2.133427     4.106832    -0.359020      27.53
 C       2.009311    -0.053177    -0.512593      21.10
 O       3.396603    -0.438105    -0.628970     200.25
 C       1.163491    -1.105812    -0.060106      86.79
 H       1.416571    -2.033678     0.272531      24.65
 C      -0.662814     0.476788     0.136399      61.49
 C      -2.092852     0.840986     0.601859      88.82
 H      -2.396106    -0.078872     1.032141      25.51
 O      -1.884845     1.959251     1.617220     263.49
 H      -1.604826     1.602641     2.365332      30.05
 C      -3.090397     1.353397    -0.402097      74.04
 H      -2.453372     1.995800    -1.216291      21.39
 O      -3.800724     0.283006    -1.189147     290.50
 H      -3.301950     0.199864    -1.907830      31.43
 C      -4.033084     2.417279     0.054029     121.24
 O      -4.598257     3.145680    -0.985560     345.36
 H      -4.368014     4.046469    -0.936058      31.06
 H      -3.496272     3.060022     0.939095      23.27
 H      -4.779011     2.140118     0.728587      28.15
55
name = lig-etoh-Waterframe_601
 C       6.127780    -1.160961     1.368372      34.87
 H       6.231476    -0.133213     1.200910      23.28
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 C       5.641999    -3.515872     0.802352      70.52
 H       5.259530    -4.098219     0.001930      24.29
 C       6.004699    -4.015047     2.029358      40.29
 O       6.067073    -5.300814     2.382672     324.00
 C       5.136741    -6.221731     1.861689     127.32
 H       5.482706    -6.659853     0.927357      26.87
 H       4.244920    -5.769976     1.785084      30.95
 H       5.295674    -7.019364     2.712624      23.13
 C       6.456645    -3.018350     2.921963       0.12
 O       6.923534    -3.402548     4.222856     300.09
 H       6.516679    -4.232509     4.439658      23.60
 C       6.579779    -1.654243     2.620168      23.52
 H       6.992891    -0.960888     3.466441      21.46
 C       5.729385    -2.173626     0.432348      14.36
 C       5.327185    -1.836595    -1.077737      74.08
 H       5.356183    -2.937592    -1.600479      23.69
 O       6.051188    -0.778424    -1.674849     245.37
 H       5.757964     0.073384    -1.269978      25.62
 C       3.778502    -1.650171    -1.226794      81.43
 H       3.237397    -2.478306    -0.593349      23.34
 C       3.328444    -1.732402    -2.666705      88.88
 O       3.421112    -3.177184    -3.175279     255.66
 H       4.210163    -3.201328    -3.819441      26.38
 H       3.940219    -0.918610    -3.256242      24.04
 H       2.239873    -1.406967    -2.919481      25.31
 C      -0.212990    -0.785245     0.273511      31.65
 H      -0.878369    -1.702245     0.836154      18.13
 C       0.221184     1.609277    -0.284657      59.95
 H      -0.073939     2.566348    -0.612649      19.26
 C       1.582259     1.255421    -0.646448      -7.02
 O       2.603339     2.220334    -1.000086     163.67
 C       2.210548     3.659493    -1.212280      95.84
 H       2.873844     3.971495    -2.036500      25.25
 H       1.077591     3.347686    -1.526749      22.27
 H       2.378313     4.349866    -0.439844      27.06
 C       2.081367    -0.131633    -0.406325      19.86
 O       3.366671    -0.346219    -0.658717     191.72
 C       1.099086    -1.083113    -0.117795      64.89
 H       1.569014    -2.103628    -0.011436      23.21
 C      -0.709479     0.484100     0.083101      37.78
 C      -2.139760     0.795184     0.662602      81.45
 H      -2.732464     0.049097     1.079255      24.70
 O      -1.928486     1.975737     1.609426     250.81
 H      -1.548944     1.673600     2.366636      31.00
 C      -3.032974     1.393231    -0.473456      64.24
 H      -2.227946     1.925316    -1.099261      21.10
 O      -3.787187     0.299795    -1.158537     293.71
 H      -3.478335     0.142253    -1.980515      30.95
 C      -4.087195     2.440361     0.183741     105.59
 O      -4.613097     3.127185    -0.996275     307.27
 H      -4.316228     4.000232    -0.833810      31.26
 H      -3.354073     3.232205     0.600603      22.76
 H      -4.858737     2.073825     0.757684      28.00
55
name = lig-etoh-Waterframe_602
 C       6.108627    -1.184954     1.384557      53.50
 H       6.070172    -0.136383     1.216766      25.00
 C       5.656365    -3.535860     0.707119      71.56
 H       5.289841    -4.235397     0.006187      21.65
 C       5.986472    -3.965358     1.991007      13.17
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 O       6.074507    -5.282970     2.413643     347.35
 C       5.181034    -6.212373     1.872487     144.24
 H       5.368662    -6.523447     0.933225      33.41
 H       4.162710    -5.834171     1.782836      28.10
 H       4.866127    -7.228861     2.522949      26.33
 C       6.438738    -3.037096     2.992722     -10.99
 O       6.867937    -3.368783     4.228919     267.68
 H       6.361472    -4.191146     4.590483      24.15
 C       6.573503    -1.671349     2.633416      31.99
 H       7.176180    -1.021769     3.358731      21.09
 C       5.657736    -2.144365     0.410803      -5.78
 C       5.263654    -1.853289    -1.069762      61.90
 H       5.638413    -2.725706    -1.764345      22.62
 O       6.078228    -0.811691    -1.684690     231.01
 H       5.512935    -0.029170    -1.501746      30.28
 C       3.750699    -1.694366    -1.234781      69.57
 H       3.299619    -2.656075    -0.708291      22.86
 C       3.253467    -1.787201    -2.704976     105.36
 O       3.431486    -3.128823    -3.150454     280.76
 H       4.002463    -3.194797    -3.969570      27.82
 H       3.877858    -1.043165    -3.322040      24.17
 H       2.208799    -1.530627    -2.658136      26.42
 C      -0.211740    -0.745614     0.195443      41.27
 H      -0.837098    -1.484531     0.777745      19.83
 C       0.199924     1.558174    -0.283329      68.47
 H      -0.109458     2.474467    -0.591895      20.42
 C       1.594074     1.270038    -0.582089       4.29
 O       2.583601     2.193700    -0.938813     200.33
 C       2.239228     3.616509    -1.207723     118.29
 H       2.685332     4.117479    -1.949064      28.73
 H       1.148561     4.094314    -1.753708      23.42
 H       2.460015     4.312235    -0.326975      25.94
 C       2.026607    -0.095694    -0.355823      20.24
 O       3.418196    -0.257907    -0.705440     142.85
 C       1.105568    -1.115444    -0.124601      63.15
 H       1.369308    -2.289790    -0.262423      20.31
 C      -0.759364     0.561344     0.103919      34.64
 C      -2.124480     0.861827     0.698540      78.56
 H      -2.593805    -0.021789     1.226061      22.13
 O      -1.983320     1.941055     1.610854     260.04
 H      -1.436524     1.534134     2.349126      27.77
 C      -3.039626     1.420759    -0.485479      85.69
 H      -2.647052     1.955566    -1.311011      23.01
 O      -3.741222     0.332154    -1.109835     273.92
 H      -3.685869     0.406124    -2.095496      26.02
 C      -4.032978     2.463179     0.174560      81.24
 O      -4.664160     3.146337    -1.019176     279.30
 H      -4.545779     4.091041    -0.864535      30.07
 H      -3.607644     3.189839     0.894187      25.05
 H      -4.816880     1.757449     0.873412      26.20
55
name = lig-etoh-Waterframe_603
 C       6.083593    -1.247363     1.370817      60.98
 H       6.053285    -0.190780     1.042544      22.34
 C       5.644108    -3.538603     0.625258      34.27
 H       5.469871    -4.373130    -0.025719      20.41
 C       6.003190    -3.904060     2.009053     -14.00
 O       6.109913    -5.294396     2.468870     211.43
 C       5.086490    -6.253115     1.821869     114.57
 H       5.509385    -6.475567     0.806546      33.25
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 H       4.053874    -5.645660     1.788721      21.34
 H       5.207640    -7.181910     2.584766      26.08
 C       6.431555    -3.013652     3.017356      13.36
 O       6.809829    -3.373162     4.285869     313.49
 H       6.262705    -4.279707     4.593962      21.53
 C       6.554488    -1.690287     2.623994      65.20
 H       7.016822    -0.973437     3.289885      24.59
 C       5.604165    -2.109920     0.366306      23.22
 C       5.252216    -1.876863    -1.055054     101.29
 H       5.563272    -2.737411    -1.564953      24.25
 O       6.071494    -0.809492    -1.688464     246.64
 H       5.701342     0.095456    -1.699409      29.40
 C       3.736897    -1.681392    -1.259189      82.25
 H       3.208469    -2.303435    -0.512603      21.26
 C       3.191435    -1.781516    -2.703407     107.54
 O       3.426087    -3.136546    -3.157520     282.71
 H       4.077420    -2.899197    -3.878392      26.56
 H       3.678169    -1.191210    -3.458278      24.23
 H       2.182895    -1.631937    -2.680581      26.56
 C      -0.261922    -0.735256     0.155135      40.60
 H      -0.883529    -1.429832     0.396172      24.64
 C       0.196430     1.540835    -0.350259     101.66
 H      -0.228160     2.521550    -0.265282      20.75
 C       1.529285     1.277521    -0.442536      22.71
 O       2.527602     2.205465    -0.914846     172.44
 C       2.242672     3.647725    -1.217823      87.86
 H       3.192224     3.747670    -1.977402      20.30
 H       1.136923     3.840396    -1.367836      24.34
 H       2.310222     3.965076    -0.065145      23.64
 C       2.041800    -0.031722    -0.404256      12.46
 O       3.443670    -0.278858    -0.757082     152.40
 C       1.115368    -1.123071    -0.130061      51.74
 H       1.219372    -2.327703    -0.138710      17.55
 C      -0.687422     0.585434     0.155399      23.75
 C      -2.086092     0.979366     0.613644      76.21
 H      -2.376052    -0.121961     0.972526      20.00
 O      -2.023528     1.904631     1.675397     258.24
 H      -1.444031     1.564112     2.551887      22.93
 C      -3.084904     1.480325    -0.438834      91.95
 H      -2.520137     2.010315    -1.170384      24.09
 O      -3.715660     0.335488    -1.063546     249.71
 H      -3.775390     0.681332    -2.027145      24.41
 C      -4.018481     2.465648     0.087480      95.07
 O      -4.729994     3.170750    -0.998606     282.36
 H      -4.663764     4.118512    -0.745512      28.65
 H      -3.754150     3.045661     0.852688      26.25
 H      -4.977370     1.764334     0.654971      24.32
55
name = lig-etoh-Waterframe_604
 C       6.042301    -1.269340     1.302113      48.71
 H       6.258031    -0.160602     1.122185      21.66
 C       5.666669    -3.538268     0.728928      54.91
 H       5.579381    -4.189492    -0.163964      21.59
 C       6.020668    -3.962911     1.993365       5.46
 O       6.095022    -5.294997     2.461388     218.79
 C       5.090702    -6.217389     1.810304     113.50
 H       5.402982    -6.604310     0.691810      26.39
 H       3.937925    -5.825704     1.815797      24.24
 H       5.136002    -7.091840     2.423124      26.84
 C       6.420899    -2.995447     3.015840      -3.60
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 O       6.738386    -3.401143     4.359112     300.38
 H       6.350975    -4.425530     4.485570      18.66
 C       6.513337    -1.641243     2.603086      44.01
 H       6.740480    -0.917110     3.304261      22.58
 C       5.594186    -2.210452     0.360743      35.39
 C       5.252839    -1.823208    -1.100768     105.78
 H       5.349648    -2.723347    -1.566270      25.44
 O       6.072737    -0.814272    -1.708019     279.19
 H       5.676145     0.060802    -1.462890      26.78
 C       3.706408    -1.579627    -1.252640      98.72
 H       3.221211    -2.294896    -0.658605      23.99
 C       3.128162    -1.776784    -2.671543     100.50
 O       3.434463    -3.168362    -3.209904     260.59
 H       4.322468    -3.173405    -3.662485      27.10
 H       3.515815    -0.986340    -3.228587      26.72
 H       2.048057    -1.591470    -2.766074      25.70
 C      -0.260973    -0.784251     0.129270      61.69
 H      -1.006053    -1.518951     0.186662      22.96
 C       0.160228     1.627312    -0.338544      94.41
 H      -0.069905     2.750209    -0.158595      20.32
 C       1.584106     1.331879    -0.411485       1.59
 O       2.452092     2.183009    -0.905387     183.45
 C       2.229436     3.578804    -1.101278     111.25
 H       3.216099     4.016465    -1.900521      22.61
 H       1.438623     3.669939    -1.686893      27.88
 H       2.480364     4.420269    -0.300804      23.96
 C       2.084245    -0.126232    -0.463561      12.89
 O       3.403311    -0.293687    -0.800923     211.94
 C       1.075398    -1.042368    -0.128973      58.77
 H       1.517932    -2.052326    -0.060103      20.96
 C      -0.633745     0.587845     0.149270      21.06
 C      -2.030869     0.967615     0.574057      81.44
 H      -2.732408     0.110979     0.873092      20.56
 O      -2.053725     1.910515     1.781106     176.44
 H      -1.600580     1.292479     2.686801      20.90
 C      -3.024545     1.545266    -0.447429      74.86
 H      -2.313370     2.057224    -1.147067      22.37
 O      -3.695657     0.349763    -1.026708     212.55
 H      -3.876569     0.413321    -2.076147      24.55
 C      -4.188875     2.465612     0.045995     106.98
 O      -4.791763     3.220782    -0.972508     313.07
 H      -4.513620     4.165797    -0.733161      27.90
 H      -3.632092     3.134535     0.661528      24.91
 H      -4.936041     1.835671     0.470014      27.17
55
name = lig-etoh-Waterframe_605
 C       6.045882    -1.241571     1.280820      54.25
 H       6.101171    -0.154060     0.902260      21.44
 C       5.683777    -3.591559     0.781795      37.67
 H       5.479594    -4.421031     0.011590      20.49
 C       6.074920    -4.013748     2.073529      18.32
 O       6.032437    -5.320752     2.392860     337.82
 C       5.125796    -6.212130     1.830371     126.62
 H       5.337956    -6.377081     0.670320      24.03
 H       4.101090    -5.758854     1.895334      28.44
 H       5.053235    -7.032876     2.336201      25.95
 C       6.406558    -3.023670     3.039176      -0.56
 O       6.658093    -3.413092     4.351231     406.54
 H       6.256985    -4.364419     4.575167      27.12
 C       6.418371    -1.624087     2.595858      59.70
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 H       6.592021    -0.879154     3.292734      23.93
 C       5.636082    -2.215157     0.358080      30.50
 C       5.213981    -1.822453    -1.138470      97.96
 H       5.412979    -2.654791    -1.919051      22.06
 O       6.066496    -0.804067    -1.721110     248.03
 H       5.853881    -0.012632    -1.140387      27.02
 C       3.690473    -1.583966    -1.247334      87.46
 H       3.394151    -2.421297    -0.667932      22.10
 C       3.119598    -1.792619    -2.695131      91.63
 O       3.438063    -3.157614    -3.236207     232.20
 H       4.379781    -3.102017    -3.554687      25.86
 H       3.602164    -1.049376    -3.336339      24.15
 H       1.937379    -1.842408    -2.581994      23.81
 C      -0.255263    -0.752616     0.101157      37.48
 H      -1.050834    -1.641347     0.462995      20.95
 C       0.275102     1.686375    -0.216868      73.59
 H      -0.161756     2.807081    -0.304070      17.21
 C       1.558441     1.264443    -0.471768      19.24
 O       2.513228     2.209115    -0.894805     200.51
 C       2.245237     3.589546    -1.073367     121.74
 H       3.087368     3.881171    -1.784109      24.33
 H       1.475746     3.845717    -1.832515      25.32
 H       1.995131     4.237849    -0.216037      26.37
 C       1.986326    -0.018867    -0.470229      27.89
 O       3.336168    -0.257252    -0.818556     179.18
 C       1.136996    -1.060492    -0.139038      61.21
 H       1.406325    -2.028077    -0.064508      21.59
 C      -0.701965     0.587074     0.118630      44.15
 C      -2.099790     0.949393     0.670327      67.91
 H      -2.527535     0.015813     1.016013      22.91
 O      -2.058310     1.884070     1.846496     157.63
 H      -1.729177     1.256055     2.800609      20.94
 C      -2.975023     1.598471    -0.537960      67.65
 H      -2.642481     2.204896    -1.476941      21.45
 O      -3.662848     0.352549    -1.010302     207.27
 H      -3.548977     0.403206    -2.119122      22.54
 C      -4.261180     2.453920     0.057570      90.16
 O      -4.873977     3.308518    -0.994782     294.31
 H      -4.423998     4.239500    -0.982578      27.41
 H      -3.866805     3.205031     0.959334      23.68
 H      -4.872046     1.905449     0.587136      29.38
55
name = lig-etoh-Waterframe_606
 C       6.045575    -1.231990     1.268609      42.56
 H       5.902592    -0.150591     1.026424      20.04
 C       5.696273    -3.615595     0.767796      39.16
 H       5.276729    -4.501535     0.202891      18.79
 C       6.083278    -3.989022     2.073693       7.10
 O       6.048028    -5.370745     2.408223     305.65
 C       5.071370    -6.199636     1.793084     121.94
 H       5.351256    -6.404672     0.774611      28.33
 H       4.179001    -5.747634     1.874271      31.23
 H       5.224325    -7.184792     2.357539      25.37
 C       6.375780    -3.022263     3.053601       6.08
 O       6.586375    -3.398857     4.341993     301.37
 H       6.086888    -4.202490     4.564485      28.57
 C       6.311886    -1.663964     2.628745      52.12
 H       6.566795    -0.903348     3.364754      23.84
 C       5.691369    -2.251404     0.307198      18.77
 C       5.226238    -1.853587    -1.148201      88.04
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 H       5.536952    -2.864678    -1.810676      22.88
 O       6.040990    -0.754263    -1.703857     193.99
 H       6.255166     0.019354    -1.115769      29.59
 C       3.691567    -1.650327    -1.277715      76.71
 H       3.167266    -2.297799    -0.497100      21.75
 C       3.148421    -1.853190    -2.704281      99.89
 O       3.454235    -3.130107    -3.229172     254.28
 H       4.244466    -2.935212    -3.812114      26.33
 H       3.358194    -1.096741    -3.538244      24.14
 H       1.943246    -1.742117    -2.661559      23.48
 C      -0.236434    -0.684118     0.099620      39.83
 H      -0.849944    -1.588720     0.746594      19.19
 C       0.248170     1.615891    -0.054679      75.71
 H      -0.029349     2.728314    -0.310170      19.08
 C       1.528597     1.377468    -0.579626       8.76
 O       2.619064     2.219180    -0.882649     193.79
 C       2.228397     3.651081    -1.122616     109.44
 H       3.090802     4.045848    -1.289953      26.41
 H       1.130540     3.713065    -1.727767      23.37
 H       1.941169     3.823055    -0.149085      28.38
 C       1.958552    -0.029867    -0.473617       7.58
 O       3.276361    -0.212854    -0.817981     121.84
 C       1.096249    -1.104273    -0.139780      61.52
 H       1.356796    -2.080599    -0.114766      21.85
 C      -0.722431     0.653872     0.114410      50.96
 C      -2.139697     0.997392     0.743642      65.65
 H      -2.574969     0.066264     0.930860      23.91
 O      -2.062119     1.839234     1.862087     248.97
 H      -1.605225     1.447485     2.794582      23.42
 C      -3.119665     1.605283    -0.508805      74.46
 H      -2.447969     2.154674    -1.301992      21.71
 O      -3.606856     0.365590    -1.057970     217.89
 H      -3.207148     0.253436    -2.126904      20.44
 C      -4.214899     2.513913     0.054780      79.35
 O      -4.954168     3.340168    -1.014914     252.73
 H      -4.492304     4.288281    -0.857804      25.31
 H      -4.047273     3.185863     1.063109      23.35
 H      -5.095368     1.695486     0.381399      24.51
55
name = lig-etoh-Waterframe_607
 C       5.997870    -1.306657     1.297894      41.10
 H       5.907263    -0.257737     1.212749      21.99
 C       5.695981    -3.603929     0.724090      68.78
 H       5.266312    -4.253030    -0.043178      23.41
 C       6.044292    -4.011847     2.006838       1.15
 O       6.110878    -5.359999     2.469729     254.21
 C       5.033202    -6.216561     1.743411     108.73
 H       5.234719    -6.443335     0.765185      28.86
 H       3.982530    -5.936391     1.842139      27.43
 H       5.109170    -7.336376     2.407740      25.85
 C       6.313679    -3.017912     3.026369     -11.52
 O       6.522747    -3.367127     4.372038     269.31
 H       6.160095    -4.209425     4.569066      28.09
 C       6.238835    -1.673280     2.641387      35.78
 H       6.441253    -0.915691     3.475456      20.67
 C       5.736469    -2.267312     0.288452      10.65
 C       5.299027    -1.865890    -1.091067      83.57
 H       5.476522    -2.786415    -1.810213      24.93
 O       6.016667    -0.729799    -1.705501     188.20
 H       6.138323    -0.151437    -0.895450      28.23
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 C       3.684417    -1.624972    -1.281452      72.58
 H       3.087534    -2.415226    -0.615292      23.77
 C       3.103527    -1.854273    -2.711892     100.55
 O       3.505456    -3.143883    -3.243142     276.73
 H       4.124569    -3.072703    -4.002701      28.52
 H       3.562425    -0.942612    -3.260685      24.45
 H       2.007335    -1.803121    -2.636473      25.47
 C      -0.265739    -0.654625     0.186961      33.27
 H      -1.110218    -1.401637     0.495451      18.31
 C       0.234979     1.695995    -0.035978      58.16
 H      -0.185099     2.666162     0.227067      19.50
 C       1.571294     1.377305    -0.607436      -1.96
 O       2.657423     2.233222    -0.915680     179.22
 C       2.176115     3.642787    -1.052610     100.42
 H       2.893608     4.482970    -1.227325      24.81
 H       1.469839     3.763339    -2.123448      22.93
 H       1.801613     4.041511    -0.022745      24.93
 C       1.971670    -0.070298    -0.524526      13.31
 O       3.289456    -0.235056    -0.848429     147.76
 C       1.016012    -1.045687    -0.162689      73.51
 H       1.322665    -2.104889    -0.084106      23.44
 C      -0.748349     0.646767     0.200651      38.68
 C      -2.154585     1.020073     0.717398      79.61
 H      -2.740584     0.120769     0.962328      21.94
 O      -2.070750     1.853228     1.886195     291.61
 H      -1.547335     1.379112     2.539501      29.62
 C      -3.161354     1.594077    -0.385330      85.87
 H      -2.399298     2.142383    -0.940860      23.51
 O      -3.563573     0.382044    -1.138337     222.50
 H      -3.133225     0.307703    -2.208078      20.78
 C      -4.300216     2.530817     0.000795      86.61
 O      -4.976216     3.344480    -0.982471     246.04
 H      -4.737010     4.368432    -0.880348      27.54
 H      -3.844647     3.074367     0.864734      24.82
 H      -5.241263     1.656441     0.208166      23.85
55
name = lig-etoh-Waterframe_608
 C       5.934012    -1.328367     1.365636      64.28
 H       5.947591    -0.341224     1.031236      25.73
 C       5.686001    -3.617201     0.619551      -5.85
 H       5.525809    -4.334775    -0.150773      18.44
 C       6.011782    -4.046168     2.001313       0.85
 O       6.081575    -5.356321     2.455724     267.49
 C       5.060423    -6.261371     1.770254      92.59
 H       5.314071    -6.320512     0.713273      25.99
 H       3.994939    -5.708131     1.937055      23.96
 H       5.068117    -7.380842     2.354951      24.33
 C       6.229358    -3.069768     3.014943     -10.09
 O       6.457836    -3.329112     4.373698     268.43
 H       6.321529    -4.245819     4.616284      22.27
 C       6.199995    -1.695700     2.667462      45.75
 H       6.201223    -0.835849     3.451033      20.07
 C       5.756648    -2.233172     0.328087      45.64
 C       5.293488    -1.856141    -1.122367      99.51
 H       5.491105    -2.611900    -1.788540      26.66
 O       5.994279    -0.733736    -1.662266     288.10
 H       5.952202     0.031072    -0.995840      27.13
 C       3.687174    -1.623231    -1.244853      94.34
 H       3.348772    -2.457760    -0.541652      25.32
 C       3.130522    -1.808800    -2.693434      99.80
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 O       3.540856    -3.177368    -3.260980     241.58
 H       4.316876    -2.957282    -3.847928      26.20
 H       3.623708    -1.050441    -3.359517      25.07
 H       2.127646    -1.807296    -2.739979      27.69
 C      -0.402390    -0.672884     0.274997      38.31
 H      -1.041052    -1.428937     0.258508      20.09
 C       0.266086     1.775180    -0.082515     113.19
 H       0.088136     2.644279     0.393927      21.04
 C       1.558472     1.310540    -0.518601      -3.92
 O       2.620665     2.292614    -0.956802     147.35
 C       2.136692     3.660760    -0.969059      96.35
 H       3.180945     4.295654    -1.375392      21.76
 H       1.546435     3.676637    -1.910921      26.31
 H       1.213566     4.025650    -0.321238      24.20
 C       1.940388    -0.011490    -0.599256      19.66
 O       3.342933    -0.323627    -0.893322     171.67
 C       0.985185    -0.973658    -0.187581      54.62
 H       1.212239    -2.141760    -0.054337      22.68
 C      -0.725382     0.698734     0.296189      43.35
 C      -2.218501     0.986879     0.721198      74.40
 H      -2.568625    -0.041874     1.132214      23.22
 O      -2.080959     1.902089     1.898991     305.61
 H      -1.655426     1.465611     2.534535      31.07
 C      -3.070494     1.592711    -0.383346      83.66
 H      -2.632096     2.296315    -1.004513      25.03
 O      -3.528399     0.408884    -1.202290     231.20
 H      -3.343145     0.702145    -2.248640      22.19
 C      -4.428783     2.449326    -0.009184     114.94
 O      -4.989972     3.351242    -0.972960     311.30
 H      -4.453860     4.253343    -0.787144      27.24
 H      -4.141543     3.048847     0.726428      26.90
 H      -5.193540     1.981950     0.640471      27.30
55
name = lig-etoh-Waterframe_609
 C       5.883203    -1.268349     1.370994      37.11
 H       5.916971    -0.201917     1.136735      22.76
 C       5.740660    -3.666763     0.617300      50.02
 H       5.752898    -4.425005    -0.118688      17.10
 C       5.958668    -4.049656     1.956455      -3.27
 O       6.018292    -5.398766     2.405446     301.86
 C       5.112745    -6.249969     1.831736     117.27
 H       5.337006    -6.412021     0.687930      26.22
 H       4.031120    -5.712853     1.910589      25.88
 H       5.188349    -7.210714     2.268344      27.35
 C       6.146636    -3.095925     3.041201     -10.92
 O       6.395399    -3.312495     4.353750     190.53
 H       6.232413    -4.276468     4.637003      18.54
 C       6.140709    -1.723949     2.705855      19.48
 H       6.205570    -0.984832     3.578534      22.91
 C       5.693158    -2.269570     0.305857     -12.68
 C       5.254693    -1.804532    -1.143774      95.78
 H       5.526423    -2.609301    -1.715053      27.27
 O       6.000761    -0.705540    -1.611789     298.67
 H       5.657467     0.218258    -1.355735      25.89
 C       3.724690    -1.714959    -1.232582     103.60
 H       3.231537    -2.331466    -0.544141      27.72
 C       3.236058    -1.851652    -2.701883     109.44
 O       3.572682    -3.169851    -3.262941     254.47
 H       4.496676    -3.062997    -3.608660      26.64
 H       3.548524    -1.091025    -3.384079      27.15
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 H       2.176199    -1.673749    -2.756650      27.26
 C      -0.382038    -0.645707     0.249150      48.13
 H      -1.035869    -1.413492     0.385856      22.79
 C       0.266762     1.703643    -0.063959      81.88
 H       0.282253     2.739936     0.106202      19.34
 C       1.584402     1.406463    -0.459785      14.90
 O       2.496466     2.291106    -0.922272     218.71
 C       2.066308     3.675891    -1.065837     107.54
 H       3.107348     4.294159    -0.711976      24.83
 H       1.580391     3.827160    -1.874132      29.64
 H       1.568781     3.993086    -0.035925      26.14
 C       1.929392    -0.051308    -0.630156      20.82
 O       3.327513    -0.340257    -0.891921     169.36
 C       0.904757    -0.940046    -0.169655      51.98
 H       1.327206    -2.059699    -0.323215      21.66
 C      -0.719142     0.774728     0.349298      27.60
 C      -2.167647     1.008183     0.806903      63.16
 H      -2.710175    -0.031041     0.984283      21.71
 O      -2.122987     1.959227     1.887718     314.36
 H      -1.834820     1.627761     2.659828      30.17
 C      -3.140433     1.594130    -0.458498      58.30
 H      -2.524121     2.325783    -1.046670      21.64
 O      -3.474576     0.470806    -1.248069     249.23
 H      -3.573493     0.651905    -2.282419      22.85
 C      -4.471853     2.382098     0.133285      95.57
 O      -4.989340     3.333182    -0.998032     279.12
 H      -4.411174     4.146192    -0.815469      29.11
 H      -4.128083     3.109351     0.865429      24.55
 H      -5.214529     1.782361     0.432844      28.98
55
name = lig-etoh-Waterframe_610
 C       5.838772    -1.287381     1.350610      43.46
 H       5.745639    -0.162229     1.250184      20.33
 C       5.820213    -3.663139     0.645384      69.31
 H       5.755047    -4.407033    -0.148227      23.90
 C       5.922184    -4.060950     1.997764      13.91
 O       6.027677    -5.379869     2.383350     293.16
 C       5.081838    -6.284100     1.809606     132.62
 H       5.299806    -6.581597     0.704354      27.13
 H       4.024369    -6.117958     1.916808      29.82
 H       5.177165    -7.067223     2.370168      27.64
 C       6.062208    -3.081203     2.999588       6.07
 O       6.334689    -3.352927     4.362181     185.35
 H       6.026889    -4.346226     4.643529      21.79
 C       6.051803    -1.722778     2.683678      49.49
 H       6.325182    -1.132788     3.541496      22.72
 C       5.612199    -2.248069     0.321134     -13.79
 C       5.261664    -1.808782    -1.069264      81.51
 H       5.576867    -2.682035    -1.836823      23.62
 O       6.017206    -0.635142    -1.593111     267.70
 H       5.309734     0.080077    -1.451227      24.56
 C       3.714206    -1.737555    -1.271352      76.25
 H       3.235889    -2.481673    -0.709441      26.66
 C       3.324780    -1.913925    -2.729926     105.61
 O       3.602137    -3.171204    -3.248581     267.79
 H       4.456683    -3.187615    -3.769370      27.15
 H       3.861438    -1.113958    -3.176442      24.24
 H       2.130781    -1.854594    -2.656584      24.05
 C      -0.336759    -0.538110     0.195655      46.52
 H      -1.092499    -1.265968     0.729940      20.48
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 C       0.273881     1.685360     0.008426     121.71
 H      -0.268703     2.716366    -0.251892      16.97
 C       1.569932     1.316592    -0.456246      15.09
 O       2.410039     2.311789    -0.899443     239.80
 C       2.056496     3.714203    -1.025693     119.83
 H       2.938127     4.374244    -1.152991      24.94
 H       1.625922     4.154228    -1.930493      24.58
 H       1.451770     3.966214    -0.162508      26.85
 C       1.913292    -0.010592    -0.569829      26.68
 O       3.255489    -0.319009    -0.867392     175.27
 C       0.962383    -0.974742    -0.222564      75.98
 H       0.980643    -2.103135    -0.339390      20.99
 C      -0.729640     0.726902     0.366332      69.05
 C      -2.122447     1.097548     0.817775      73.86
 H      -2.636166     0.173595     1.143098      23.24
 O      -2.204333     2.036140     1.881550     267.76
 H      -1.903167     1.603695     2.753067      25.78
 C      -3.229090     1.644230    -0.437011      66.43
 H      -2.483011     2.383233    -0.957090      20.37
 O      -3.447816     0.497203    -1.278051     255.10
 H      -3.401362     0.688331    -2.270539      23.40
 C      -4.433802     2.362782     0.168085      83.14
 O      -4.969782     3.256158    -0.981140     246.28
 H      -4.689575     4.159971    -0.843670      30.02
 H      -4.123798     2.846789     1.306417      23.25
 H      -5.184014     1.555366     0.120892      27.45
55
name = lig-etoh-Waterframe_611
 C       5.762731    -1.307349     1.366581      60.00
 H       5.628562    -0.237405     0.976672      19.10
 C       5.845676    -3.579753     0.660321      61.04
 H       5.711831    -4.354418    -0.149890      20.55
 C       5.903744    -4.048961     2.010424      10.40
 O       6.041725    -5.356259     2.373594     297.13
 C       5.023157    -6.407899     1.783664     103.53
 H       5.355198    -6.614529     0.745987      28.83
 H       4.101270    -5.980127     1.887455      29.24
 H       5.256148    -7.307053     2.518862      25.71
 C       6.000118    -3.078347     3.030888       2.43
 O       6.255457    -3.404766     4.349489     182.64
 H       6.102783    -4.482846     4.592521      19.32
 C       5.986856    -1.712182     2.653817      72.50
 H       6.235211    -0.954015     3.309958      26.39
 C       5.601851    -2.246554     0.385260      19.53
 C       5.290888    -1.831103    -1.039002      73.15
 H       5.621361    -2.762155    -1.817409      23.70
 O       5.977589    -0.592598    -1.557206     263.36
 H       5.412042     0.238997    -1.375668      24.79
 C       3.690315    -1.695822    -1.271042      78.17
 H       3.298743    -2.545540    -0.645536      22.91
 C       3.369973    -1.889803    -2.729097      95.06
 O       3.647481    -3.255583    -3.253989     264.19
 H       4.376594    -3.068023    -3.911542      25.60
 H       3.892612    -1.162797    -3.394035      22.64
 H       2.195841    -1.675965    -3.030666      22.03
 C      -0.300064    -0.582224     0.205312      34.81
 H      -1.007175    -1.545428     0.624010      16.68
 C       0.211719     1.710396     0.035560      47.12
 H      -0.262504     2.788673    -0.362431      16.26
 C       1.433837     1.342257    -0.446782      22.25
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 O       2.415107     2.347049    -0.928024     190.54
 C       2.045799     3.784667    -0.957906     107.55
 H       2.935466     4.086688    -1.145195      24.28
 H       1.246632     3.734172    -2.052533      22.42
 H       1.370916     4.166930    -0.305264      28.97
 C       1.946737    -0.066691    -0.483577      12.22
 O       3.218982    -0.330327    -0.862726     186.38
 C       0.945104    -1.029833    -0.275374      60.16
 H       1.135992    -2.049581    -0.305661      19.61
 C      -0.714010     0.783592     0.359886      66.93
 C      -2.193343     1.163741     0.779732      79.37
 H      -2.494074     0.251090     1.145313      23.89
 O      -2.279385     2.142012     1.902686     230.29
 H      -1.756709     1.597871     2.736204      22.27
 C      -3.112180     1.690706    -0.340649      86.12
 H      -2.779175     2.579241    -1.028001      20.83
 O      -3.454737     0.521973    -1.273401     256.75
 H      -3.032081     0.673615    -2.106119      25.67
 C      -4.416463     2.304274     0.066528      96.49
 O      -4.953329     3.169529    -0.904905     274.61
 H      -4.667743     4.025618    -0.647381      31.11
 H      -4.512486     2.775713     1.225073      24.45
 H      -5.300685     1.444337     0.304572      25.40
55
name = lig-etoh-Waterframe_612
 C       5.657118    -1.266794     1.357892      46.87
 H       5.697385    -0.149861     1.138032      22.05
 C       5.804589    -3.585519     0.687463      56.54
 H       5.811584    -4.330161    -0.179651      20.62
 C       5.891721    -4.014464     1.979619      11.66
 O       6.022919    -5.411382     2.357128     270.76
 C       5.061468    -6.436037     1.807458      90.25
 H       5.281870    -6.696122     0.795042      26.54
 H       4.079270    -5.960697     1.805418      26.92
 H       5.079546    -7.597160     2.485139      22.53
 C       5.966616    -3.072627     3.082958       8.29
 O       6.174095    -3.437657     4.343185     171.22
 H       6.204259    -4.496822     4.515628      18.50
 C       5.951067    -1.668173     2.708736      41.16
 H       6.013234    -0.894426     3.433722      21.47
 C       5.630020    -2.236878     0.348546      39.37
 C       5.266641    -1.776702    -1.058905      92.36
 H       5.662974    -2.604923    -1.739123      23.07
 O       5.927220    -0.601227    -1.515142     300.52
 H       5.658430     0.237294    -0.959061      23.22
 C       3.713970    -1.662249    -1.250126      83.24
 H       3.083167    -2.379533    -0.554382      21.75
 C       3.363087    -1.856766    -2.819156      82.31
 O       3.671486    -3.318254    -3.241155     238.00
 H       4.585960    -3.324520    -3.761660      23.74
 H       4.093503    -1.215098    -3.444546      22.18
 H       2.318729    -1.489599    -2.973956      24.95
 C      -0.331604    -0.666429     0.263210      41.35
 H      -1.182095    -1.524058     0.286407      18.90
 C       0.145519     1.816416    -0.040961      31.98
 H       0.067036     2.978914     0.088894      15.99
 C       1.481370     1.411596    -0.475013      -2.25
 O       2.396224     2.317507    -0.898321     182.04
 C       1.976808     3.756748    -0.992514      93.63
 H       2.880430     4.388009    -1.155445      24.77
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 H       1.207776     3.864462    -2.059427      21.68
 H       1.700107     4.282664    -0.056270      25.64
 C       1.900566    -0.066204    -0.427582       6.35
 O       3.254123    -0.349807    -0.872074     168.97
 C       0.925347    -1.063525    -0.276628      69.49
 H       1.267877    -1.996791    -0.329892      22.79
 C      -0.782935     0.751005     0.377144      29.43
 C      -2.218301     1.195780     0.799706      77.42
 H      -2.800150     0.272625     1.006596      22.87
 O      -2.322538     2.213229     1.906189     201.06
 H      -1.653289     1.884790     2.809363      22.47
 C      -3.015242     1.702076    -0.344431      86.06
 H      -2.427707     2.460911    -0.892543      23.73
 O      -3.440711     0.589083    -1.212060     291.78
 H      -2.904293     0.361488    -1.887523      30.08
 C      -4.503902     2.188707     0.089717      89.73
 O      -4.966791     3.127375    -0.859951     277.12
 H      -4.467756     3.913497    -0.732167      31.40
 H      -4.324771     2.844397     0.884316      25.48
 H      -5.172414     1.173939     0.140347      25.61
55
name = lig-etoh-Waterframe_613
 C       5.621057    -1.235589     1.426807      46.40
 H       5.553267    -0.155177     1.293922      21.78
 C       5.740207    -3.615284     0.639670      -3.05
 H       5.855546    -4.421588    -0.136612      16.19
 C       5.880015    -4.055397     2.026427      -3.41
 O       6.001321    -5.467441     2.345230     261.52
 C       5.101158    -6.389361     1.801274     109.83
 H       5.374312    -6.729779     0.839664      26.54
 H       3.959886    -6.131093     1.831106      24.42
 H       5.097837    -7.324123     2.658068      24.10
 C       5.949902    -3.042338     3.033455      -6.01
 O       6.110414    -3.438688     4.376757     200.61
 H       6.036953    -4.415563     4.600159      19.90
 C       5.882974    -1.648821     2.759015      45.96
 H       5.839218    -1.040078     3.697954      21.82
 C       5.639765    -2.168857     0.311088      12.81
 C       5.232113    -1.748329    -1.076948     106.89
 H       5.489549    -2.415943    -1.759654      27.97
 O       5.899397    -0.580805    -1.477045     273.79
 H       5.899812     0.046395    -0.671894      25.93
 C       3.687168    -1.645910    -1.302416      76.99
 H       3.203172    -2.545557    -0.738496      25.28
 C       3.424091    -1.881597    -2.861305     100.69
 O       3.633251    -3.322992    -3.195111     246.26
 H       4.578004    -3.323256    -3.601139      23.74
 H       4.178474    -1.188930    -3.344618      25.17
 H       2.458267    -1.741365    -3.084964      28.71
 C      -0.451697    -0.652472     0.270191      34.81
 H      -1.234580    -1.342629     0.382975      20.97
 C       0.162720     1.800714    -0.091259     123.53
 H      -0.111657     2.683969     0.368090      20.81
 C       1.481085     1.383556    -0.456546       5.88
 O       2.416795     2.336309    -0.869326     174.94
 C       1.963616     3.727271    -1.040607      90.92
 H       2.869498     4.387303    -1.601583      23.99
 H       1.069637     4.004685    -1.540564      27.25
 H       1.653274     3.945321     0.082565      26.01
 C       1.874625     0.023307    -0.471027      11.19
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 O       3.268014    -0.298613    -0.860718     134.21
 C       0.915972    -1.028841    -0.203947      54.09
 H       1.063217    -2.098984    -0.376734      22.90
 C      -0.799538     0.706266     0.385257      53.24
 C      -2.201707     1.150570     0.904704      67.71
 H      -2.902340     0.306730     1.323375      22.68
 O      -2.326545     2.251390     1.877163     198.39
 H      -1.689883     1.864600     2.795040      22.01
 C      -3.037572     1.719208    -0.411805     101.19
 H      -2.412965     2.410167    -0.841734      28.29
 O      -3.407688     0.626507    -1.155581     316.15
 H      -2.855204     0.310199    -1.748294      32.23
 C      -4.441886     2.137746     0.148284      94.35
 O      -5.033020     3.104594    -0.888846     260.64
 H      -4.420820     3.829549    -0.950636      31.97
 H      -4.425113     2.375889     1.145160      28.53
 H      -5.098106     1.286424     0.112654      27.93
55
name = lig-etoh-Waterframe_614
 C       5.634569    -1.227027     1.485223      49.55
 H       5.303858    -0.262815     1.263438      23.26
 C       5.705172    -3.582828     0.648755      89.96
 H       5.651727    -4.282598    -0.171934      27.64
 C       5.856885    -4.079475     1.970417      -4.54
 O       6.012547    -5.416630     2.361193     320.96
 C       5.084477    -6.400086     1.814626     116.75
 H       5.443835    -6.772865     0.839126      31.92
 H       4.036354    -5.868295     1.725287      26.63
 H       5.242435    -7.119841     2.462349      32.16
 C       5.944880    -3.113178     3.053063      -0.41
 O       6.046275    -3.382324     4.390414     107.48
 H       6.022962    -4.284926     4.620697      16.58
 C       5.787562    -1.708399     2.787623      26.84
 H       5.758771    -0.964655     3.683370      21.55
 C       5.606777    -2.192775     0.388445      -3.94
 C       5.203044    -1.744859    -1.085113      88.24
 H       5.522046    -2.553216    -1.734718      27.12
 O       5.909912    -0.531308    -1.461108     265.32
 H       5.944079     0.225116    -0.764735      26.61
 C       3.639586    -1.633067    -1.372884      83.66
 H       3.186003    -2.434175    -0.819915      28.14
 C       3.473468    -1.904819    -2.838944     116.31
 O       3.599871    -3.295376    -3.136510     272.79
 H       4.370992    -3.388707    -3.797194      26.55
 H       4.047575    -1.306035    -3.540016      27.58
 H       2.507968    -1.610911    -3.191561      28.21
 C      -0.492411    -0.614558     0.223283      56.36
 H      -1.056847    -1.322607     0.587183      24.85
 C       0.124312     1.628407    -0.017503      83.49
 H      -0.129205     2.590679     0.128594      23.09
 C       1.450278     1.399224    -0.443868       4.88
 O       2.450793     2.350571    -0.886615     175.10
 C       1.936710     3.687628    -1.007233      95.89
 H       2.872459     4.146923    -1.692949      22.37
 H       0.976421     3.650580    -1.404919      27.45
 H       1.909737     4.346761     0.034000      24.73
 C       1.871961    -0.016340    -0.554003      10.94
 O       3.216840    -0.234362    -0.841581     133.63
 C       0.834107    -0.914804    -0.106260      58.28
 H       1.050732    -2.061269    -0.373396      23.43
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 C      -0.780695     0.745601     0.398359      24.61
 C      -2.223319     1.150484     0.941248      74.73
 H      -2.497281     0.154430     1.478402      21.32
 O      -2.260263     2.254207     1.850352     232.58
 H      -1.902483     1.884498     2.869871      23.96
 C      -3.066117     1.695356    -0.303764      89.85
 H      -2.661660     2.532315    -0.912464      24.81
 O      -3.381203     0.568720    -1.190179     277.80
 H      -2.735805     0.560987    -1.811365      30.97
 C      -4.393541     2.177801     0.131110     105.49
 O      -5.093719     3.054008    -0.875439     218.83
 H      -4.570687     3.885273    -0.916498      30.61
 H      -4.625256     2.405939     1.225936      27.31
 H      -4.942144     1.353812    -0.045505      29.04
55
name = lig-etoh-Waterframe_615
 C       5.616229    -1.280828     1.477586      60.46
 H       5.319633    -0.279197     1.335965      23.10
 C       5.681910    -3.552369     0.666223      85.64
 H       5.446604    -4.145669    -0.157503      25.74
 C       5.857944    -4.040706     1.964006      16.49
 O       6.038865    -5.345360     2.365608     248.17
 C       5.091126    -6.384355     1.814897     114.02
 H       5.368035    -6.665728     0.719824      28.53
 H       4.042646    -5.951110     1.736506      27.90
 H       4.981172    -7.200197     2.422268      30.15
 C       5.909918    -3.151791     3.065908       3.86
 O       5.991613    -3.346042     4.415661     148.71
 H       6.147268    -4.286881     4.647947      18.18
 C       5.716048    -1.791026     2.790971      31.38
 H       5.713506    -1.029002     3.658487      22.89
 C       5.516089    -2.180937     0.453601       8.10
 C       5.207379    -1.704400    -0.999966      73.53
 H       5.723672    -2.558727    -1.712622      22.56
 O       5.942221    -0.517110    -1.483571     264.15
 H       5.526551     0.308481    -0.992711      23.82
 C       3.665230    -1.580886    -1.349278      84.89
 H       3.027719    -2.194663    -0.837036      27.25
 C       3.424497    -1.832236    -2.895654      92.33
 O       3.573178    -3.299513    -3.098719     264.35
 H       4.262904    -3.393496    -3.821256      26.47
 H       4.252638    -1.409778    -3.429840      25.81
 H       2.326065    -1.372052    -3.056302      24.46
 C      -0.487318    -0.585772     0.228862      45.45
 H      -1.076844    -1.404991     0.641527      22.20
 C       0.181419     1.670507     0.052187      51.21
 H      -0.102659     2.683576    -0.194811      17.71
 C       1.496004     1.332748    -0.471954       8.24
 O       2.427728     2.306747    -0.860234     191.16
 C       1.965960     3.689261    -0.967043     103.73
 H       2.367113     4.217154    -1.864686      25.77
 H       0.829221     3.546413    -1.625093      21.77
 H       2.084606     4.395011    -0.152704      26.85
 C       1.796590     0.007643    -0.576867      31.56
 O       3.151393    -0.247128    -0.866637     160.12
 C       0.838486    -0.881401    -0.123750      59.01
 H       1.133211    -2.057666    -0.007650      21.73
 C      -0.886768     0.723630     0.443089      44.74
 C      -2.172954     1.173211     0.915215      99.45
 H      -2.719008     0.277426     1.280072      23.55
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 O      -2.168117     2.252600     1.866315     251.24
 H      -1.898458     1.820761     2.795181      25.75
 C      -3.088451     1.623438    -0.176982      67.89
 H      -2.422566     2.467763    -0.729792      23.35
 O      -3.326508     0.502981    -1.244869     226.05
 H      -2.839271     0.624044    -2.030585      27.80
 C      -4.526078     2.182805     0.100237      93.31
 O      -5.121030     3.015452    -0.844586     214.06
 H      -4.816084     3.955441    -0.726788      30.10
 H      -4.412500     2.967779     1.066244      24.30
 H      -5.112410     1.185055     0.108807      26.89
55
name = lig-etoh-Waterframe_616
 C       5.544002    -1.292489     1.529425      73.05
 H       5.619091    -0.195055     1.406054      25.33
 C       5.631703    -3.545259     0.666676      34.05
 H       5.508627    -4.302502    -0.060420      22.64
 C       5.871245    -4.013391     2.019998       1.05
 O       6.044934    -5.377269     2.349098     350.95
 C       5.090062    -6.291591     1.790876     102.86
 H       5.443528    -6.622465     0.721640      27.38
 H       4.123177    -5.879734     1.794094      29.81
 H       4.988314    -7.306963     2.579545      24.45
 C       5.848892    -3.103665     3.089159       2.45
 O       5.958094    -3.374262     4.461372     185.46
 H       6.083374    -4.408812     4.715511      19.99
 C       5.684779    -1.792673     2.776115      68.11
 H       5.666215    -1.203490     3.706630      22.93
 C       5.427878    -2.141434     0.407322       4.74
 C       5.225749    -1.649112    -0.933841      70.37
 H       5.505223    -2.558308    -1.725513      22.25
 O       5.949886    -0.521179    -1.482180     270.82
 H       5.411003     0.338845    -1.319989      24.87
 C       3.663746    -1.528510    -1.306886      83.17
 H       3.180748    -2.416966    -0.827891      26.33
 C       3.410181    -1.744192    -2.874001      84.26
 O       3.511316    -3.283456    -3.088267     244.03
 H       4.339385    -3.341124    -3.634958      25.65
 H       4.169788    -1.173552    -3.433207      26.38
 H       2.304028    -1.500177    -3.358403      24.67
 C      -0.469165    -0.603207     0.311184      35.31
 H      -1.314203    -1.487290     0.445575      19.67
 C       0.229410     1.764903     0.067602      79.01
 H      -0.178303     2.877389     0.020419      19.21
 C       1.422670     1.381057    -0.460838      20.80
 O       2.414329     2.278187    -0.823830     207.68
 C       1.951888     3.678017    -1.067158     117.45
 H       2.476329     3.993928    -1.840801      28.46
 H       0.653095     3.999112    -1.003401      21.02
 H       2.055903     4.072441    -0.151016      28.67
 C       1.795279    -0.023633    -0.571332      20.71
 O       3.127286    -0.271184    -0.928665     175.24
 C       0.852905    -0.977165    -0.167607      70.39
 H       1.223549    -2.003677     0.158309      23.75
 C      -0.808189     0.748127     0.412381      68.21
 C      -2.250534     1.137971     0.949950      86.63
 H      -2.788785     0.387284     1.429289      27.72
 O      -2.064762     2.242303     1.916990     292.00
 H      -1.668713     1.814274     2.648037      30.05
 C      -3.134489     1.589463    -0.279351      71.75
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 H      -2.501628     2.504270    -0.684008      22.64
 O      -3.267276     0.474422    -1.218435     255.58
 H      -2.988310     0.560854    -2.182308      24.45
 C      -4.599481     2.148652     0.155150      96.44
 O      -5.176173     2.998897    -0.887527     225.85
 H      -4.751330     3.889274    -0.627989      29.25
 H      -4.319008     2.738067     1.170198      26.45
 H      -5.465299     1.536415     0.767114      26.52
55
name = lig-etoh-Waterframe_617
 C       5.472818    -1.226228     1.520654      42.74
 H       5.682570    -0.112146     1.318293      19.44
 C       5.574987    -3.545057     0.725431      54.17
 H       5.723703    -4.295676    -0.070125      20.12
 C       5.859362    -4.019568     2.032723       4.00
 O       6.066910    -5.392489     2.337943     236.70
 C       5.063970    -6.228832     1.766223     100.23
 H       5.337410    -6.610107     0.768991      24.35
 H       4.139563    -5.765573     1.734577      27.40
 H       5.320636    -7.247541     2.562335      22.10
 C       5.797543    -3.133037     3.170446      -1.58
 O       5.937846    -3.423163     4.489608     197.11
 H       5.845077    -4.514833     4.651443      18.86
 C       5.672030    -1.720047     2.861244      35.45
 H       5.698085    -0.997011     3.633201      24.43
 C       5.412670    -2.153779     0.439782       7.24
 C       5.147927    -1.604345    -1.047513      92.05
 H       5.447823    -2.501159    -1.583933      23.79
 O       5.965450    -0.535768    -1.472278     301.20
 H       5.623746     0.405678    -1.230617      24.24
 C       3.623774    -1.536645    -1.329388      82.21
 H       3.257481    -2.482552    -0.710818      23.88
 C       3.418038    -1.741607    -2.813221      99.66
 O       3.474380    -3.200379    -3.108688     261.56
 H       4.342723    -3.420700    -3.494223      26.49
 H       4.060535    -1.180812    -3.517816      25.86
 H       2.341109    -1.415764    -3.069665      26.52
 C      -0.397996    -0.615097     0.343472      53.18
 H      -1.344703    -1.419715     0.486436      18.16
 C       0.113464     1.799573     0.095463      72.54
 H      -0.019596     2.928986     0.562690      17.91
 C       1.388235     1.402437    -0.454373       2.73
 O       2.373102     2.283759    -0.837548     201.30
 C       1.947490     3.679235    -1.064818     111.73
 H       2.575456     4.023196    -1.846437      26.44
 H       0.867585     3.738792    -1.284879      25.85
 H       2.479894     4.232107    -0.193514      24.92
 C       1.779923    -0.064941    -0.534372      11.95
 O       3.116339    -0.245821    -0.971254     169.31
 C       0.850384    -1.088875    -0.150688      57.08
 H       1.170077    -2.068695    -0.182827      24.84
 C      -0.717241     0.761419     0.389203      42.90
 C      -2.285027     1.122449     0.974652      63.69
 H      -2.550434     0.218688     1.533531      25.91
 O      -1.979671     2.213579     1.956468     319.93
 H      -1.530812     1.863882     2.598947      33.16
 C      -3.241949     1.583150    -0.382481      79.78
 H      -2.994293     2.451186    -0.934538      24.03
 O      -3.232263     0.439532    -1.145435     269.44
 H      -2.920815     0.568077    -2.145286      22.71
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 C      -4.582273     2.141468     0.282826      89.44
 O      -5.223257     2.982217    -0.899529     196.36
 H      -4.653795     3.857662    -0.938726      29.83
 H      -4.267589     2.836457     0.956034      28.00
 H      -5.445398     1.379624     0.525533      25.62
55
name = lig-etoh-Waterframe_618
 C       5.466111    -1.213540     1.537631      52.49
 H       5.294811    -0.103245     1.263694      23.07
 C       5.563110    -3.525153     0.782879      24.67
 H       5.721830    -4.157037    -0.148597      18.43
 C       5.817508    -4.006315     2.088071      11.76
 O       6.098254    -5.338395     2.320724     259.18
 C       5.082079    -6.250808     1.750182     121.64
 H       5.230825    -6.423934     0.744023      26.61
 H       4.052351    -5.853045     1.878582      26.67
 H       4.820188    -7.182949     2.315431      25.95
 C       5.750795    -3.081489     3.189562      -2.88
 O       5.909027    -3.482005     4.513464     149.70
 H       6.011851    -4.547264     4.772846      17.14
 C       5.659529    -1.666741     2.895301      52.60
 H       5.799794    -0.937065     3.609009      27.02
 C       5.401216    -2.125820     0.480454      -2.76
 C       5.107189    -1.655310    -1.079597      89.39
 H       5.463929    -2.322137    -1.730640      26.66
 O       5.993453    -0.540409    -1.477866     262.25
 H       5.818368     0.246169    -0.881843      25.47
 C       3.629009    -1.545763    -1.351146      89.04
 H       2.919310    -2.211998    -0.732650      25.56
 C       3.349645    -1.776921    -2.798662     118.41
 O       3.453260    -3.123362    -3.142329     279.48
 H       4.301837    -3.225206    -3.607644      27.18
 H       4.135439    -1.212372    -3.344698      26.32
 H       2.418440    -1.436117    -2.856303      29.32
 C      -0.353633    -0.623974     0.316215      41.02
 H      -1.098719    -1.380980     0.743481      22.26
 C       0.125532     1.785532     0.109208      91.16
 H      -0.123688     2.799552     0.662381      18.18
 C       1.357463     1.335592    -0.416427      11.50
 O       2.336640     2.292698    -0.874798     173.96
 C       2.043934     3.664630    -1.051987     114.53
 H       2.409362     4.018051    -2.182621      24.71
 H       1.138831     3.738563    -1.324088      29.60
 H       2.197304     4.614530    -0.220495      24.31
 C       1.739660    -0.027120    -0.502114      14.25
 O       3.086641    -0.194408    -0.983959     108.81
 C       0.890988    -1.117898    -0.134591      72.94
 H       0.917218    -2.073439    -0.465361      24.49
 C      -0.830295     0.713603     0.439547      66.06
 C      -2.123838     1.173964     0.931728      81.72
 H      -2.728485     0.195717     1.309315      23.12
 O      -1.955269     2.173765     1.956387     273.75
 H      -1.591664     1.719084     2.763655      27.51
 C      -3.307760     1.597995    -0.285127      83.69
 H      -2.876198     2.303034    -0.910060      25.72
 O      -3.252389     0.345946    -1.093399     233.75
 H      -2.795251     0.531700    -2.062382      23.19
 C      -4.565284     2.180506     0.227632     112.49
 O      -5.252030     2.938301    -0.861076     243.31
 H      -4.628681     3.782713    -0.975340      29.84
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 H      -4.403616     2.783196     1.032832      28.96
 H      -5.176204     1.314533     0.477985      27.93
55
name = lig-etoh-Waterframe_619
 C       5.453883    -1.216678     1.577331      50.94
 H       5.075039    -0.173915     1.505458      24.37
 C       5.594789    -3.453453     0.791743      54.89
 H       5.531148    -4.287846     0.014776      25.09
 C       5.743473    -3.932933     2.121385       8.14
 O       6.100642    -5.327784     2.315404     223.29
 C       5.040590    -6.256036     1.743757     117.07
 H       5.255899    -6.355946     0.696132      28.75
 H       4.076000    -5.593518     1.895530      24.04
 H       5.109589    -7.119190     2.189505      30.26
 C       5.739946    -3.031763     3.211510       4.12
 O       5.883199    -3.494990     4.534715     138.51
 H       6.117157    -4.438823     4.526212      23.90
 C       5.653809    -1.649597     2.878846      53.23
 H       5.781973    -1.042425     3.683092      24.24
 C       5.378229    -2.123583     0.457766      17.62
 C       5.180775    -1.725918    -0.972961      77.10
 H       5.443079    -2.556755    -1.693527      25.27
 O       5.988729    -0.561071    -1.464945     249.78
 H       5.924010     0.205006    -0.841415      26.35
 C       3.556617    -1.490140    -1.295801      79.59
 H       3.114452    -2.317239    -0.725370      26.32
 C       3.263015    -1.715462    -2.806963     105.11
 O       3.461316    -3.129391    -3.200769     274.78
 H       4.219112    -3.146402    -3.815645      27.47
 H       3.906769    -1.011971    -3.394030      26.35
 H       2.295157    -1.430411    -3.179507      27.41
 C      -0.428792    -0.656382     0.337155      52.32
 H      -0.934202    -1.425820     0.693810      24.32
 C       0.128978     1.656717     0.155648      71.29
 H      -0.084179     2.705980     0.134665      20.91
 C       1.359112     1.372827    -0.368969      12.33
 O       2.346957     2.261320    -0.880402     185.35
 C       2.042465     3.697954    -1.134867      78.31
 H       2.855448     3.926820    -2.067634      21.20
 H       0.793996     3.891840    -1.221320      22.63
 H       2.307833     4.222742    -0.082916      24.45
 C       1.797157    -0.031212    -0.525583      23.74
 O       3.065778    -0.132956    -0.995084     164.11
 C       0.896243    -1.022342    -0.151847      69.77
 H       0.964418    -2.082987    -0.465455      23.63
 C      -0.795805     0.687296     0.430831      45.74
 C      -2.131338     1.191113     0.903712      86.49
 H      -2.763582     0.322270     1.394011      21.69
 O      -1.954543     2.142264     1.953940     223.02
 H      -1.869643     1.583302     2.910251      23.70
 C      -3.112961     1.596499    -0.198416      72.81
 H      -2.519669     2.348673    -0.810235      23.08
 O      -3.333496     0.260842    -1.013215     199.47
 H      -2.798671     0.423656    -1.977084      22.78
 C      -4.597200     2.166664     0.146200     108.61
 O      -5.255436     2.894250    -0.809135     259.65
 H      -4.772853     3.851724    -0.786647      27.75
 H      -4.545875     2.685546     1.215214      26.74
 H      -5.216903     1.425419     0.450675      29.32
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name = lig-etoh-Waterframe_620
 C       5.393198    -1.195878     1.582076      55.26
 H       5.263720    -0.147768     1.469786      22.31
 C       5.615348    -3.450631     0.806303      54.88
 H       5.526424    -4.247544     0.025888      23.93
 C       5.713147    -3.898512     2.117067       9.03
 O       6.055617    -5.296637     2.314820     221.93
 C       5.045041    -6.176167     1.739384     113.57
 H       5.194247    -6.396912     0.608497      26.38
 H       3.868161    -5.875946     1.916685      23.75
 H       5.338590    -7.086386     2.284442      26.31
 C       5.763441    -3.043924     3.241407      19.88
 O       5.864559    -3.448215     4.515059     152.42
 H       6.004112    -4.370151     4.532811      22.91
 C       5.655073    -1.675652     2.921392      39.93
 H       5.594087    -0.944068     3.677073      26.58
 C       5.390808    -2.088083     0.499152      18.39
 C       5.187640    -1.686264    -0.927834      73.40
 H       5.452002    -2.764093    -1.464195      23.39
 O       5.976215    -0.635059    -1.434978     287.30
 H       5.789903     0.209717    -0.968245      26.82
 C       3.528005    -1.465686    -1.273725      86.59
 H       3.075955    -2.157560    -0.645400      27.10
 C       3.194805    -1.633888    -2.837323      85.29
 O       3.490817    -3.134015    -3.253039     241.70
 H       4.313716    -3.193043    -3.806957      26.02
 H       3.870050    -1.010712    -3.456855      25.92
 H       2.004256    -1.496589    -3.096935      25.08
 C      -0.453803    -0.728109     0.348495      47.98
 H      -1.157607    -1.433602     0.541100      21.34
 C       0.175932     1.657614     0.131271      69.11
 H      -0.253227     2.526421    -0.084219      19.96
 C       1.470733     1.360394    -0.367860      16.61
 O       2.340429     2.239518    -0.887118     203.68
 C       2.052112     3.660005    -1.126082     103.33
 H       2.766743     4.135501    -1.873842      25.52
 H       0.858203     4.036721    -1.641137      22.46
 H       2.401248     4.124685    -0.311773      28.38
 C       1.803251     0.044053    -0.517841      30.10
 O       3.112482    -0.128981    -1.008599     178.55
 C       0.835797    -0.938579    -0.190227      65.87
 H       1.342410    -2.018050    -0.133801      23.03
 C      -0.786839     0.619268     0.443336      41.26
 C      -2.239616     1.096805     1.000242      79.61
 H      -2.575112     0.212379     1.436124      25.59
 O      -1.989290     2.157457     1.958483     205.79
 H      -1.650796     1.590276     2.962532      22.12
 C      -2.963245     1.570613    -0.225741      74.35
 H      -2.541886     2.401933    -0.956431      22.41
 O      -3.399338     0.256910    -0.902453     200.98
 H      -2.911791     0.122379    -1.936575      22.07
 C      -4.549188     2.051226     0.206149      73.42
 O      -5.250535     2.911092    -0.811749     190.52
 H      -4.945711     3.924271    -0.707651      28.59
 H      -4.411209     2.884491     1.112724      24.50
 H      -5.155823     1.167624     0.207636      27.93
55
name = lig-etoh-Waterframe_621
 C       5.370502    -1.167692     1.645642      61.61
 H       5.424185    -0.175776     1.367977      21.42
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 C       5.594624    -3.446685     0.804401      41.84
 H       5.730601    -4.061872    -0.068171      19.89
 C       5.762117    -3.934214     2.104928      25.68
 O       5.959050    -5.220518     2.318518     267.74
 C       5.075078    -6.160860     1.751196     110.50
 H       5.165031    -6.242395     0.578744      23.82
 H       4.031284    -5.994199     2.071651      26.79
 H       5.159797    -7.275359     2.348261      23.07
 C       5.775482    -3.028156     3.200355       7.19
 O       5.861734    -3.416704     4.537195     229.03
 H       5.880375    -4.321247     4.735013      23.39
 C       5.613504    -1.647410     2.936991      39.68
 H       5.476979    -0.919141     3.768819      27.00
 C       5.407936    -2.056115     0.569654       3.77
 C       5.064063    -1.667144    -0.927835      88.17
 H       5.452609    -2.506541    -1.700213      20.84
 O       5.987068    -0.689611    -1.415100     288.57
 H       5.605993     0.172649    -1.180498      27.88
 C       3.583621    -1.486349    -1.329205      93.98
 H       2.927764    -2.102343    -0.772496      25.29
 C       3.195552    -1.700512    -2.839152      93.37
 O       3.501371    -3.084345    -3.271439     262.18
 H       4.448720    -3.041354    -3.629522      24.59
 H       3.709274    -0.942936    -3.449305      24.96
 H       1.988073    -1.460027    -2.769062      24.09
 C      -0.437660    -0.757679     0.321355      36.42
 H      -1.247311    -1.577610     0.458759      19.45
 C       0.166295     1.670708     0.065312      78.19
 H      -0.238851     2.647920     0.075821      20.41
 C       1.461950     1.416292    -0.364366       8.46
 O       2.379909     2.286343    -0.948513     227.68
 C       2.099047     3.655462    -1.110841     126.48
 H       2.685257     3.836381    -1.847932      27.44
 H       0.987569     3.737123    -1.566010      25.58
 H       2.030811     4.294624    -0.261587      28.70
 C       1.799726     0.040431    -0.484374      24.06
 O       3.168582    -0.137028    -0.992197     152.31
 C       0.870628    -0.960689    -0.203979      74.16
 H       1.274911    -2.075208     0.016636      22.14
 C      -0.819926     0.611304     0.514500      48.24
 C      -2.154549     0.990263     1.086900      71.46
 H      -2.778847     0.224863     1.443712      25.89
 O      -2.059047     2.159840     1.979593     199.36
 H      -1.313712     1.874054     2.823326      23.83
 C      -3.105269     1.492477    -0.264682      80.77
 H      -2.402782     2.145273    -0.938660      22.56
 O      -3.419093     0.277402    -0.819475     209.28
 H      -2.943228     0.044619    -1.836389      21.34
 C      -4.405185     2.041180     0.202451      82.14
 O      -5.232382     2.898684    -0.821446     215.44
 H      -4.718363     3.829243    -0.648969      26.06
 H      -4.466119     2.349314     1.359963      26.23
 H      -4.924164     1.015814     0.361388      26.79
55
name = lig-etoh-Waterframe_622
 C       5.399573    -1.118635     1.667331      55.26
 H       5.248160    -0.064932     1.539898      23.42
 C       5.585599    -3.398566     0.767874      52.77
 H       5.757070    -4.057387    -0.030396      22.87
 C       5.805889    -3.880142     2.069242      12.02
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 O       5.912664    -5.240382     2.384289     300.81
 C       5.022748    -6.197528     1.778005     101.88
 H       5.165218    -6.187651     0.664692      24.40
 H       4.122461    -5.830681     1.969422      31.61
 H       5.537274    -7.260626     2.168118      22.70
 C       5.762293    -3.006448     3.185701     -21.50
 O       5.866450    -3.379964     4.573366     239.87
 H       5.884249    -4.359304     4.579561      27.69
 C       5.549235    -1.610474     2.971137      26.17
 H       5.535663    -1.026616     3.959081      19.53
 C       5.354810    -2.065606     0.545398      18.42
 C       5.018101    -1.716300    -0.942463     102.61
 H       5.201809    -2.668402    -1.397535      24.65
 O       5.989541    -0.671451    -1.407363     277.73
 H       5.699903     0.241236    -1.333306      26.82
 C       3.607775    -1.502927    -1.366296      82.51
 H       3.115532    -2.424101    -0.833554      21.57
 C       3.231019    -1.759976    -2.789146     114.34
 O       3.507838    -3.007452    -3.257978     271.47
 H       4.414404    -3.079926    -3.768532      25.67
 H       3.521117    -1.008967    -3.496570      25.18
 H       2.118022    -1.737611    -2.919320      24.98
 C      -0.409763    -0.679712     0.265508      51.25
 H      -0.929895    -1.718999     0.662448      20.64
 C       0.044598     1.679049     0.057856     102.40
 H      -0.048768     2.783434     0.406281      19.27
 C       1.400998     1.443512    -0.403041      -5.95
 O       2.434367     2.297842    -0.961720     172.36
 C       2.068297     3.670156    -1.153392     104.10
 H       2.858067     4.096313    -1.809491      24.19
 H       1.217488     3.640404    -1.538031      31.08
 H       1.909701     4.391733    -0.085274      24.02
 C       1.876082    -0.001079    -0.481967       4.32
 O       3.166905    -0.134205    -0.941779     148.25
 C       0.938357    -1.052989    -0.157123      55.39
 H       1.137832    -2.147995    -0.374995      19.90
 C      -0.757952     0.607620     0.559482      27.42
 C      -2.106979     1.020648     1.093450      73.20
 H      -2.698236     0.170911     1.630380      19.69
 O      -2.119965     2.145664     1.976703     275.14
 H      -1.481402     1.913452     2.844840      24.65
 C      -3.133490     1.420284    -0.198746      72.52
 H      -2.518206     2.047067    -0.859476      23.02
 O      -3.443891     0.184745    -0.838102     230.38
 H      -2.829854     0.279098    -1.787306      20.89
 C      -4.399173     2.043184     0.218643      96.67
 O      -5.132809     2.843731    -0.751597     291.88
 H      -4.621133     3.752036    -0.844554      28.81
 H      -4.279672     2.551131     1.125765      26.32
 H      -5.198418     1.157022     0.296274      24.32
55
name = lig-etoh-Waterframe_623
 C       5.399635    -1.095043     1.638897      46.89
 H       4.981074    -0.053301     1.565589      22.04
 C       5.613535    -3.395698     0.758784      36.66
 H       5.553867    -4.128300    -0.014913      17.65
 C       5.807362    -3.848992     2.091018       1.54
 O       5.925785    -5.259284     2.471418     254.29
 C       5.014718    -6.193669     1.757380     125.37
 H       5.131493    -6.220780     0.729556      29.36
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 H       3.911418    -6.147382     2.016025      28.88
 H       5.247710    -7.189283     2.241271      25.60
 C       5.739791    -2.960741     3.239316      18.77
 O       5.872953    -3.368143     4.540779     186.35
 H       5.962515    -4.393100     4.571285      23.59
 C       5.519799    -1.626059     2.989137      42.27
 H       5.497407    -0.865551     3.875402      20.29
 C       5.267074    -1.974365     0.524416      14.22
 C       5.108658    -1.717816    -0.942608     111.30
 H       5.365586    -2.576001    -1.410947      27.36
 O       5.989370    -0.686514    -1.429607     304.39
 H       5.638337     0.151474    -1.094152      27.31
 C       3.590353    -1.511947    -1.307303      83.49
 H       3.041883    -2.300049    -0.600631      22.33
 C       3.186176    -1.692255    -2.812699     105.66
 O       3.558168    -3.054851    -3.253653     255.97
 H       4.449234    -2.994618    -3.819803      24.68
 H       3.675804    -0.940432    -3.430354      24.63
 H       2.191972    -1.663492    -2.767877      27.40
 C      -0.273875    -0.699250     0.250169      37.81
 H      -1.137495    -1.391398     0.753684      19.03
 C       0.098455     1.725708     0.082434      89.11
 H      -0.390404     2.772408     0.495828      14.65
 C       1.373454     1.332151    -0.469150       8.83
 O       2.444950     2.272758    -0.914941     156.35
 C       2.015570     3.710861    -1.198377      77.07
 H       2.877392     4.481053    -1.652689      22.63
 H       1.071776     3.876891    -1.864803      23.83
 H       2.054887     4.104032     0.015346      21.97
 C       1.851632     0.015916    -0.481310      21.34
 O       3.163146    -0.184131    -0.895651     168.93
 C       0.995568    -1.062252    -0.152686      83.21
 H       1.131549    -1.992425    -0.544860      21.63
 C      -0.711411     0.672655     0.545201      31.05
 C      -2.175814     1.054817     1.078297      85.13
 H      -2.320753     0.019852     1.639610      18.92
 O      -2.153163     2.154973     1.983310     332.87
 H      -1.947038     1.739041     2.833158      27.60
 C      -3.044802     1.333075    -0.090550      65.85
 H      -2.688945     2.059552    -0.707941      24.98
 O      -3.444001     0.062026    -0.920997     205.33
 H      -2.891480     0.020544    -1.899048      21.28
 C      -4.506391     2.062239     0.303694     103.45
 O      -5.017943     2.800032    -0.732620     328.47
 H      -4.587374     3.727005    -0.703543      28.75
 H      -4.242873     2.752108     0.984951      26.28
 H      -5.277687     1.273544     0.634204      25.84
55
name = lig-etoh-Waterframe_624
 C       5.310885    -1.112431     1.636092      59.99
 H       5.062356     0.003779     1.442030      20.95
 C       5.605998    -3.359623     0.834338      44.75
 H       5.447784    -4.053260    -0.006659      17.79
 C       5.771052    -3.877576     2.149587      14.02
 O       5.911847    -5.234674     2.507574     281.97
 C       5.027441    -6.203481     1.784625     130.46
 H       5.202950    -6.204101     0.753521      30.06
 H       3.830261    -5.921116     2.125077      25.51
 H       5.240304    -7.099539     2.127771      28.43
 C       5.732338    -2.954018     3.241661       3.12
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 O       5.887668    -3.385925     4.519302     198.53
 H       5.952154    -4.446152     4.630462      22.62
 C       5.513357    -1.566858     2.927696      56.42
 H       5.370996    -0.788904     3.752687      22.79
 C       5.294417    -2.000330     0.564809      15.06
 C       5.160836    -1.682695    -0.969796      88.07
 H       5.567547    -2.516087    -1.614122      25.32
 O       5.985692    -0.674594    -1.460015     292.68
 H       5.828475     0.131784    -0.944269      27.78
 C       3.584772    -1.524369    -1.237885      86.21
 H       2.971276    -2.249451    -0.660550      22.99
 C       3.169492    -1.657800    -2.788151      86.74
 O       3.589962    -3.105387    -3.244457     232.84
 H       4.544296    -2.986657    -3.598340      25.18
 H       3.748872    -0.868098    -3.347975      23.86
 H       2.111325    -1.418751    -2.940653      25.38
 C      -0.277119    -0.648362     0.366431      36.96
 H      -0.970094    -1.526395     0.362019      17.85
 C       0.212244     1.732842     0.131841      67.18
 H      -0.093210     2.868055    -0.056231      15.75
 C       1.410511     1.376450    -0.517107      16.79
 O       2.394203     2.263649    -0.903641     195.47
 C       1.995996     3.718027    -1.129967      74.76
 H       3.039420     3.985417    -1.741194      20.62
 H       0.905718     3.930242    -1.860327      22.51
 H       1.555717     4.221454    -0.272290      25.07
 C       1.831449     0.002649    -0.511145      14.18
 O       3.182444    -0.215721    -0.856324     188.41
 C       0.995815    -1.042097    -0.193068      64.85
 H       1.263099    -2.004788    -0.337568      20.85
 C      -0.666438     0.702726     0.470154      75.11
 C      -2.110212     0.955078     1.071625      84.09
 H      -2.676542     0.108507     1.615619      22.37
 O      -2.188864     2.157509     2.009753     284.13
 H      -2.095973     1.838557     2.826346      29.09
 C      -3.156000     1.243362    -0.074182      63.68
 H      -2.612724     1.972576    -0.693528      21.41
 O      -3.410403    -0.012632    -0.962975     219.64
 H      -2.914003     0.049247    -1.903918      21.98
 C      -4.491085     2.010748     0.448481      93.18
 O      -4.951110     2.788808    -0.807374     306.15
 H      -4.657855     3.637687    -0.504234      29.44
 H      -4.239815     2.719565     1.406484      25.15
 H      -5.186718     1.408356     0.975351      28.78
55
name = lig-etoh-Waterframe_625
 C       5.206921    -1.104899     1.597878      39.94
 H       5.206960     0.026936     1.395839      20.72
 C       5.552916    -3.384669     0.919147      50.37
 H       5.639807    -4.106724     0.045102      20.03
 C       5.713520    -3.884163     2.193058      27.90
 O       5.891527    -5.216840     2.503705     261.79
 C       5.045659    -6.165235     1.845556     121.09
 H       5.201546    -6.092129     0.728897      24.93
 H       3.928534    -5.701832     1.945076      23.88
 H       5.319623    -7.076663     2.239623      27.63
 C       5.729399    -2.938230     3.205424       4.10
 O       5.906594    -3.399943     4.546550     166.65
 H       5.889765    -4.482449     4.410980      17.26
 C       5.506967    -1.542947     2.908885      31.48
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 H       5.326933    -0.872143     3.781909      22.27
 C       5.397965    -2.070086     0.547069      34.34
 C       5.135155    -1.690019    -0.956160      73.01
 H       5.374135    -2.769795    -1.500811      22.96
 O       6.001318    -0.598686    -1.489291     293.94
 H       5.951356     0.262574    -1.040326      27.38
 C       3.579383    -1.551189    -1.265297      92.52
 H       3.262442    -2.383519    -0.748290      25.90
 C       3.242578    -1.697389    -2.721092      97.83
 O       3.568428    -3.076231    -3.198835     254.22
 H       4.458575    -3.055742    -3.630102      27.96
 H       3.905769    -1.018803    -3.348933      23.27
 H       2.135274    -1.590755    -3.149761      23.91
 C      -0.289101    -0.652401     0.411539      46.21
 H      -0.980349    -1.391558     0.511756      21.03
 C       0.304343     1.751075     0.093097      61.82
 H       0.022836     2.791324    -0.053023      17.14
 C       1.479459     1.397086    -0.490866      18.84
 O       2.332210     2.317524    -0.920574     233.22
 C       1.957089     3.662269    -1.091315     108.41
 H       2.899160     4.198367    -1.503207      23.81
 H       1.185153     3.480756    -2.025695      23.20
 H       1.794689     4.306439    -0.395142      28.95
 C       1.883591     0.000199    -0.569804      18.15
 O       3.209866    -0.201218    -0.813165     178.94
 C       0.921913    -0.992261    -0.194405      70.68
 H       1.228832    -2.022136     0.011480      22.03
 C      -0.710357     0.684861     0.487693      52.04
 C      -2.088679     0.888811     1.078188      84.95
 H      -2.320507    -0.012228     1.637071      25.51
 O      -2.207638     2.113457     2.003401     281.45
 H      -1.854163     1.880562     2.802056      31.38
 C      -3.270214     1.180277    -0.105102      61.26
 H      -2.760246     1.954086    -0.845632      19.68
 O      -3.381001    -0.030121    -0.939612     264.08
 H      -2.991877     0.334937    -1.761635      23.50
 C      -4.420443     1.924263     0.504581      99.56
 O      -4.904255     2.749846    -0.798095     218.15
 H      -4.745841     3.669528    -0.744818      29.45
 H      -3.967133     2.805603     1.313019      21.46
 H      -5.263874     1.353655     0.699096      27.77
55
name = lig-etoh-Waterframe_626
 C       5.214033    -1.129153     1.562388      51.47
 H       4.974997    -0.066124     1.327678      23.00
 C       5.524224    -3.482468     0.877237      18.81
 H       5.778845    -4.303268     0.129721      18.39
 C       5.659947    -3.857915     2.215647       7.41
 O       5.908510    -5.197517     2.519162     287.26
 C       5.032762    -6.078841     1.850380     125.92
 H       5.324302    -6.300140     0.710422      23.81
 H       4.016481    -6.022915     2.005635      27.24
 H       5.063366    -7.107466     2.453724      25.63
 C       5.718822    -2.900577     3.276737       5.55
 O       5.916749    -3.393650     4.530154     144.36
 H       5.988303    -4.486370     4.537027      19.44
 C       5.463734    -1.567501     2.922280      57.10
 H       5.399574    -0.901928     3.757049      23.13
 C       5.426024    -2.025645     0.513542      13.64
 C       5.126704    -1.691661    -0.920140      92.21
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 H       5.492802    -2.549337    -1.664759      22.81
 O       6.009933    -0.579039    -1.518931     290.53
 H       5.582347     0.201310    -1.067307      27.23
 C       3.647943    -1.559562    -1.257691      95.73
 H       3.097554    -2.289507    -0.669777      24.23
 C       3.353414    -1.761606    -2.763005      99.96
 O       3.547533    -3.060767    -3.143724     282.51
 H       4.348355    -3.032826    -3.704888      27.09
 H       3.953714    -0.989256    -3.307571      22.99
 H       2.155934    -1.494530    -2.704171      23.44
 C      -0.347912    -0.639942     0.388783      36.97
 H      -0.953264    -1.276315     0.906485      18.64
 C       0.190455     1.705430     0.072073      70.46
 H      -0.067965     2.629680     0.324871      19.93
 C       1.517463     1.329105    -0.427119       9.62
 O       2.404008     2.358308    -0.926018     201.22
 C       1.936742     3.661065    -1.177390     117.51
 H       2.685170     4.193122    -1.507817      27.24
 H       1.178441     3.864601    -1.839905      29.45
 H       1.647099     4.156466    -0.108300      25.66
 C       1.866038     0.005014    -0.576770      35.25
 O       3.248240    -0.230330    -0.791384     197.96
 C       0.939551    -0.943313    -0.154637      58.45
 H       1.256370    -2.073943    -0.050409      19.25
 C      -0.685499     0.736397     0.522876      39.50
 C      -2.131778     0.915014     1.077813      90.26
 H      -2.192731     0.032543     1.593966      24.05
 O      -2.198945     2.015086     1.978480     315.21
 H      -1.531143     1.819676     2.651500      29.80
 C      -3.185188     1.111766    -0.074548      65.60
 H      -2.846135     2.033622    -0.743703      21.09
 O      -3.382791    -0.014836    -0.897520     286.13
 H      -3.196267     0.117307    -1.807723      26.88
 C      -4.415269     1.907796     0.366541     106.58
 O      -4.889979     2.678647    -0.748000     300.09
 H      -4.571098     3.572122    -0.685203      29.89
 H      -4.015921     2.533325     1.333602      23.40
 H      -5.282102     1.335662     0.731139      27.20
55
name = lig-etoh-Waterframe_627
 C       5.283833    -1.177752     1.588941      45.04
 H       4.830949    -0.243471     1.406907      22.34
 C       5.548676    -3.461641     0.806769      79.17
 H       5.603039    -4.249507     0.022825      23.44
 C       5.639463    -3.813575     2.183178      12.98
 O       5.916463    -5.163110     2.546662     243.68
 C       4.990296    -6.122419     1.871830     102.89
 H       5.348881    -6.367447     0.778186      26.68
 H       4.035057    -5.710276     1.871478      26.92
 H       5.262423    -7.149308     2.514982      25.11
 C       5.679051    -2.923509     3.285816      11.06
 O       5.934242    -3.364554     4.561046     144.42
 H       6.093327    -4.432143     4.497895      22.75
 C       5.402928    -1.558038     2.952763      42.83
 H       5.406337    -0.776089     3.625414      23.34
 C       5.393485    -2.108347     0.507126      -4.45
 C       5.232115    -1.687750    -0.973536      90.78
 H       5.558057    -2.544111    -1.519869      26.18
 O       5.955386    -0.601251    -1.501393     334.36
 H       5.616051     0.356758    -1.288640      25.49
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 C       3.723712    -1.554567    -1.214666      87.49
 H       3.021724    -2.312838    -0.696738      26.03
 C       3.387981    -1.684704    -2.715721      99.81
 O       3.563875    -3.126522    -3.143356     261.23
 H       4.397671    -3.156872    -3.661926      27.84
 H       3.884241    -1.046479    -3.428478      25.65
 H       2.306707    -1.408807    -2.903502      26.68
 C      -0.344100    -0.602741     0.357918      58.36
 H      -0.824939    -1.413348     0.944319      20.96
 C       0.143845     1.702396     0.054804      90.17
 H      -0.039845     2.666253     0.397715      20.34
 C       1.468315     1.421496    -0.402464      -0.21
 O       2.492268     2.297700    -0.927057     151.44
 C       1.901724     3.762312    -1.205368      84.99
 H       2.743135     4.243404    -1.518997      25.47
 H       1.015284     3.850583    -1.739524      27.51
 H       1.345678     3.975981    -0.052067      22.43
 C       1.883404    -0.003497    -0.531934      10.20
 O       3.257368    -0.261508    -0.798339     176.32
 C       0.935793    -0.979511    -0.077020      63.71
 H       1.251196    -2.098061    -0.340717      21.21
 C      -0.725693     0.689642     0.540719      32.36
 C      -2.114411     0.908066     1.062557      86.29
 H      -2.623620    -0.020769     1.565059      21.35
 O      -2.180281     1.951584     1.977015     292.00
 H      -1.478991     1.806344     2.706013      27.53
 C      -3.056505     1.167281    -0.070649      71.15
 H      -2.363169     1.754873    -0.670172      23.49
 O      -3.402715    -0.052040    -0.869738     277.15
 H      -3.195008     0.089031    -1.722389      30.12
 C      -4.442009     1.849146     0.294999     110.78
 O      -4.911156     2.643757    -0.732218     341.68
 H      -4.457523     3.475173    -0.614902      30.44
 H      -4.325852     2.488375     1.049784      27.65
 H      -5.203214     1.107080     0.771129      26.74
55
name = lig-etoh-Waterframe_628
 C       5.315322    -1.229492     1.613285      53.59
 H       5.095330    -0.241421     1.384176      21.92
 C       5.587190    -3.449382     0.796225      58.80
 H       5.471682    -4.126709    -0.019562      17.85
 C       5.668593    -3.842851     2.138657      10.68
 O       5.897641    -5.136131     2.542904     312.13
 C       5.020896    -6.166839     1.910460     106.48
 H       5.316053    -6.299260     0.899498      31.11
 H       4.009162    -5.638218     1.818432      27.59
 H       4.928490    -7.130352     2.596356      25.43
 C       5.624236    -2.919069     3.244842     -12.25
 O       5.955137    -3.335360     4.595390     217.82
 H       6.004198    -4.378557     4.540128      25.23
 C       5.372862    -1.553952     2.974129      59.19
 H       5.279316    -0.807927     3.709916      23.81
 C       5.376652    -2.121129     0.509336       0.47
 C       5.292008    -1.719015    -0.980103      88.80
 H       5.535856    -2.533437    -1.525756      29.98
 O       5.943994    -0.617301    -1.507347     340.18
 H       5.652322     0.281331    -1.008220      24.49
 C       3.714058    -1.560808    -1.246015      72.95
 H       3.450114    -2.553687    -0.679674      22.44
 C       3.378098    -1.642386    -2.718861      97.81
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 O       3.591739    -3.176735    -3.156136     229.43
 H       4.502615    -3.104123    -3.574815      27.27
 H       4.119025    -1.120948    -3.274697      23.79
 H       2.425493    -1.515762    -2.972184      28.28
 C      -0.279941    -0.690670     0.383806       8.16
 H      -1.150174    -1.560888     0.505892      15.23
 C       0.180593     1.766092     0.069389      75.56
 H      -0.188402     2.876313     0.102246      16.82
 C       1.473706     1.426937    -0.443158       8.17
 O       2.469103     2.288891    -0.930416     181.30
 C       1.862830     3.753631    -1.138830      78.68
 H       2.711073     4.530152    -1.478162      22.39
 H       1.170421     3.400225    -2.042995      21.55
 H       1.690707     4.443584    -0.136343      22.10
 C       1.880247     0.014073    -0.422853      22.31
 O       3.229672    -0.236757    -0.797106     170.20
 C       1.002486    -1.002499    -0.097178      70.31
 H       1.034916    -2.134310    -0.211976      18.89
 C      -0.760608     0.609604     0.534239      76.09
 C      -2.123690     0.811642     1.096572      65.38
 H      -2.546751    -0.269054     1.526464      22.44
 O      -2.160686     1.974230     2.014056     212.84
 H      -1.708301     1.643621     2.999094      23.52
 C      -3.004775     1.257489    -0.164447      83.49
 H      -2.538228     1.845082    -0.886918      24.18
 O      -3.395643    -0.089782    -0.838404     244.42
 H      -3.123047     0.111964    -1.634525      28.41
 C      -4.378337     1.782871     0.342525      85.73
 O      -4.985815     2.640514    -0.802395     279.12
 H      -4.625008     3.543494    -0.825247      30.16
 H      -4.356874     2.374480     1.185767      27.92
 H      -5.029224     0.828195     0.216481      25.92
55
name = lig-etoh-Waterframe_629
 C       5.303604    -1.173288     1.589341      69.69
 H       5.388667    -0.157367     1.362916      26.09
 C       5.591723    -3.493602     0.805818      27.34
 H       5.647380    -4.249328     0.073812      20.40
 C       5.711642    -3.874756     2.152177      -6.63
 O       5.879021    -5.183061     2.538814     358.81
 C       5.033566    -6.135402     1.938219     134.13
 H       5.408293    -6.530551     1.073982      24.72
 H       3.839782    -5.886973     1.898891      23.91
 H       4.980719    -6.926267     2.600569      24.30
 C       5.612827    -2.930993     3.264165     -10.85
 O       5.947281    -3.309717     4.555276     310.84
 H       5.830839    -4.284327     4.704881      27.21
 C       5.368702    -1.596197     2.975289      56.78
 H       5.173446    -0.950028     3.851370      21.75
 C       5.426575    -2.053127     0.521968      18.26
 C       5.204447    -1.740148    -0.961462      93.94
 H       5.576039    -2.572677    -1.621640      20.33
 O       6.004108    -0.596094    -1.507268     282.36
 H       5.676845     0.164030    -0.874755      23.41
 C       3.699781    -1.600558    -1.270755      74.92
 H       3.034442    -2.314497    -0.678667      16.70
 C       3.398167    -1.739213    -2.773884      94.21
 O       3.630050    -3.146845    -3.167275     268.73
 H       4.514006    -3.071046    -3.694376      25.05
 H       4.111457    -1.018909    -3.223666      20.50
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 H       2.422129    -1.391265    -2.967949      25.34
 C      -0.271196    -0.769259     0.394480      29.25
 H      -1.077433    -1.662334     0.200942      16.18
 C       0.173679     1.702243     0.114827      56.90
 H      -0.332467     2.781432    -0.187803      15.43
 C       1.465871     1.373473    -0.443989       6.52
 O       2.392573     2.371076    -0.904915     210.25
 C       1.927538     3.683689    -1.094071      97.62
 H       2.816983     4.209092    -1.813444      20.90
 H       0.895341     3.769719    -1.939151      22.50
 H       1.405988     4.116362    -0.337246      26.89
 C       1.923707     0.019479    -0.344782      10.98
 O       3.210026    -0.217195    -0.784269     185.11
 C       1.017169    -1.056345    -0.118654      68.13
 H       1.512442    -2.006823    -0.195059      17.25
 C      -0.636227     0.612279     0.500185      41.48
 C      -2.130153     0.827828     1.064969      67.65
 H      -2.464145    -0.131376     1.602945      20.78
 O      -2.132988     1.962032     2.066805     204.59
 H      -2.158051     1.552383     3.156160      22.55
 C      -3.042116     1.234560    -0.189440      96.08
 H      -2.706356     1.992210    -0.882759      21.38
 O      -3.339166    -0.073826    -0.836509     251.57
 H      -3.207348    -0.138581    -1.728322      26.86
 C      -4.339242     1.798648     0.247051      79.63
 O      -5.064760     2.617853    -0.857235     258.10
 H      -4.757373     3.563332    -0.730570      28.41
 H      -4.431260     1.976313     1.467327      24.91
 H      -5.000797     0.867119     0.212872      26.07
55
name = lig-etoh-Waterframe_630
 C       5.314459    -1.101869     1.607665      32.96
 H       5.112001    -0.016344     1.421439      17.23
 C       5.589146    -3.463686     0.849329      90.87
 H       5.818792    -4.191449     0.104066      37.30
 C       5.733317    -3.876564     2.186754       2.83
 O       5.878785    -5.226693     2.553914     382.78
 C       5.008311    -6.200106     1.984066     105.75
 H       5.402224    -6.631775     1.009059      21.20
 H       3.996845    -5.652923     1.697704      26.95
 H       5.155184    -6.908677     2.690894      22.62
 C       5.643762    -2.982172     3.240048       2.14
 O       5.915929    -3.297597     4.532997     300.27
 H       5.771361    -4.234362     4.626115      29.18
 C       5.360261    -1.621734     2.930770      57.73
 H       5.234105    -0.878346     3.804246      22.66
 C       5.481023    -2.103784     0.520769      35.48
 C       5.141165    -1.718159    -0.951394      98.47
 H       5.528744    -2.730225    -1.517254      17.45
 O       6.036610    -0.603409    -1.458351     269.81
 H       5.840297     0.365476    -1.200814      23.61
 C       3.619527    -1.583615    -1.261559      72.55
 H       3.028364    -2.342296    -0.764685      16.99
 C       3.427800    -1.789369    -2.796318      86.33
 O       3.667269    -3.090349    -3.206768     261.08
 H       4.526176    -3.034476    -3.801826      24.44
 H       4.031823    -1.106794    -3.489215      18.95
 H       2.279183    -1.489357    -3.049011      20.77
 C      -0.239480    -0.797996     0.315902      45.53
 H      -0.996575    -1.573003     0.633583      16.04
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 C       0.198456     1.577292     0.083258      47.68
 H      -0.349116     2.643625     0.054898      15.35
 C       1.453059     1.367190    -0.381729      32.33
 O       2.310285     2.364071    -0.858389     285.34
 C       1.899027     3.651163    -1.158796     112.57
 H       2.902886     4.212469    -1.480943      20.43
 H       0.991636     3.765293    -1.763889      25.56
 H       1.660457     4.068908    -0.168108      25.41
 C       1.956639     0.004453    -0.343711      27.82
 O       3.257071    -0.217771    -0.799570     197.60
 C       1.063480    -1.068583    -0.096518      59.68
 H       1.425361    -2.034257    -0.160144      15.89
 C      -0.632547     0.557516     0.531528      69.10
 C      -2.053691     0.941745     1.013714      86.30
 H      -2.489507     0.092946     1.383961      19.74
 O      -2.121284     1.925358     2.077494     230.92
 H      -2.143464     1.377766     3.103210      21.20
 C      -3.070279     1.179033    -0.191365      69.87
 H      -2.353360     1.848765    -0.818980      19.37
 O      -3.261550    -0.071337    -0.860831     260.35
 H      -3.196854     0.094120    -1.837052      23.91
 C      -4.479875     1.755862     0.119989      90.00
 O      -5.097005     2.601361    -0.835083     275.62
 H      -4.879233     3.570218    -0.648881      27.66
 H      -4.397593     2.548514     1.197627      21.75
 H      -5.143824     0.949052     0.319597      26.97
55
name = lig-etoh-Waterframe_631
 C       5.329182    -1.147942     1.595593      41.19
 H       4.737053    -0.172919     1.404245      17.79
 C       5.636268    -3.424913     0.883422      17.12
 H       5.741362    -4.103464     0.013372      17.24
 C       5.726089    -3.938543     2.191391       8.41
 O       5.918544    -5.226988     2.576732     373.60
 C       5.011585    -6.275041     1.991440      89.94
 H       5.430907    -6.583538     0.911048      27.41
 H       4.004664    -5.856539     1.894484      29.66
 H       4.729411    -7.143655     2.740733      24.10
 C       5.677563    -2.938578     3.199565       3.38
 O       5.871170    -3.322049     4.556984     230.71
 H       5.942755    -4.243834     4.562593      27.17
 C       5.377614    -1.598992     2.883388      67.50
 H       5.308364    -0.879459     3.781894      22.35
 C       5.445691    -2.054777     0.549709      56.37
 C       5.167642    -1.690182    -0.897354     115.03
 H       5.416779    -2.560064    -1.679694      20.64
 O       6.051693    -0.657826    -1.419713     306.83
 H       5.551875     0.180478    -1.178956      25.51
 C       3.625888    -1.530164    -1.273256      93.73
 H       3.286554    -2.357829    -0.782870      20.27
 C       3.368187    -1.698577    -2.812377      78.00
 O       3.703452    -3.118443    -3.266497     234.98
 H       4.680083    -2.988720    -3.647161      23.84
 H       4.035799    -0.956877    -3.377908      19.39
 H       2.191972    -1.721202    -3.058963      20.66
 C      -0.262610    -0.791103     0.303953      60.96
 H      -0.716639    -1.543526     0.793151      20.70
 C       0.155428     1.533725     0.070880      74.07
 H      -0.027873     2.568837     0.328456      18.99
 C       1.502135     1.319626    -0.321659      14.06
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 O       2.295902     2.254055    -0.836139     178.38
 C       1.838589     3.708504    -1.123180     102.54
 H       2.663148     4.149620    -1.644569      25.03
 H       1.179134     3.707840    -1.800218      28.41
 H       1.897567     4.400394    -0.099723      22.69
 C       1.974451    -0.016118    -0.412439      17.74
 O       3.298790    -0.227379    -0.830488     199.01
 C       1.120650    -1.072057    -0.065932      70.29
 H       1.158030    -2.088943    -0.116852      18.56
 C      -0.701822     0.482303     0.543574      27.53
 C      -2.052028     0.933449     1.013235      87.96
 H      -2.434683    -0.008584     1.371615      21.04
 O      -2.112334     1.912106     2.050834     252.87
 H      -1.712569     1.352391     2.971034      21.62
 C      -3.041039     1.202398    -0.196861      52.94
 H      -2.615199     1.949981    -1.049517      20.88
 O      -3.176939    -0.100793    -0.935907     243.12
 H      -3.114333     0.319928    -1.871569      22.25
 C      -4.578609     1.778584     0.115114     105.07
 O      -5.150869     2.603850    -0.872080     291.03
 H      -4.801842     3.557371    -0.703889      27.69
 H      -4.312261     2.475860     0.911641      24.65
 H      -5.207238     1.026229     0.419963      28.38
55
name = lig-etoh-Waterframe_632
 C       5.253454    -1.157896     1.567431      45.59
 H       4.868426    -0.081092     1.316371      20.25
 C       5.698275    -3.423642     0.850354      51.34
 H       5.604076    -4.168715    -0.007300      15.96
 C       5.710334    -3.919026     2.165259       4.95
 O       5.947023    -5.294305     2.599844     294.89
 C       4.993200    -6.278366     1.998639     102.04
 H       5.450477    -6.726725     1.003284      29.34
 H       4.076544    -5.888880     1.869135      30.45
 H       4.995498    -7.288709     2.791064      25.10
 C       5.714675    -2.926036     3.242266      -6.77
 O       5.820988    -3.346145     4.558573     181.55
 H       6.043864    -4.233043     4.572597      23.46
 C       5.445282    -1.581740     2.935187      57.18
 H       5.248881    -0.863742     3.769614      21.29
 C       5.386748    -2.061466     0.545226      36.46
 C       5.210628    -1.715056    -0.935816     118.12
 H       5.538833    -2.669456    -1.350663      27.68
 O       6.037078    -0.688670    -1.378631     315.36
 H       5.735961     0.212147    -1.084512      27.54
 C       3.747677    -1.525035    -1.300477      92.31
 H       3.127138    -2.196365    -0.693361      23.16
 C       3.304841    -1.671502    -2.810022      86.75
 O       3.719024    -3.112773    -3.291939     257.24
 H       4.621450    -3.032274    -3.761105      26.14
 H       3.747380    -0.823041    -3.344650      24.44
 H       2.228988    -1.399866    -2.960075      25.11
 C      -0.239338    -0.841014     0.371008      42.49
 H      -0.767010    -1.680736     0.600132      20.51
 C       0.159604     1.542506     0.126427      74.22
 H      -0.061888     2.475536     0.355219      20.96
 C       1.460111     1.224223    -0.284004      10.37
 O       2.350959     2.261553    -0.838743     132.34
 C       1.891334     3.707130    -1.069940      95.56
 H       2.538506     3.910867    -1.761824      25.24
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 H       0.821065     3.677114    -1.646002      23.91
 H       1.321781     4.381602    -0.192770      22.67
 C       1.985284    -0.088988    -0.481735      22.28
 O       3.294279    -0.209252    -0.854781     189.17
 C       1.066766    -1.085296    -0.047138      52.35
 H       1.523084    -2.094281    -0.164285      18.24
 C      -0.728881     0.541979     0.473716      32.99
 C      -2.160499     0.801411     1.015766      69.04
 H      -2.646562    -0.140282     1.559151      20.14
 O      -2.085826     1.908003     2.013938     250.48
 H      -1.459954     1.761212     2.876242      25.46
 C      -3.093754     1.238508    -0.254350      62.00
 H      -2.750609     2.144390    -0.822994      22.18
 O      -3.088020    -0.081380    -1.018904     222.72
 H      -3.055646    -0.119972    -2.131916      21.44
 C      -4.509689     1.814828     0.214202      93.16
 O      -5.219544     2.613592    -0.966346     224.84
 H      -4.746788     3.551336    -0.950021      28.20
 H      -4.433228     2.248761     1.096807      28.77
 H      -5.249205     1.032336     0.442071      27.58
55
name = lig-etoh-Waterframe_633
 C       5.168107    -1.141376     1.631803      51.35
 H       5.169370    -0.048151     1.394289      21.00
 C       5.695646    -3.467598     0.817430      37.34
 H       5.771569    -4.271429     0.005827      19.81
 C       5.752870    -3.875865     2.185324       6.15
 O       5.942074    -5.321478     2.580739     234.70
 C       5.040504    -6.291274     2.018531     119.76
 H       5.351643    -6.630005     1.051822      29.13
 H       4.069068    -5.904079     1.888750      27.39
 H       5.180857    -7.100175     2.885596      25.50
 C       5.727109    -2.975928     3.265686       3.31
 O       5.784014    -3.360769     4.563995     244.45
 H       5.847907    -4.320352     4.657749      20.71
 C       5.494170    -1.549310     2.955770      42.58
 H       5.283547    -0.882303     3.766178      21.00
 C       5.348448    -2.131469     0.524069      24.25
 C       5.240007    -1.806198    -0.951982     110.21
 H       5.598745    -2.581324    -1.503226      24.12
 O       6.071514    -0.666508    -1.372720     279.81
 H       5.874646     0.189009    -0.958805      26.62
 C       3.773950    -1.551049    -1.343236      76.42
 H       3.165857    -2.388144    -0.738775      19.26
 C       3.319076    -1.690326    -2.795633     104.66
 O       3.650705    -3.022718    -3.289350     267.24
 H       4.467347    -2.855212    -3.813749      27.03
 H       3.799307    -1.078884    -3.502173      22.70
 H       2.299788    -1.665719    -2.750429      25.75
 C      -0.244958    -0.854344     0.439315      33.17
 H      -1.074565    -1.615113     0.410059      17.05
 C       0.186156     1.575529     0.208748      49.32
 H      -0.200650     2.539398     0.223825      17.26
 C       1.479470     1.245197    -0.355353      -6.30
 O       2.377947     2.299315    -0.782626     172.74
 C       1.832471     3.587892    -1.069512      83.53
 H       2.556813     4.269362    -1.629731      22.44
 H       0.665279     3.384985    -1.629792      20.91
 H       1.991837     4.220338    -0.078487      22.66
 C       1.908524    -0.105137    -0.476111      14.95
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 O       3.297016    -0.180322    -0.890802     146.70
 C       1.076685    -1.140345    -0.077122      67.03
 H       1.475696    -2.266698    -0.000545      18.63
 C      -0.772673     0.455768     0.437957      46.14
 C      -2.229085     0.746678     1.007275      71.08
 H      -2.757550    -0.236719     1.478196      21.68
 O      -2.087899     1.923700     1.930311     252.80
 H      -1.517951     1.632493     2.719117      27.42
 C      -3.158898     1.240672    -0.281953      84.89
 H      -2.478644     1.903256    -0.632550      25.03
 O      -3.030511    -0.027737    -1.074115     228.98
 H      -2.963490     0.276515    -2.227335      19.42
 C      -4.473193     1.807682     0.212760      81.17
 O      -5.214462     2.582064    -0.971108     223.08
 H      -4.825887     3.552290    -1.123917      28.18
 H      -4.469464     2.513351     1.203534      24.17
 H      -5.216989     0.895764     0.222367      24.66
55
name = lig-etoh-Waterframe_634
 C       5.189129    -1.219098     1.643682      60.23
 H       5.038104    -0.183783     1.450597      22.04
 C       5.649470    -3.519748     0.858514      54.90
 H       5.999094    -4.192290     0.050947      23.36
 C       5.825698    -3.933791     2.196067       3.43
 O       5.957254    -5.244366     2.542310     261.90
 C       5.100663    -6.298276     2.044947     127.33
 H       5.339381    -6.604570     1.101478      24.66
 H       3.942610    -6.016995     2.168356      24.48
 H       5.014289    -7.121032     2.639435      26.51
 C       5.699002    -2.965942     3.249299      -5.46
 O       5.761559    -3.376543     4.596929     288.10
 H       5.544593    -4.382448     4.769797      23.01
 C       5.495917    -1.595741     2.950704      52.57
 H       5.448823    -0.942273     3.765374      20.85
 C       5.333574    -2.165359     0.566189      24.25
 C       5.256515    -1.795508    -0.975132      99.62
 H       5.545214    -2.525007    -1.688531      22.37
 O       6.139173    -0.648705    -1.376089     260.27
 H       5.708843     0.035409    -0.877017      27.31
 C       3.735499    -1.557866    -1.350476      73.73
 H       3.255389    -2.508232    -0.827821      19.22
 C       3.341798    -1.717250    -2.792689     105.32
 O       3.576900    -2.971070    -3.295656     256.23
 H       4.504380    -2.997823    -3.690225      25.68
 H       3.712817    -0.899700    -3.425346      23.62
 H       2.257553    -1.652275    -2.785551      25.14
 C      -0.278037    -0.867646     0.398436      20.42
 H      -1.030396    -1.814908     0.619542      16.50
 C       0.176983     1.513547     0.232175      62.58
 H      -0.197935     2.614393     0.203739      16.94
 C       1.442353     1.354640    -0.408378       5.47
 O       2.403882     2.260808    -0.727982     232.38
 C       1.804240     3.511954    -1.008533     101.92
 H       2.452556     4.161988    -1.894800      21.75
 H       0.720049     3.568484    -1.507976      24.24
 H       1.826908     3.970458    -0.135308      27.90
 C       1.916066    -0.076915    -0.460980       0.62
 O       3.266816    -0.213035    -0.921715     135.06
 C       1.052254    -1.197627    -0.066105      56.27
 H       1.266499    -2.374998    -0.001173      18.67
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 C      -0.764643     0.415031     0.482746      51.43
 C      -2.231636     0.786250     0.947097      95.36
 H      -2.609147    -0.106441     1.492102      23.02
 O      -2.121694     1.896020     1.828487     310.65
 H      -1.835067     1.526670     2.637641      30.17
 C      -3.054904     1.184992    -0.217859      86.03
 H      -2.487103     1.992246    -0.749298      21.74
 O      -3.032760     0.083248    -1.129135     253.23
 H      -3.045866     0.510632    -2.201359      20.19
 C      -4.526887     1.796208     0.046960      82.83
 O      -5.159209     2.510986    -0.926141     273.91
 H      -4.778908     3.502894    -0.834087      27.21
 H      -4.234510     2.602084     1.044328      22.60
 H      -5.195480     0.886591     0.497075      25.30
55
name = lig-etoh-Waterframe_635
 C       5.254017    -1.294992     1.593182      50.67
 H       4.799980    -0.393556     1.396202      22.54
 C       5.639984    -3.537148     0.894375      50.82
 H       5.887195    -4.186117     0.088496      21.37
 C       5.824056    -3.939251     2.190847      15.50
 O       6.020182    -5.247188     2.549808     244.07
 C       5.096315    -6.291880     2.069152     106.96
 H       5.295206    -6.510686     0.978197      22.81
 H       3.955551    -5.809377     2.084626      23.42
 H       5.372626    -7.103707     2.642537      25.22
 C       5.671708    -3.029327     3.287305      -3.96
 O       5.736449    -3.349227     4.609771     221.21
 H       5.633761    -4.457877     4.810724      18.86
 C       5.473867    -1.685081     2.963233      60.86
 H       5.507583    -0.954577     3.697359      23.34
 C       5.352663    -2.199299     0.555379      17.83
 C       5.240289    -1.710717    -0.987464      85.11
 H       5.584912    -2.756976    -1.438205      19.82
 O       6.160676    -0.657886    -1.343133     254.00
 H       5.892369     0.231887    -1.088436      27.56
 C       3.720600    -1.568024    -1.311086      90.73
 H       3.134250    -2.229012    -0.691499      20.75
 C       3.285464    -1.636196    -2.798052      76.41
 O       3.561707    -3.028218    -3.336745     249.49
 H       4.522386    -2.968434    -3.735423      24.62
 H       3.809701    -0.752615    -3.320518      22.15
 H       2.148634    -1.365438    -2.915501      23.90
 C      -0.292115    -0.932109     0.313622      49.34
 H      -0.911229    -1.840151     0.810253      22.28
 C       0.138445     1.463728     0.169880      57.51
 H      -0.301496     2.553593     0.546634      15.69
 C       1.404439     1.219262    -0.365254      13.54
 O       2.392963     2.200766    -0.710015     192.06
 C       1.789508     3.564275    -0.973887     100.51
 H       2.534589     3.820164    -1.875838      21.46
 H       0.878825     3.354867    -1.269560      30.40
 H       1.626584     4.217641    -0.257498      27.53
 C       1.905369    -0.087832    -0.442675      16.81
 O       3.206049    -0.277927    -0.927815     182.16
 C       1.015678    -1.143121    -0.051278      64.90
 H       1.462596    -2.148955    -0.231282      18.39
 C      -0.715921     0.453505     0.536498      45.17
 C      -2.130184     0.781197     0.928015     106.51
 H      -2.614779    -0.007841     1.362235      23.38
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 O      -2.173164     1.894570     1.789701     346.55
 H      -2.094974     1.701220     2.631270      33.64
 C      -2.993153     1.210221    -0.288071      69.91
 H      -2.650167     2.283258    -0.675947      20.99
 O      -3.063867     0.171074    -1.179671     282.78
 H      -3.096164     0.259286    -2.237981      22.26
 C      -4.455458     1.703395     0.059630     104.40
 O      -5.113447     2.480457    -0.952189     254.61
 H      -4.945014     3.506360    -0.740283      27.75
 H      -4.310074     2.454104     0.926789      25.11
 H      -5.229437     1.049733     0.485851      27.35
55
name = lig-etoh-Waterframe_636
 C       5.286685    -1.321569     1.605289      55.49
 H       4.922129    -0.340453     1.409273      23.79
 C       5.667822    -3.546250     0.829846      28.56
 H       5.637170    -4.358140     0.163286      19.71
 C       5.771520    -3.943097     2.236863      12.43
 O       6.112177    -5.321800     2.577015     278.40
 C       5.114304    -6.238757     2.053246     113.04
 H       5.275146    -6.439008     0.877020      28.80
 H       4.015285    -5.987060     2.365552      25.23
 H       5.388306    -7.160338     2.709007      25.91
 C       5.657101    -3.088860     3.318978       6.75
 O       5.719828    -3.322629     4.634429     226.97
 H       5.813303    -4.362353     4.946774      19.96
 C       5.439465    -1.729230     2.925276      55.04
 H       5.314248    -1.010964     3.691338      23.40
 C       5.388783    -2.203250     0.485451      19.66
 C       5.196601    -1.695948    -0.892892      87.92
 H       5.613837    -2.556673    -1.693060      21.40
 O       6.166132    -0.681805    -1.318990     239.55
 H       5.860155     0.222297    -1.201331      29.49
 C       3.653029    -1.565652    -1.291610      87.19
 H       3.310712    -2.388730    -0.758477      24.27
 C       3.266804    -1.588497    -2.804059      86.10
 O       3.565283    -3.039903    -3.370353     217.59
 H       4.354462    -2.807048    -4.001693      24.71
 H       4.029858    -1.064867    -3.436428      21.24
 H       2.103425    -1.447441    -2.968323      23.05
 C      -0.320699    -0.915268     0.304746      61.00
 H      -1.018719    -1.772608     0.557593      23.41
 C       0.118939     1.463105     0.128705     110.56
 H      -0.088032     2.576450     0.528488      18.45
 C       1.445134     1.150933    -0.294104       8.36
 O       2.319027     2.165499    -0.658858     176.23
 C       1.791017     3.541655    -1.002766      95.27
 H       2.390568     4.074544    -1.728758      25.41
 H       0.864101     3.332294    -1.446012      26.67
 H       2.038202     4.378961    -0.195010      22.54
 C       1.877955    -0.164311    -0.441484      35.32
 O       3.158079    -0.273444    -0.897259     196.94
 C       1.039539    -1.133196    -0.100965      73.88
 H       1.359895    -2.109397    -0.215222      22.33
 C      -0.684316     0.362492     0.532817      30.81
 C      -2.070418     0.748247     0.935302      75.31
 H      -2.595261    -0.143234     1.247919      22.02
 O      -2.225109     1.960905     1.814989     317.79
 H      -2.100545     1.712099     2.640758      31.68
 C      -3.036806     1.330676    -0.404976      57.01
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 H      -2.321779     2.146565    -0.789536      22.21
 O      -3.084531     0.163797    -1.261196     304.96
 H      -2.969726     0.410113    -2.122924      27.28
 C      -4.379582     1.655020     0.212982      96.39
 O      -5.083039     2.467434    -1.030889     208.42
 H      -5.002490     3.511159    -0.861684      27.00
 H      -4.296512     2.205282     0.988304      29.00
 H      -4.912858     0.791340     0.216693      29.59
55
name = lig-etoh-Waterframe_637
 C       5.292123    -1.308684     1.593388      45.45
 H       5.308703    -0.191261     1.463133      20.67
 C       5.678439    -3.590901     0.828067      33.51
 H       5.607469    -4.348826     0.054903      19.79
 C       5.765991    -4.036094     2.222715       5.69
 O       6.174320    -5.349696     2.576005     336.28
 C       5.159074    -6.246510     2.091664     113.77
 H       5.105454    -6.323716     0.922684      28.30
 H       4.269617    -5.930174     2.416514      29.92
 H       5.190040    -7.429801     2.402159      24.94
 C       5.640442    -3.065346     3.295861       4.40
 O       5.729710    -3.288086     4.694546     264.82
 H       5.502504    -4.214708     4.932644      25.40
 C       5.385740    -1.746247     2.916428      45.75
 H       5.081698    -1.076410     3.739029      22.41
 C       5.438765    -2.219439     0.506660      15.68
 C       5.166277    -1.730019    -0.931300      90.95
 H       5.304166    -2.589030    -1.666039      22.90
 O       6.149290    -0.679481    -1.294971     253.64
 H       5.707833     0.127572    -1.019113      28.23
 C       3.634999    -1.558251    -1.309294      76.55
 H       3.154807    -2.448718    -0.915202      23.89
 C       3.339258    -1.697155    -2.837165     103.14
 O       3.559676    -2.988837    -3.382478     268.86
 H       4.335148    -3.004638    -4.070257      24.91
 H       3.818255    -0.845914    -3.377750      25.07
 H       2.286269    -1.330064    -3.010858      25.62
 C      -0.301300    -0.957138     0.311261      49.90
 H      -0.989189    -1.710992     0.356163      21.67
 C       0.183539     1.434828     0.152433      73.38
 H      -0.135182     2.475835     0.213417      20.51
 C       1.424087     1.236513    -0.236620      22.69
 O       2.284784     2.182534    -0.630684     217.82
 C       1.832180     3.497540    -1.049179      91.07
 H       2.449522     3.759084    -1.800538      24.47
 H       0.663232     3.843844    -1.366281      22.76
 H       1.910509     4.008801     0.121429      21.58
 C       1.877206    -0.164623    -0.445596       1.94
 O       3.166125    -0.264554    -0.847690     142.49
 C       0.973803    -1.306147    -0.149991      59.92
 H       1.176441    -2.299540    -0.170994      23.96
 C      -0.739221     0.408082     0.501034      41.01
 C      -2.151471     0.796341     0.895431      76.97
 H      -2.666195    -0.128789     1.445190      20.78
 O      -2.245959     1.980024     1.861011     252.94
 H      -1.862569     1.676660     2.686934      28.44
 C      -2.941672     1.323347    -0.393785      81.83
 H      -2.497419     2.119692    -1.004270      23.28
 O      -3.113754     0.166634    -1.324843     272.50
 H      -2.974841     0.354743    -2.197225      27.18
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 C      -4.354503     1.692880     0.165956      86.69
 O      -5.049822     2.423091    -1.035397     241.73
 H      -4.744299     3.397191    -0.839808      27.85
 H      -4.448319     2.097066     1.181057      27.06
 H      -4.705823     0.651204     0.163978      28.10
55
name = lig-etoh-Waterframe_638
 C       5.338336    -1.284619     1.573110      41.67
 H       5.349520    -0.146772     1.295006      21.24
 C       5.651326    -3.638254     0.888945      38.39
 H       5.884890    -4.254839    -0.025244      21.71
 C       5.825614    -4.069533     2.204462       2.45
 O       6.215894    -5.377015     2.558016     315.33
 C       5.143750    -6.305916     2.094524     109.30
 H       5.079103    -6.128859     1.062191      28.15
 H       4.247695    -5.903376     2.482622      29.68
 H       5.626738    -7.320537     2.440425      23.97
 C       5.617839    -3.087279     3.277230      -4.41
 O       5.735317    -3.224001     4.685747     289.81
 H       5.545411    -4.129498     5.021595      24.33
 C       5.302572    -1.731022     2.930258      39.30
 H       5.105265    -0.995886     3.792521      20.54
 C       5.452052    -2.250426     0.557842      20.24
 C       5.161509    -1.831338    -1.002874     104.29
 H       5.519725    -2.633458    -1.473697      25.65
 O       6.068387    -0.676657    -1.273632     240.48
 H       5.824785     0.159470    -0.850177      26.69
 C       3.680287    -1.566073    -1.339538      87.99
 H       2.979131    -2.215916    -0.715678      21.97
 C       3.392242    -1.676757    -2.872044     107.13
 O       3.575217    -2.977375    -3.403295     262.87
 H       4.535682    -2.923747    -3.784679      24.22
 H       4.015157    -0.926716    -3.360567      25.20
 H       2.361276    -1.591170    -2.925854      26.84
 C      -0.351512    -0.968952     0.316378      34.97
 H      -1.030087    -1.694013     0.496501      19.54
 C       0.100165     1.467635     0.244074      46.40
 H      -0.329793     2.341728     0.109869      16.38
 C       1.464027     1.144373    -0.247399       2.40
 O       2.294805     2.199119    -0.662670     185.90
 C       1.872900     3.502717    -1.016867      88.04
 H       2.587315     3.745700    -1.768901      24.08
 H       0.623754     3.504161    -1.347214      21.81
 H       2.186455     4.405724    -0.177533      22.20
 C       1.794891    -0.191554    -0.398685      13.33
 O       3.217024    -0.281124    -0.815427     143.17
 C       0.948799    -1.359057    -0.198889      59.27
 H       1.230782    -2.389690    -0.335665      20.66
 C      -0.777764     0.428042     0.467892      49.41
 C      -2.211183     0.900179     0.871278      79.61
 H      -2.870367     0.000250     1.329215      21.33
 O      -2.238323     1.945645     1.891841     241.31
 H      -1.603083     1.684855     2.696440      27.14
 C      -2.893372     1.264479    -0.361317     106.19
 H      -2.476113     2.139091    -0.762329      24.47
 O      -3.142287     0.172170    -1.309127     236.70
 H      -3.066260     0.354772    -2.382456      20.33
 C      -4.348834     1.690012    -0.041441      81.69
 O      -4.999847     2.376294    -0.954227     272.33
 H      -4.711495     3.336633    -1.001160      29.86
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 H      -4.534469     2.361877     1.081264      23.06
 H      -5.086573     0.730635     0.198597      24.87
55
name = lig-etoh-Waterframe_639
 C       5.380886    -1.289624     1.589058      42.14
 H       5.070377    -0.223325     1.259201      19.26
 C       5.652568    -3.623328     0.901780      38.70
 H       6.028688    -4.426279     0.174791      20.95
 C       5.898284    -4.028919     2.274508       2.20
 O       6.233551    -5.392077     2.531306     212.13
 C       5.179770    -6.320518     2.096223     128.68
 H       5.028118    -6.364528     1.077184      27.45
 H       4.132722    -6.390230     2.785526      24.68
 H       5.532528    -7.315352     2.379986      26.34
 C       5.577879    -3.081669     3.277910       5.26
 O       5.737502    -3.170953     4.627903     214.52
 H       5.848799    -4.097979     4.970584      24.52
 C       5.257634    -1.718440     2.897398      46.04
 H       5.242740    -0.972942     3.778727      22.70
 C       5.404076    -2.288512     0.545897      33.10
 C       5.245135    -1.892864    -0.922873     109.91
 H       5.725702    -2.582999    -1.604760      24.43
 O       5.979194    -0.697746    -1.285256     276.37
 H       5.632833     0.040930    -0.738202      27.15
 C       3.708152    -1.590952    -1.331355      81.52
 H       3.253717    -2.567742    -0.820869      22.60
 C       3.384595    -1.593655    -2.843314      97.26
 O       3.660307    -3.017023    -3.430179     240.97
 H       4.602525    -3.015832    -3.823129      25.78
 H       4.010394    -1.001431    -3.463104      24.70
 H       2.365464    -1.363891    -3.052215      26.73
 C      -0.427866    -0.960693     0.300753      21.55
 H      -1.098715    -1.746830     0.715732      18.33
 C       0.102088     1.477798     0.253639      43.58
 H      -0.231683     2.470751     0.304478      16.71
 C       1.353241     1.150184    -0.234842      -1.85
 O       2.348005     2.133664    -0.679008     184.36
 C       1.926677     3.555001    -0.992532     106.73
 H       2.375744     3.919343    -2.037491      23.18
 H       0.916521     3.425424    -1.396205      25.65
 H       2.068056     4.304221    -0.360380      27.41
 C       1.860248    -0.280163    -0.401219      16.85
 O       3.236220    -0.298136    -0.792665     179.13
 C       0.877927    -1.247813    -0.196317      58.18
 H       1.211828    -2.308068    -0.489984      19.85
 C      -0.814858     0.359778     0.491646      49.86
 C      -2.199281     0.856715     0.932909      76.52
 H      -2.744538    -0.038518     1.223812      22.56
 O      -2.213799     1.922856     1.886147     245.93
 H      -1.638865     1.474566     2.766952      23.86
 C      -3.009681     1.290994    -0.413655      87.69
 H      -2.339884     2.060141    -0.790960      21.98
 O      -3.128003     0.138477    -1.266826     212.73
 H      -3.059218     0.649798    -2.268844      18.75
 C      -4.361807     1.649112    -0.023595      79.20
 O      -5.038135     2.421380    -1.041540     287.85
 H      -4.721669     3.351898    -0.922579      30.02
 H      -4.036182     2.406658     0.865607      22.29
 H      -5.031489     0.664127     0.167560      25.56
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name = lig-etoh-Waterframe_640
 C       5.314528    -1.332066     1.549243      42.11
 H       5.044570    -0.269122     1.409245      18.12
 C       5.732014    -3.624669     0.953496      44.24
 H       5.761406    -4.426798     0.151638      19.64
 C       5.897315    -3.973076     2.292296      23.81
 O       6.217152    -5.388221     2.511138     209.75
 C       5.230739    -6.413135     2.138439     122.53
 H       4.848023    -6.364388     1.080255      25.86
 H       4.183002    -6.209877     2.873753      22.11
 H       5.662478    -7.322919     2.239441      25.73
 C       5.562871    -3.017494     3.278668      16.08
 O       5.754109    -3.149541     4.607397     225.11
 H       5.735869    -4.156444     4.850638      26.56
 C       5.292503    -1.723623     2.874396      53.98
 H       5.154602    -0.973027     3.698835      23.72
 C       5.384693    -2.320395     0.537777      40.35
 C       5.303948    -1.869397    -0.881435     111.64
 H       5.508433    -2.790093    -1.653989      24.35
 O       5.929263    -0.697823    -1.285848     311.26
 H       5.471129     0.105725    -0.872684      25.53
 C       3.755784    -1.687313    -1.318321      74.05
 H       3.075472    -2.546208    -0.983071      22.48
 C       3.425298    -1.605101    -2.859335      87.80
 O       3.724651    -3.026974    -3.417720     271.60
 H       4.471402    -2.829586    -4.054426      26.28
 H       4.049061    -0.810130    -3.301363      23.63
 H       2.376198    -1.213799    -3.087805      24.50
 C      -0.483960    -0.932858     0.294481      36.25
 H      -1.129733    -1.929098     0.558759      17.03
 C       0.094800     1.421560     0.224092      72.78
 H      -0.041473     2.488574     0.663000      16.75
 C       1.379331     1.165458    -0.272753      26.95
 O       2.378042     2.086012    -0.678618     207.06
 C       1.922697     3.520137    -1.051898     106.42
 H       2.619586     3.736134    -2.032345      20.75
 H       0.957015     3.636824    -1.160405      30.27
 H       2.106908     4.061704    -0.236714      26.26
 C       1.878229    -0.191028    -0.404417      21.62
 O       3.212250    -0.384296    -0.761969     180.57
 C       0.857184    -1.174898    -0.201197      82.69
 H       0.975931    -2.350523    -0.370242      18.76
 C      -0.834162     0.394512     0.549602      45.06
 C      -2.216282     0.710039     0.937665      84.41
 H      -2.663132    -0.055657     1.447087      22.88
 O      -2.166369     1.882268     1.878082     230.51
 H      -2.037432     1.530773     2.998415      22.08
 C      -3.031771     1.256234    -0.414786      65.99
 H      -2.594319     2.115464    -1.093796      19.13
 O      -3.077108     0.105714    -1.241862     217.80
 H      -3.159888     0.207280    -2.380252      19.37
 C      -4.386707     1.720558     0.072820      90.73
 O      -5.116022     2.482914    -1.174256     269.00
 H      -4.910879     3.389311    -0.969496      29.58
 H      -4.421425     2.188368     0.958100      28.71
 H      -4.863834     0.810809     0.403070      29.07
55
name = lig-etoh-Waterframe_641
 C       5.181753    -1.349608     1.513582      55.48
 H       5.137217    -0.353591     1.187098      21.95
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 C       5.784198    -3.618662     0.931727      47.10
 H       5.715918    -4.393828     0.167237      21.05
 C       5.841458    -4.017026     2.264977       7.61
 O       6.208769    -5.358805     2.519186     265.55
 C       5.239231    -6.444478     2.182602     112.30
 H       4.859887    -6.146515     1.111887      25.37
 H       4.418950    -6.378785     2.929351      25.05
 H       5.775195    -7.335797     2.274306      23.61
 C       5.617750    -2.994297     3.286356      -3.55
 O       5.773322    -3.179104     4.646217     298.20
 H       5.423927    -4.115697     5.037535      22.34
 C       5.336191    -1.673106     2.868918      51.68
 H       5.014482    -0.958798     3.600710      21.65
 C       5.435342    -2.309341     0.556643      22.10
 C       5.175556    -1.880476    -0.941477      86.09
 H       5.816977    -2.784987    -1.505472      21.50
 O       5.948804    -0.671652    -1.288659     267.77
 H       5.471900     0.208384    -1.049006      22.40
 C       3.696007    -1.769864    -1.323401      86.41
 H       3.116534    -2.500722    -0.822809      23.27
 C       3.529537    -1.663142    -2.855552      96.36
 O       3.746954    -2.957928    -3.403988     274.00
 H       4.525568    -2.906575    -4.034178      26.03
 H       4.287273    -0.915542    -3.247691      22.21
 H       2.368625    -1.570742    -2.940089      23.11
 C      -0.428209    -0.902975     0.263414      40.90
 H      -1.282001    -1.769549     0.222119      16.87
 C       0.117948     1.397789     0.232438     116.75
 H      -0.185635     2.498491     0.697332      17.11
 C       1.485575     1.156928    -0.334608      17.27
 O       2.346410     2.100909    -0.694788     258.22
 C       1.951701     3.405489    -1.064617     105.27
 H       2.654969     3.779635    -1.919239      22.59
 H       0.859267     3.631848    -1.206032      24.79
 H       2.525515     4.083279    -0.168582      20.87
 C       1.801220    -0.168466    -0.417955      23.73
 O       3.190783    -0.489059    -0.727660     175.31
 C       0.834654    -1.165575    -0.186707      69.56
 H       1.222900    -2.255394    -0.314971      20.99
 C      -0.816195     0.399466     0.566811      57.10
 C      -2.251490     0.709111     0.946279      79.18
 H      -2.806599    -0.166873     1.382416      22.17
 O      -2.154125     1.844218     1.871788     268.02
 H      -2.090540     1.372177     2.929672      23.51
 C      -3.019703     1.200622    -0.364958      64.56
 H      -2.454849     2.161417    -0.800089      20.21
 O      -3.054129     0.002938    -1.240406     240.58
 H      -3.076157     0.447142    -2.293687      19.15
 C      -4.514283     1.811373     0.070680     102.33
 O      -5.160212     2.457896    -1.186600     291.57
 H      -4.983457     3.430347    -1.119471      29.30
 H      -4.641534     2.513819     0.837075      27.37
 H      -5.148022     1.024383     0.154308      28.58
55
name = lig-etoh-Waterframe_642
 C       5.106315    -1.316677     1.512421      46.13
 H       4.888780    -0.374194     1.146367      23.36
 C       5.771867    -3.620879     0.852730      46.49
 H       6.050242    -4.356763     0.142887      22.40
 C       5.788307    -4.041886     2.263368      -4.92
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 O       6.208980    -5.338037     2.569690     261.87
 C       5.247199    -6.380619     2.235650     120.01
 H       4.779232    -6.364610     1.151522      25.73
 H       4.558598    -6.591680     2.873614      30.09
 H       5.787931    -7.404481     2.175195      23.59
 C       5.693326    -3.031885     3.291217     -22.06
 O       5.780113    -3.214684     4.705145     318.35
 H       5.444459    -4.214966     4.998606      22.58
 C       5.338139    -1.625658     2.878261      35.84
 H       5.113286    -0.951007     3.633347      20.13
 C       5.453148    -2.281248     0.493533      26.26
 C       5.139328    -1.906019    -0.931620      87.11
 H       5.561165    -2.561369    -1.731915      22.15
 O       5.976012    -0.666939    -1.313289     208.16
 H       5.494408     0.160076    -0.917528      24.37
 C       3.612258    -1.798165    -1.289031      94.59
 H       3.249035    -2.715092    -0.965307      25.28
 C       3.560164    -1.739570    -2.785058     109.52
 O       3.773239    -2.958698    -3.430582     281.13
 H       4.669922    -2.959851    -3.857340      24.92
 H       4.172607    -0.913281    -3.269128      23.71
 H       2.579191    -1.269459    -3.177038      24.55
 C      -0.429541    -0.913636     0.211325       9.28
 H      -1.242689    -1.703418     0.203802      16.83
 C       0.208583     1.428621     0.269735      54.42
 H      -0.175958     2.554398     0.277449      15.26
 C       1.378096     1.159636    -0.312363      22.59
 O       2.366519     2.099701    -0.739361     228.62
 C       2.053581     3.402028    -1.035984     108.67
 H       2.350688     3.568744    -2.003486      24.12
 H       0.827455     3.449223    -1.358129      23.17
 H       2.213125     4.412953    -0.185507      22.11
 C       1.824082    -0.277418    -0.474424      26.69
 O       3.160017    -0.558571    -0.695482     195.69
 C       0.895223    -1.228679    -0.177727      44.91
 H       1.233770    -2.248992    -0.325823      19.81
 C      -0.769195     0.382274     0.518099      73.49
 C      -2.260051     0.782776     0.944953      76.49
 H      -2.799793    -0.245790     1.279704      20.55
 O      -2.200533     1.800891     1.885029     287.05
 H      -1.706341     1.429274     2.779716      25.33
 C      -3.072962     1.177446    -0.232399      61.39
 H      -2.330151     1.850868    -0.697697      20.68
 O      -3.058314    -0.030737    -1.238096     228.07
 H      -2.960596     0.489783    -2.183659      20.84
 C      -4.651366     1.844328    -0.075873      82.82
 O      -5.181031     2.402006    -1.156875     309.66
 H      -4.798812     3.393191    -1.155197      25.78
 H      -4.375012     2.733727     0.762548      21.80
 H      -5.422893     1.042216     0.251860      24.00
55
name = lig-etoh-Waterframe_643
 C       5.111799    -1.310773     1.527595      40.06
 H       4.544295    -0.400311     1.447647      19.24
 C       5.755995    -3.616709     0.843360      54.39
 H       6.235856    -4.220134     0.119681      21.90
 C       5.785131    -3.972299     2.234530     -22.81
 O       6.178898    -5.329832     2.630743     223.47
 C       5.267519    -6.382197     2.249575      88.13
 H       4.715363    -6.085481     1.325349      27.92
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 H       4.424462    -6.471944     3.098089      23.68
 H       6.030971    -7.304702     2.116796      20.75
 C       5.704769    -3.007197     3.300166      -8.50
 O       5.782362    -3.252450     4.696997     185.42
 H       5.745062    -4.251577     4.923739      26.10
 C       5.335041    -1.687944     2.886763      33.44
 H       5.286761    -0.979268     3.660650      23.56
 C       5.405365    -2.290717     0.466184       8.13
 C       5.195771    -1.873299    -0.961641     104.04
 H       5.355267    -2.658400    -1.534959      27.66
 O       5.958197    -0.692462    -1.334114     219.74
 H       5.701652     0.135762    -0.762277      24.66
 C       3.624201    -1.809536    -1.240660      86.03
 H       3.044621    -2.708614    -0.940895      25.66
 C       3.499040    -1.672407    -2.808238      96.49
 O       3.794790    -3.049802    -3.457456     266.82
 H       4.558814    -2.821306    -4.103107      24.05
 H       4.414213    -1.056006    -2.945937      23.10
 H       2.535111    -1.318122    -3.127807      25.63
 C      -0.445105    -0.964379     0.164288      18.47
 H      -1.081032    -1.722545     0.380657      19.29
 C       0.172509     1.479647     0.302207      49.90
 H      -0.066205     2.525485     0.204764      15.01
 C       1.428191     1.067490    -0.323494       9.23
 O       2.413866     2.019072    -0.749819     168.02
 C       2.009747     3.497517    -1.110190      85.80
 H       2.544891     3.707974    -1.964610      23.71
 H       0.818656     3.426297    -1.147076      22.89
 H       2.298793     4.172913    -0.227532      23.71
 C       1.825851    -0.283206    -0.493039      25.04
 O       3.142221    -0.602053    -0.674707     187.93
 C       0.931438    -1.366960    -0.191684      42.10
 H       1.035092    -2.364452    -0.269537      20.20
 C      -0.771846     0.421820     0.451175      48.96
 C      -2.207425     0.721234     0.951642      83.77
 H      -2.552507    -0.179913     1.584297      19.63
 O      -2.259228     1.798831     1.947641     311.57
 H      -1.643456     1.588454     2.644170      30.64
 C      -3.180125     1.169080    -0.266109      79.27
 H      -2.811706     1.979742    -0.801801      20.22
 O      -3.087610     0.001349    -1.195827     263.14
 H      -2.954003     0.283858    -2.166272      21.96
 C      -4.616151     1.761164    -0.073313      87.00
 O      -5.219660     2.402668    -1.231403     313.88
 H      -4.900269     3.449909    -1.282607      27.12
 H      -4.404425     2.576178     0.884200      22.73
 H      -5.249232     1.058945     0.653617      25.40
55
name = lig-etoh-Waterframe_644
 C       5.129566    -1.384125     1.579220      54.59
 H       4.579938    -0.406591     1.370093      18.34
 C       5.770618    -3.564521     0.883833      39.58
 H       6.050261    -4.320429     0.123493      23.29
 C       5.846423    -3.954150     2.243324      -4.27
 O       6.154563    -5.254289     2.682064     265.20
 C       5.258744    -6.355255     2.255005      95.49
 H       4.745056    -6.025336     1.426029      32.23
 H       4.481715    -6.546205     3.283036      21.08
 H       5.723676    -7.438875     2.020423      25.57
 C       5.669922    -3.011763     3.301905       7.08
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 O       5.808810    -3.267718     4.617873     308.54
 H       5.665344    -4.207003     4.850118      21.53
 C       5.347375    -1.745683     2.892515      62.50
 H       5.193883    -0.964381     3.655645      24.39
 C       5.329589    -2.255470     0.539216      27.55
 C       5.196512    -1.882925    -0.960863      99.26
 H       5.717289    -2.703744    -1.504081      25.76
 O       5.938135    -0.736799    -1.370347     254.26
 H       5.721947     0.032673    -0.710901      26.52
 C       3.649367    -1.805373    -1.283428      83.92
 H       3.100720    -2.629280    -0.663246      21.95
 C       3.490236    -1.672265    -2.828156      93.36
 O       3.777540    -3.074949    -3.463795     275.25
 H       4.382204    -3.019823    -4.274560      27.43
 H       4.255938    -0.975762    -3.216345      23.11
 H       2.541775    -1.367404    -3.107582      26.62
 C      -0.396962    -0.981904     0.156142      43.59
 H      -1.058188    -1.659182     0.489680      19.77
 C       0.174682     1.442657     0.224699      43.73
 H      -0.097146     2.356607     0.542633      16.42
 C       1.499670     1.052314    -0.329499       2.18
 O       2.430375     1.973086    -0.771408     175.07
 C       1.955855     3.470756    -1.125276     100.35
 H       2.621252     3.902886    -1.917739      24.20
 H       0.935379     3.722612    -1.390296      25.74
 H       2.290687     3.899519    -0.374984      27.93
 C       1.782407    -0.378323    -0.455706      24.92
 O       3.173622    -0.576580    -0.658455     186.75
 C       0.826403    -1.408767    -0.207497      24.90
 H       1.129318    -2.397397    -0.262817      17.97
 C      -0.804920     0.425260     0.391129      67.39
 C      -2.183246     0.694698     0.992607      67.41
 H      -2.547351    -0.244369     1.342889      23.56
 O      -2.306819     1.822386     1.983361     321.25
 H      -1.902844     1.598813     2.728410      33.24
 C      -3.237171     1.161388    -0.389141      76.17
 H      -2.778931     2.090645    -0.788874      19.24
 O      -3.152840     0.023202    -1.158502     284.93
 H      -3.086412     0.316341    -2.054189      23.33
 C      -4.541807     1.663165     0.102271      96.41
 O      -5.249493     2.379733    -1.293339     136.10
 H      -5.023282     3.404116    -1.066040      25.69
 H      -4.435257     2.570560     0.632254      25.38
 H      -5.415885     0.943459     0.144150      24.43
55
name = lig-etoh-Waterframe_645
 C       5.095459    -1.379098     1.616525      51.75
 H       4.963882    -0.266643     1.282428      20.54
 C       5.785650    -3.542781     0.933183      47.97
 H       5.715637    -4.352830     0.131488      21.03
 C       5.911273    -3.965975     2.260940      20.50
 O       6.163982    -5.233150     2.715958     271.44
 C       5.200693    -6.297694     2.279505     122.98
 H       4.590299    -6.088855     1.475529      28.75
 H       4.462818    -6.650458     3.160829      24.20
 H       5.824852    -7.134751     2.005633      25.65
 C       5.645382    -3.056143     3.261194       1.37
 O       5.843748    -3.289975     4.579961     331.25
 H       5.504662    -4.128448     4.867593      27.03
 C       5.335273    -1.703271     2.947595      38.63
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 H       5.004421    -0.994987     3.792274      16.66
 C       5.316888    -2.282834     0.559692      40.49
 C       5.174423    -1.947169    -0.897192      85.09
 H       5.738404    -2.763408    -1.637845      22.07
 O       5.933084    -0.758647    -1.395494     255.90
 H       5.619405     0.125838    -0.932242      23.51
 C       3.708795    -1.774346    -1.349727      74.60
 H       3.255448    -2.811843    -1.022616      22.24
 C       3.503000    -1.765367    -2.884359     111.15
 O       3.702230    -3.046962    -3.451353     278.02
 H       4.616645    -2.948787    -3.939519      23.67
 H       3.972759    -0.968366    -3.407240      25.05
 H       2.446912    -1.500630    -3.083123      25.69
 C      -0.504844    -0.941074     0.222280      51.52
 H      -1.266166    -1.742543     0.465578      17.27
 C       0.213653     1.354561     0.111049      77.82
 H       0.069449     2.246531     0.644662      18.02
 C       1.445551     1.027301    -0.320785      -0.53
 O       2.404238     1.992835    -0.837728     188.32
 C       1.971081     3.380896    -1.099637      87.56
 H       2.676079     3.603506    -2.082743      21.56
 H       1.020058     3.474965    -1.460911      27.86
 H       2.069416     4.019418    -0.122654      23.74
 C       1.812608    -0.404920    -0.422988      20.27
 O       3.197103    -0.538903    -0.662355     164.58
 C       0.826147    -1.386023    -0.251314      65.50
 H       1.113125    -2.486045    -0.250721      22.03
 C      -0.780096     0.372598     0.370666      39.63
 C      -2.230362     0.753320     0.964916      73.85
 H      -2.714598    -0.129104     1.231728      24.65
 O      -2.337760     1.804206     1.972943     329.36
 H      -2.169572     1.456265     2.837979      27.02
 C      -3.149077     1.189130    -0.327572      74.91
 H      -2.437304     1.920980    -0.901506      19.50
 O      -3.252985     0.008806    -1.201348     261.17
 H      -3.251861     0.282485    -2.036032      27.93
 C      -4.590158     1.636865     0.086100      87.00
 O      -5.235037     2.328051    -1.253149     245.18
 H      -5.007377     3.365569    -1.221710      26.84
 H      -4.575117     2.216250     0.894324      28.64
 H      -5.295991     0.801404     0.304137      27.77
55
name = lig-etoh-Waterframe_646
 C       5.099529    -1.284552     1.617492      23.24
 H       5.013784    -0.154510     1.423315      21.15
 C       5.752093    -3.618926     0.927291      44.84
 H       5.812887    -4.401074     0.089364      19.12
 C       5.939028    -3.963860     2.266483      15.16
 O       6.163079    -5.295497     2.723293     304.39
 C       5.168996    -6.256828     2.306674     133.66
 H       4.515865    -5.854834     1.459689      25.95
 H       4.613338    -6.506393     3.102819      27.55
 H       5.757231    -6.993313     1.969498      24.87
 C       5.642030    -2.991790     3.273232     -11.70
 O       5.868851    -3.328206     4.609523     239.00
 H       5.606818    -4.234415     4.924079      21.91
 C       5.270508    -1.674396     2.983251      44.01
 H       5.073978    -1.015238     3.920151      20.58
 C       5.353699    -2.303817     0.591362       9.40
 C       5.181287    -1.930229    -0.909793      86.47
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 H       5.387140    -3.011595    -1.413985      21.99
 O       5.947830    -0.778798    -1.394372     257.64
 H       5.435745     0.083374    -1.164777      23.98
 C       3.763135    -1.775033    -1.395436      83.65
 H       3.063780    -2.571542    -1.139358      25.12
 C       3.426111    -1.760372    -2.931408     100.93
 O       3.680901    -3.046236    -3.468491     277.38
 H       4.661411    -3.165878    -3.740886      24.08
 H       4.076088    -1.050859    -3.443148      25.70
 H       2.266925    -1.696087    -2.892646      25.01
 C      -0.541159    -1.008299     0.236182      41.30
 H      -1.434858    -1.846742     0.358701      16.86
 C       0.172189     1.321770     0.089504      52.29
 H       0.078944     2.486914     0.254804      16.92
 C       1.473564     0.971226    -0.391709      14.83
 O       2.353203     1.954507    -0.867570     218.19
 C       1.976364     3.258820    -1.097610      90.48
 H       2.844755     3.749427    -1.838927      21.86
 H       0.977308     3.094195    -1.486018      25.72
 H       1.901376     4.257602    -0.190660      22.21
 C       1.869810    -0.354148    -0.427764      27.18
 O       3.208937    -0.568596    -0.705576     169.09
 C       0.815466    -1.328411    -0.238110      76.89
 H       0.958935    -2.514177    -0.331134      24.00
 C      -0.837633     0.378509     0.444340      51.14
 C      -2.280981     0.797051     0.876343      90.22
 H      -2.725927    -0.106051     1.394841      22.87
 O      -2.352625     1.773328     1.938870     267.77
 H      -2.144279     1.270602     2.838261      24.70
 C      -3.056899     1.205300    -0.245459      80.35
 H      -2.662917     2.093425    -0.891296      22.01
 O      -3.350226    -0.012158    -1.249159     198.13
 H      -3.286053     0.324726    -2.057979      26.92
 C      -4.626281     1.666602    -0.042737     101.08
 O      -5.195600     2.256031    -1.123985     311.20
 H      -4.750979     3.172601    -1.203504      30.34
 H      -4.775981     2.155531     0.992564      26.97
 H      -4.970184     0.705237     0.187083      29.42
55
name = lig-etoh-Waterframe_647
 C       5.172030    -1.254967     1.634555      58.80
 H       4.779547    -0.286316     1.300380      22.47
 C       5.700172    -3.673677     0.908302      33.02
 H       6.066573    -4.390221     0.142426      18.11
 C       5.911669    -3.968227     2.299748     -18.82
 O       6.186184    -5.313184     2.716679     213.49
 C       5.149625    -6.241212     2.309545      95.82
 H       4.443932    -5.631340     1.505772      24.79
 H       4.590385    -6.482503     3.118014      27.06
 H       5.408153    -7.229658     1.826444      23.88
 C       5.678447    -2.981707     3.351288      -9.72
 O       5.883932    -3.336718     4.656645     204.47
 H       5.773855    -4.376137     4.725759      22.96
 C       5.202791    -1.658092     2.975722      42.46
 H       5.146104    -0.891233     3.798239      21.42
 C       5.372406    -2.222674     0.622453      -6.35
 C       5.175995    -1.940194    -0.927721      90.01
 H       5.734472    -2.679081    -1.483233      23.42
 O       5.977153    -0.827748    -1.391277     259.46
 H       5.395693    -0.033862    -1.169045      26.71
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 C       3.668977    -1.785010    -1.388764     103.33
 H       3.244358    -2.592953    -0.857502      26.53
 C       3.383200    -1.716632    -2.917619      95.60
 O       3.674150    -3.107441    -3.500936     246.64
 H       4.540900    -3.070129    -4.086651      23.38
 H       3.835267    -0.883996    -3.546575      24.97
 H       2.257638    -1.436909    -3.148378      24.76
 C      -0.484875    -1.012829     0.206629      41.59
 H      -1.273070    -1.933966     0.305794      19.50
 C       0.133897     1.325534     0.096990      72.27
 H      -0.349302     2.418336    -0.184880      16.48
 C       1.426940     0.983522    -0.439074      15.74
 O       2.376532     1.845509    -0.849958     223.14
 C       1.907891     3.241216    -1.152798      98.62
 H       2.683819     3.738525    -1.729065      24.51
 H       0.986191     3.443767    -1.865450      24.80
 H       1.816780     3.621369     0.008858      22.98
 C       1.858787    -0.389950    -0.458941      18.43
 O       3.233752    -0.596819    -0.772043     187.62
 C       0.774674    -1.298698    -0.178938      56.25
 H       1.122740    -2.377847    -0.489313      21.23
 C      -0.872527     0.373359     0.502339      58.92
 C      -2.263765     0.744675     0.903637      64.76
 H      -2.787891    -0.326354     1.169783      21.80
 O      -2.362617     1.768835     1.904693     222.42
 H      -1.771340     1.394765     2.835119      21.97
 C      -3.184506     1.254874    -0.366768      75.10
 H      -2.549369     2.059312    -0.814799      22.61
 O      -3.383578     0.027067    -1.256533     232.62
 H      -3.139762     0.328310    -2.126635      24.49
 C      -4.551224     1.572181     0.008778      96.81
 O      -5.174952     2.240151    -1.077019     306.94
 H      -4.780933     3.142940    -1.160292      31.38
 H      -4.767838     2.480752     0.865229      22.43
 H      -5.147525     0.657470    -0.099122      26.07
55
name = lig-etoh-Waterframe_648
 C       5.204813    -1.291969     1.613588      41.39
 H       4.765056    -0.380016     1.356578      21.84
 C       5.683518    -3.562577     0.973872      63.22
 H       5.941489    -4.256128     0.209498      24.33
 C       5.843644    -3.964861     2.318183      -8.85
 O       6.226301    -5.305418     2.694289     230.62
 C       5.076711    -6.226992     2.301806      66.12
 H       4.276464    -5.649810     1.597959      25.51
 H       4.425059    -6.488938     3.256139      23.19
 H       5.567890    -7.204084     1.703559      22.53
 C       5.697925    -2.987596     3.364855       1.93
 O       5.903398    -3.319469     4.696162     175.56
 H       5.726674    -4.379271     4.878458      22.96
 C       5.229370    -1.678306     3.007837      36.02
 H       5.004948    -0.893218     3.691649      20.56
 C       5.388999    -2.263334     0.571504      14.03
 C       5.229732    -1.953865    -0.952346      89.07
 H       5.614429    -2.750086    -1.456736      26.79
 O       5.990589    -0.826227    -1.384277     245.28
 H       5.757136     0.091438    -1.067782      25.95
 C       3.602623    -1.854340    -1.365001      80.75
 H       3.178949    -2.797555    -0.995423      26.57
 C       3.345594    -1.753310    -2.930641      96.76
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 O       3.665032    -3.101318    -3.543672     269.85
 H       4.196150    -2.855631    -4.351409      25.93
 H       4.089162    -0.941272    -3.295762      23.99
 H       2.276270    -1.586540    -3.138097      25.43
 C      -0.484358    -0.949637     0.230151      64.45
 H      -1.127352    -1.827332     0.420310      22.61
 C       0.062981     1.325156     0.054919      90.35
 H      -0.405895     2.396209    -0.124821      17.55
 C       1.329219     0.946585    -0.418832      14.19
 O       2.387259     1.816709    -0.904234     178.18
 C       1.881384     3.220028    -1.157873     117.55
 H       2.693728     3.646006    -1.441214      26.72
 H       0.942616     3.317312    -1.897218      24.62
 H       1.517487     3.575891    -0.313957      28.92
 C       1.775357    -0.380829    -0.474952      19.82
 O       3.189277    -0.569846    -0.811351     134.04
 C       0.897168    -1.361195    -0.193534      63.95
 H       0.989543    -2.453380    -0.338122      21.71
 C      -0.813392     0.312781     0.474372      38.90
 C      -2.293218     0.666696     0.893755      55.75
 H      -2.886374    -0.267135     1.260098      20.65
 O      -2.359661     1.752256     1.877441     220.75
 H      -1.634128     1.696150     2.809305      23.49
 C      -3.198844     1.178046    -0.452305      74.41
 H      -2.749323     2.003256    -0.959584      22.68
 O      -3.357694     0.114339    -1.263774     269.27
 H      -3.035372     0.196059    -2.265851      22.10
 C      -4.574550     1.545255     0.095861      72.76
 O      -5.195293     2.292505    -1.146722     269.46
 H      -5.009979     3.235569    -1.066267      30.60
 H      -4.309038     1.945224     1.262545      22.99
 H      -5.252214     0.684865     0.524866      26.88
55
name = lig-etoh-Waterframe_649
 C       5.174237    -1.354472     1.608371      43.64
 H       4.970601    -0.346881     1.460762      24.01
 C       5.715834    -3.516225     1.025089      43.01
 H       5.685012    -4.292695     0.315613      23.26
 C       5.807562    -3.945773     2.368319      -2.67
 O       6.186158    -5.272422     2.631505     286.82
 C       5.027518    -6.195400     2.305323      76.21
 H       4.343949    -5.751517     1.603001      29.06
 H       4.564688    -6.665214     3.359264      20.62
 H       5.678213    -7.056721     1.775850      22.60
 C       5.681480    -3.010393     3.380594     -20.41
 O       5.925475    -3.286043     4.728932     396.18
 H       5.506618    -4.234511     5.034054      23.61
 C       5.314945    -1.695609     2.978599      46.09
 H       4.950628    -1.125496     3.763250      21.47
 C       5.386270    -2.253016     0.528838      15.22
 C       5.209445    -1.960580    -0.951698      91.33
 H       5.456257    -2.864090    -1.499522      26.38
 O       6.026119    -0.794626    -1.401304     186.58
 H       5.785160    -0.085630    -0.749943      26.62
 C       3.629908    -1.913930    -1.373129      67.34
 H       2.896873    -2.675723    -0.954523      23.54
 C       3.358714    -1.853549    -2.899212     116.64
 O       3.639954    -3.041231    -3.586697     299.15
 H       4.244132    -2.996318    -4.375398      26.40
 H       4.097898    -1.098680    -3.241214      25.03
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 H       2.386096    -1.519989    -3.043730      27.26
 C      -0.376532    -1.071865     0.258068      31.34
 H      -1.109174    -1.660692     0.582790      19.98
 C       0.018831     1.355445    -0.019733      85.20
 H      -0.153794     2.391967     0.189554      18.22
 C       1.320450     0.980263    -0.418380      14.12
 O       2.296149     1.835660    -0.965721     194.50
 C       1.872753     3.168593    -1.144077     118.67
 H       2.726142     3.845976    -1.331316      25.38
 H       1.245762     2.975680    -2.078364      25.20
 H       1.346618     3.733956    -0.392369      27.37
 C       1.792840    -0.393641    -0.503278      18.19
 O       3.074255    -0.550740    -0.830789     132.69
 C       0.863712    -1.472384    -0.186915      59.73
 H       1.141755    -2.474176    -0.131610      21.58
 C      -0.875569     0.324433     0.437777      46.69
 C      -2.296217     0.640803     0.844537      90.06
 H      -2.696585    -0.160364     1.351702      21.24
 O      -2.354766     1.754133     1.824668     210.26
 H      -1.727200     1.330241     2.728613      22.14
 C      -3.165856     1.107356    -0.367553      87.72
 H      -2.890498     2.006772    -0.828007      24.05
 O      -3.318176     0.069493    -1.342611     265.10
 H      -3.026807     0.539917    -2.384324      17.36
 C      -4.601487     1.593656     0.167139      83.20
 O      -5.228587     2.328611    -1.125338     270.27
 H      -5.117323     3.219767    -0.892153      31.71
 H      -4.434388     2.366899     0.847605      26.82
 H      -5.247859     0.633980     0.377185      26.45
55
name = lig-etoh-Waterframe_650
 C       5.140429    -1.326380     1.624082      56.47
 H       5.005722    -0.271521     1.401911      24.56
 C       5.723131    -3.581367     0.997369      33.41
 H       5.750300    -4.447544     0.334573      20.91
 C       5.824437    -3.932100     2.371936      20.69
 O       6.083334    -5.242898     2.571216     282.64
 C       5.093434    -6.201855     2.304487     110.53
 H       4.357458    -5.849291     1.782763      33.33
 H       4.532191    -6.570965     3.297051      22.89
 H       5.399714    -7.074064     1.794695      24.26
 C       5.664571    -3.017334     3.440128       3.78
 O       5.919669    -3.241673     4.761056     302.51
 H       5.609615    -4.195357     4.969772      22.51
 C       5.383562    -1.731671     2.959375      47.42
 H       5.144204    -1.016269     3.727832      23.56
 C       5.380101    -2.228733     0.568640      -4.65
 C       5.123741    -1.974902    -0.947027      76.14
 H       5.755452    -2.752841    -1.593961      21.36
 O       6.023219    -0.802813    -1.398121     157.93
 H       5.769796    -0.077245    -0.779941      28.67
 C       3.636046    -1.869980    -1.348402      86.00
 H       3.225544    -2.716896    -0.665989      23.21
 C       3.430496    -1.844574    -2.864709     117.05
 O       3.606061    -3.065892    -3.640903     279.88
 H       4.517000    -2.945604    -4.012108      25.32
 H       3.924411    -1.033402    -3.321240      26.72
 H       2.425350    -1.492699    -3.014137      26.86
 C      -0.426064    -1.118485     0.350478      57.62
 H      -1.001095    -1.936164     0.668951      19.51
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 C       0.012423     1.354555    -0.040379      55.26
 H      -0.174277     2.269809     0.266402      18.99
 C       1.336318     0.959402    -0.463900       7.17
 O       2.229240     1.852472    -0.956562     218.25
 C       1.842381     3.171429    -1.227003      95.65
 H       2.876351     3.904793    -1.466100      22.55
 H       1.355547     3.402404    -2.143664      26.00
 H       1.069021     3.561475    -0.265616      21.89
 C       1.707860    -0.444412    -0.507035      20.21
 O       3.055822    -0.578433    -0.890051     157.17
 C       0.875486    -1.510906    -0.169164      63.52
 H       1.270168    -2.441636    -0.054729      24.47
 C      -0.849624     0.284115     0.328247      38.13
 C      -2.279724     0.634077     0.824665      99.49
 H      -2.641931    -0.278002     1.215393      25.45
 O      -2.323905     1.736411     1.768553     262.73
 H      -2.055328     1.287377     2.764507      24.08
 C      -3.221546     1.099519    -0.245294      73.80
 H      -2.540082     1.953164    -0.603816      22.62
 O      -3.265580     0.000924    -1.397955     206.18
 H      -3.260396     0.485658    -2.472750      18.77
 C      -4.604779     1.687070     0.082944     124.51
 O      -5.255266     2.318204    -1.030140     331.42
 H      -5.040129     3.221543    -1.028559      34.03
 H      -4.718612     2.430426     0.715574      28.77
 H      -5.372016     0.919254     0.354929      27.74
55
name = lig-etoh-Waterframe_651
 C       5.166096    -1.297422     1.630804      35.68
 H       4.805475    -0.237269     1.400290      21.05
 C       5.683986    -3.587144     0.956259      45.54
 H       5.993028    -4.341677     0.173245      17.54
 C       5.826020    -3.914863     2.304626       4.18
 O       6.061054    -5.277649     2.570882     337.69
 C       5.064676    -6.258964     2.302916     126.79
 H       4.199910    -5.778431     1.750178      29.40
 H       4.696286    -6.525460     3.250272      27.24
 H       5.491526    -7.037588     1.815166      24.44
 C       5.678909    -3.000939     3.420258     -11.46
 O       5.893026    -3.225541     4.799593     261.98
 H       5.846298    -4.147569     5.036982      24.83
 C       5.391955    -1.673849     2.996069      36.81
 H       5.514430    -0.803711     3.675453      22.59
 C       5.356972    -2.301786     0.603008       3.98
 C       5.165261    -1.908346    -0.912825      80.22
 H       5.472909    -2.955774    -1.496570      21.57
 O       5.979819    -0.825095    -1.366438     218.92
 H       5.748776     0.085653    -1.149049      26.30
 C       3.668624    -1.814157    -1.291104      90.97
 H       3.227129    -2.786469    -0.944162      24.42
 C       3.421704    -1.793717    -2.872456      92.59
 O       3.608842    -3.090578    -3.655259     260.97
 H       4.523547    -3.197273    -4.073341      24.02
 H       4.087393    -1.027210    -3.230271      24.96
 H       2.283111    -1.734698    -2.982751      24.68
 C      -0.481256    -1.125239     0.398135      49.09
 H      -1.137123    -1.989692     0.738585      17.31
 C       0.054466     1.253686    -0.033417      83.56
 H      -0.383725     2.209380     0.053224      18.77
 C       1.260577     0.904604    -0.520927      12.65
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 O       2.237055     1.851718    -0.959886     166.60
 C       1.791000     3.278994    -1.335239      87.31
 H       2.910195     3.696453    -1.043866      20.83
 H       1.186298     3.429783    -2.177349      25.35
 H       1.157301     3.717014    -0.279581      21.38
 C       1.678446    -0.456736    -0.544948      15.41
 O       3.087731    -0.612751    -0.945507     174.37
 C       0.852172    -1.479239    -0.086944      58.58
 H       1.177450    -2.505039    -0.079457      22.61
 C      -0.847016     0.184803     0.257800      61.72
 C      -2.274882     0.556335     0.856263      76.36
 H      -2.731896    -0.413226     1.340469      22.15
 O      -2.278089     1.699244     1.750782     280.03
 H      -2.174424     1.553264     2.757295      26.75
 C      -3.236252     1.111296    -0.313525      79.70
 H      -2.606857     1.986515    -0.842008      21.21
 O      -3.244735    -0.019394    -1.327799     264.36
 H      -3.060868     0.370956    -2.262647      22.34
 C      -4.646951     1.739408     0.032499     103.14
 O      -5.301889     2.334642    -1.021003     347.30
 H      -4.800755     3.097463    -1.233760      35.37
 H      -4.407422     2.245389     1.201178      24.64
 H      -5.222588     0.969349     0.429477      28.89
55
name = lig-etoh-Waterframe_652
 C       5.209494    -1.341722     1.650763      51.45
 H       4.828982    -0.288278     1.330233      20.59
 C       5.674568    -3.576587     0.925839      25.53
 H       6.006202    -4.281302     0.083103      19.86
 C       5.798573    -3.963998     2.305946      -8.72
 O       6.121247    -5.306812     2.604425     269.89
 C       4.986765    -6.314017     2.318674      99.55
 H       4.092528    -5.840708     1.530740      24.30
 H       4.659340    -6.769223     3.153163      26.55
 H       5.555503    -7.086909     1.730591      24.51
 C       5.708737    -2.967392     3.360251     -35.63
 O       5.867515    -3.213293     4.779971     228.10
 H       5.800694    -4.172144     4.940799      27.57
 C       5.411422    -1.575305     2.998194      45.51
 H       5.541235    -0.852430     3.827318      22.77
 C       5.295910    -2.248181     0.600926      35.20
 C       5.180442    -1.880579    -0.820549      98.65
 H       5.514309    -2.743678    -1.468019      23.75
 O       5.973098    -0.835221    -1.363846     251.40
 H       5.428772    -0.068176    -1.195863      28.59
 C       3.696729    -1.850169    -1.350438      88.39
 H       3.050872    -2.587724    -0.912607      25.49
 C       3.422200    -1.836291    -2.904141      96.06
 O       3.623434    -3.101061    -3.601064     275.85
 H       4.292658    -3.037486    -4.359948      24.15
 H       3.980995    -0.973408    -3.399151      24.60
 H       2.289357    -1.448641    -3.044256      23.70
 C      -0.458442    -1.191031     0.369890      31.32
 H      -1.355327    -1.823158     0.773558      16.44
 C      -0.023119     1.127128    -0.034863      69.31
 H      -0.379611     2.240839    -0.273751      17.03
 C       1.289666     0.892434    -0.618716      11.41
 O       2.216753     1.864661    -0.991860     183.88
 C       1.788497     3.325997    -1.277444     111.68
 H       2.626588     4.013794    -1.564462      24.20
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 H       1.374802     3.260135    -2.284993      25.88
 H       1.115718     3.854835    -0.628908      26.69
 C       1.750485    -0.477474    -0.596699      23.58
 O       3.057233    -0.578489    -0.931638     174.56
 C       0.812561    -1.463397     0.007703      64.44
 H       1.103498    -2.574111    -0.069389      20.66
 C      -0.958261     0.141344     0.332895      44.58
 C      -2.309183     0.535197     0.846804      69.01
 H      -2.834359    -0.366867     1.470235      19.72
 O      -2.220579     1.680689     1.758839     274.81
 H      -1.941978     1.379691     2.580972      30.10
 C      -3.195286     1.090738    -0.446903      87.40
 H      -2.797292     2.005754    -0.966105      20.27
 O      -3.248409    -0.021548    -1.212902     315.78
 H      -3.055366     0.175902    -2.060999      26.79
 C      -4.614356     1.630611     0.122789      71.54
 O      -5.357274     2.392069    -1.057072     286.44
 H      -4.785696     3.137896    -1.247765      32.02
 H      -4.175604     2.650600     0.855092      20.42
 H      -5.238457     0.797824     0.324378      26.69
55
name = lig-etoh-Waterframe_653
 C       5.203644    -1.273873     1.659720      40.79
 H       5.090058    -0.178802     1.359403      21.80
 C       5.680832    -3.560481     0.955148      47.43
 H       5.750844    -4.367909     0.171274      23.12
 C       5.778288    -3.992308     2.317230     -12.87
 O       6.130076    -5.351722     2.642788     254.99
 C       5.010381    -6.358007     2.299390      80.07
 H       4.043031    -5.776250     1.686190      23.55
 H       4.497606    -6.757528     3.166810      24.31
 H       5.428718    -7.238665     1.582721      25.17
 C       5.726590    -2.932608     3.341333       6.67
 O       5.842014    -3.201078     4.668481     213.85
 H       5.703655    -4.205961     4.861772      19.93
 C       5.483894    -1.627340     2.999770      59.52
 H       5.170322    -0.843793     3.787679      20.83
 C       5.283612    -2.241490     0.641863      23.00
 C       5.130854    -1.953768    -0.870067      97.39
 H       5.668406    -2.714829    -1.216979      27.01
 O       5.958104    -0.792404    -1.355191     211.21
 H       5.577293     0.051689    -1.099387      27.85
 C       3.652277    -1.863024    -1.423093      84.69
 H       3.234739    -2.655299    -0.870775      25.27
 C       3.431766    -1.843789    -2.946122     103.19
 O       3.608206    -3.117334    -3.522711     285.66
 H       4.306460    -2.937367    -4.227312      24.61
 H       4.102261    -1.084306    -3.506221      23.63
 H       2.339793    -1.533966    -3.041197      24.25
 C      -0.551598    -1.192679     0.370969      61.32
 H      -0.949100    -2.254509     0.677484      20.07
 C      -0.074959     1.069464    -0.155757      59.36
 H      -0.469944     2.261119    -0.129169      16.57
 C       1.248627     0.856771    -0.643393      -0.20
 O       2.197957     1.940351    -1.012700     190.11
 C       1.781506     3.310926    -1.307363     118.56
 H       2.583065     3.840897    -1.523119      26.07
 H       1.136027     3.168275    -2.309735      24.23
 H       1.141712     3.661580    -0.698268      29.68
 C       1.718699    -0.476992    -0.572503      18.38
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 O       3.083714    -0.546637    -0.911722     165.05
 C       0.909769    -1.482725    -0.010784      59.83
 H       1.219725    -2.622675     0.131780      18.60
 C      -0.987218     0.117706     0.435978      36.45
 C      -2.373592     0.637636     0.812261      83.27
 H      -3.001624    -0.242731     1.129521      21.48
 O      -2.156610     1.659166     1.787520     348.88
 H      -1.686078     1.327062     2.413065      31.49
 C      -3.191155     1.114426    -0.390941      94.00
 H      -2.614981     1.831769    -0.884837      24.40
 O      -3.284414    -0.114681    -1.194651     273.08
 H      -3.243763     0.102627    -2.046103      28.13
 C      -4.523637     1.603879     0.044963     101.68
 O      -5.381955     2.373282    -1.053767     269.91
 H      -5.044920     3.368588    -0.962395      27.30
 H      -4.624247     2.320527     0.918098      24.11
 H      -5.264013     0.928410     0.590984      26.54
55
name = lig-etoh-Waterframe_654
 C       5.231867    -1.188949     1.650483      37.69
 H       5.103674    -0.121685     1.483125      22.07
 C       5.638916    -3.581767     1.033869      54.43
 H       5.560503    -4.322226     0.257508      21.88
 C       5.808160    -3.982978     2.325609      20.13
 O       6.071400    -5.396087     2.664922     268.70
 C       5.039357    -6.346288     2.275323      90.97
 H       4.312167    -5.746431     1.784952      30.12
 H       4.664236    -6.669848     3.333157      23.05
 H       5.468497    -7.238278     1.615856      23.71
 C       5.736506    -3.013708     3.295963      -1.42
 O       5.818259    -3.211124     4.602274     228.62
 H       5.903742    -4.261818     4.867686      17.36
 C       5.495903    -1.625950     2.951548      31.02
 H       5.148136    -0.992872     3.857471      22.05
 C       5.293778    -2.234602     0.651676       0.07
 C       5.121226    -1.965424    -0.954740      87.55
 H       5.554937    -2.823062    -1.450054      27.25
 O       5.930973    -0.754024    -1.340157     185.45
 H       5.740461     0.038599    -0.839190      28.06
 C       3.636481    -1.833721    -1.415948      93.76
 H       3.097615    -2.743514    -1.153867      26.34
 C       3.408073    -1.804573    -2.949959     109.09
 O       3.590362    -3.169541    -3.472797     287.80
 H       4.394844    -3.364279    -4.011267      27.66
 H       4.178206    -1.110216    -3.335455      25.60
 H       2.432137    -1.580899    -3.194753      27.83
 C      -0.455000    -1.273631     0.368456      41.45
 H      -1.125350    -2.160119     0.688954      18.91
 C      -0.121401     1.093064    -0.264537      85.03
 H      -0.511206     2.168371    -0.023364      17.26
 C       1.163351     0.900096    -0.629204       9.11
 O       2.165597     1.933283    -1.002105     203.08
 C       1.706339     3.224200    -1.401145     100.17
 H       2.636337     3.744743    -1.324102      23.63
 H       0.914212     3.460525    -2.281464      24.11
 H       1.197727     3.684674    -0.354740      24.06
 C       1.729099    -0.464998    -0.530362      16.58
 O       3.133320    -0.569167    -0.898822     185.49
 C       0.889184    -1.476348    -0.039754      54.31
 H       1.475348    -2.448719     0.179405      19.01
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 C      -0.960878     0.090841     0.416894      43.61
 C      -2.385483     0.673839     0.821914      93.35
 H      -2.930693    -0.074676     1.278423      20.02
 O      -2.122771     1.668991     1.831444     357.79
 H      -1.578364     1.385514     2.453170      31.04
 C      -3.164351     1.146964    -0.345936      82.25
 H      -2.612404     1.800517    -0.961788      25.53
 O      -3.344686    -0.217411    -1.219891     170.33
 H      -3.364277     0.209115    -2.083693      24.04
 C      -4.593692     1.699087    -0.032622      99.20
 O      -5.360293     2.292018    -1.006528     321.76
 H      -5.240613     3.326589    -0.815807      27.79
 H      -4.386501     2.182000     0.800711      28.50
 H      -5.086710     0.609766     0.263992      26.39
55
name = lig-etoh-Waterframe_655
 C       5.296578    -1.187134     1.607965      51.93
 H       4.950848    -0.228339     1.404756      21.98
 C       5.534728    -3.565389     0.993238      47.55
 H       5.589143    -4.304010     0.244981      25.25
 C       5.866973    -4.074055     2.328321      11.27
 O       6.048466    -5.366490     2.678825     393.98
 C       5.054432    -6.302658     2.287906     116.60
 H       4.305834    -5.991101     1.769549      33.19
 H       4.603404    -6.916521     3.215788      24.53
 H       5.547060    -7.054896     1.683776      22.50
 C       5.730648    -3.006408     3.259495     -14.80
 O       5.818476    -3.249651     4.640612     115.34
 H       5.903678    -4.307533     4.848506      19.81
 C       5.459619    -1.650900     2.924391      61.95
 H       5.490516    -1.038634     3.846221      22.38
 C       5.317885    -2.212643     0.579060      21.17
 C       5.139815    -1.915573    -0.944314      87.12
 H       5.496827    -2.698877    -1.768365      22.62
 O       5.907818    -0.753718    -1.328147     196.03
 H       5.568833    -0.150880    -0.682882      29.74
 C       3.612823    -1.804823    -1.408714      84.40
 H       2.938929    -2.633191    -0.982505      23.99
 C       3.436931    -1.783730    -2.960770     104.35
 O       3.559004    -3.239270    -3.432857     276.83
 H       4.355330    -3.039686    -4.094865      23.05
 H       4.095613    -1.104951    -3.472937      26.23
 H       2.510745    -1.401193    -3.247757      27.46
 C      -0.395587    -1.266764     0.389247     -13.20
 H      -1.114500    -1.947367     0.762312      15.10
 C      -0.225819     1.142970    -0.246620      91.33
 H      -0.513639     2.124935    -0.308885      17.34
 C       1.219933     0.905367    -0.641328      20.45
 O       2.080459     1.835918    -1.014054     218.83
 C       1.623672     3.205563    -1.350692      88.60
 H       2.596705     3.904651    -1.767717      21.55
 H       1.052827     3.291950    -2.319685      24.68
 H       1.118112     3.870279    -0.328502      21.87
 C       1.758772    -0.381506    -0.519333      30.27
 O       3.112733    -0.595289    -0.850205     209.04
 C       0.922332    -1.479777    -0.062297      99.75
 H       1.321974    -2.479337     0.064189      22.19
 C      -0.913455     0.049904     0.266778      29.03
 C      -2.280714     0.582489     0.921500      71.14
 H      -2.803760    -0.144624     1.468827      19.97
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 O      -2.115850     1.739668     1.847855     263.33
 H      -1.728342     1.352845     2.701757      25.36
 C      -3.176653     1.124349    -0.449569      64.73
 H      -2.644982     1.865189    -1.120279      22.38
 O      -3.407810    -0.221164    -1.229159     176.26
 H      -3.245055     0.060794    -2.250812      21.98
 C      -4.596424     1.647957     0.001363      86.88
 O      -5.377343     2.247924    -0.999035     268.22
 H      -5.071634     3.268170    -1.192732      28.74
 H      -4.387712     2.420651     0.939984      23.65
 H      -5.196436     0.669853     0.108982      25.76
55
name = lig-etoh-Waterframe_656
 C       5.331474    -1.264276     1.540930      46.72
 H       5.033999    -0.287989     1.340181      20.02
 C       5.485874    -3.605763     0.914450      45.39
 H       5.559230    -4.296791     0.106581      24.11
 C       5.832186    -3.986565     2.231733     -13.02
 O       6.056938    -5.327374     2.714828     268.23
 C       5.060451    -6.358120     2.275752     105.44
 H       4.102727    -5.931352     1.665376      25.80
 H       4.611157    -6.829084     3.227474      25.53
 H       5.599333    -6.969682     1.673729      24.62
 C       5.736159    -3.026982     3.318036      -9.13
 O       5.836862    -3.268431     4.666009     203.31
 H       5.715472    -4.252279     4.940216      20.84
 C       5.460318    -1.688505     2.912881      51.40
 H       5.558903    -0.898245     3.599014      23.73
 C       5.349164    -2.233721     0.520494      19.60
 C       5.114243    -1.888048    -0.951107      84.27
 H       5.717891    -2.858030    -1.413869      21.25
 O       5.874227    -0.734700    -1.297065     207.49
 H       5.616617     0.122068    -0.934373      26.33
 C       3.588650    -1.774622    -1.398309      79.88
 H       3.175801    -2.737557    -0.894107      21.84
 C       3.445973    -1.807288    -2.956597      98.80
 O       3.551424    -3.209274    -3.425207     244.52
 H       4.084355    -3.218004    -4.342252      24.38
 H       4.250523    -1.327869    -3.477236      24.61
 H       2.373329    -1.418529    -3.142533      23.85
 C      -0.371939    -1.189174     0.387476      28.73
 H      -0.786151    -2.015645     0.790004      16.45
 C      -0.123127     1.162040    -0.276375      96.33
 H      -0.644366     1.979165    -0.459027      18.18
 C       1.130063     0.880332    -0.600540       9.91
 O       2.052624     1.851786    -1.067573     187.74
 C       1.578571     3.212010    -1.326547      94.85
 H       2.623293     3.665251    -1.801360      20.60
 H       0.810766     3.018095    -1.937965      26.42
 H       1.006019     3.768007    -0.455794      23.30
 C       1.742390    -0.423993    -0.504771      21.03
 O       3.084211    -0.544996    -0.785123     194.89
 C       0.973992    -1.479122    -0.070675      48.51
 H       1.239565    -2.455727    -0.120487      16.91
 C      -0.954268     0.090045     0.202545     118.02
 C      -2.186525     0.531530     0.919318      62.45
 H      -2.759802    -0.370661     1.334360      22.56
 O      -2.092848     1.776776     1.817332     193.44
 H      -2.148780     1.524542     2.923220      22.19
 C      -3.225292     0.988640    -0.473363      86.73
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 H      -2.599983     1.781840    -1.057989      20.56
 O      -3.464558    -0.146436    -1.236476     224.19
 H      -3.014066    -0.098100    -2.251915      21.21
 C      -4.527591     1.529357     0.065217     100.43
 O      -5.425360     2.264492    -1.067824     232.29
 H      -4.713014     3.036439    -1.286067      28.92
 H      -4.750398     2.328672     1.034634      24.46
 H      -5.117739     0.882338     0.581941      28.66
55
name = lig-etoh-Waterframe_657
 C       5.341429    -1.370625     1.532168      62.01
 H       5.357238    -0.313143     1.312466      23.59
 C       5.512102    -3.650215     0.819009      46.64
 H       5.456912    -4.489771     0.098511      21.97
 C       5.740294    -3.901897     2.212138      -6.68
 O       6.036975    -5.283350     2.715479     181.30
 C       5.079866    -6.398024     2.258412      83.93
 H       4.190555    -5.645803     1.657527      21.90
 H       4.754108    -6.819745     3.181328      26.16
 H       5.497643    -7.178289     1.630930      27.69
 C       5.722577    -3.023092     3.318887      -1.19
 O       5.858098    -3.270736     4.678809     307.77
 H       5.875692    -4.205168     4.918150      24.27
 C       5.508399    -1.688741     2.872046      51.23
 H       5.337047    -0.912445     3.531126      22.33
 C       5.330835    -2.294858     0.504452      33.02
 C       5.098847    -1.867581    -0.914392      90.03
 H       5.500682    -2.669086    -1.633774      23.13
 O       5.884112    -0.683262    -1.306213     218.75
 H       5.415499     0.139296    -1.046077      26.08
 C       3.653771    -1.782378    -1.363169      82.40
 H       3.061118    -2.678316    -1.037472      24.96
 C       3.439737    -1.851462    -2.924028      97.70
 O       3.504620    -3.174582    -3.432628     255.98
 H       4.289323    -3.226070    -4.172763      22.74
 H       4.226209    -1.147536    -3.300516      24.89
 H       2.380359    -1.400466    -3.313592      23.63
 C      -0.340920    -1.140011     0.355877      17.33
 H      -0.884315    -1.931768     0.827406      18.05
 C      -0.155686     1.150895    -0.308912      76.43
 H      -0.535122     2.158399    -0.477165      15.60
 C       1.222307     0.882951    -0.611249      13.53
 O       2.062558     1.882762    -1.091404     267.45
 C       1.500954     3.153269    -1.321150     128.92
 H       2.249588     3.878661    -1.742237      25.89
 H       0.605813     3.264853    -1.931398      27.42
 H       1.410215     3.590642    -0.454486      31.43
 C       1.728286    -0.461198    -0.497937      41.57
 O       3.095221    -0.493317    -0.759484     196.16
 C       0.929882    -1.494561    -0.064868      -6.37
 H       1.316018    -2.447786    -0.099837      16.74
 C      -0.922101     0.131593     0.269749      73.06
 C      -2.237477     0.561669     0.823909      72.79
 H      -2.629469    -0.383654     1.479731      19.68
 O      -2.081158     1.749716     1.724410     186.04
 H      -2.078521     1.367121     2.854927      20.99
 C      -3.233418     0.901051    -0.330571      92.03
 H      -2.724846     1.741490    -0.934990      20.46
 O      -3.523561    -0.134917    -1.275058     222.91
 H      -2.907277     0.200119    -2.188898      19.75
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 C      -4.612016     1.499920     0.112634      83.55
 O      -5.391869     2.217480    -1.086218     241.71
 H      -4.821000     3.128831    -1.175982      29.04
 H      -4.002211     2.300797     0.689936      23.38
 H      -5.152754     0.655690     0.485880      27.79
55
name = lig-etoh-Waterframe_658
 C       5.369776    -1.398188     1.525632      45.22
 H       5.446317    -0.321624     1.190121      21.62
 C       5.551165    -3.700850     0.828009      31.02
 H       5.496941    -4.595344     0.127134      17.84
 C       5.676544    -4.012519     2.249203      11.97
 O       5.998881    -5.257788     2.662252     287.61
 C       5.118159    -6.326539     2.268261     123.99
 H       4.056087    -6.059040     1.692815      23.95
 H       4.718897    -6.817032     3.061506      27.82
 H       5.577078    -7.124631     1.540129      28.13
 C       5.693452    -2.978715     3.276442       3.46
 O       5.881418    -3.260119     4.651817     258.81
 H       6.047029    -4.185949     4.816659      25.03
 C       5.541920    -1.665797     2.890789      63.88
 H       5.293635    -0.992785     3.653152      22.21
 C       5.303409    -2.375998     0.463516      30.46
 C       5.128485    -1.856311    -0.964234     107.56
 H       5.448687    -2.509019    -1.644354      28.12
 O       5.885507    -0.634285    -1.322753     255.16
 H       5.352015     0.092996    -0.909427      25.65
 C       3.630552    -1.770689    -1.330162      92.27
 H       3.086607    -2.527142    -0.826757      26.10
 C       3.438673    -1.786150    -2.877007      91.54
 O       3.487721    -3.163057    -3.470887     291.21
 H       4.408660    -3.084620    -3.827249      26.12
 H       4.171410    -1.108881    -3.435944      23.27
 H       2.357975    -1.390533    -3.063553      24.00
 C      -0.408520    -1.164849     0.376437      36.17
 H      -1.232362    -1.855707     0.784865      15.20
 C      -0.141893     1.157738    -0.353766      94.89
 H      -0.404981     2.288629    -0.305184      16.96
 C       1.270801     0.890059    -0.642105      17.98
 O       2.106678     1.875575    -1.137659     191.19
 C       1.438622     3.198364    -1.276868     104.01
 H       2.052783     3.688112    -1.895191      26.37
 H       0.404702     3.316415    -1.981382      22.77
 H       1.450674     3.604125    -0.192829      26.07
 C       1.776634    -0.388178    -0.521189      23.55
 O       3.142719    -0.513938    -0.780241     212.27
 C       0.899048    -1.512533    -0.071752      77.32
 H       1.243153    -2.549103     0.173735      18.29
 C      -0.844750     0.183328     0.331857      36.26
 C      -2.325349     0.547053     0.803399      92.02
 H      -2.724278    -0.255851     1.535067      19.41
 O      -2.095971     1.700237     1.606978     223.52
 H      -1.566757     1.245359     2.572103      19.44
 C      -3.303017     0.904473    -0.253813      85.85
 H      -2.824346     1.750335    -0.711674      24.76
 O      -3.530662    -0.169329    -1.319997     186.85
 H      -3.250481     0.289922    -2.380931      17.84
 C      -4.626051     1.551025     0.090505     109.31
 O      -5.283325     2.132624    -1.025515     278.75
 H      -5.202374     3.165579    -0.984285      29.49
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 H      -4.506001     2.272989     0.877122      27.72
 H      -5.487628     0.830170     0.485001      25.76
55
name = lig-etoh-Waterframe_659
 C       5.407662    -1.378927     1.464539      34.13
 H       5.188110    -0.281012     1.169560      14.78
 C       5.550602    -3.767991     0.921926      23.18
 H       5.695508    -4.528691     0.096547      16.11
 C       5.644037    -4.029552     2.248717      30.25
 O       5.963699    -5.307778     2.632633     267.04
 C       5.086183    -6.329414     2.249660     109.56
 H       4.300664    -5.986061     1.752268      33.41
 H       4.879660    -6.884727     3.175783      25.15
 H       5.871741    -6.898375     1.572926      24.93
 C       5.679414    -3.034665     3.252845      -1.05
 O       5.905508    -3.236815     4.578888     200.70
 H       5.959157    -4.198127     4.820877      24.86
 C       5.526989    -1.635255     2.892230      56.43
 H       5.570602    -0.869956     3.646097      27.21
 C       5.341000    -2.380721     0.479418      30.83
 C       5.178641    -1.878035    -1.037940      98.04
 H       5.680443    -2.636283    -1.591744      28.57
 O       5.851504    -0.613645    -1.319831     234.42
 H       5.671987     0.248861    -0.810458      24.71
 C       3.614019    -1.750161    -1.314475     100.98
 H       3.219255    -2.601592    -0.857147      27.30
 C       3.363235    -1.725002    -2.832301      94.44
 O       3.503378    -3.102064    -3.487692     283.96
 H       4.242470    -3.239265    -4.101553      28.70
 H       4.101668    -1.108648    -3.380192      24.23
 H       2.373553    -1.422250    -2.954094      27.10
 C      -0.468708    -1.161787     0.388957      51.29
 H      -1.128128    -2.132287     0.649701      17.50
 C      -0.019994     1.184165    -0.331575      93.71
 H      -0.628685     2.184448    -0.230309      14.45
 C       1.225613     0.919484    -0.692976      14.53
 O       2.125251     1.892912    -1.195757     188.28
 C       1.451405     3.268940    -1.256309      68.48
 H       2.111273     3.784143    -1.880579      22.40
 H       0.366968     2.828890    -1.524965      18.35
 H       1.091435     3.941194    -0.184630      21.77
 C       1.782490    -0.447404    -0.512052      23.10
 O       3.186384    -0.525363    -0.805402     221.99
 C       0.888634    -1.437488    -0.048789     100.47
 H       1.280739    -2.535288     0.173398      18.10
 C      -0.898455     0.166284     0.321923     103.15
 C      -2.310404     0.456715     0.845780      85.76
 H      -2.770559    -0.363665     1.293548      27.68
 O      -2.125826     1.692005     1.538437     255.52
 H      -1.359960     1.602745     2.366277      23.70
 C      -3.371461     0.948559    -0.346648      68.20
 H      -2.850004     1.697270    -0.841512      25.06
 O      -3.512245    -0.177653    -1.327681     195.31
 H      -3.500036     0.403203    -2.307646      19.11
 C      -4.707826     1.588481     0.181272     111.32
 O      -5.199293     2.092185    -1.014814     277.85
 H      -5.211512     3.117980    -0.921941      28.23
 H      -4.891801     2.221991     0.981695      29.05
 H      -5.445940     0.693437     0.633324      26.33
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name = lig-etoh-Waterframe_660
 C       5.401343    -1.340467     1.475214      49.01
 H       5.100576    -0.284409     1.177419      16.81
 C       5.519329    -3.693965     0.878529      71.01
 H       5.783840    -4.565748     0.246517      26.58
 C       5.650633    -4.026593     2.274643      -5.38
 O       5.971523    -5.332711     2.685610     336.62
 C       5.097172    -6.416562     2.204213      80.31
 H       4.282764    -5.994560     1.762973      30.62
 H       4.826062    -7.103568     3.153227      23.00
 H       5.456580    -7.196758     1.444874      22.80
 C       5.655587    -2.987650     3.229290      13.29
 O       5.936190    -3.240848     4.542163     209.05
 H       5.869037    -4.216739     4.855610      24.40
 C       5.516956    -1.700726     2.775786      68.89
 H       5.675655    -0.858052     3.451394      25.35
 C       5.424854    -2.366038     0.498074      35.78
 C       5.210794    -1.889799    -0.988722      97.91
 H       5.726350    -2.630765    -1.809968      21.82
 O       5.859710    -0.625789    -1.344452     146.25
 H       5.547899     0.055271    -0.631655      25.52
 C       3.707346    -1.817395    -1.361089      80.50
 H       3.131842    -2.673269    -0.959072      23.16
 C       3.296449    -1.736360    -2.861365     110.42
 O       3.500248    -3.036493    -3.478143     312.34
 H       4.077645    -2.782247    -4.207442      26.79
 H       3.888585    -0.881370    -3.178084      24.42
 H       2.344336    -1.450586    -3.082072      25.95
 C      -0.420197    -1.162874     0.338264      27.74
 H      -1.025523    -2.095298     0.699384      17.46
 C      -0.113314     1.147223    -0.171679      75.32
 H      -0.428160     2.247313    -0.360945      14.20
 C       1.306037     0.895315    -0.744687      -2.66
 O       2.121320     1.951344    -1.191895     205.71
 C       1.440668     3.259655    -1.244851      93.97
 H       1.864883     4.113184    -1.901799      23.21
 H       0.505506     3.260235    -1.876658      23.92
 H       1.540373     3.733844    -0.142723      22.34
 C       1.758563    -0.430114    -0.516576      26.61
 O       3.155247    -0.514839    -0.788309     187.35
 C       0.899924    -1.381463     0.007225      32.08
 H       1.352754    -2.467591    -0.048838      17.22
 C      -0.963989     0.085653     0.234877      45.04
 C      -2.295022     0.450958     0.763060      87.23
 H      -2.618658    -0.359912     1.344400      23.51
 O      -2.189990     1.733147     1.525695     240.25
 H      -1.482371     1.626375     2.324806      26.80
 C      -3.310055     0.955761    -0.354448      73.05
 H      -2.907890     1.783018    -0.969075      21.60
 O      -3.521144    -0.131289    -1.296854     209.14
 H      -3.409975     0.256984    -2.290323      19.85
 C      -4.784921     1.489779     0.299286      82.74
 O      -5.213645     2.120719    -1.065886     201.46
 H      -4.916956     3.107051    -1.110492      28.85
 H      -4.400940     2.345421     1.044186      24.40
 H      -5.284953     0.551371     0.389639      27.63
55
name = lig-etoh-Waterframe_661
 C       5.354405    -1.323192     1.405879      48.37
 H       5.293846    -0.234335     1.250995      21.48
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 C       5.539890    -3.665549     0.874616      60.74
 H       5.571065    -4.399839     0.073510      26.17
 C       5.666081    -4.044705     2.236486      -5.97
 O       5.975179    -5.362084     2.737813     268.93
 C       5.082504    -6.516806     2.161776      84.82
 H       3.968680    -6.036679     1.850765      22.37
 H       4.696894    -7.127021     3.130792      22.55
 H       5.521959    -7.062544     1.352614      24.27
 C       5.656859    -3.026736     3.218723       6.09
 O       5.963234    -3.227745     4.557519     213.93
 H       5.986112    -4.275588     4.701191      20.96
 C       5.529841    -1.692587     2.741151      42.07
 H       5.486740    -0.893155     3.577290      19.99
 C       5.478620    -2.292957     0.425852      26.55
 C       5.242666    -1.910071    -0.967309      86.62
 H       5.649050    -2.785229    -1.754871      18.89
 O       5.879513    -0.657412    -1.349262     188.75
 H       5.424407     0.111412    -0.796520      20.08
 C       3.700227    -1.853340    -1.396426      54.20
 H       3.191609    -2.729206    -0.821008      19.59
 C       3.261938    -1.716181    -2.858948     104.26
 O       3.504843    -2.957821    -3.506777     274.62
 H       4.283570    -2.893045    -4.158380      25.21
 H       3.848793    -0.981170    -3.417003      23.75
 H       2.125486    -1.498556    -2.814026      22.98
 C      -0.376124    -1.235643     0.292470      37.42
 H      -1.040291    -1.984319     0.718886      17.99
 C      -0.060848     1.103586    -0.147069      73.72
 H      -0.519920     2.126139    -0.124798      15.31
 C       1.191863     0.926465    -0.671407      18.58
 O       2.099985     1.997911    -1.187290     204.23
 C       1.450028     3.297664    -1.253956     107.45
 H       2.368564     3.846015    -1.861616      21.50
 H       0.527573     3.429643    -1.616685      28.35
 H       1.360411     3.537795    -0.294386      28.58
 C       1.810533    -0.320533    -0.557027      21.07
 O       3.127436    -0.557073    -0.761150     164.84
 C       0.984256    -1.411955     0.013206      48.95
 H       1.306166    -2.486118     0.090427      19.28
 C      -0.961383     0.097170     0.144804      70.19
 C      -2.319238     0.546842     0.682257      97.95
 H      -2.749198    -0.236309     1.361295      19.68
 O      -2.255485     1.762961     1.534293     273.48
 H      -1.840975     1.418409     2.357518      26.60
 C      -3.290267     0.926375    -0.305408      91.42
 H      -2.851878     1.957061    -0.699624      20.42
 O      -3.540303    -0.091510    -1.278085     257.57
 H      -3.180618     0.214186    -2.126889      24.44
 C      -4.671615     1.400030     0.169699      86.71
 O      -5.272195     2.171699    -1.046506     221.72
 H      -4.631282     2.921125    -1.130936      30.65
 H      -4.512308     2.089187     1.288831      24.74
 H      -5.448481     0.842895     0.521275      27.72
55
name = lig-etoh-Waterframe_662
 C       5.355680    -1.276006     1.401337      44.13
 H       5.384643    -0.260381     1.105627      22.27
 C       5.584796    -3.653195     0.834238      61.57
 H       5.408964    -4.368790     0.067875      24.12
 C       5.700019    -4.092853     2.193371       0.05
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 O       5.910598    -5.407552     2.730310     276.04
 C       5.042145    -6.516243     2.173266     105.36
 H       3.971965    -5.992368     1.669331      22.89
 H       5.074381    -7.315275     2.984170      24.72
 H       5.675095    -6.846297     1.449248      28.06
 C       5.700678    -3.043189     3.196073      -2.82
 O       5.973859    -3.222137     4.553422     204.72
 H       6.172976    -4.233265     4.863886      19.36
 C       5.519102    -1.672639     2.797693      38.83
 H       5.295649    -0.903776     3.660141      21.64
 C       5.475717    -2.285791     0.410393      16.69
 C       5.210468    -1.909231    -1.074589      96.71
 H       5.784896    -2.714450    -1.594153      22.98
 O       5.911607    -0.691635    -1.356773     204.99
 H       5.418512     0.197684    -1.144368      21.74
 C       3.654195    -1.805248    -1.345234      79.83
 H       3.207253    -2.806285    -0.940040      22.37
 C       3.267803    -1.702629    -2.832178      94.36
 O       3.498827    -2.940524    -3.588769     264.92
 H       4.461393    -2.970436    -3.955031      25.65
 H       3.706843    -0.844780    -3.396496      24.28
 H       2.044051    -1.560406    -2.786632      22.43
 C      -0.391909    -1.231271     0.251155      25.71
 H      -0.888490    -2.069093     0.540683      18.17
 C      -0.087387     1.169912    -0.192364      71.93
 H      -0.452278     2.096098     0.102321      16.50
 C       1.241753     1.010444    -0.627845       2.80
 O       1.998178     1.956799    -1.168706     249.36
 C       1.526715     3.350706    -1.222766     105.80
 H       2.425822     4.035459    -1.627997      22.98
 H       0.573323     3.288326    -1.779507      26.55
 H       1.301338     3.878228    -0.288215      28.18
 C       1.790527    -0.381474    -0.527182      28.83
 O       3.179777    -0.589389    -0.751648     200.70
 C       1.056038    -1.430987    -0.033400      56.06
 H       1.562019    -2.291162     0.257786      17.78
 C      -0.905857     0.055414     0.140471      67.56
 C      -2.316796     0.590258     0.748524      80.07
 H      -2.806254    -0.365422     1.219294      22.69
 O      -2.281535     1.760800     1.570404     323.04
 H      -2.168187     1.546404     2.403410      31.49
 C      -3.354127     0.954834    -0.348136     106.84
 H      -2.823138     1.834536    -0.884569      23.55
 O      -3.522379    -0.076451    -1.306761     278.99
 H      -3.101847     0.195099    -2.042293      28.67
 C      -4.644188     1.408138     0.037426     118.61
 O      -5.290807     2.217451    -0.934734     273.46
 H      -4.727177     2.967772    -1.194655      32.94
 H      -4.600547     2.186693     0.883276      26.88
 H      -5.377480     0.628857     0.298278      27.12
55
name = lig-etoh-Waterframe_663
 C       5.424999    -1.282747     1.486470      47.40
 H       5.258257    -0.309150     1.175850      21.18
 C       5.604908    -3.677928     0.782977      28.33
 H       5.546228    -4.490911     0.103104      18.94
 C       5.748312    -4.085422     2.189793      10.21
 O       5.801133    -5.411747     2.700830     295.07
 C       5.099355    -6.458072     2.145947     146.40
 H       3.973657    -6.291207     1.891621      27.46
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 H       4.998829    -7.248965     2.797407      28.43
 H       5.520183    -6.916185     1.207865      29.73
 C       5.770909    -3.028395     3.165391       5.55
 O       5.981728    -3.215833     4.538961     170.58
 H       6.035491    -4.254564     4.824205      21.98
 C       5.470614    -1.675726     2.803427      59.99
 H       5.383073    -0.919616     3.646894      24.00
 C       5.422748    -2.301990     0.456215      36.55
 C       5.183911    -1.898940    -1.104904     106.92
 H       5.492276    -2.550717    -1.797694      26.46
 O       5.963586    -0.702911    -1.415220     221.58
 H       5.336673     0.087287    -1.166881      24.52
 C       3.660332    -1.780087    -1.351329      94.52
 H       3.129572    -2.634328    -0.881929      22.99
 C       3.247912    -1.722921    -2.837681      97.13
 O       3.497459    -2.941239    -3.653512     288.15
 H       4.367480    -2.678614    -4.133268      24.46
 H       3.685201    -0.736955    -3.122021      22.83
 H       2.105760    -1.608408    -3.043608      22.06
 C      -0.332712    -1.249842     0.194720       1.72
 H      -0.918507    -2.068557     0.415667      17.33
 C      -0.123474     1.233349    -0.221390      75.24
 H      -0.388260     2.185988     0.001288      15.48
 C       1.274909     0.935009    -0.571347       5.27
 O       1.988372     1.982929    -1.145786     196.20
 C       1.569450     3.394850    -1.187256      94.39
 H       2.335007     3.961458    -1.666873      25.09
 H       0.909795     3.521561    -2.201943      23.04
 H       1.261122     3.941106    -0.064632      24.59
 C       1.803849    -0.380080    -0.501971      28.64
 O       3.236171    -0.569610    -0.722288     217.69
 C       1.001668    -1.442654    -0.048433      42.65
 H       1.556719    -2.235830     0.258169      15.09
 C      -0.905596     0.103827     0.225162      52.41
 C      -2.332598     0.523516     0.791460      76.46
 H      -2.653106    -0.334538     1.510133      17.30
 O      -2.275954     1.750978     1.624326     303.07
 H      -2.176652     1.579528     2.464837      30.84
 C      -3.256647     1.014102    -0.470619      91.10
 H      -2.870413     1.801118    -1.077882      26.37
 O      -3.484940    -0.115514    -1.389554     266.42
 H      -3.160735     0.097309    -2.154704      29.10
 C      -4.748293     1.509453     0.053164     105.76
 O      -5.350938     2.292490    -0.909011     329.88
 H      -4.922516     3.146541    -0.997407      32.39
 H      -4.536375     1.891403     0.927969      30.60
 H      -5.125888     0.442436    -0.029176      27.16
55
name = lig-etoh-Waterframe_664
 C       5.457247    -1.338542     1.477579      46.48
 H       5.176171    -0.327123     1.380984      22.08
 C       5.607539    -3.725639     0.816338      31.70
 H       5.751353    -4.410941    -0.013893      20.54
 C       5.771088    -4.014798     2.155646      21.71
 O       5.737026    -5.345841     2.693770     190.97
 C       5.067321    -6.476494     2.046460     133.63
 H       4.136635    -6.213855     2.041829      31.13
 H       5.154997    -7.161563     2.799232      28.63
 H       5.441169    -6.804402     0.947842      27.36
 C       5.819579    -3.022397     3.170103      11.60
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 O       5.983627    -3.225301     4.513219     186.22
 H       5.938929    -4.244348     4.656682      21.40
 C       5.480034    -1.714052     2.841255      56.86
 H       5.518259    -0.986368     3.616172      24.81
 C       5.391814    -2.332321     0.444127      35.78
 C       5.179995    -1.905682    -1.046267     101.54
 H       5.419709    -2.699726    -1.729469      26.24
 O       5.962314    -0.706509    -1.485050     184.30
 H       5.661624     0.172961    -0.990977      24.54
 C       3.644234    -1.792637    -1.368298      78.67
 H       3.265022    -2.569484    -0.799557      24.46
 C       3.191516    -1.723192    -2.883124     106.07
 O       3.533749    -2.899402    -3.693398     291.76
 H       4.272604    -2.908250    -4.371483      27.61
 H       3.802429    -0.975186    -3.391848      22.75
 H       2.163374    -1.523404    -2.823333      25.70
 C      -0.389179    -1.197365     0.183353      43.40
 H      -1.067062    -2.025515     0.480432      17.91
 C      -0.084785     1.173012    -0.194975      54.33
 H      -0.450426     2.188416    -0.339694      15.58
 C       1.191225     0.915091    -0.543460      11.74
 O       2.077615     2.030087    -1.117246     163.67
 C       1.626845     3.426498    -1.234069      98.22
 H       2.563563     3.785945    -1.271964      22.93
 H       0.642152     3.735936    -1.855875      22.17
 H       1.070120     3.639764    -0.109185      22.50
 C       1.882131    -0.334417    -0.480329      15.53
 O       3.232101    -0.492040    -0.676906     179.61
 C       1.009134    -1.448645    -0.061997      52.10
 H       1.228172    -2.532480     0.043937      18.14
 C      -0.907655     0.189861     0.313228      42.34
 C      -2.313825     0.506277     0.767461      79.85
 H      -2.955938    -0.302155     1.209523      18.91
 O      -2.257416     1.732315     1.660389     262.58
 H      -1.835487     1.363337     2.513317      24.32
 C      -3.205771     1.037045    -0.531372      64.61
 H      -2.615063     1.810469    -0.910816      24.10
 O      -3.438467    -0.161801    -1.478691     233.00
 H      -3.199191     0.130290    -2.306372      26.31
 C      -4.676218     1.495332     0.064350      79.81
 O      -5.460297     2.431606    -0.928987     240.23
 H      -5.136448     3.292430    -0.794754      31.48
 H      -4.786736     1.665350     1.222145      26.44
 H      -5.574106     0.644166     0.082792      24.57
55
name = lig-etoh-Waterframe_665
 C       5.400953    -1.395695     1.454320      58.06
 H       5.262207    -0.340224     1.141199      22.47
 C       5.608789    -3.675560     0.792545      35.92
 H       5.746147    -4.518623     0.052151      21.51
 C       5.761337    -4.027197     2.161824      21.59
 O       5.737330    -5.270681     2.684225     334.74
 C       4.990037    -6.457595     1.965572     112.36
 H       3.907027    -6.203859     1.893432      26.49
 H       5.358671    -7.343642     2.553012      26.33
 H       5.542541    -6.560716     0.911540      27.64
 C       5.820496    -3.016104     3.188876       5.12
 O       5.987177    -3.285002     4.503541     126.67
 H       6.140047    -4.231084     4.743506      18.93
 C       5.574716    -1.713734     2.832396      67.74
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 H       5.514229    -1.022170     3.576112      25.97
 C       5.414983    -2.337168     0.432499      43.27
 C       5.168670    -1.897869    -1.002287      83.26
 H       5.791740    -2.796340    -1.519704      23.22
 O       5.924872    -0.731091    -1.534329      74.74
 H       5.900134     0.007593    -0.812776      28.18
 C       3.662215    -1.757606    -1.345441      79.48
 H       3.141852    -2.588526    -0.954077      25.38
 C       3.227823    -1.703886    -2.936653     103.11
 O       3.511896    -2.919397    -3.703141     287.71
 H       4.453111    -2.666358    -4.034361      25.13
 H       3.646051    -0.802816    -3.425436      24.51
 H       2.220918    -1.559197    -2.960674      26.83
 C      -0.451075    -1.078646     0.240862      61.59
 H      -1.079623    -2.019909     0.524184      19.85
 C      -0.072349     1.172866    -0.155049      84.75
 H      -0.578739     2.159160    -0.544104      14.95
 C       1.297054     1.006883    -0.612958       4.11
 O       2.128288     1.994035    -1.082876     228.49
 C       1.642028     3.400767    -1.150456     107.14
 H       2.482287     4.186193    -1.126218      23.55
 H       1.057684     3.613459    -2.087314      23.81
 H       1.281993     3.687289    -0.235578      27.11
 C       1.846604    -0.376921    -0.400728      22.19
 O       3.219557    -0.434041    -0.676001     173.89
 C       0.972476    -1.402134    -0.096884      80.13
 H       1.203463    -2.520585    -0.380945      18.85
 C      -0.924254     0.132776     0.366795      22.87
 C      -2.343293     0.588398     0.678348      89.69
 H      -2.795872    -0.308567     1.037656      21.54
 O      -2.239698     1.655067     1.679803     245.66
 H      -1.472157     1.391388     2.455931      22.41
 C      -3.246632     0.981339    -0.490868      83.75
 H      -2.727034     1.827315    -1.008143      20.63
 O      -3.374510    -0.141526    -1.517294     226.63
 H      -3.139003     0.372327    -2.482565      18.20
 C      -4.645897     1.454329    -0.016154      63.03
 O      -5.518771     2.551742    -0.872891     224.51
 H      -5.163535     3.411720    -0.881874      31.43
 H      -4.639874     2.230972     1.016104      21.73
 H      -5.349146     0.484793    -0.090010      24.25
55
name = lig-etoh-Waterframe_666
 C       5.335996    -1.373513     1.459021      56.89
 H       5.261135    -0.289898     1.104992      21.81
 C       5.630416    -3.668426     0.787719      34.43
 H       5.503355    -4.515007     0.029320      19.39
 C       5.716419    -4.001216     2.156170      14.00
 O       5.730242    -5.331164     2.665731     264.50
 C       5.006698    -6.338142     1.897675     109.99
 H       3.739421    -6.365481     1.777955      25.06
 H       5.102082    -7.443037     2.368868      24.17
 H       5.320567    -6.338802     0.843560      27.43
 C       5.805981    -3.055416     3.181527       2.07
 O       6.006948    -3.350401     4.537832     270.49
 H       6.160743    -4.282846     4.671830      23.67
 C       5.678604    -1.648312     2.774902      53.42
 H       5.549594    -0.916484     3.515259      20.44
 C       5.448292    -2.310477     0.433540      34.76
 C       5.198738    -1.916697    -1.008485      90.78
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 H       5.493322    -2.816000    -1.825532      22.52
 O       5.886822    -0.765206    -1.540941     131.04
 H       5.843187    -0.012737    -0.836905      24.50
 C       3.670329    -1.695024    -1.372588      87.65
 H       3.029340    -2.533406    -0.969026      21.45
 C       3.261964    -1.662705    -2.923079      93.52
 O       3.520201    -2.915213    -3.678611     269.69
 H       4.497294    -2.957495    -4.080107      25.01
 H       3.751635    -0.733005    -3.309041      23.87
 H       2.149657    -1.645358    -3.047180      24.30
 C      -0.396500    -1.161572     0.327204      23.52
 H      -1.178190    -2.040008     0.474470      16.80
 C       0.000871     1.233552    -0.192967      34.98
 H      -0.612236     2.257301    -0.293369      14.26
 C       1.314019     1.013887    -0.573397      17.46
 O       2.201153     1.986001    -1.060740     222.90
 C       1.686748     3.374069    -1.048159     108.11
 H       2.643150     4.084789    -1.364461      21.67
 H       1.230436     3.348458    -1.960875      26.14
 H       1.016022     3.605993    -0.327918      27.92
 C       1.795513    -0.298849    -0.371180      19.53
 O       3.200961    -0.468948    -0.718240     187.95
 C       0.839161    -1.343160    -0.150339      81.42
 H       1.309018    -2.405347    -0.367263      18.15
 C      -0.919209     0.233738     0.302231      36.88
 C      -2.350186     0.586778     0.674193      86.65
 H      -2.716521    -0.244177     1.188463      21.74
 O      -2.242726     1.601443     1.639346     211.72
 H      -1.569820     1.228645     2.558736      21.09
 C      -3.300363     0.993253    -0.545803      88.28
 H      -2.961172     1.923516    -1.171502      20.31
 O      -3.313555    -0.086958    -1.473426     238.93
 H      -3.073644     0.424607    -2.564134      15.54
 C      -4.683529     1.541186    -0.143052      89.68
 O      -5.519733     2.591900    -0.806352     314.54
 H      -4.914658     3.310052    -0.917674      33.96
 H      -4.232138     1.925926     0.936245      24.52
 H      -5.268434     0.685158     0.091595      28.17
55
name = lig-etoh-Waterframe_667
 C       5.351261    -1.284381     1.436076      41.39
 H       5.024794    -0.186243     1.347523      20.68
 C       5.621460    -3.669956     0.800996      40.66
 H       5.463838    -4.376820    -0.055035      18.97
 C       5.669460    -4.030338     2.161939       9.42
 O       5.709674    -5.420373     2.627732     292.14
 C       4.971942    -6.269571     1.783470     125.18
 H       3.896499    -5.759765     2.011020      23.32
 H       5.303458    -7.285837     2.320967      23.55
 H       5.273475    -6.298152     0.821014      30.45
 C       5.807720    -2.999329     3.195463       4.40
 O       6.026016    -3.371438     4.522195     202.60
 H       5.972435    -4.341045     4.739857      23.60
 C       5.737193    -1.662962     2.777926      50.35
 H       5.797243    -0.825807     3.535263      20.98
 C       5.461435    -2.313735     0.401538      17.35
 C       5.138855    -1.937181    -1.098392      91.98
 H       5.376602    -2.811012    -1.770716      23.74
 O       5.894620    -0.779868    -1.523610     216.54
 H       5.538388     0.066382    -1.054702      23.68
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 C       3.610213    -1.689756    -1.394639      84.60
 H       3.201211    -2.648201    -0.837921      20.02
 C       3.308520    -1.637103    -2.893219      88.41
 O       3.563672    -2.912415    -3.622803     266.35
 H       4.278896    -2.721587    -4.369762      24.98
 H       3.885792    -0.890147    -3.470316      21.67
 H       2.118586    -1.369525    -2.886246      22.27
 C      -0.464044    -1.120788     0.376048      31.76
 H      -1.118880    -2.053391     0.519594      17.21
 C      -0.044350     1.310928    -0.208454      50.10
 H      -0.216917     2.429765    -0.102569      13.31
 C       1.323870     1.037627    -0.488587      -0.35
 O       2.278798     1.978831    -0.987761     207.23
 C       1.736615     3.315979    -1.082219      84.07
 H       2.751696     3.956046    -0.860820      21.20
 H       1.013609     3.463845    -1.906959      24.07
 H       0.998871     3.621714    -0.163217      21.86
 C       1.789380    -0.266263    -0.435868      20.35
 O       3.145902    -0.508464    -0.758922     205.99
 C       0.874633    -1.333355    -0.197323      78.59
 H       1.179466    -2.415018    -0.080357      19.83
 C      -0.841347     0.244739     0.171873      27.59
 C      -2.322346     0.545427     0.672680      62.90
 H      -2.895732    -0.350888     1.018217      21.39
 O      -2.252489     1.630726     1.610917     205.11
 H      -2.073594     1.138094     2.671303      20.86
 C      -3.333151     1.110656    -0.680627      65.84
 H      -2.594391     1.939055    -0.955693      21.82
 O      -3.273116    -0.072901    -1.429788     295.08
 H      -3.010077     0.168989    -2.426537      21.38
 C      -4.724412     1.598954    -0.109123     128.91
 O      -5.450891     2.585195    -0.758105     327.06
 H      -4.962426     3.454721    -0.885127      31.18
 H      -4.575585     1.951883     0.815326      30.55
 H      -5.490571     0.990748     0.118062      27.94
55
name = lig-etoh-Waterframe_668
 C       5.444089    -1.284121     1.434987      49.16
 H       5.038036    -0.273665     1.176319      21.14
 C       5.572218    -3.635678     0.803646      51.40
 H       5.681558    -4.429597     0.078199      20.18
 C       5.662853    -4.065086     2.202715       8.06
 O       5.753735    -5.385409     2.583507     301.00
 C       4.901761    -6.232648     1.718205     132.23
 H       3.859272    -6.006897     1.684754      26.94
 H       4.874555    -7.298979     2.003257      26.88
 H       5.224574    -6.234333     0.711313      28.31
 C       5.820408    -3.041594     3.177378       2.73
 O       6.043417    -3.327432     4.486019     142.25
 H       5.950514    -4.314742     4.750859      22.95
 C       5.739226    -1.659698     2.768454      50.52
 H       6.025597    -0.901980     3.634877      23.73
 C       5.406845    -2.241989     0.390838      16.37
 C       5.072635    -1.926766    -1.125641     108.96
 H       5.480334    -2.644376    -1.657187      26.78
 O       5.913105    -0.774164    -1.515282     196.46
 H       5.346491     0.023105    -1.291290      27.78
 C       3.590772    -1.772422    -1.382526      85.93
 H       2.960405    -2.685229    -1.060449      23.45
 C       3.328810    -1.633964    -2.898664     100.53
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 O       3.579052    -2.903463    -3.561883     301.76
 H       4.257294    -2.523982    -4.204360      24.73
 H       3.976840    -0.834258    -3.286103      22.96
 H       2.242701    -1.223322    -3.150946      23.11
 C      -0.404089    -1.016325     0.256592       5.35
 H      -1.078573    -1.709636     0.707333      17.64
 C      -0.005849     1.376918    -0.207043      94.29
 H      -0.463987     2.337109    -0.034651      15.03
 C       1.338627     1.091632    -0.457222       3.37
 O       2.303459     1.956194    -0.882839     224.30
 C       1.779112     3.301702    -1.053089     105.52
 H       2.544547     4.090727    -1.107692      25.73
 H       1.343162     3.695787    -2.087862      23.65
 H       1.405149     3.554726     0.104689      24.45
 C       1.769570    -0.376465    -0.535496      33.76
 O       3.101621    -0.502950    -0.785991     213.63
 C       0.899794    -1.366997    -0.120580      31.09
 H       1.318400    -2.335627    -0.069040      17.23
 C      -0.956593     0.225732     0.142993      87.94
 C      -2.322699     0.608418     0.577070      65.00
 H      -2.777127    -0.431113     0.956944      20.03
 O      -2.279107     1.659289     1.597352     216.74
 H      -2.163877     1.416461     2.682759      22.98
 C      -3.262522     1.185424    -0.610930      81.48
 H      -2.755101     2.016699    -1.183615      24.11
 O      -3.270832    -0.094392    -1.430885     267.29
 H      -3.054908     0.160546    -2.259258      25.86
 C      -4.714757     1.628857     0.018873      86.22
 O      -5.415379     2.639064    -0.812712     257.82
 H      -5.073587     3.632609    -0.650533      27.87
 H      -4.548389     2.033580     0.966394      27.26
 H      -5.381884     0.626328    -0.128392      25.76
55
name = lig-etoh-Waterframe_669
 C       5.524180    -1.298391     1.435585      46.43
 H       5.515957    -0.246800     1.162329      24.00
 C       5.524143    -3.584329     0.826257      55.92
 H       5.732119    -4.300752     0.094446      23.19
 C       5.676497    -3.994288     2.131211      23.32
 O       5.767402    -5.382661     2.521034     198.54
 C       4.808203    -6.247744     1.639673     122.58
 H       3.857291    -5.899991     1.554210      27.75
 H       4.859927    -7.198387     2.033883      29.18
 H       5.331758    -6.154876     0.595658      27.30
 C       5.825916    -3.064006     3.134188      14.98
 O       6.065904    -3.263743     4.487230     129.29
 H       6.151363    -4.294653     4.686769      21.80
 C       5.751737    -1.700074     2.760345      47.10
 H       5.903383    -0.877125     3.595226      23.64
 C       5.328272    -2.264839     0.421120      25.26
 C       5.103518    -1.916317    -1.037433      96.37
 H       5.448950    -2.723547    -1.642560      27.78
 O       5.878105    -0.753977    -1.521224     168.09
 H       5.534180     0.153821    -1.323018      27.51
 C       3.525751    -1.816750    -1.427057      82.12
 H       2.952020    -2.640338    -1.016826      25.94
 C       3.333581    -1.597235    -2.913693     112.47
 O       3.593776    -2.873430    -3.535184     317.91
 H       4.452918    -3.050899    -3.932917      30.80
 H       4.104239    -0.889092    -3.114555      23.91
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 H       2.335033    -1.354874    -3.195335      26.88
 C      -0.413280    -0.984871     0.152255      56.80
 H      -0.936553    -1.679796     0.668336      22.08
 C      -0.038141     1.345059    -0.164472      63.15
 H      -0.434897     2.292802    -0.217332      18.91
 C       1.314140     0.995700    -0.484106      10.11
 O       2.328963     1.970536    -0.803429     188.64
 C       1.917688     3.397399    -0.971829      93.27
 H       2.779318     3.788781    -1.221856      25.45
 H       1.071284     3.151960    -1.821859      23.20
 H       1.074763     3.752539    -0.272287      24.18
 C       1.709818    -0.343593    -0.588371      22.16
 O       3.107806    -0.528606    -0.820825     173.82
 C       0.954423    -1.405147    -0.039256      52.89
 H       1.213428    -2.397324     0.051717      21.31
 C      -0.931220     0.370677     0.094065      33.16
 C      -2.347533     0.719843     0.532525      89.64
 H      -2.911995    -0.205730     0.989508      20.49
 O      -2.311511     1.724277     1.576929     241.96
 H      -1.831830     1.242743     2.317409      25.42
 C      -3.198564     1.180209    -0.491836      95.08
 H      -3.039476     1.928358    -1.172706      25.44
 O      -3.322833    -0.072297    -1.412495     188.59
 H      -3.086280     0.261530    -2.299678      23.18
 C      -4.647365     1.665452     0.038670      64.35
 O      -5.395168     2.664591    -0.867531     224.36
 H      -4.902923     3.579323    -0.569133      26.39
 H      -4.576803     1.857884     1.228270      24.85
 H      -5.157686     0.493972    -0.042878      25.39
55
name = lig-etoh-Waterframe_670
 C       5.583673    -1.281040     1.436095      59.76
 H       5.868094    -0.290197     1.264050      23.55
 C       5.478785    -3.595927     0.762228      47.61
 H       5.455878    -4.259664    -0.064999      18.85
 C       5.707648    -4.007056     2.099868      27.05
 O       5.718499    -5.395895     2.414037     241.15
 C       4.802589    -6.223079     1.585649     117.78
 H       3.867497    -5.607128     1.669670      25.39
 H       4.883510    -7.114796     2.134955      26.99
 H       5.279026    -6.473608     0.450553      25.65
 C       5.836682    -3.006826     3.165020      24.83
 O       6.092648    -3.234950     4.486948     181.87
 H       6.207294    -4.256678     4.755259      24.89
 C       5.772063    -1.701641     2.746798      58.68
 H       5.786882    -0.930796     3.545806      23.11
 C       5.291040    -2.244985     0.467433      34.90
 C       5.097738    -1.895141    -0.977374      73.58
 H       5.500352    -2.839472    -1.637030      24.58
 O       5.836849    -0.743466    -1.531559     174.96
 H       5.526317     0.001483    -0.965530      27.13
 C       3.504515    -1.764721    -1.414494      90.44
 H       3.066860    -2.600439    -1.005336      26.03
 C       3.385852    -1.605834    -2.938447     109.57
 O       3.590841    -2.910345    -3.544303     311.23
 H       4.554077    -2.767452    -3.764412      26.99
 H       4.012817    -0.819438    -3.391495      24.10
 H       2.438391    -1.291027    -3.128595      27.70
 C      -0.465467    -1.000414     0.138828      35.30
 H      -1.169607    -1.774580     0.369754      17.93
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 C       0.021266     1.406140    -0.190588      47.22
 H      -0.117719     2.412067    -0.293825      15.44
 C       1.294887     0.995146    -0.552552      19.41
 O       2.318827     1.960932    -0.680056     192.56
 C       1.930702     3.380460    -0.959504     115.35
 H       2.853411     3.881373    -1.222781      24.26
 H       1.332550     3.380011    -1.922321      25.65
 H       1.670141     4.093067    -0.203716      26.76
 C       1.780384    -0.353768    -0.570974      28.89
 O       3.099396    -0.554712    -0.849857     219.40
 C       0.894023    -1.345832    -0.026648      44.95
 H       1.147509    -2.343275     0.207719      18.80
 C      -0.903707     0.338414     0.084668      57.06
 C      -2.311531     0.788506     0.610746      79.27
 H      -2.761778    -0.120165     0.958391      22.62
 O      -2.302398     1.799888     1.575144     295.08
 H      -1.656018     1.569174     2.186209      29.86
 C      -3.303813     1.199277    -0.567737      93.51
 H      -2.687236     2.009088    -1.013790      23.59
 O      -3.414950    -0.005555    -1.346638     258.70
 H      -3.042752     0.316424    -2.413945      18.21
 C      -4.587753     1.621757    -0.012702      96.63
 O      -5.317210     2.614606    -0.844892     219.69
 H      -4.923769     3.627839    -0.931404      27.74
 H      -4.744477     2.228912     1.090581      23.82
 H      -5.557332     0.976343    -0.021460      23.84
55
name = lig-etoh-Waterframe_671
 C       5.642691    -1.241393     1.443639      64.68
 H       5.694408    -0.252453     1.122713      23.57
 C       5.419762    -3.624292     0.734487      32.02
 H       5.153894    -4.386455    -0.013860      17.69
 C       5.724754    -4.043937     2.091183      18.35
 O       5.692979    -5.389223     2.309066     274.04
 C       4.840946    -6.189954     1.591888     119.76
 H       3.665981    -5.805806     1.426232      25.09
 H       4.508062    -7.110769     2.163190      25.71
 H       5.104389    -6.521616     0.502404      25.08
 C       5.850498    -3.048367     3.143257       0.90
 O       6.124120    -3.240145     4.509681     192.42
 H       6.029616    -4.282505     4.657128      25.20
 C       5.794453    -1.632715     2.789712      57.17
 H       5.931834    -0.944001     3.541238      25.69
 C       5.322484    -2.184001     0.453690      23.32
 C       5.034895    -1.876668    -1.020449      92.24
 H       5.566999    -2.824062    -1.615118      23.54
 O       5.787754    -0.737829    -1.493604     177.63
 H       5.641944    -0.015684    -0.861218      29.47
 C       3.626299    -1.724617    -1.401054      99.05
 H       2.987590    -2.541251    -1.161911      25.16
 C       3.372263    -1.639163    -2.952702      93.05
 O       3.612168    -2.949290    -3.563704     264.97
 H       4.367927    -2.797044    -4.292737      24.79
 H       4.070925    -0.884539    -3.451239      22.90
 H       2.317723    -1.315583    -3.118295      24.94
 C      -0.545512    -1.003795     0.159064      37.03
 H      -1.386902    -1.775084     0.135291      18.98
 C       0.081764     1.427100    -0.256653      78.05
 H      -0.215853     2.464211    -0.059596      17.91
 C       1.359902     1.041229    -0.603938       7.54
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 O       2.306199     1.991230    -0.566508     229.25
 C       1.991004     3.367598    -0.992492     113.80
 H       3.097212     3.785418    -1.452662      23.49
 H       1.380831     3.719941    -1.720549      29.45
 H       1.911857     3.797735    -0.034307      25.85
 C       1.776635    -0.380696    -0.482179      33.08
 O       3.098598    -0.520990    -0.837845     199.83
 C       0.829344    -1.274083    -0.078707      68.96
 H       1.262349    -2.280734     0.144037      21.65
 C      -0.942347     0.348494     0.122589      56.71
 C      -2.292979     0.746282     0.642816      81.39
 H      -2.635205    -0.090188     1.148122      26.88
 O      -2.253164     1.913266     1.595865     313.67
 H      -1.727060     1.925194     2.264030      35.17
 C      -3.309609     1.198866    -0.583574      72.56
 H      -2.732927     2.108876    -1.133421      22.87
 O      -3.518890     0.064122    -1.329564     247.46
 H      -3.077263     0.225100    -2.419720      18.15
 C      -4.714173     1.710217    -0.040563     107.55
 O      -5.263097     2.601132    -0.894939     290.05
 H      -4.678191     3.502379    -0.799782      28.10
 H      -4.156278     2.093915     0.919194      25.06
 H      -5.212637     0.809254     0.139479      29.93
55
name = lig-etoh-Waterframe_672
 C       5.663370    -1.210385     1.440773      27.82
 H       5.374842    -0.211870     1.222658      21.15
 C       5.355561    -3.538483     0.795973      62.70
 H       5.143719    -4.351324     0.037362      23.23
 C       5.685815    -3.995872     2.023204      14.22
 O       5.719852    -5.392881     2.291708     219.24
 C       4.729047    -6.245875     1.559815     103.00
 H       3.819363    -5.535141     1.280547      25.68
 H       4.671834    -7.160716     2.325031      24.15
 H       5.371811    -6.530887     0.789054      27.20
 C       5.882150    -3.034292     3.099866       3.63
 O       6.139008    -3.303499     4.495461     147.97
 H       6.018077    -4.309122     4.757952      22.46
 C       5.843754    -1.638348     2.816677      47.02
 H       6.074669    -0.986462     3.546750      22.75
 C       5.386795    -2.245919     0.414375      19.13
 C       5.080833    -1.869215    -1.040223     104.21
 H       5.356888    -2.707962    -1.753130      26.33
 O       5.777092    -0.705053    -1.451388     233.16
 H       5.594162     0.123338    -1.003622      28.07
 C       3.619770    -1.729780    -1.468211      79.58
 H       3.041752    -2.615697    -1.012839      22.70
 C       3.368856    -1.668626    -2.974042      87.42
 O       3.607227    -2.991207    -3.594737     272.12
 H       4.237181    -2.985189    -4.414138      28.05
 H       4.082796    -0.858224    -3.372295      22.18
 H       2.207473    -1.452555    -3.136819      23.37
 C      -0.610945    -0.938474     0.134777      56.81
 H      -1.270102    -1.882763     0.418050      19.45
 C      -0.016672     1.327958    -0.266042      82.64
 H      -0.277251     2.424442     0.052132      15.99
 C       1.365094     1.041570    -0.564656      20.57
 O       2.352246     2.038498    -0.541790     195.83
 C       2.141422     3.407106    -0.971387      83.86
 H       3.235409     3.575055    -1.557144      19.60
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 H       1.146020     3.427415    -1.445749      26.13
 H       1.828468     4.003634    -0.026532      23.56
 C       1.733569    -0.264408    -0.441691      19.75
 O       3.125144    -0.464858    -0.784936     167.21
 C       0.787406    -1.318248    -0.130488      65.89
 H       1.101795    -2.442241    -0.116724      18.56
 C      -0.903526     0.438102     0.142060      46.06
 C      -2.301910     0.773064     0.665198      78.94
 H      -2.848868    -0.034064     1.192202      22.78
 O      -2.213572     2.034805     1.570605     300.19
 H      -1.806444     1.683919     2.294946      28.39
 C      -3.274401     1.218812    -0.480827      72.41
 H      -2.981911     1.986472    -1.275826      22.06
 O      -3.621795     0.060601    -1.395114     204.15
 H      -3.070624     0.275731    -2.356525      19.52
 C      -4.633216     1.719613     0.043088     106.51
 O      -5.267326     2.659817    -0.999634     244.91
 H      -4.788249     3.581347    -0.757580      26.78
 H      -4.628319     2.308713     0.939397      28.08
 H      -5.219726     0.909516     0.239224      30.49
55
name = lig-etoh-Waterframe_673
 C       5.618655    -1.262207     1.439604      59.93
 H       5.409858    -0.184718     1.362135      22.31
 C       5.307684    -3.520795     0.784966      46.91
 H       5.326598    -4.239273    -0.108448      23.10
 C       5.639886    -3.980666     2.101677       6.39
 O       5.740146    -5.353933     2.326692     256.24
 C       4.733928    -6.281382     1.549895     100.75
 H       3.815641    -5.751689     1.324457      26.20
 H       4.384162    -7.093840     2.331867      25.03
 H       5.144914    -6.744283     0.731440      26.04
 C       5.934302    -3.036341     3.117608      10.11
 O       6.143110    -3.385638     4.431113     170.25
 H       6.155002    -4.415979     4.522211      22.46
 C       5.912308    -1.676125     2.742735      51.47
 H       6.031018    -1.002573     3.559427      24.44
 C       5.437337    -2.153955     0.406438      21.63
 C       5.135893    -1.847279    -1.069653      96.73
 H       5.568891    -2.534691    -1.651697      25.43
 O       5.830836    -0.635453    -1.445034     282.32
 H       5.258777     0.011107    -1.064769      27.51
 C       3.519532    -1.721843    -1.441697      67.71
 H       3.056643    -2.657019    -0.902407      21.95
 C       3.358057    -1.708494    -3.002224      95.42
 O       3.550555    -3.042070    -3.623577     281.85
 H       4.470617    -2.694440    -4.002712      23.44
 H       3.951549    -0.921910    -3.493154      23.55
 H       2.253559    -1.367592    -3.252978      24.39
 C      -0.531079    -0.946408     0.110053      39.49
 H      -1.296647    -1.572088     0.703289      21.26
 C      -0.022409     1.379710    -0.249395      68.41
 H      -0.343921     2.531401    -0.219926      18.09
 C       1.283856     1.130120    -0.441955      19.01
 O       2.402060     2.023951    -0.527457     197.52
 C       2.203432     3.430752    -0.912699     105.85
 H       2.888635     3.868295    -1.657835      24.83
 H       1.336396     3.315283    -1.754600      23.19
 H       2.334326     4.395408    -0.227047      22.94
 C       1.760960    -0.282979    -0.479711      11.26
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 O       3.127660    -0.448349    -0.735348     170.93
 C       0.720035    -1.312552    -0.202087      68.81
 H       0.924181    -2.435625    -0.366145      21.13
 C      -0.996801     0.370202     0.192589      42.05
 C      -2.328003     0.937644     0.653896      90.04
 H      -2.822490    -0.009355     1.188497      22.17
 O      -2.164762     2.085187     1.533048     272.22
 H      -2.043858     1.606640     2.393249      25.00
 C      -3.297156     1.220341    -0.449995      84.50
 H      -2.718545     2.011547    -0.915514      24.44
 O      -3.694824     0.059791    -1.432381     186.79
 H      -3.213310     0.343729    -2.298125      23.59
 C      -4.591945     1.786878     0.134115      99.39
 O      -5.260736     2.688744    -1.065941     185.11
 H      -5.146818     3.697066    -1.075539      27.37
 H      -4.778286     2.386572     0.890637      29.56
 H      -5.452799     1.139970     0.071722      27.94
55
name = lig-etoh-Waterframe_674
 C       5.572845    -1.231736     1.467236      49.46
 H       5.730587    -0.140263     1.213791      22.49
 C       5.359130    -3.511152     0.764144      55.53
 H       5.423875    -4.314777    -0.015091      22.70
 C       5.571625    -3.977282     2.090296       7.57
 O       5.706911    -5.364551     2.352205     214.99
 C       4.770374    -6.275683     1.626684     119.84
 H       3.941863    -5.782167     1.368735      28.53
 H       4.416863    -6.976172     2.381873      26.82
 H       5.075996    -6.799095     0.707336      26.73
 C       5.965657    -3.074720     3.114773      16.63
 O       6.167430    -3.484393     4.378183     202.44
 H       6.176555    -4.485203     4.441226      20.56
 C       5.976318    -1.724941     2.718948      43.89
 H       5.969498    -0.888728     3.515993      20.38
 C       5.398993    -2.132329     0.384071      15.65
 C       5.161026    -1.786415    -1.094867      93.11
 H       5.644736    -2.592267    -1.599223      24.36
 O       5.862809    -0.547493    -1.451003     267.40
 H       5.414686     0.251632    -1.158988      25.70
 C       3.553013    -1.713002    -1.369740      74.24
 H       2.854748    -2.533269    -1.002835      22.81
 C       3.253091    -1.721747    -2.991541     101.67
 O       3.544796    -3.022111    -3.654093     278.47
 H       4.511701    -3.166028    -3.919524      28.95
 H       4.029320    -1.156078    -3.393635      23.67
 H       2.248350    -1.417690    -3.276058      26.83
 C      -0.594560    -0.925652     0.193229      40.85
 H      -1.154115    -1.833177     0.495216      19.52
 C      -0.093223     1.494597    -0.185541      78.74
 H      -0.455380     2.548451    -0.439579      18.00
 C       1.341151     1.125304    -0.324663      -1.00
 O       2.415485     2.036166    -0.504487     180.82
 C       2.233742     3.462670    -0.992655      88.65
 H       3.026425     3.495089    -1.589401      24.08
 H       1.166425     3.900312    -1.454563      23.12
 H       2.207244     3.982186     0.048067      23.91
 C       1.702043    -0.299129    -0.515830      28.70
 O       3.091317    -0.494378    -0.724663     197.61
 C       0.815317    -1.274664    -0.341619      68.31
 H       1.013328    -2.358456    -0.411198      20.54
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 C      -0.996323     0.411141     0.164971      25.17
 C      -2.343575     0.922041     0.696484      87.98
 H      -2.760635     0.191371     1.478492      23.40
 O      -2.121830     2.098280     1.502211     240.06
 H      -2.173391     2.016971     2.527923      26.17
 C      -3.360000     1.274167    -0.482827      92.72
 H      -2.919855     2.027739    -1.078619      25.34
 O      -3.703829     0.137807    -1.397322     222.25
 H      -3.442513     0.396636    -2.220100      26.92
 C      -4.707840     1.959536     0.045969      85.11
 O      -5.256319     2.671767    -1.105544     280.67
 H      -4.918465     3.588831    -0.984556      28.89
 H      -4.288314     2.390524     1.065099      25.07
 H      -5.378417     0.907630     0.206324      26.09
55
name = lig-etoh-Waterframe_675
 C       5.597490    -1.214850     1.442142      38.27
 H       5.795684    -0.109464     1.199701      21.87
 C       5.453419    -3.518137     0.726304      62.26
 H       5.305708    -4.274219    -0.014203      22.38
 C       5.550370    -3.988787     2.011510      13.75
 O       5.656376    -5.386128     2.363265     226.73
 C       4.767734    -6.251213     1.746577     125.19
 H       3.946451    -5.642369     1.379257      26.73
 H       4.622237    -7.009438     2.419627      28.14
 H       5.528980    -6.723012     0.915549      28.06
 C       5.937963    -3.125481     3.052768      -8.00
 O       6.222292    -3.583831     4.368534     203.09
 H       6.001850    -4.504882     4.591545      21.94
 C       5.983256    -1.711259     2.757740      30.23
 H       6.302847    -0.967572     3.653962      20.37
 C       5.323223    -2.165814     0.403978      19.60
 C       5.136273    -1.690160    -1.052672      91.76
 H       5.497839    -2.522609    -1.868269      24.74
 O       5.880908    -0.483807    -1.485705     236.24
 H       5.630534     0.317936    -0.975242      25.79
 C       3.584200    -1.714888    -1.390090      82.23
 H       3.285011    -2.625607    -0.864144      24.21
 C       3.255443    -1.728448    -2.958172     101.43
 O       3.508712    -3.031837    -3.653989     258.20
 H       4.410114    -2.806937    -4.126453      26.55
 H       3.840580    -0.894716    -3.346233      24.63
 H       2.272570    -1.525346    -3.153531      28.20
 C      -0.536833    -0.931134     0.191458      44.40
 H      -1.210736    -1.734019     0.272118      20.83
 C      -0.022708     1.505607    -0.141787      60.00
 H      -0.426756     2.476582    -0.242934      19.35
 C       1.320045     1.141752    -0.275650      14.63
 O       2.344138     2.031010    -0.509813     205.33
 C       2.234265     3.474591    -0.977973     101.88
 H       3.196983     3.580318    -1.503311      23.13
 H       1.233816     3.730504    -1.412145      24.82
 H       2.474873     3.983215    -0.061798      25.15
 C       1.710499    -0.201076    -0.526795      10.13
 O       3.055237    -0.529090    -0.743208     183.73
 C       0.714815    -1.271221    -0.387861      56.53
 H       1.173133    -2.222652    -0.462278      20.60
 C      -0.978145     0.491736     0.154048      41.11
 C      -2.372274     0.846935     0.753275      70.42
 H      -2.898097     0.044172     1.284841      23.94
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 O      -2.093220     2.177372     1.463163     209.13
 H      -2.136588     1.802449     2.497953      23.08
 C      -3.445160     1.358852    -0.516313      84.52
 H      -3.002146     2.072629    -1.224676      23.53
 O      -3.683590     0.233751    -1.330429     260.36
 H      -3.479580     0.475410    -2.132592      29.18
 C      -4.732827     1.979236    -0.082909      97.99
 O      -5.267181     2.682505    -1.092144     290.93
 H      -4.864985     3.534145    -1.152114      31.71
 H      -4.370294     2.902315     0.804781      23.49
 H      -5.524550     1.314899     0.634642      25.46
55
name = lig-etoh-Waterframe_676
 C       5.689470    -1.265859     1.472533      51.27
 H       5.594769    -0.149414     1.299860      21.04
 C       5.475942    -3.568855     0.623243      47.91
 H       5.355609    -4.169355    -0.229098      18.61
 C       5.617186    -4.050525     2.001168      16.26
 O       5.643635    -5.310957     2.427099     239.69
 C       4.795391    -6.292042     1.798398     113.54
 H       3.697316    -5.984104     1.357496      25.61
 H       4.462461    -7.048991     2.487459      26.24
 H       5.239131    -6.806030     0.790696      25.93
 C       5.893049    -3.135069     3.069562      -8.91
 O       6.276518    -3.634086     4.325949     236.83
 H       5.920731    -4.496620     4.513657      26.38
 C       5.958051    -1.723830     2.770208      55.73
 H       6.564918    -1.141308     3.581772      21.98
 C       5.321719    -2.118577     0.429679      16.49
 C       5.088425    -1.606125    -1.053691     100.62
 H       5.637266    -2.457367    -1.785618      23.85
 O       5.889023    -0.443176    -1.499065     237.70
 H       5.604812     0.199300    -0.804856      27.65
 C       3.619371    -1.713047    -1.421539      84.45
 H       3.395659    -2.621616    -0.957076      22.83
 C       3.258354    -1.726407    -2.889118     101.70
 O       3.512432    -2.985009    -3.656832     267.68
 H       4.142557    -2.643185    -4.354175      27.74
 H       3.624427    -0.839375    -3.489583      23.71
 H       2.178358    -1.618162    -2.843519      26.09
 C      -0.549758    -0.865290     0.096204      17.47
 H      -1.338266    -1.479310     0.311875      17.55
 C      -0.010666     1.472885    -0.070931     109.62
 H      -0.116918     2.467025     0.124283      19.57
 C       1.314617     1.166004    -0.339903      17.94
 O       2.309227     2.062368    -0.537340     274.27
 C       2.264094     3.435570    -0.869423     124.87
 H       2.954161     3.826683    -1.870824      22.48
 H       1.484499     3.551874    -1.466440      28.76
 H       2.375482     4.231122    -0.221335      27.01
 C       1.667144    -0.220443    -0.515984      32.76
 O       3.024347    -0.508706    -0.771242     185.19
 C       0.710956    -1.203324    -0.381115      69.04
 H       0.891826    -2.232737    -0.511905      21.51
 C      -0.963655     0.442544     0.213657      64.52
 C      -2.393034     0.936685     0.645045      82.21
 H      -2.822977     0.127639     1.146509      23.16
 O      -2.124206     2.177958     1.461528     201.81
 H      -1.744147     1.834693     2.510105      23.08
 C      -3.415398     1.393598    -0.474839      94.04
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 H      -2.753829     2.256832    -0.838995      22.81
 O      -3.670815     0.263249    -1.312953     275.81
 H      -3.345713     0.469576    -2.167002      26.21
 C      -4.682204     2.045869     0.011792     106.60
 O      -5.374689     2.736807    -1.185527     263.65
 H      -5.041262     3.626040    -1.185240      32.80
 H      -4.441886     2.970585     0.625135      25.89
 H      -5.535470     1.497514     0.348286      27.47
55
name = lig-etoh-Waterframe_677
 C       5.740568    -1.290011     1.517196      47.94
 H       5.641368    -0.200010     1.449227      19.42
 C       5.449400    -3.556975     0.597780      51.71
 H       5.485944    -4.246842    -0.209128      22.63
 C       5.683858    -3.995252     1.921460     -14.40
 O       5.617523    -5.329144     2.484747     229.02
 C       4.750951    -6.396286     1.785158      93.93
 H       3.740808    -5.733191     1.608789      23.46
 H       4.688793    -7.083693     2.706040      23.73
 H       5.244647    -6.872204     0.927293      25.41
 C       5.875042    -3.125100     3.080642      10.77
 O       6.317754    -3.630824     4.262766     253.64
 H       6.076987    -4.590653     4.393872      24.54
 C       5.987079    -1.812368     2.815311      65.35
 H       6.342881    -1.043554     3.485859      25.59
 C       5.402549    -2.122194     0.408220      17.44
 C       5.157878    -1.610670    -1.066306     102.77
 H       5.592256    -2.492366    -1.574563      23.24
 O       5.861524    -0.421422    -1.461498     268.24
 H       5.588538     0.479047    -1.045705      23.51
 C       3.655268    -1.672651    -1.410554      81.16
 H       3.076848    -2.497906    -1.046753      21.91
 C       3.166835    -1.717503    -2.868986      93.33
 O       3.521301    -2.898964    -3.658759     260.02
 H       4.217696    -2.827465    -4.354781      29.34
 H       3.666002    -0.851793    -3.459207      22.20
 H       2.001051    -1.700479    -2.789417      23.03
 C      -0.694528    -0.826987     0.000102      49.95
 H      -1.268304    -1.714504     0.270918      19.73
 C       0.005408     1.484899     0.033504      55.05
 H      -0.207283     2.449725     0.411963      15.68
 C       1.295030     1.131443    -0.444845      11.44
 O       2.390001     2.096992    -0.539727     196.53
 C       2.198337     3.467848    -0.900329      88.88
 H       3.230192     3.423119    -1.602908      17.88
 H       1.175211     3.648844    -1.304860      24.60
 H       2.152455     4.138822     0.052522      23.18
 C       1.700082    -0.251853    -0.542947      25.91
 O       3.005186    -0.465156    -0.808489     191.60
 C       0.706831    -1.218542    -0.350022      65.25
 H       0.815640    -2.251805    -0.570299      19.48
 C      -0.990170     0.518675     0.250888      34.32
 C      -2.349560     1.031249     0.609885     101.02
 H      -2.842071     0.319844     1.257763      21.04
 O      -2.197768     2.139759     1.482986     217.13
 H      -1.453032     1.786804     2.314707      22.75
 C      -3.296838     1.447617    -0.407364      77.85
 H      -2.858854     2.253869    -1.145272      21.68
 O      -3.644261     0.289702    -1.337279     206.15
 H      -3.152206     0.489182    -2.217356      22.68
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 C      -4.694049     2.188891     0.055527      89.48
 O      -5.471524     2.777423    -1.254893     249.56
 H      -5.211240     3.717371    -1.148375      28.89
 H      -4.338139     2.638176     0.849763      29.87
 H      -5.213968     1.404961     0.358216      30.86
55
name = lig-etoh-Waterframe_678
 C       5.733602    -1.306929     1.520897      54.61
 H       5.882648    -0.272996     1.383020      25.07
 C       5.444912    -3.516848     0.638125      68.95
 H       5.406769    -4.294233    -0.137673      23.66
 C       5.688950    -4.003772     1.923356       6.69
 O       5.594979    -5.380076     2.446938     263.57
 C       4.748989    -6.398299     1.858953     115.52
 H       3.710447    -6.019772     1.585279      27.36
 H       4.699825    -7.315850     2.604093      23.95
 H       5.179913    -6.764141     1.047373      27.09
 C       5.925540    -3.190118     3.023203       1.92
 O       6.351632    -3.630542     4.242473     209.76
 H       6.184913    -4.649592     4.305968      19.83
 C       6.027006    -1.762548     2.831615      46.27
 H       6.020001    -1.188662     3.681790      22.28
 C       5.522145    -2.123616     0.389956      41.69
 C       5.237722    -1.668636    -1.031243     100.19
 H       5.593958    -2.256418    -1.746918      22.66
 O       5.852967    -0.422187    -1.450133     321.19
 H       5.256690     0.311831    -0.980661      21.17
 C       3.590837    -1.637944    -1.380283      68.27
 H       3.262592    -2.541703    -0.702679      20.15
 C       3.124783    -1.675996    -2.924239      89.36
 O       3.516685    -2.861548    -3.656210     267.50
 H       4.436408    -2.535092    -3.841438      26.02
 H       3.461711    -0.660389    -3.327563      22.27
 H       1.957466    -1.609732    -3.062708      22.77
 C      -0.715100    -0.862072    -0.086208      15.98
 H      -1.547980    -1.705621     0.038091      17.25
 C       0.087949     1.518541     0.126665      56.54
 H      -0.244780     2.572300     0.364332      16.25
 C       1.317024     1.146641    -0.485127      15.07
 O       2.419375     2.024750    -0.522320     188.72
 C       2.121937     3.496515    -0.920949      92.16
 H       2.915643     4.073265    -1.388911      23.59
 H       1.088046     3.763791    -1.536491      22.79
 H       2.315167     3.968542     0.163617      22.31
 C       1.687392    -0.239930    -0.595526      13.80
 O       3.061706    -0.406628    -0.859286     187.03
 C       0.576522    -1.249942    -0.317419      45.33
 H       0.954153    -2.261004    -0.465606      18.39
 C      -1.005702     0.574993     0.208216      47.89
 C      -2.335292     1.044966     0.728497      68.77
 H      -2.940110     0.121953     1.124043      20.45
 O      -2.252794     2.172851     1.550297     225.61
 H      -1.525348     1.768151     2.378785      23.52
 C      -3.306999     1.574989    -0.562510      66.91
 H      -2.752944     2.230844    -1.301622      22.23
 O      -3.598691     0.344313    -1.330029     197.71
 H      -3.079564     0.534981    -2.289074      19.58
 C      -4.669607     2.220251    -0.025285      89.05
 O      -5.485377     2.792246    -1.145341     292.87
 H      -5.235589     3.766541    -1.341797      29.30
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 H      -4.604757     2.920837     0.843344      25.71
 H      -5.279116     1.292281     0.406945      26.73
55
name = lig-etoh-Waterframe_679
 C       5.771280    -1.242278     1.506778      56.74
 H       5.903520    -0.252088     1.238878      27.89
 C       5.470510    -3.538728     0.681759      64.01
 H       5.114754    -4.147643    -0.214236      20.03
 C       5.632933    -4.124524     1.986738      10.31
 O       5.588685    -5.403049     2.375982     352.42
 C       4.746561    -6.398119     1.889068     129.49
 H       3.781709    -6.229626     1.727908      31.99
 H       4.695543    -7.262240     2.653289      25.90
 H       5.129513    -6.725746     0.894827      29.37
 C       6.062105    -3.156800     2.988348      -4.41
 O       6.380533    -3.654974     4.249740     235.24
 H       6.014905    -4.657000     4.406128      21.21
 C       5.998861    -1.765984     2.813328      59.21
 H       5.967567    -1.235483     3.711667      18.93
 C       5.623561    -2.157158     0.390783      -0.24
 C       5.248302    -1.682998    -1.085605      81.46
 H       5.655536    -2.443497    -1.812910      22.05
 O       5.829569    -0.431208    -1.430594     296.37
 H       5.476137     0.350563    -0.771506      17.45
 C       3.541343    -1.643439    -1.344694      59.65
 H       3.176403    -2.578828    -0.693715      17.94
 C       3.075258    -1.624880    -2.910362      91.13
 O       3.571551    -2.789765    -3.659809     272.46
 H       4.546327    -2.786610    -3.729843      28.64
 H       3.567672    -0.784494    -3.376004      21.21
 H       1.962541    -1.600617    -2.948343      22.32
 C      -0.754206    -0.793449    -0.116892      43.30
 H      -1.770759    -1.414777    -0.217660      14.48
 C       0.097373     1.509005     0.152944      62.79
 H       0.084071     2.661898     0.268145      11.06
 C       1.365509     1.147842    -0.426525      16.28
 O       2.414541     2.013863    -0.580882     211.48
 C       2.102474     3.525729    -0.843548      85.65
 H       2.706922     4.010519    -1.461414      23.61
 H       1.094570     3.463845    -1.563800      23.81
 H       1.718252     4.104764     0.091831      23.71
 C       1.559853    -0.231091    -0.624292      21.66
 O       3.098172    -0.358744    -0.890702     162.62
 C       0.625328    -1.228417    -0.372320      63.99
 H       0.762306    -2.357292    -0.257712      16.99
 C      -0.933267     0.547209     0.149654      61.06
 C      -2.426180     1.076022     0.698009      40.73
 H      -2.958896     0.130549     1.162993      19.18
 O      -2.278791     2.212254     1.676065     236.33
 H      -1.954214     2.007757     2.736005      25.30
 C      -3.314014     1.663899    -0.665045      85.54
 H      -2.674105     2.395845    -1.043904      22.39
 O      -3.552552     0.425103    -1.321923     232.01
 H      -3.264592     0.461418    -2.466418      18.12
 C      -4.622419     2.194745    -0.139261      89.04
 O      -5.493511     2.781277    -1.020655     281.73
 H      -4.981727     3.700072    -1.168166      28.15
 H      -4.503622     3.143258     0.575955      21.51
 H      -5.443358     1.329043     0.325014      23.02
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name = lig-etoh-Waterframe_680
 C       5.854867    -1.213481     1.437404      43.57
 H       5.742652    -0.151681     1.393782      18.58
 C       5.475493    -3.600635     0.705750      61.86
 H       4.979006    -4.221032    -0.112354      20.34
 C       5.611824    -4.080175     1.981307       7.69
 O       5.611123    -5.433746     2.360697     210.78
 C       4.702716    -6.453838     1.852198     107.41
 H       3.708649    -5.971550     1.911724      25.78
 H       4.992245    -7.174321     2.586992      25.05
 H       5.096315    -6.966589     0.759629      25.37
 C       6.150394    -3.200866     2.997410      -7.04
 O       6.412695    -3.668660     4.271871     214.35
 H       5.859830    -4.565841     4.482626      20.18
 C       5.960175    -1.786964     2.767898      38.74
 H       6.213670    -1.034208     3.571781      21.50
 C       5.649342    -2.173848     0.415765       8.94
 C       5.181701    -1.679398    -1.113587      89.56
 H       5.675018    -2.590878    -1.755387      24.09
 O       5.824728    -0.440597    -1.421243     261.00
 H       5.638002     0.330051    -0.715141      22.99
 C       3.562729    -1.648379    -1.361566      76.60
 H       2.892967    -2.402005    -0.947435      23.29
 C       3.137521    -1.624704    -2.839619     110.07
 O       3.609360    -2.749085    -3.660217     279.65
 H       4.521684    -2.582452    -4.007421      29.38
 H       3.461739    -0.718361    -3.265078      23.61
 H       2.098885    -1.657370    -2.920638      27.03
 C      -0.725247    -0.706841    -0.164528      42.27
 H      -1.541181    -1.499793    -0.217837      15.45
 C       0.141280     1.520081     0.091897      83.17
 H      -0.203495     2.526599     0.568571      14.99
 C       1.340861     1.149237    -0.312803      13.59
 O       2.409549     2.092449    -0.660500     181.88
 C       1.973451     3.463579    -0.788803      90.97
 H       3.000859     3.730782    -1.306841      20.91
 H       1.145513     3.334903    -1.477735      25.09
 H       1.685410     4.073203     0.048111      25.25
 C       1.634008    -0.235829    -0.647028      53.28
 O       3.022839    -0.354601    -0.877064     195.59
 C       0.598709    -1.202338    -0.436658      43.72
 H       0.874106    -2.343605    -0.432753      14.81
 C      -0.998509     0.631024     0.185665      70.41
 C      -2.427995     1.169311     0.618900      75.18
 H      -3.053542     0.416295     1.139261      18.98
 O      -2.319620     2.233664     1.771983     242.31
 H      -2.394672     1.510321     2.518028      21.01
 C      -3.258937     1.663080    -0.579100      96.36
 H      -2.750485     2.425593    -1.144985      23.50
 O      -3.511406     0.479317    -1.380802     197.44
 H      -3.272439     0.805201    -2.512325      17.07
 C      -4.596044     2.187751    -0.118700      80.96
 O      -5.534136     2.823226    -1.028094     316.25
 H      -5.287138     3.855021    -1.258891      28.89
 H      -3.977956     2.580156     0.820046      23.81
 H      -4.894049     1.254155     0.475821      29.77
55
name = lig-etoh-Waterframe_681
 C       5.909385    -1.300009     1.422873      48.50
 H       5.729450    -0.206123     1.335087      19.30
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 C       5.442471    -3.562990     0.667374      51.59
 H       5.185099    -4.390301    -0.042553      22.29
 C       5.678341    -4.049510     1.994380       7.78
 O       5.658302    -5.447391     2.350186     195.39
 C       4.707650    -6.485001     1.836225     103.71
 H       3.512931    -6.142307     1.939866      23.70
 H       4.725327    -7.349067     2.431323      25.17
 H       4.779131    -6.777653     0.632898      25.09
 C       6.113274    -3.210707     3.028606       1.24
 O       6.445242    -3.662857     4.297852     214.87
 H       6.022474    -4.601792     4.501188      22.64
 C       6.026257    -1.801081     2.709511      47.33
 H       6.385992    -1.080123     3.575237      22.60
 C       5.551884    -2.184113     0.351746      35.50
 C       5.114748    -1.707116    -1.009804     114.73
 H       5.469691    -2.316727    -1.968073      21.78
 O       5.836773    -0.468505    -1.441387     290.88
 H       5.408432     0.230152    -0.817381      24.21
 C       3.584014    -1.636887    -1.374343      85.37
 H       3.233771    -2.481346    -0.852604      22.49
 C       3.237609    -1.624634    -2.837676     111.06
 O       3.658649    -2.721389    -3.673139     297.57
 H       4.304895    -2.292694    -4.219690      28.19
 H       3.425617    -0.619317    -3.194625      23.31
 H       2.178601    -1.706995    -2.834071      25.27
 C      -0.698519    -0.674877    -0.193217      67.40
 H      -1.359771    -1.466383    -0.052520      18.24
 C      -0.000791     1.585345     0.119449      81.54
 H      -0.042844     2.614085     0.597802      16.70
 C       1.424942     1.148018    -0.293225      12.02
 O       2.352110     2.091766    -0.666441     209.37
 C       1.877105     3.396051    -0.816817     109.89
 H       2.863957     4.254072    -1.085029      23.18
 H       1.220291     3.697128    -1.509689      27.59
 H       1.777321     3.765320     0.149550      27.30
 C       1.701595    -0.200569    -0.594104      32.46
 O       2.969961    -0.396814    -0.857862     208.08
 C       0.604784    -1.115323    -0.515600      41.27
 H       0.728268    -2.200491    -0.850636      18.08
 C      -1.047521     0.702339     0.219125      17.15
 C      -2.363429     1.264215     0.608169      91.55
 H      -2.908862     0.395513     0.838483      19.47
 O      -2.365869     2.178183     1.795833     290.17
 H      -2.390977     1.570888     2.557416      25.16
 C      -3.210424     1.670512    -0.572999      80.48
 H      -2.718783     2.406959    -1.288412      22.42
 O      -3.463097     0.519125    -1.484923     229.63
 H      -3.046323     0.833525    -2.440693      20.04
 C      -4.507200     2.177478     0.048764     104.09
 O      -5.557291     2.848131    -1.031591     226.05
 H      -5.200613     3.862543    -0.973734      26.11
 H      -4.714566     3.057979     0.754364      22.75
 H      -5.168323     1.417126     0.210758      28.12
55
name = lig-etoh-Waterframe_682
 C       5.877404    -1.400496     1.391780      44.69
 H       6.084484    -0.297008     1.113880      21.64
 C       5.414970    -3.572126     0.664071      64.65
 H       5.372983    -4.243695    -0.181450      23.38
 C       5.737168    -4.100885     1.968959      -7.82
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 O       5.692900    -5.478267     2.319794     221.35
 C       4.674700    -6.438257     1.815593     111.46
 H       3.531279    -6.069785     2.036236      24.03
 H       4.921252    -7.338611     2.360414      23.81
 H       4.896629    -6.498614     0.768659      27.08
 C       6.026766    -3.184706     3.065630       4.24
 O       6.469269    -3.641645     4.314354     260.56
 H       6.208139    -4.574567     4.468762      23.06
 C       6.199326    -1.850889     2.720741      46.14
 H       6.349158    -1.095908     3.605843      19.05
 C       5.427929    -2.216572     0.322759      25.31
 C       5.102448    -1.665888    -1.045018     107.28
 H       5.379556    -2.576031    -1.601214      21.57
 O       5.819629    -0.500853    -1.431011     347.08
 H       5.507985     0.371221    -1.110320      25.70
 C       3.621173    -1.660805    -1.297519      81.65
 H       3.270244    -2.588176    -0.829438      19.93
 C       3.238903    -1.609211    -2.867150      91.49
 O       3.717363    -2.685284    -3.705315     263.51
 H       4.474488    -2.554288    -4.271595      29.53
 H       3.711823    -0.676386    -3.342557      21.60
 H       2.100527    -1.620936    -2.841768      22.87
 C      -0.714726    -0.630620    -0.161194       7.65
 H      -1.465646    -1.302848    -0.059081      16.94
 C       0.068578     1.650867     0.145985      61.41
 H      -0.088314     2.692566     0.310893      16.30
 C       1.291738     1.209072    -0.269821      21.50
 O       2.332517     2.054636    -0.689977     222.51
 C       1.856667     3.492208    -0.773819      85.38
 H       2.824459     4.132918    -1.126012      21.19
 H       0.984504     3.672410    -1.551805      24.26
 H       1.314388     3.674786     0.202281      24.11
 C       1.638853    -0.141029    -0.493654       8.79
 O       3.051039    -0.462332    -0.847930     191.19
 C       0.596376    -1.017604    -0.611218      95.66
 H       0.633641    -1.978525    -1.054739      18.69
 C      -0.969784     0.695821     0.205164      76.88
 C      -2.338619     1.204259     0.668683      74.34
 H      -2.866459     0.287812     0.913552      22.85
 O      -2.407492     2.102698     1.777494     327.28
 H      -2.081531     1.777675     2.509612      32.53
 C      -3.199648     1.755837    -0.629117      64.58
 H      -2.665919     2.702968    -1.084800      20.99
 O      -3.412635     0.577153    -1.535933     262.51
 H      -3.106760     0.676741    -2.377551      26.12
 C      -4.618663     2.217731     0.088783      89.46
 O      -5.507555     2.841875    -1.008225     263.48
 H      -5.160466     3.821908    -1.212950      28.32
 H      -4.660433     3.019855     0.948665      23.92
 H      -5.232585     1.373047     0.347683      27.66
55
name = lig-etoh-Waterframe_683
 C       5.867978    -1.423029     1.399841      51.05
 H       6.292118    -0.395145     1.127524      21.86
 C       5.403952    -3.675592     0.666726      57.19
 H       5.291035    -4.322230    -0.152464      22.48
 C       5.728925    -4.138751     1.939225       8.87
 O       5.733510    -5.489371     2.293997     194.56
 C       4.690612    -6.332801     1.789081     130.34
 H       3.735392    -5.966633     2.139250      26.56
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 H       5.041076    -7.279752     2.260172      24.36
 H       4.742195    -6.489350     0.823944      30.11
 C       6.006147    -3.236070     3.067826      -0.32
 O       6.470385    -3.615941     4.314727     245.09
 H       6.158960    -4.497937     4.502387      24.07
 C       6.310376    -1.869231     2.698779      35.20
 H       6.595456    -1.089550     3.436091      20.78
 C       5.361612    -2.224050     0.429799      21.63
 C       5.123790    -1.693685    -1.081598     114.26
 H       5.576058    -2.383379    -1.697659      24.30
 O       5.834740    -0.528896    -1.455610     336.69
 H       5.400374     0.201003    -0.982014      25.81
 C       3.580205    -1.711764    -1.328413      77.22
 H       2.958627    -2.564603    -0.901567      19.23
 C       3.279115    -1.599056    -2.890127      85.24
 O       3.736130    -2.713053    -3.746312     249.87
 H       4.750971    -2.512594    -3.782548      25.03
 H       3.749336    -0.558025    -3.199817      20.69
 H       2.160457    -1.451870    -3.207162      22.26
 C      -0.733358    -0.591307    -0.130743      31.06
 H      -1.585756    -1.231162    -0.276172      17.56
 C       0.079991     1.726509     0.176356      58.44
 H      -0.322640     2.649446     0.119874      17.24
 C       1.327476     1.272205    -0.301473       6.39
 O       2.307010     2.102619    -0.710725     176.61
 C       1.833161     3.550430    -0.732777      92.11
 H       2.684581     4.035694    -0.912924      25.32
 H       1.088703     3.301928    -1.645222      21.42
 H       1.403784     4.164653     0.240185      23.63
 C       1.662261    -0.154477    -0.465435       1.16
 O       3.060831    -0.421908    -0.763249     176.05
 C       0.515269    -0.993175    -0.679186      69.46
 H       0.754524    -1.911604    -1.042664      18.53
 C      -0.910430     0.727220     0.251240      51.76
 C      -2.367487     1.051074     0.662639      67.73
 H      -2.989250     0.167719     1.065333      21.19
 O      -2.424466     2.062603     1.749374     321.44
 H      -1.829211     1.716563     2.322841      30.85
 C      -3.244181     1.804991    -0.546694      68.15
 H      -2.751625     2.715756    -1.038133      22.72
 O      -3.381009     0.681540    -1.501369     272.49
 H      -3.149549     0.925805    -2.431648      22.02
 C      -4.735217     2.261654     0.002188     110.31
 O      -5.452545     2.815329    -0.990726     354.76
 H      -5.126992     3.731812    -1.141974      31.59
 H      -4.207493     2.622835     0.810040      27.45
 H      -5.005992     1.299591     0.537155      29.58
55
name = lig-etoh-Waterframe_684
 C       5.942808    -1.372620     1.470813      42.61
 H       6.027408    -0.314790     1.170344      19.56
 C       5.374375    -3.701289     0.660532      48.32
 H       5.084413    -4.457382    -0.012982      17.50
 C       5.690537    -4.139454     1.985788      16.68
 O       5.802654    -5.482525     2.263014     265.70
 C       4.723849    -6.274502     1.785229     135.06
 H       3.855262    -5.941553     2.166665      28.81
 H       4.692309    -7.310654     2.221110      25.96
 H       4.489140    -6.361238     0.671728      26.52
 C       6.096884    -3.240552     3.006231      16.69
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 O       6.439178    -3.619792     4.307393     230.19
 H       6.047960    -4.479969     4.617280      23.85
 C       6.321745    -1.911205     2.659611      78.99
 H       6.943060    -1.373387     3.284857      25.18
 C       5.344206    -2.308988     0.442015       5.59
 C       5.139036    -1.836918    -1.040021     123.93
 H       5.579913    -2.454059    -1.793011      30.74
 O       5.827077    -0.519943    -1.457647     257.58
 H       5.517640     0.154765    -0.860544      26.52
 C       3.465924    -1.698993    -1.447641      69.29
 H       3.029741    -2.591838    -0.868401      21.38
 C       3.309601    -1.564137    -2.937341      94.68
 O       3.751692    -2.719493    -3.744529     234.14
 H       4.832503    -2.697962    -3.845309      25.88
 H       3.911113    -0.659452    -3.186623      21.72
 H       2.200941    -1.447080    -3.170816      23.90
 C      -0.721997    -0.589116    -0.168609      40.77
 H      -1.657929    -1.244810    -0.373489      16.65
 C       0.017165     1.745585     0.178114      37.89
 H      -0.212045     2.762546     0.188718      16.18
 C       1.423715     1.247304    -0.324419      -5.65
 O       2.318876     2.248016    -0.678791     218.09
 C       1.854313     3.557417    -0.765168     113.68
 H       2.661739     4.121017    -1.063730      25.40
 H       1.143917     4.016249    -1.610088      24.08
 H       1.515579     3.930775     0.312962      24.32
 C       1.666537    -0.137701    -0.510319      18.20
 O       3.020309    -0.370355    -0.660435     140.89
 C       0.535443    -0.999422    -0.677173      84.37
 H       0.593315    -2.025336    -0.982784      19.25
 C      -0.985386     0.740441     0.341247      34.57
 C      -2.439384     1.052578     0.629707      73.09
 H      -2.887824    -0.021322     0.836279      22.78
 O      -2.408884     2.021676     1.717917     276.70
 H      -1.906400     1.646512     2.504427      26.81
 C      -3.300735     1.712414    -0.438412     107.00
 H      -2.742063     2.542539    -0.776632      24.68
 O      -3.375071     0.790063    -1.445213     281.95
 H      -3.231143     1.226035    -2.439028      19.76
 C      -4.583205     2.179016     0.011800      95.56
 O      -5.467732     2.822454    -1.015809     268.66
 H      -5.265094     3.716426    -0.971240      32.89
 H      -4.585416     3.120021     0.753982      23.63
 H      -5.468916     1.340675     0.225751      24.94
55
name = lig-etoh-Waterframe_685
 C       5.928443    -1.395862     1.379477      38.28
 H       5.902259    -0.335454     1.337665      21.41
 C       5.324405    -3.681757     0.731171      55.53
 H       4.954178    -4.335593    -0.061214      18.79
 C       5.667260    -4.117015     2.011219      24.45
 O       5.866258    -5.511898     2.226270     166.14
 C       4.648764    -6.257335     1.811234     100.87
 H       3.780774    -5.711453     2.225898      25.61
 H       4.989781    -7.301113     2.200840      23.97
 H       4.717145    -6.146571     0.535004      23.24
 C       6.204773    -3.291777     2.978052      -5.30
 O       6.405702    -3.622941     4.290068     127.54
 H       5.978752    -4.585481     4.491941      25.16
 C       6.373228    -1.907824     2.677461      30.43
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 H       6.999777    -1.462411     3.376072      19.38
 C       5.420420    -2.309475     0.405828      28.51
 C       5.075015    -1.870602    -1.023346     109.49
 H       5.437748    -2.814854    -1.602557      25.74
 O       5.787376    -0.562500    -1.411869     250.78
 H       5.636231     0.175519    -0.849727      28.24
 C       3.492534    -1.650811    -1.426939      70.58
 H       2.833017    -2.533490    -1.132006      22.85
 C       3.326769    -1.516352    -3.015418     108.78
 O       3.749241    -2.731391    -3.702743     269.49
 H       4.595179    -2.528109    -4.298475      27.45
 H       3.895830    -0.738434    -3.385130      25.09
 H       2.302284    -1.345307    -3.248854      26.74
 C      -0.706404    -0.545774    -0.225999      45.56
 H      -1.553558    -1.393529    -0.250140      18.86
 C       0.066117     1.635017     0.119896      81.89
 H      -0.018733     2.704087     0.477662      19.01
 C       1.266768     1.311021    -0.276468      18.88
 O       2.366205     2.327974    -0.664802     166.74
 C       1.902153     3.698801    -0.786834     101.84
 H       2.974977     4.332528    -1.068340      22.10
 H       1.007389     3.840521    -1.347329      27.39
 H       1.608235     3.893790     0.196514      27.90
 C       1.651959    -0.067862    -0.590483      21.68
 O       3.011847    -0.419688    -0.628273     136.99
 C       0.571763    -1.009902    -0.599285      61.20
 H       0.615911    -2.096227    -0.979970      19.86
 C      -1.030931     0.706623     0.303202      37.89
 C      -2.454308     1.062299     0.704534      91.03
 H      -3.016472     0.135508     0.980214      22.00
 O      -2.405788     1.993210     1.723707     260.32
 H      -2.378512     1.411373     2.720019      21.27
 C      -3.225951     1.689599    -0.370048      94.71
 H      -2.693264     2.596512    -0.542909      26.08
 O      -3.416816     0.814456    -1.438521     242.62
 H      -3.212112     1.134592    -2.543157      18.17
 C      -4.629548     2.168257     0.078270      71.95
 O      -5.482529     2.821949    -1.090506     234.20
 H      -5.318536     3.787613    -1.111046      29.34
 H      -4.827063     2.910252     1.064001      24.23
 H      -5.203477     1.158715     0.511017      26.72
55
name = lig-etoh-Waterframe_686
 C       5.931765    -1.442541     1.380467      54.57
 H       5.974627    -0.418382     1.154190      24.52
 C       5.268061    -3.611447     0.781868      55.76
 H       4.967497    -4.326248    -0.050126      23.99
 C       5.711820    -4.174537     1.982867       4.42
 O       5.856506    -5.519474     2.200558     225.09
 C       4.669705    -6.224937     1.831802     112.81
 H       3.611931    -5.885891     2.294530      22.57
 H       4.752066    -7.330385     2.126511      23.67
 H       4.525104    -6.369495     0.580712      24.38
 C       6.274028    -3.257168     2.991902      -5.71
 O       6.396038    -3.645911     4.280292     240.05
 H       6.068471    -4.666532     4.548919      21.20
 C       6.426647    -1.911019     2.634184      51.92
 H       6.621623    -1.094474     3.400568      21.65
 C       5.467921    -2.259616     0.378648      30.92
 C       4.964521    -1.791199    -0.997483     112.52
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 H       5.402521    -2.540992    -1.859125      20.02
 O       5.750495    -0.682309    -1.375941     306.24
 H       5.432017    -0.029228    -0.785280      27.38
 C       3.542597    -1.595665    -1.384954      84.62
 H       2.911880    -2.440651    -1.234653      21.73
 C       3.354835    -1.444495    -3.061330      98.01
 O       3.701861    -2.751354    -3.679003     266.31
 H       4.574936    -2.439788    -4.157647      25.24
 H       3.904558    -0.632390    -3.456231      23.59
 H       2.352081    -1.246702    -3.293814      25.17
 C      -0.728289    -0.599089    -0.264514      43.80
 H      -1.498056    -1.444397    -0.137733      18.55
 C      -0.027162     1.610919     0.159483      72.48
 H      -0.210701     2.637424     0.739659      18.37
 C       1.349235     1.361903    -0.358712       5.90
 O       2.357452     2.305618    -0.643399     146.06
 C       1.939264     3.828396    -0.719448      85.75
 H       2.968408     4.559175    -1.216073      22.05
 H       1.235827     3.684744    -1.424996      26.79
 H       1.757755     4.393098     0.140588      26.13
 C       1.623969    -0.033943    -0.648171      27.48
 O       3.016700    -0.484701    -0.656051     179.83
 C       0.617791    -0.965942    -0.530163      53.55
 H       0.951184    -2.064322    -0.834390      18.30
 C      -1.008891     0.654182     0.179216      17.26
 C      -2.409187     0.985668     0.808604      74.50
 H      -2.954301     0.188306     1.197347      20.37
 O      -2.426925     2.014648     1.843975     228.48
 H      -2.411432     1.340222     2.853312      19.91
 C      -3.203323     1.817618    -0.378899      52.54
 H      -2.597015     2.727238    -0.791255      22.81
 O      -3.476319     0.771397    -1.470717     175.55
 H      -3.003160     1.229149    -2.410069      19.34
 C      -4.808482     2.178772     0.140905      86.80
 O      -5.462643     2.745574    -1.106161     280.35
 H      -5.072530     3.747900    -1.111419      26.47
 H      -4.443664     2.746143     1.031488      25.30
 H      -5.119048     1.231113     0.287929      30.41
55
name = lig-etoh-Waterframe_687
 C       5.992806    -1.409407     1.382168      37.71
 H       6.185360    -0.385847     1.141074      22.04
 C       5.247685    -3.597068     0.759089      57.25
 H       4.856288    -4.394785     0.030046      22.37
 C       5.834195    -4.106666     1.955308      12.34
 O       5.790604    -5.532453     2.192491     180.05
 C       4.649584    -6.304613     1.818176     124.22
 H       3.736551    -5.760418     2.392823      24.08
 H       4.844633    -7.224147     2.338953      24.56
 H       4.431823    -6.279437     0.812015      28.51
 C       6.259366    -3.264624     2.973167      -7.40
 O       6.440757    -3.654797     4.305550     262.71
 H       5.947522    -4.546541     4.540550      19.66
 C       6.427889    -1.882332     2.605232      42.98
 H       6.354280    -1.032842     3.432305      19.85
 C       5.396472    -2.286491     0.383376      29.38
 C       4.961731    -1.780465    -1.018325     103.24
 H       5.157466    -2.662830    -1.751898      22.82
 O       5.743559    -0.704855    -1.341558     286.24
 H       5.467970     0.132337    -0.992294      27.47
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 C       3.470747    -1.566342    -1.448874      89.02
 H       3.127045    -2.526288    -1.118531      21.95
 C       3.374324    -1.395629    -3.012393      93.21
 O       3.653803    -2.708077    -3.683563     274.43
 H       4.607447    -2.877247    -3.876002      28.99
 H       4.108870    -0.623102    -3.423789      22.68
 H       2.295151    -1.192598    -3.185418      24.26
 C      -0.720668    -0.776005    -0.289490      14.09
 H      -1.484343    -1.519168    -0.224041      18.51
 C      -0.007632     1.669730     0.190828      46.41
 H      -0.426351     2.653576     0.705309      16.38
 C       1.385329     1.381696    -0.453669       3.16
 O       2.345936     2.344149    -0.575534     169.37
 C       1.998424     3.864156    -0.697158      88.98
 H       2.912899     4.140019    -1.319271      22.23
 H       1.203209     4.097121    -1.486863      24.72
 H       1.708467     4.470557     0.255521      23.55
 C       1.681701     0.013790    -0.663881      30.53
 O       2.996534    -0.462547    -0.683909     193.61
 C       0.632030    -0.954266    -0.516746      37.38
 H       0.985780    -2.058886    -0.475820      18.84
 C      -1.042246     0.637591     0.140933      38.37
 C      -2.385046     1.035997     0.799264      63.28
 H      -2.821607     0.072584     1.004743      22.36
 O      -2.444446     2.019556     1.993988     246.04
 H      -1.814201     1.691948     2.882386      24.37
 C      -3.322570     1.786971    -0.381697      60.20
 H      -2.683723     2.663642    -0.865233      22.38
 O      -3.504053     0.785515    -1.459019     189.58
 H      -3.023435     0.965935    -2.463239      20.29
 C      -4.779642     2.171785     0.065757     120.84
 O      -5.419693     2.667078    -1.027868     257.46
 H      -5.259157     3.766529    -1.199973      25.72
 H      -4.933688     2.873712     0.837488      28.11
 H      -5.369760     1.349109     0.278417      29.99
55
name = lig-etoh-Waterframe_688
 C       6.039842    -1.379500     1.286518      42.94
 H       6.207463    -0.293921     1.155808      23.07
 C       5.277191    -3.662678     0.735136      44.72
 H       4.715147    -4.334275     0.035144      19.48
 C       5.879843    -4.115129     1.893555      18.88
 O       5.779779    -5.503128     2.200135     188.83
 C       4.590791    -6.340027     1.873550     127.68
 H       3.685845    -5.904552     2.322020      27.73
 H       4.843680    -7.267834     2.243532      26.43
 H       4.461190    -6.472336     0.884151      30.43
 C       6.242906    -3.240262     3.000086      -8.35
 O       6.496220    -3.629030     4.300508     250.64
 H       6.063775    -4.460514     4.561600      24.63
 C       6.348513    -1.866866     2.649251      29.09
 H       6.795115    -1.259108     3.566029      18.29
 C       5.297243    -2.248907     0.428684      19.72
 C       4.947527    -1.833048    -1.025726      97.07
 H       5.389867    -2.627110    -1.556762      26.39
 O       5.821284    -0.631481    -1.363334     201.03
 H       5.412822     0.190072    -1.060453      27.66
 C       3.437848    -1.596967    -1.473947      80.85
 H       2.753428    -2.486206    -1.191003      21.84
 C       3.384610    -1.414233    -2.946547      98.53
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 O       3.584891    -2.652700    -3.689928     283.92
 H       4.564860    -2.553754    -3.790800      28.04
 H       4.168940    -0.576396    -3.285578      22.79
 H       2.368435    -1.008732    -3.353316      24.62
 C      -0.725393    -0.757782    -0.245793       7.44
 H      -1.305236    -1.591047    -0.309005      18.20
 C       0.049892     1.614875     0.115930      60.23
 H      -0.088507     2.672584     0.370441      18.20
 C       1.249946     1.429081    -0.440137      17.65
 O       2.334202     2.441909    -0.508170     222.25
 C       2.068906     3.822764    -0.748877     106.69
 H       2.910820     4.162472    -0.993273      24.38
 H       1.011061     4.125118    -1.252061      23.51
 H       2.056397     4.130580     0.452351      22.13
 C       1.669375     0.027013    -0.646540      20.15
 O       2.995098    -0.371261    -0.712727     157.90
 C       0.669589    -1.015580    -0.522627      45.61
 H       1.002297    -2.033485    -0.442168      18.87
 C      -1.000135     0.647180     0.158640      66.18
 C      -2.425402     1.141687     0.740298      63.46
 H      -2.980561     0.166901     1.050579      21.77
 O      -2.428230     2.036310     2.009920     256.68
 H      -1.910879     1.348668     2.591489      23.42
 C      -3.378181     1.664971    -0.348493     100.83
 H      -2.972298     2.683121    -0.639780      21.39
 O      -3.542619     0.774709    -1.425551     239.87
 H      -3.071649     1.159655    -2.321221      20.26
 C      -4.712723     2.146627     0.057102     105.92
 O      -5.461530     2.646782    -1.069432     260.33
 H      -5.296222     3.773366    -1.079380      25.36
 H      -4.849896     2.843306     0.846865      26.94
 H      -5.313211     1.216600     0.605748      27.06
55
name = lig-etoh-Waterframe_689
 C       6.031779    -1.397044     1.325000      39.26
 H       6.139017    -0.342458     0.918375      23.54
 C       5.298468    -3.636250     0.699183      44.05
 H       4.838615    -4.345556     0.027460      21.99
 C       5.816475    -4.190978     1.900649      17.62
 O       5.790021    -5.503897     2.229500     202.79
 C       4.569093    -6.332125     1.936956     111.87
 H       3.642155    -6.077570     2.285628      28.36
 H       4.789813    -7.287257     2.408919      26.82
 H       4.511001    -6.588480     0.712100      25.26
 C       6.217738    -3.214614     2.972156      -8.84
 O       6.555593    -3.597346     4.278020     203.47
 H       6.243359    -4.442512     4.523901      25.43
 C       6.297347    -1.856313     2.658948      65.98
 H       7.004029    -1.245331     3.206128      21.29
 C       5.258310    -2.211256     0.465491      32.57
 C       4.978243    -1.822028    -1.004802      96.80
 H       5.415045    -2.446911    -1.663560      27.31
 O       5.866794    -0.590785    -1.408310     193.48
 H       5.412438     0.116036    -0.901251      26.57
 C       3.438266    -1.619903    -1.401944      75.87
 H       2.609843    -2.388209    -1.168663      23.10
 C       3.345733    -1.370386    -2.964244      96.51
 O       3.563226    -2.591190    -3.693661     276.56
 H       4.361210    -2.476165    -4.265831      28.52
 H       4.247613    -0.688834    -3.141804      22.02
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 H       2.341956    -0.856070    -3.234326      24.95
 C      -0.656937    -0.621982    -0.169572      44.20
 H      -1.417380    -1.362011    -0.147107      20.38
 C      -0.006789     1.625039     0.028373      82.22
 H      -0.217609     2.598210     0.263575      20.75
 C       1.327231     1.403878    -0.444410       3.21
 O       2.285423     2.394347    -0.482309     273.14
 C       2.119650     3.799720    -0.644174     105.07
 H       2.955554     4.466234    -1.184842      22.96
 H       1.172582     3.998701    -1.356523      25.18
 H       2.025247     4.454016     0.299339      24.63
 C       1.598376    -0.002598    -0.612340      31.97
 O       3.034498    -0.262618    -0.768763     142.49
 C       0.686263    -1.023341    -0.517039      38.01
 H       0.945585    -1.983589    -0.696138      20.67
 C      -1.014168     0.643759     0.206613      41.27
 C      -2.470100     1.146037     0.730325      74.33
 H      -2.974835     0.223088     1.224509      21.87
 O      -2.386817     2.017228     1.881432     282.89
 H      -2.383901     1.573853     2.681972      29.62
 C      -3.341416     1.699873    -0.338135      99.20
 H      -2.870382     2.514892    -0.787060      26.23
 O      -3.567870     0.723484    -1.411295     201.40
 H      -3.260955     1.250024    -2.243653      21.83
 C      -4.779488     2.114686     0.174196      78.92
 O      -5.520772     2.639834    -1.115182     220.66
 H      -5.237621     3.696020    -1.175895      26.34
 H      -4.237964     2.814742     0.895427      24.10
 H      -5.296253     1.030899     0.471817      26.84
55
name = lig-etoh-Waterframe_690
 C       5.918838    -1.413135     1.384393      39.80
 H       6.352705    -0.385234     1.120135      23.97
 C       5.291321    -3.609905     0.704355      59.76
 H       5.065455    -4.229330    -0.108740      22.78
 C       5.698836    -4.123316     1.968941       5.42
 O       5.768980    -5.566591     2.278685     211.00
 C       4.609303    -6.356238     1.981067      96.39
 H       3.748754    -5.778368     2.304506      26.08
 H       4.847335    -7.269624     2.637892      23.95
 H       4.515775    -6.473430     0.660671      22.82
 C       6.174143    -3.264487     2.927830     -22.57
 O       6.616062    -3.570764     4.230984     280.35
 H       6.242937    -4.413823     4.465598      30.20
 C       6.342370    -1.822076     2.601990      45.64
 H       6.828744    -1.158056     3.216082      23.58
 C       5.312449    -2.251083     0.433104      12.43
 C       5.029194    -1.742477    -1.001781     110.29
 H       5.219630    -2.592193    -1.705799      27.42
 O       5.825811    -0.595736    -1.420578     254.88
 H       5.739741     0.258282    -0.877086      26.53
 C       3.458696    -1.524535    -1.363963      82.99
 H       3.084555    -2.426737    -0.821013      24.60
 C       3.348723    -1.296199    -2.939759      97.72
 O       3.542639    -2.557443    -3.727413     296.34
 H       4.120281    -2.417249    -4.494288      31.38
 H       4.094850    -0.597315    -3.211781      24.71
 H       2.357426    -0.904176    -3.132869      27.25
 C      -0.629246    -0.600084    -0.079510      35.93
 H      -1.492555    -1.325331     0.033972      19.99
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 C      -0.070224     1.732140    -0.044825      91.70
 H      -0.424128     2.661075     0.240543      19.92
 C       1.303728     1.348047    -0.401985      15.15
 O       2.324750     2.297633    -0.465184     184.47
 C       2.095338     3.859054    -0.565542      83.33
 H       3.075449     3.901685    -1.452454      20.08
 H       1.243085     3.956633    -1.218370      27.03
 H       1.876224     4.396922     0.272891      26.98
 C       1.718435     0.002300    -0.598611      29.12
 O       3.047110    -0.205032    -0.844496     189.12
 C       0.623822    -0.985301    -0.506556      62.89
 H       0.714242    -1.947144    -0.900543      23.18
 C      -1.041625     0.736617     0.246507      69.41
 C      -2.431532     1.000573     0.791361      72.17
 H      -2.940774     0.028395     0.960328      24.82
 O      -2.343757     2.059601     1.726632     310.72
 H      -2.534835     1.780104     2.546113      32.27
 C      -3.366411     1.747812    -0.412459      77.08
 H      -2.812530     2.543929    -0.838269      27.53
 O      -3.563429     0.669887    -1.404488     209.17
 H      -3.565368     0.852230    -2.357466      25.04
 C      -4.749352     2.109678     0.158785      95.61
 O      -5.540532     2.631711    -1.040798     253.76
 H      -5.299416     3.585501    -1.248773      30.45
 H      -4.961641     2.952320     1.079826      25.09
 H      -5.504223     1.394522     0.610646      27.33
55
name = lig-etoh-Waterframe_691
 C       5.831553    -1.351023     1.389098      36.39
 H       6.069333    -0.274068     1.168288      21.89
 C       5.267855    -3.641367     0.707936      48.63
 H       5.172324    -4.325074    -0.103735      23.69
 C       5.573952    -4.137815     2.019213      -3.47
 O       5.779974    -5.543342     2.325331     213.32
 C       4.645545    -6.334660     2.016792     114.73
 H       3.688832    -5.752674     2.332142      25.43
 H       4.577542    -7.401425     2.492603      24.19
 H       4.532177    -6.728142     0.974116      26.82
 C       6.177263    -3.190125     2.969165      12.26
 O       6.648657    -3.579911     4.165665     220.73
 H       6.181329    -4.346751     4.571855      22.47
 C       6.390913    -1.900951     2.605686      50.36
 H       6.628743    -1.291326     3.427285      26.51
 C       5.399493    -2.245602     0.356347      11.36
 C       5.023630    -1.637395    -1.016535     110.82
 H       5.358748    -2.563595    -1.748738      22.35
 O       5.816599    -0.614000    -1.437599     283.95
 H       5.620552     0.183850    -0.782856      24.36
 C       3.585080    -1.402401    -1.351414      95.33
 H       2.969034    -2.186171    -0.907964      24.59
 C       3.345129    -1.290070    -2.904078     102.39
 O       3.480678    -2.520942    -3.751223     291.52
 H       4.232290    -2.207709    -4.290678      27.88
 H       3.932375    -0.509553    -3.228248      25.89
 H       2.367576    -0.994893    -3.100290      28.16
 C      -0.691141    -0.576567     0.034591      49.03
 H      -1.293525    -1.573523     0.081030      19.13
 C      -0.095667     1.809713    -0.079196      65.79
 H      -0.162798     2.917873     0.046236      17.11
 C       1.206147     1.372969    -0.314164      18.02
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 O       2.379922     2.257327    -0.430145     177.62
 C       2.046871     3.750521    -0.610216     108.97
 H       3.183146     4.262809    -0.836327      21.64
 H       1.207624     3.991270    -1.112495      29.35
 H       2.152608     4.145986     0.357781      27.05
 C       1.704607    -0.000891    -0.572026      14.03
 O       3.067180    -0.181160    -0.906200     194.79
 C       0.638941    -0.921400    -0.525574      68.09
 H       0.691652    -1.988128    -0.909154      21.11
 C      -1.004389     0.760040     0.234176      53.44
 C      -2.405375     0.954320     0.688088      85.60
 H      -2.881282     0.094167     1.122698      26.22
 O      -2.334356     2.132643     1.625941     287.87
 H      -2.225517     1.713163     2.449024      28.10
 C      -3.373313     1.656029    -0.435257      84.23
 H      -2.893881     2.657821    -0.759073      24.96
 O      -3.568207     0.600228    -1.391479     249.43
 H      -3.657287     0.918701    -2.249882      26.77
 C      -4.806915     2.192518     0.096144     106.35
 O      -5.563139     2.628350    -0.954175     296.54
 H      -5.320026     3.518050    -1.017731      33.20
 H      -4.898144     3.075675     0.902525      26.02
 H      -5.155148     1.279033     0.420054      30.40
55
name = lig-etoh-Waterframe_692
 C       5.829386    -1.329294     1.388258      48.96
 H       5.603614    -0.298212     1.260399      22.14
 C       5.272746    -3.672817     0.712054      34.65
 H       5.016847    -4.491811     0.001751      21.73
 C       5.544803    -4.132341     2.033441       9.08
 O       5.781003    -5.468575     2.366564     256.32
 C       4.605437    -6.363043     2.035391     110.66
 H       3.538176    -5.898795     2.246073      24.41
 H       4.821934    -7.159003     2.825629      24.32
 H       4.667095    -6.540086     1.089860      31.05
 C       6.132034    -3.234045     2.954968      -7.44
 O       6.678085    -3.621738     4.175111     295.16
 H       6.091803    -4.387702     4.535144      24.75
 C       6.353098    -1.864548     2.598158      44.39
 H       6.706897    -1.224083     3.469201      24.60
 C       5.443711    -2.204260     0.366271      17.60
 C       5.050604    -1.695784    -1.032203      99.22
 H       5.315614    -2.470450    -1.898540      21.83
 O       5.880329    -0.539652    -1.448612     240.28
 H       5.514329     0.335161    -0.956976      22.33
 C       3.587606    -1.383251    -1.403082      84.43
 H       2.911877    -2.157670    -1.126447      22.53
 C       3.296589    -1.304714    -2.901939      98.18
 O       3.451408    -2.449222    -3.762596     269.29
 H       4.410373    -2.601973    -3.995746      27.70
 H       3.934495    -0.506006    -3.354941      23.00
 H       2.241867    -1.028372    -2.880603      25.72
 C      -0.595020    -0.601561     0.054211      33.74
 H      -1.482013    -1.313303     0.331883      18.31
 C      -0.044586     1.820746    -0.076201      74.08
 H      -0.358942     2.979456    -0.059580      17.70
 C       1.294702     1.421862    -0.274626       8.14
 O       2.359782     2.259857    -0.421561     232.58
 C       2.117517     3.617210    -0.549492     120.04
 H       2.755759     4.225335    -1.011214      27.41
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 H       1.313209     3.938059    -1.210910      26.94
 H       1.804887     3.965108     0.629909      24.31
 C       1.592569     0.050199    -0.537639      17.49
 O       3.054748    -0.072196    -0.904094     135.57
 C       0.626610    -0.906555    -0.516398      74.54
 H       0.977039    -2.020923    -0.725547      19.43
 C      -1.025606     0.721257     0.187793      55.05
 C      -2.442643     1.120060     0.585725      99.70
 H      -2.775964     0.300878     1.176794      24.65
 O      -2.349940     2.168540     1.592206     272.26
 H      -1.748571     1.859883     2.279938      29.56
 C      -3.363910     1.575235    -0.401669      94.95
 H      -2.709042     2.352744    -1.063251      23.21
 O      -3.589131     0.539674    -1.403552     242.68
 H      -3.586822     1.029329    -2.131142      28.14
 C      -4.774294     2.164998     0.127352     104.39
 O      -5.634462     2.681302    -0.961505     321.23
 H      -5.522632     3.564163    -1.065770      34.85
 H      -4.343452     2.734938     0.809250      29.42
 H      -5.225204     1.241790     0.508932      29.54
55
name = lig-etoh-Waterframe_693
 C       5.841275    -1.347940     1.399351      40.83
 H       5.682274    -0.322922     1.349979      21.57
 C       5.297843    -3.618880     0.713538      56.39
 H       4.844991    -4.292172    -0.089240      18.58
 C       5.614471    -4.093024     1.995340      28.07
 O       5.695655    -5.411100     2.402462     293.04
 C       4.615853    -6.374061     2.104485     112.61
 H       3.629709    -5.860371     2.248793      27.32
 H       4.838211    -7.229671     2.737112      26.04
 H       4.785007    -6.723535     0.961115      28.27
 C       6.138425    -3.215769     2.956702      -4.52
 O       6.668199    -3.681393     4.197279     231.74
 H       6.220823    -4.594968     4.537667      25.25
 C       6.244331    -1.816778     2.630183      42.13
 H       6.844824    -1.045872     3.299556      21.92
 C       5.398951    -2.293501     0.388146      32.22
 C       5.103914    -1.716495    -1.075028      96.73
 H       5.376210    -2.545360    -1.688663      28.58
 O       5.954594    -0.464763    -1.453349     163.29
 H       5.564773     0.441806    -1.049071      21.72
 C       3.492516    -1.406305    -1.438318      60.01
 H       3.068868    -2.280777    -0.928033      21.63
 C       3.252932    -1.255748    -2.959163      92.66
 O       3.440547    -2.433825    -3.764326     277.20
 H       4.411213    -2.623936    -3.805987      28.49
 H       3.808185    -0.291518    -3.420918      22.82
 H       2.114181    -1.045961    -3.079728      24.39
 C      -0.606801    -0.600160     0.057998      35.90
 H      -1.319965    -1.420463     0.353292      19.10
 C      -0.020053     1.740878    -0.045263      82.32
 H      -0.570955     2.797963    -0.017372      18.43
 C       1.329245     1.459940    -0.268186      20.80
 O       2.405533     2.247345    -0.439965     220.48
 C       2.105836     3.610154    -0.448238      98.69
 H       2.978367     3.947285    -0.868366      24.34
 H       1.178138     3.518490    -1.232383      23.72
 H       1.523363     4.219511     0.466643      24.19
 C       1.644330     0.136197    -0.546278      15.60
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 O       2.991630     0.005860    -0.867957     105.99
 C       0.664816    -0.979302    -0.460175      59.66
 H       1.028754    -2.101392    -0.525363      18.56
 C      -0.975170     0.786180     0.093936      53.67
 C      -2.402781     1.203189     0.664610      73.17
 H      -2.931911     0.221836     0.969644      22.52
 O      -2.354167     2.242629     1.590840     296.10
 H      -1.553229     2.005191     2.112023      28.65
 C      -3.418565     1.567234    -0.537247      86.31
 H      -2.949270     2.462691    -1.077748      22.85
 O      -3.617183     0.465907    -1.437340     259.08
 H      -3.496736     0.713044    -2.273863      28.26
 C      -4.651943     2.071256     0.135648      99.47
 O      -5.685045     2.740511    -0.953200     255.39
 H      -5.485167     3.651959    -1.054209      32.92
 H      -4.426442     2.831111     0.886116      26.48
 H      -5.533067     1.594599     0.736562      25.52
55
name = lig-etoh-Waterframe_694
 C       5.811069    -1.386302     1.374933      56.48
 H       6.118031    -0.422018     1.069199      25.55
 C       5.283575    -3.617149     0.682193      43.75
 H       4.895571    -4.326804    -0.127110      18.60
 C       5.704930    -4.064610     1.966111       4.00
 O       5.602626    -5.401078     2.446338     271.56
 C       4.664912    -6.358377     2.127671     123.20
 H       3.676963    -6.029488     2.286649      28.97
 H       4.662690    -7.172246     2.760757      27.19
 H       4.621790    -6.958299     0.951643      25.45
 C       6.203671    -3.159821     3.031748      -1.91
 O       6.619590    -3.708348     4.189482     282.62
 H       6.180049    -4.672926     4.411114      26.11
 C       6.173112    -1.817804     2.710303      53.55
 H       6.655600    -1.048752     3.448130      19.96
 C       5.343921    -2.205309     0.374004      36.68
 C       5.113322    -1.623534    -1.089804     110.42
 H       5.487415    -2.296395    -1.734038      26.24
 O       6.001558    -0.478635    -1.454860     179.42
 H       5.596689     0.251714    -0.814827      24.34
 C       3.490280    -1.379321    -1.430101      63.19
 H       2.819199    -2.151428    -0.903449      21.81
 C       3.144570    -1.194851    -3.015259      85.60
 O       3.454221    -2.452463    -3.750997     268.51
 H       4.384287    -2.285532    -4.109950      25.95
 H       3.827160    -0.272024    -3.300059      22.09
 H       2.048524    -0.969395    -3.308746      24.09
 C      -0.625250    -0.606381     0.013937      27.60
 H      -1.227038    -1.426455     0.227580      19.29
 C      -0.006111     1.773799    -0.025454      87.64
 H      -0.168908     2.870398     0.153282      17.59
 C       1.305224     1.407766    -0.289865      15.35
 O       2.482121     2.243847    -0.389452     179.30
 C       2.021399     3.692479    -0.463117      91.58
 H       3.102644     4.287536    -0.493411      23.45
 H       1.346088     4.024702    -1.448600      24.20
 H       1.849403     4.047130     0.539487      27.38
 C       1.675125     0.046144    -0.564681      29.93
 O       2.992155    -0.048416    -0.857811     165.21
 C       0.757800    -0.941100    -0.340822      66.56
 H       0.922984    -2.026089    -0.418718      20.31
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 C      -1.010549     0.739064     0.090751      49.33
 C      -2.351499     1.157824     0.617518      67.76
 H      -2.832413     0.241123     1.221432      22.52
 O      -2.340986     2.335143     1.599222     227.67
 H      -1.626224     2.176783     2.300308      28.16
 C      -3.445205     1.611214    -0.653766      81.41
 H      -3.259559     2.460079    -1.181144      25.88
 O      -3.638243     0.379416    -1.475141     219.40
 H      -3.321590     0.488783    -2.309883      26.63
 C      -4.703197     2.123659     0.097756      77.02
 O      -5.674187     2.766462    -0.900293     242.95
 H      -5.240702     3.660377    -0.993794      29.86
 H      -4.465312     3.143830     0.686654      22.46
 H      -5.185661     1.099472     0.666134      24.81
55
name = lig-etoh-Waterframe_695
 C       5.832766    -1.358244     1.400821      48.45
 H       6.363735    -0.450936     1.060240      22.90
 C       5.257371    -3.622515     0.670879      30.03
 H       5.033813    -4.474579    -0.002701      21.21
 C       5.740112    -4.041323     1.942031       0.63
 O       5.597230    -5.374796     2.498536     209.26
 C       4.581282    -6.403418     2.113399     108.03
 H       3.606260    -6.003286     2.156249      27.03
 H       4.893893    -7.062227     2.912153      24.36
 H       4.913157    -6.631677     1.021398      24.51
 C       6.195800    -3.188129     2.999863      -7.87
 O       6.578024    -3.704582     4.215048     312.50
 H       5.957455    -4.576295     4.393459      23.44
 C       6.145120    -1.787292     2.757073      56.51
 H       6.322505    -1.088188     3.573871      21.19
 C       5.297615    -2.124191     0.320577      27.79
 C       5.075983    -1.548043    -1.113543     108.21
 H       5.302753    -2.318630    -1.889739      22.43
 O       5.983002    -0.505680    -1.406482     200.55
 H       5.977527     0.365384    -0.869886      23.69
 C       3.495195    -1.297247    -1.460789      87.56
 H       2.918628    -2.258936    -1.119052      19.69
 C       3.096791    -1.193157    -3.018957      99.35
 O       3.494888    -2.432583    -3.739887     281.72
 H       4.133055    -2.263809    -4.467390      28.92
 H       3.735860    -0.455408    -3.445739      23.37
 H       2.045673    -0.877342    -3.066941      24.21
 C      -0.587250    -0.615344    -0.053432      51.69
 H      -1.319988    -1.311986     0.053699      19.96
 C       0.039157     1.810178    -0.013082      47.76
 H      -0.109709     2.783777     0.309395      16.57
 C       1.349452     1.351583    -0.345783       1.88
 O       2.445343     2.312252    -0.344244     168.59
 C       2.087003     3.783616    -0.442548      95.81
 H       3.062941     4.598780    -0.591826      22.01
 H       1.429556     4.168583    -1.237872      26.25
 H       1.531411     3.857185     0.394125      27.19
 C       1.708139     0.001623    -0.546123      22.00
 O       3.081237    -0.170786    -0.865089     207.41
 C       0.733062    -0.954202    -0.208841      58.51
 H       1.015949    -1.931491    -0.357224      19.88
 C      -1.020578     0.718742     0.148762      30.66
 C      -2.388750     1.180710     0.533522      82.51
 H      -2.836503     0.396963     1.206266      20.22
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 O      -2.318974     2.393296     1.546493     195.91
 H      -1.967562     1.955457     2.465035      23.73
 C      -3.425751     1.621779    -0.663607      75.04
 H      -2.913241     2.216213    -1.427692      24.63
 O      -3.654137     0.334835    -1.485771     228.09
 H      -3.169743     0.567693    -2.239598      27.51
 C      -4.783984     2.188440    -0.007682     102.38
 O      -5.645030     2.752215    -0.832962     301.00
 H      -5.369956     3.753085    -1.156030      26.58
 H      -4.221341     2.699718     0.955632      22.86
 H      -5.149145     1.237908     0.515096      27.30
55
name = lig-etoh-Waterframe_696
 C       5.889524    -1.298599     1.413516      30.97
 H       6.011166    -0.143046     1.342355      23.01
 C       5.250714    -3.549255     0.673143      53.91
 H       4.946311    -4.242544    -0.077373      22.31
 C       5.690966    -4.069120     1.933730       6.77
 O       5.615294    -5.324477     2.535875     232.71
 C       4.582234    -6.367332     2.078475     116.34
 H       3.500581    -6.021831     2.089684      27.21
 H       4.751507    -7.370220     2.714436      25.52
 H       4.837121    -6.763230     1.209145      30.41
 C       6.144945    -3.171555     2.946836       3.31
 O       6.532898    -3.670169     4.232459     246.90
 H       6.020340    -4.462575     4.732146      22.64
 C       6.124505    -1.796961     2.734362      56.90
 H       6.243882    -1.135131     3.501641      20.25
 C       5.301821    -2.193920     0.347666       8.38
 C       4.994095    -1.542369    -1.134634      93.83
 H       5.287132    -2.493000    -1.839857      23.73
 O       5.993826    -0.501301    -1.388032     169.51
 H       5.704570     0.312582    -0.827535      24.89
 C       3.556061    -1.351084    -1.569987      91.65
 H       3.229523    -2.315704    -1.177728      23.16
 C       3.176434    -1.203236    -3.018152     117.25
 O       3.461095    -2.422641    -3.724066     294.31
 H       4.169690    -2.160233    -4.367224      27.95
 H       3.508631    -0.371364    -3.505715      26.64
 H       2.120440    -1.122716    -3.019447      26.45
 C      -0.647353    -0.585899    -0.057103      50.06
 H      -1.387109    -1.386744    -0.104375      20.46
 C       0.061592     1.702525     0.013519      61.81
 H      -0.252302     2.615115     0.288311      21.90
 C       1.400692     1.439520    -0.374731      15.00
 O       2.393361     2.400163    -0.353626     200.88
 C       2.107252     3.835265    -0.391012     102.48
 H       3.204442     4.231479    -0.288483      22.42
 H       1.595021     3.810570    -1.253757      27.54
 H       1.390901     4.252056     0.401251      25.40
 C       1.776779     0.027972    -0.493799      14.58
 O       3.104951    -0.205750    -0.796932     167.30
 C       0.769747    -1.032016    -0.175123      36.07
 H       1.003269    -2.034850    -0.203436      20.71
 C      -0.911237     0.818457     0.158718      22.78
 C      -2.482302     1.260830     0.513391      84.73
 H      -3.023689     0.445678     0.878131      23.98
 O      -2.291266     2.376297     1.461081     253.05
 H      -2.465513     1.746554     2.324857      22.59
 C      -3.373768     1.557747    -0.654019      78.66
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 H      -2.657815     2.298714    -1.293364      22.29
 O      -3.649001     0.348546    -1.461432     219.28
 H      -3.247623     0.435264    -2.350840      26.09
 C      -4.648326     2.124164    -0.016308     108.69
 O      -5.701650     2.793739    -0.845442     230.24
 H      -5.366757     3.872964    -1.038457      24.58
 H      -4.632866     2.804498     0.879896      25.11
 H      -5.352446     1.455823     0.222184      27.66
55
name = lig-etoh-Waterframe_697
 C       5.861008    -1.274225     1.390944      59.97
 H       5.490640    -0.192861     1.315887      22.49
 C       5.238777    -3.541600     0.668043      67.34
 H       4.781907    -4.061409    -0.118039      22.41
 C       5.606849    -4.065809     1.972826       7.77
 O       5.578847    -5.366500     2.523530     233.50
 C       4.656838    -6.320090     2.029320     115.11
 H       3.559253    -5.843205     2.115462      26.57
 H       4.567510    -7.188500     2.859626      25.40
 H       4.758330    -6.671614     1.013897      28.50
 C       6.075693    -3.198264     2.981982      10.10
 O       6.498480    -3.576747     4.230402     271.96
 H       6.012307    -4.323629     4.625589      25.12
 C       6.129318    -1.790668     2.657106      34.09
 H       6.409622    -1.185145     3.461981      21.96
 C       5.375249    -2.122637     0.430220     -12.18
 C       5.057996    -1.645304    -1.113826      64.24
 H       5.582502    -2.424507    -1.839761      22.77
 O       5.963104    -0.493273    -1.379333     162.68
 H       5.528533     0.266963    -0.909577      27.28
 C       3.634065    -1.430572    -1.565363      75.88
 H       3.005862    -2.232435    -1.294180      25.05
 C       3.197443    -1.203194    -3.033293     102.98
 O       3.437812    -2.429010    -3.753765     272.82
 H       4.395773    -2.454406    -4.081575      26.59
 H       3.527014    -0.233006    -3.474271      25.57
 H       2.109618    -1.220871    -2.981234      26.50
 C      -0.603427    -0.575305    -0.033406      33.92
 H      -1.482753    -1.347237    -0.029503      19.75
 C       0.130516     1.730824     0.046515      77.23
 H      -0.124130     2.768426     0.167596      22.83
 C       1.416305     1.458133    -0.343151      13.16
 O       2.384116     2.442960    -0.340293     216.83
 C       2.089414     3.829237    -0.375659     125.48
 H       3.020559     4.238124    -0.300964      25.92
 H       1.945688     4.236111    -1.473459      25.22
 H       1.662681     4.469069     0.594297      24.08
 C       1.762206     0.030990    -0.416246      22.50
 O       3.115303    -0.205685    -0.703286     126.87
 C       0.780980    -0.967859    -0.224231      66.15
 H       0.995333    -2.035248    -0.125729      22.89
 C      -0.993696     0.732243     0.132077      55.59
 C      -2.405979     1.237102     0.515814      95.88
 H      -2.834253     0.400365     1.030298      25.71
 O      -2.317175     2.299528     1.385424     246.33
 H      -2.531529     2.125447     2.430680      26.34
 C      -3.302444     1.574368    -0.697488      91.93
 H      -3.110009     2.563384    -1.353353      22.05
 O      -3.630395     0.380143    -1.417199     233.65
 H      -3.398697     0.538485    -2.416721      23.19
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 C      -4.646343     2.078189    -0.031672      72.21
 O      -5.731040     2.864053    -0.902574     223.34
 H      -5.304156     3.899224    -1.115111      25.63
 H      -4.389048     2.749527     0.717119      25.60
 H      -5.116170     1.037806     0.289739      26.52
55
name = lig-etoh-Waterframe_698
 C       5.747545    -1.225993     1.411234      39.33
 H       5.687240    -0.118584     1.205171      21.50
 C       5.233375    -3.535965     0.712509      55.57
 H       4.801919    -4.233912     0.003250      24.51
 C       5.509694    -4.064595     2.011672     -11.61
 O       5.572987    -5.407218     2.477521     288.24
 C       4.615900    -6.275791     1.994642     112.78
 H       3.637012    -5.707333     1.950072      26.87
 H       4.764566    -7.151281     2.696897      24.32
 H       4.944383    -6.586578     0.812713      26.44
 C       6.013839    -3.128537     2.982845       5.65
 O       6.462248    -3.470193     4.237474     267.24
 H       6.064672    -4.264367     4.516296      22.24
 C       6.170856    -1.806905     2.644635      52.78
 H       6.586667    -1.113151     3.431319      26.65
 C       5.401495    -2.141122     0.371885      18.85
 C       5.246776    -1.729262    -1.044796      88.86
 H       5.548268    -2.541884    -1.679432      25.73
 O       5.887909    -0.487594    -1.380827     209.24
 H       5.661894     0.353670    -0.970788      26.74
 C       3.597803    -1.452931    -1.454288      62.97
 H       2.963881    -2.310326    -1.179522      25.13
 C       3.186867    -1.212167    -3.015646      85.35
 O       3.441730    -2.453111    -3.815391     266.52
 H       4.418618    -2.492343    -4.082613      26.31
 H       3.823601    -0.341987    -3.553137      23.43
 H       2.073265    -0.932993    -2.983659      25.02
 C      -0.556110    -0.606180    -0.007572      35.54
 H      -1.283559    -1.520931     0.207873      19.50
 C       0.059884     1.777827     0.063053      87.59
 H      -0.081075     2.926623     0.129700      19.82
 C       1.389046     1.401503    -0.249034       7.41
 O       2.408602     2.433403    -0.332718     199.45
 C       2.188364     3.915509    -0.395944      92.47
 H       3.123267     4.287918    -0.257501      24.23
 H       1.521602     4.584199    -1.258990      24.14
 H       1.352680     3.952509     0.473136      22.84
 C       1.780638     0.048095    -0.380067      25.47
 O       3.161566    -0.233435    -0.627578     147.32
 C       0.750427    -0.869060    -0.282906      66.33
 H       1.151279    -1.960368    -0.291775      22.32
 C      -0.958060     0.734104     0.089243      58.60
 C      -2.286229     1.105922     0.507375      79.12
 H      -2.816435     0.249513     1.091159      23.86
 O      -2.341489     2.321694     1.349960     193.53
 H      -2.284957     1.962817     2.409172      24.76
 C      -3.375182     1.677272    -0.720832      78.27
 H      -2.845066     2.298287    -1.485371      23.95
 O      -3.589210     0.400418    -1.424657     175.89
 H      -3.426790     0.711168    -2.464101      22.17
 C      -4.720851     2.090500    -0.093366      92.20
 O      -5.674703     2.853357    -0.931874     318.40
 H      -5.285176     3.714254    -1.152072      32.18
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 H      -4.336257     2.588332     0.719274      27.58
 H      -5.119129     1.089476     0.546982      27.02
55
name = lig-etoh-Waterframe_699
 C       5.665848    -1.235411     1.427226      44.34
 H       6.158373    -0.302700     1.221925      20.97
 C       5.218273    -3.562935     0.771764      61.09
 H       5.068096    -4.354259    -0.030668      23.15
 C       5.464902    -4.014433     2.074191      23.44
 O       5.617026    -5.352228     2.438592     200.80
 C       4.538283    -6.285441     1.893309     118.88
 H       3.531379    -6.017685     1.893520      27.90
 H       4.478108    -7.179367     2.360371      26.99
 H       4.923765    -6.702334     0.795244      25.02
 C       5.969844    -3.078308     2.978738      24.49
 O       6.423496    -3.386545     4.259929     210.38
 H       6.147881    -4.201471     4.644701      21.92
 C       6.184853    -1.707369     2.625720       8.38
 H       6.687724    -1.034833     3.467476      23.35
 C       5.401809    -2.221775     0.379496       8.96
 C       5.241843    -1.707361    -1.028791      98.43
 H       5.596182    -2.400800    -1.680798      26.52
 O       5.876120    -0.492764    -1.421563     256.96
 H       5.520015     0.101095    -0.770612      27.44
 C       3.540322    -1.460022    -1.349392      65.42
 H       3.161159    -2.422239    -0.870040      22.72
 C       3.254331    -1.254389    -2.951297      88.29
 O       3.413029    -2.467959    -3.837849     273.21
 H       4.169052    -2.182371    -4.444892      25.49
 H       4.040764    -0.440170    -3.348864      21.99
 H       2.217639    -0.854333    -3.244984      24.08
 C      -0.545903    -0.615463     0.016675      44.57
 H      -1.174258    -1.517533     0.312244      18.76
 C       0.020121     1.776020     0.016322      55.62
 H      -0.517709     2.841543     0.204182      13.72
 C       1.397337     1.476596    -0.147060      20.95
 O       2.450338     2.385767    -0.379596     189.08
 C       2.174302     3.951149    -0.338876      85.89
 H       3.164890     4.474609    -0.091410      22.92
 H       1.647566     3.979285    -1.361079      23.79
 H       1.643133     4.164286     0.586464      28.40
 C       1.844317     0.104499    -0.389791      22.84
 O       3.207496    -0.283984    -0.569533     181.51
 C       0.819878    -0.892344    -0.335917      71.21
 H       1.069720    -2.035933    -0.559619      19.23
 C      -0.862606     0.775402     0.086127      52.95
 C      -2.362539     1.122671     0.473649      57.63
 H      -2.891582     0.113534     0.845132      22.07
 O      -2.339478     2.324983     1.371439     210.66
 H      -1.800225     1.832030     2.215799      23.06
 C      -3.394616     1.612870    -0.709055      87.22
 H      -2.794219     2.333387    -1.121840      26.09
 O      -3.564494     0.417498    -1.501276     224.44
 H      -3.343741     0.520352    -2.602925      20.90
 C      -4.724915     2.165104    -0.081997     104.86
 O      -5.601816     2.770044    -0.953619     304.98
 H      -5.307659     3.606986    -1.128877      33.88
 H      -4.667690     2.896311     0.800019      25.82
 H      -5.530750     1.370783     0.076466      25.03
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name = lig-etoh-Waterframe_700
 C       5.728264    -1.277668     1.385006      74.52
 H       6.016766    -0.378975     0.926591      24.16
 C       5.211551    -3.600421     0.767133      62.66
 H       5.242941    -4.366450    -0.096752      23.83
 C       5.468030    -3.955980     2.119476       5.78
 O       5.576972    -5.346214     2.396126     189.83
 C       4.511529    -6.330341     1.775404     109.20
 H       3.600861    -5.795231     1.803237      24.98
 H       4.557870    -7.098126     2.498875      25.13
 H       4.713067    -6.447960     0.726007      26.48
 C       5.960197    -2.998115     3.068548      20.00
 O       6.398087    -3.314917     4.303723     243.51
 H       5.992526    -4.160492     4.659165      24.88
 C       6.130508    -1.654072     2.657975      31.62
 H       6.683234    -0.903671     3.376971      22.83
 C       5.366299    -2.224313     0.456621       9.69
 C       5.085064    -1.693932    -1.101863      93.37
 H       5.444908    -2.412699    -1.848816      23.69
 O       5.881651    -0.482048    -1.417170     255.37
 H       5.642499     0.241865    -0.847324      26.01
 C       3.575455    -1.514925    -1.292864      75.82
 H       2.941249    -2.380280    -0.858022      20.52
 C       3.344054    -1.307317    -2.877241      98.23
 O       3.379325    -2.454022    -3.817265     298.88
 H       3.988408    -2.359588    -4.598728      27.16
 H       4.148125    -0.599509    -2.992981      21.86
 H       2.366889    -0.816160    -3.019107      25.19
 C      -0.447221    -0.591656     0.007832      10.75
 H      -1.251219    -1.259394     0.136800      18.00
 C       0.083632     1.814039    -0.040994      96.65
 H      -0.388478     2.894792     0.093111      15.15
 C       1.481626     1.556281    -0.126286       2.06
 O       2.509547     2.396796    -0.390762     229.65
 C       2.149766     3.845968    -0.256031     123.18
 H       3.214187     4.484429    -0.515010      23.21
 H       1.785183     4.126315    -1.169246      29.03
 H       1.655748     4.304102     0.463326      31.54
 C       1.826245     0.107209    -0.392358      23.70
 O       3.229694    -0.294240    -0.528338     166.66
 C       0.882157    -0.930540    -0.366006      46.63
 H       1.115051    -2.007195    -0.668104      17.27
 C      -0.973173     0.692631     0.135023      55.11
 C      -2.452075     1.191494     0.419571      97.99
 H      -2.845695     0.337336     1.036429      20.45
 O      -2.331705     2.243547     1.416851     231.00
 H      -1.569503     2.100731     2.175148      25.55
 C      -3.325259     1.528988    -0.640496      99.78
 H      -3.079290     2.475049    -1.140791      21.61
 O      -3.578983     0.418035    -1.596909     256.06
 H      -3.113253     0.887197    -2.549114      17.54
 C      -4.754314     2.152062    -0.029176      84.83
 O      -5.580079     2.751662    -1.087615     277.51
 H      -5.323146     3.729195    -1.286202      29.15
 H      -4.494401     2.834374     0.966364      24.21
 H      -5.090036     1.239116     0.388622      28.77
55
name = lig-etoh-Waterframe_701
 C       5.854459    -1.282441     1.305194      35.09
 H       5.702218    -0.272449     1.025823      25.97
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 C       5.246419    -3.571374     0.775503      55.19
 H       5.063248    -4.404733     0.031055      23.15
 C       5.495389    -3.963834     2.094991       3.45
 O       5.500386    -5.369808     2.366298     148.73
 C       4.520523    -6.245970     1.706409     112.59
 H       3.543396    -5.660768     1.833957      23.85
 H       4.665865    -7.217125     2.396541      24.06
 H       4.738862    -6.562931     0.769838      28.10
 C       5.933162    -2.930709     3.131386      10.44
 O       6.379992    -3.273122     4.405242     170.28
 H       5.911711    -4.158272     4.736591      23.20
 C       6.066862    -1.612356     2.710082      50.21
 H       6.498357    -0.839319     3.363500      20.67
 C       5.281603    -2.224812     0.368710      16.98
 C       5.002914    -1.712027    -1.052329      89.54
 H       5.294034    -2.572075    -1.835425      24.71
 O       5.865088    -0.487985    -1.398403     159.60
 H       5.641805     0.357225    -1.065467      27.32
 C       3.575967    -1.559051    -1.296205      82.16
 H       2.981727    -2.436220    -0.943384      24.22
 C       3.415058    -1.304877    -2.797832     109.09
 O       3.326364    -2.454161    -3.750234     280.04
 H       4.225502    -2.349751    -4.215009      25.56
 H       4.154628    -0.728534    -3.179111      25.83
 H       2.511632    -0.763287    -2.830899      28.05
 C      -0.459350    -0.587739    -0.022455      29.02
 H      -1.048131    -1.429997    -0.124085      18.89
 C       0.098815     1.781413    -0.051393      82.59
 H       0.035236     2.851303    -0.214088      13.57
 C       1.494307     1.453587    -0.198053       3.50
 O       2.560972     2.463390    -0.340810     218.82
 C       2.199753     3.788458    -0.314376      93.12
 H       3.357788     4.253766    -0.297037      20.02
 H       1.452842     4.187785    -1.001996      27.62
 H       1.658873     3.968866     0.702280      27.11
 C       1.859479     0.081086    -0.375220      26.55
 O       3.212058    -0.257819    -0.519165     132.15
 C       0.890020    -0.904661    -0.365698      54.68
 H       1.190047    -1.908718    -0.555932      20.19
 C      -0.930009     0.762214     0.130035      65.41
 C      -2.360736     1.117504     0.554392      74.60
 H      -2.934682     0.344272     0.965181      25.09
 O      -2.347991     2.228646     1.451377     218.36
 H      -1.553988     1.805865     2.067030      22.89
 C      -3.406492     1.594720    -0.668204      69.90
 H      -2.907116     2.385570    -1.465278      17.75
 O      -3.579728     0.470721    -1.644953     208.62
 H      -3.201489     0.777822    -2.672245      18.83
 C      -4.715215     2.039799    -0.010487      90.20
 O      -5.566117     2.711637    -1.186241     199.07
 H      -5.066686     3.741188    -1.231833      25.49
 H      -4.371339     2.954938     0.682328      23.84
 H      -5.251783     1.298755     0.594648      28.19
55
name = lig-etoh-Waterframe_702
 C       5.872929    -1.295123     1.278330      58.09
 H       5.793127    -0.218683     1.204319      26.18
 C       5.259048    -3.540283     0.770316      56.57
 H       4.809682    -4.288895     0.147516      22.55
 C       5.556293    -3.951780     2.102052      12.41
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 O       5.457774    -5.353042     2.372251     189.61
 C       4.532551    -6.139368     1.693553     132.57
 H       3.355720    -5.970317     1.670136      24.75
 H       4.380433    -7.238577     2.223469      25.02
 H       4.859388    -6.420660     0.657658      26.51
 C       5.898215    -2.997720     3.142543     -15.01
 O       6.337806    -3.237178     4.492418     227.54
 H       6.009170    -4.175778     4.989532      19.22
 C       6.019832    -1.571513     2.664311      27.63
 H       6.200304    -0.886295     3.399041      22.86
 C       5.317384    -2.178837     0.356011      27.37
 C       5.057413    -1.725327    -0.962141      80.53
 H       5.498695    -2.530032    -1.718679      23.37
 O       5.829603    -0.553536    -1.400344     161.08
 H       5.307196     0.113096    -1.017634      31.11
 C       3.535060    -1.510555    -1.309075      86.25
 H       3.060221    -2.387363    -0.964314      26.76
 C       3.389890    -1.241474    -2.798357     111.11
 O       3.306445    -2.453812    -3.640474     278.14
 H       4.221515    -2.608448    -4.045973      26.91
 H       4.207819    -0.649879    -3.184308      26.16
 H       2.488551    -0.704180    -3.030817      27.29
 C      -0.497110    -0.584826    -0.097368      42.44
 H      -1.173566    -1.442988    -0.056049      19.02
 C       0.176293     1.748006    -0.065935      60.67
 H      -0.206532     2.684029    -0.167460      19.12
 C       1.499179     1.373679    -0.306761      21.35
 O       2.559541     2.363095    -0.317847     201.48
 C       2.241077     3.828798    -0.274169      92.77
 H       3.030308     4.574090    -0.374798      23.43
 H       1.402574     4.063041    -1.129180      23.46
 H       1.996604     3.890518     0.913365      23.07
 C       1.931950     0.061356    -0.357628      36.19
 O       3.212805    -0.253775    -0.552447     196.29
 C       0.845060    -0.869998    -0.330121      69.58
 H       1.059351    -1.855825    -0.385115      22.80
 C      -0.833204     0.807425     0.107275     100.94
 C      -2.311900     1.056293     0.578619      59.14
 H      -2.683712     0.081740     0.888428      25.39
 O      -2.329062     2.215254     1.503279     250.75
 H      -1.972687     1.943242     2.500925      25.25
 C      -3.423230     1.579572    -0.761899      61.43
 H      -2.787561     2.608044    -0.991672      19.10
 O      -3.599482     0.515336    -1.637494     279.87
 H      -3.343879     0.745450    -2.564681      22.91
 C      -4.674925     2.042151    -0.106625     116.13
 O      -5.520192     2.629269    -1.181649     212.81
 H      -5.206719     3.736608    -1.379106      27.78
 H      -4.521007     2.870235     0.525962      28.24
 H      -5.513909     1.434972     0.292644      27.27
55
name = lig-etoh-Waterframe_703
 C       5.823450    -1.216793     1.382929      60.61
 H       6.106387    -0.283911     0.846816      19.51
 C       5.232823    -3.504295     0.790181      68.40
 H       4.773661    -4.110852     0.079442      23.93
 C       5.591258    -3.948197     2.114029       4.38
 O       5.434672    -5.291498     2.447411     171.48
 C       4.465895    -6.153471     1.622165     103.47
 H       3.531474    -5.493860     1.559192      25.84
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 H       4.650554    -7.062532     2.272203      24.76
 H       4.943640    -6.087003     0.537869      25.85
 C       5.917606    -3.019188     3.144711       9.66
 O       6.270920    -3.195689     4.516870     239.17
 H       5.805718    -4.098869     4.881284      19.73
 C       5.981392    -1.700939     2.667424      57.36
 H       6.041071    -0.916104     3.343840      23.66
 C       5.448635    -2.195261     0.470743      16.43
 C       5.103381    -1.752852    -1.049770     100.81
 H       5.388400    -2.618268    -1.649128      25.40
 O       5.773138    -0.608312    -1.385641     224.54
 H       5.446260     0.173583    -0.978710      25.56
 C       3.560127    -1.452550    -1.303083      90.79
 H       2.880069    -2.182966    -0.985238      26.38
 C       3.321235    -1.164558    -2.884710      95.29
 O       3.310843    -2.479148    -3.514216     277.66
 H       4.050547    -2.551814    -4.210000      26.68
 H       4.273658    -0.495130    -3.033198      23.58
 H       2.357172    -0.620252    -3.126157      25.28
 C      -0.521212    -0.535548    -0.161129      30.72
 H      -1.392310    -1.194118     0.142671      19.06
 C       0.192542     1.757079    -0.090472      66.35
 H      -0.132203     2.709125     0.137092      20.90
 C       1.557970     1.445129    -0.377857      14.09
 O       2.584806     2.257462    -0.342516     167.16
 C       2.253630     3.817301    -0.167526      97.45
 H       3.005463     4.245829    -0.631957      26.50
 H       1.344947     4.054622    -0.987372      25.24
 H       1.760706     4.355059     0.717249      25.64
 C       1.856718     0.008536    -0.370720      24.07
 O       3.280483    -0.289208    -0.598395     183.01
 C       0.842950    -0.924608    -0.288175      71.65
 H       1.034589    -1.946444    -0.304208      22.83
 C      -0.831812     0.740974     0.079515      52.38
 C      -2.270738     1.084261     0.498208      74.10
 H      -2.544596     0.143625     1.117527      20.53
 O      -2.314639     2.177478     1.562162     251.66
 H      -2.525111     1.687010     2.454724      26.01
 C      -3.285027     1.534818    -0.656848      92.48
 H      -2.912882     2.402215    -1.224787      25.27
 O      -3.624908     0.541382    -1.642162     274.83
 H      -3.261204     0.799282    -2.404744      28.32
 C      -4.726284     2.126063    -0.211149     112.38
 O      -5.507047     2.587241    -1.212204     270.82
 H      -5.221821     3.644433    -1.384551      27.53
 H      -4.529288     2.637979     0.635419      30.20
 H      -5.084294     1.075013     0.204189      28.58
55
name = lig-etoh-Waterframe_704
 C       5.786950    -1.208668     1.428069      38.32
 H       6.211109    -0.254468     1.036847      17.97
 C       5.216949    -3.510221     0.870705      62.52
 H       4.941347    -4.154923     0.080549      26.17
 C       5.566458    -3.987769     2.117252      16.63
 O       5.402877    -5.258067     2.543535     182.78
 C       4.499361    -6.053534     1.576639     114.25
 H       3.525305    -5.603571     1.657520      27.46
 H       4.333548    -7.012704     1.938542      28.51
 H       4.888116    -6.378244     0.497235      26.58
 C       5.957298    -3.025173     3.142778      19.60
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 O       6.170902    -3.178546     4.478805     192.21
 H       5.767516    -4.005246     4.889143      20.66
 C       5.975226    -1.695405     2.771929      36.00
 H       6.233185    -1.024654     3.658254      20.21
 C       5.506571    -2.168948     0.427130       9.58
 C       5.056060    -1.847651    -1.045231      97.73
 H       5.329739    -2.513606    -1.780368      27.38
 O       5.795139    -0.597511    -1.422800     153.97
 H       5.649118     0.142242    -0.841084      24.05
 C       3.570661    -1.451362    -1.368106      79.20
 H       2.919530    -2.315937    -1.089898      25.26
 C       3.300141    -1.129738    -2.875222      90.49
 O       3.336869    -2.505167    -3.445174     267.91
 H       3.811321    -2.250730    -4.276259      27.48
 H       4.108109    -0.515671    -3.548248      23.06
 H       2.273224    -0.615323    -3.027722      23.58
 C      -0.527728    -0.578327    -0.162045      49.23
 H      -1.259679    -1.469182    -0.003231      18.25
 C       0.172328     1.786152    -0.097023      56.44
 H       0.156097     2.790379     0.346074      15.48
 C       1.495511     1.383640    -0.365309       5.89
 O       2.638310     2.310171    -0.340698     179.36
 C       2.235963     3.759932    -0.185621      95.91
 H       3.281305     4.024614    -0.553134      22.03
 H       1.388887     3.856030    -0.889402      28.15
 H       2.148835     4.052578     0.868483      27.69
 C       1.841497     0.003682    -0.448809      15.91
 O       3.273849    -0.253725    -0.584013     156.94
 C       0.827826    -1.034386    -0.268962      42.67
 H       1.117710    -2.127549    -0.272869      19.16
 C      -0.840417     0.828923     0.016118      49.78
 C      -2.247314     1.153514     0.481077      76.47
 H      -2.860916     0.211043     0.881381      19.81
 O      -2.315955     2.127538     1.576698     278.89
 H      -2.500301     1.451681     2.280664      23.09
 C      -3.178496     1.599434    -0.592032      87.65
 H      -2.623343     2.132988    -1.205095      25.80
 O      -3.626729     0.526996    -1.642641     197.70
 H      -3.112511     0.669603    -2.422627      27.22
 C      -4.647748     2.037053    -0.158137      82.53
 O      -5.526208     2.612166    -1.290098     258.41
 H      -5.189955     3.525822    -1.411726      30.43
 H      -4.736432     2.799546     0.738474      25.56
 H      -5.205651     1.015134     0.061907      27.16
55
name = lig-etoh-Waterframe_705
 C       5.811510    -1.271883     1.461501      33.47
 H       5.827593    -0.143313     1.373643      25.23
 C       5.248496    -3.500403     0.861001      61.95
 H       5.062101    -4.346960     0.186786      23.84
 C       5.539724    -3.951891     2.193370      25.44
 O       5.325004    -5.329633     2.585047     236.47
 C       4.524145    -6.002074     1.610471     126.57
 H       3.594315    -5.549532     1.407906      29.33
 H       4.275827    -6.892400     2.039736      28.52
 H       5.032616    -6.000754     0.606221      27.31
 C       5.940896    -3.018730     3.114146     -11.28
 O       6.077160    -3.216159     4.474808     147.18
 H       5.812897    -4.055264     4.813814      25.45
 C       6.006040    -1.582836     2.819692      10.34
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 H       6.449013    -0.960289     3.734182      14.25
 C       5.431408    -2.186179     0.387972      32.79
 C       5.041206    -1.800814    -1.027556      95.33
 H       5.380062    -2.574628    -1.711973      26.34
 O       5.862626    -0.591516    -1.486100      81.55
 H       5.682677    -0.029285    -0.737282      30.68
 C       3.590832    -1.431777    -1.407775      72.72
 H       2.943766    -2.382055    -1.211462      25.69
 C       3.292106    -1.167226    -2.848475     105.08
 O       3.351232    -2.497214    -3.451675     280.13
 H       3.744238    -2.537793    -4.360723      28.51
 H       3.960544    -0.448592    -3.432886      24.33
 H       2.235430    -0.816742    -2.850988      25.07
 C      -0.475467    -0.638438    -0.130859      64.97
 H      -1.324429    -1.399157    -0.182862      19.59
 C       0.193950     1.810536    -0.066625      82.31
 H      -0.100643     2.881698     0.320303      16.64
 C       1.496475     1.319124    -0.318620      -1.53
 O       2.608891     2.309181    -0.333186     205.16
 C       2.321185     3.640155    -0.231061     112.00
 H       3.119392     4.677678    -0.474409      22.93
 H       1.551411     4.077600    -0.703641      29.17
 H       2.233315     3.692741     0.819606      28.31
 C       1.859055    -0.037552    -0.522488      44.08
 O       3.188827    -0.225642    -0.553213     177.23
 C       0.834715    -1.030483    -0.296143      40.26
 H       1.067822    -2.200756    -0.261509      19.44
 C      -0.862173     0.837322    -0.037126     111.95
 C      -2.290146     1.157985     0.500492      69.28
 H      -2.617899     0.115959     0.642389      25.87
 O      -2.321470     2.066437     1.586399     320.60
 H      -1.972206     1.753244     2.407328      30.01
 C      -3.194348     1.692893    -0.711763      79.21
 H      -2.588771     2.622658    -1.144720      22.18
 O      -3.575635     0.505406    -1.582418     210.09
 H      -3.076587     0.564169    -2.491182      22.85
 C      -4.584218     1.969357    -0.137460      90.30
 O      -5.488550     2.629179    -1.316029     229.42
 H      -5.172620     3.434274    -1.474096      35.73
 H      -4.765346     2.849736     0.699011      25.04
 H      -5.251488     1.170110     0.150598      28.28
55
name = lig-etoh-Waterframe_706
 C       5.811622    -1.252020     1.478523      33.19
 H       5.500921    -0.226509     1.192174      22.44
 C       5.324009    -3.542610     0.832578      55.78
 H       4.985371    -4.255215    -0.015694      20.29
 C       5.487156    -3.927686     2.210656     -15.02
 O       5.252059    -5.319413     2.622392     195.14
 C       4.507399    -5.991223     1.626266     125.71
 H       3.683705    -5.331453     1.318387      25.99
 H       4.435766    -7.048829     2.068384      25.77
 H       5.199057    -6.151926     0.857855      29.32
 C       5.891434    -2.918854     3.197682      29.59
 O       6.017633    -3.272861     4.497507     186.91
 H       5.662072    -4.178315     4.733178      22.10
 C       6.077166    -1.620316     2.786782      71.05
 H       6.307493    -0.664188     3.398047      22.15
 C       5.327975    -2.181549     0.481505     -18.50
 C       5.100174    -1.674796    -1.069844      92.45
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 H       5.320659    -2.691112    -1.591935      25.29
 O       5.918630    -0.615918    -1.507611     174.35
 H       5.858852     0.212582    -0.984283      28.08
 C       3.615925    -1.411548    -1.341541      91.83
 H       2.946056    -2.250323    -0.948583      25.53
 C       3.270911    -1.212356    -2.863303     117.21
 O       3.344446    -2.514531    -3.512316     286.78
 H       3.983563    -2.398102    -4.285587      27.64
 H       3.892070    -0.441088    -3.122655      27.70
 H       2.259686    -0.920255    -2.939789      28.10
 C      -0.488371    -0.555948    -0.120580      30.91
 H      -1.298801    -1.275947    -0.073475      17.58
 C       0.168293     1.732629    -0.021936     127.92
 H      -0.144632     2.897343    -0.024144      18.54
 C       1.524576     1.393434    -0.282450      18.92
 O       2.593480     2.182077    -0.400036     247.19
 C       2.359511     3.674755    -0.153017      87.80
 H       3.433633     4.110576    -0.715100      20.58
 H       1.448692     3.978716    -0.720125      27.89
 H       1.993077     3.978002     0.849216      28.04
 C       1.797738    -0.031589    -0.505397      58.92
 O       3.168344    -0.288396    -0.573112     218.67
 C       0.860974    -0.997927    -0.354248      50.12
 H       1.106680    -2.152450    -0.386404      18.22
 C      -0.823088     0.735281    -0.031857      63.17
 C      -2.287964     1.098842     0.425007      64.40
 H      -2.749053     0.252247     0.854575      23.52
 O      -2.334340     2.044766     1.588051     297.45
 H      -1.625880     1.749206     2.081085      32.03
 C      -3.265920     1.695031    -0.757147      76.26
 H      -3.159797     2.805248    -1.394267      19.02
 O      -3.456117     0.521512    -1.515541     228.64
 H      -3.105511     0.706040    -2.569516      18.25
 C      -4.641953     2.063594    -0.210203      99.05
 O      -5.416151     2.602328    -1.285539     280.02
 H      -5.096902     3.493141    -1.429710      33.57
 H      -4.271060     2.680535     0.723962      25.98
 H      -4.922324     1.159881     0.179440      31.83
55
name = lig-etoh-Waterframe_707
 C       5.712873    -1.227971     1.409200      55.05
 H       5.779677    -0.153309     1.184184      21.30
 C       5.362103    -3.567188     0.831876      61.79
 H       5.046128    -4.278046    -0.023955      21.94
 C       5.444109    -3.911948     2.185881       9.97
 O       5.211819    -5.185181     2.693004     129.98
 C       4.543071    -6.046751     1.613039     112.03
 H       3.504061    -5.599303     1.293003      24.50
 H       3.963725    -7.061934     2.091994      24.88
 H       5.131707    -6.371806     0.785410      27.40
 C       5.809335    -2.935475     3.247936     -25.60
 O       5.997500    -3.297746     4.546136     237.01
 H       5.438831    -4.182448     4.919149      16.75
 C       6.143719    -1.601306     2.734958      47.64
 H       6.227476    -0.865836     3.557581      23.84
 C       5.306436    -2.128082     0.531605      34.59
 C       5.118511    -1.640269    -0.987907      82.53
 H       5.464085    -2.421164    -1.822281      23.18
 O       6.002016    -0.609910    -1.531487     186.06
 H       5.710692     0.274344    -1.163392      26.65
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 C       3.574403    -1.446934    -1.277471      93.59
 H       3.288576    -2.417279    -0.864687      26.33
 C       3.228776    -1.257738    -2.818010     113.97
 O       3.374106    -2.516686    -3.625638     270.57
 H       4.148081    -2.323280    -4.210312      27.01
 H       3.907272    -0.619780    -3.295147      26.59
 H       2.261644    -0.847421    -3.024839      27.48
 C      -0.495950    -0.620696    -0.139943      14.34
 H      -1.191203    -1.363677     0.091699      17.05
 C       0.176509     1.699677    -0.029260      70.34
 H      -0.165168     2.802062    -0.116221      17.75
 C       1.465577     1.362020    -0.262489      25.42
 O       2.609301     2.148158    -0.439208     200.91
 C       2.373245     3.671391    -0.148458     114.56
 H       3.338484     3.894446    -0.370607      23.59
 H       1.689370     3.838168    -1.078449      23.05
 H       2.391442     4.030657     0.962158      26.55
 C       1.802754     0.036507    -0.433818      38.33
 O       3.187000    -0.310284    -0.596933     211.53
 C       0.798743    -0.977574    -0.410744      52.66
 H       1.108020    -2.033971    -0.567324      18.68
 C      -0.867968     0.750189     0.052844     115.43
 C      -2.304352     1.135601     0.338020      65.57
 H      -2.911394     0.277634     0.634367      23.58
 O      -2.314029     2.058319     1.510896     249.89
 H      -1.763244     1.641120     2.126457      28.23
 C      -3.311352     1.671481    -0.728289      79.34
 H      -2.659846     2.273347    -1.457472      20.63
 O      -3.336357     0.507274    -1.531122     209.44
 H      -3.085896     0.769675    -2.626974      19.16
 C      -4.613227     2.126940    -0.200869     110.11
 O      -5.385018     2.600698    -1.251172     282.18
 H      -5.141087     3.663005    -1.380748      27.73
 H      -4.600750     2.912996     0.537782      26.79
 H      -5.216377     1.226504     0.166420      28.30
55
name = lig-etoh-Waterframe_708
 C       5.688480    -1.146900     1.488581      34.90
 H       6.143008    -0.201337     1.162926      19.98
 C       5.333525    -3.484154     0.832009      74.76
 H       5.265100    -4.366871     0.158260      23.84
 C       5.429077    -3.863348     2.206762      26.14
 O       5.140794    -5.128266     2.685690     100.40
 C       4.495013    -6.127994     1.663886     100.55
 H       3.693019    -5.485884     1.090639      23.45
 H       4.228926    -6.913572     2.525995      23.47
 H       5.243813    -6.391949     0.841113      25.70
 C       5.755200    -2.951608     3.173056      11.19
 O       5.986933    -3.267443     4.586516     186.35
 H       5.594390    -4.206469     5.004111      17.98
 C       6.099012    -1.637974     2.767942      34.29
 H       6.462804    -1.014000     3.522825      23.77
 C       5.346804    -2.163434     0.404468      11.80
 C       5.122055    -1.673974    -0.957883      86.58
 H       5.396622    -2.623865    -1.529034      23.63
 O       6.049736    -0.550603    -1.515954     150.98
 H       5.645512     0.303678    -1.147974      24.93
 C       3.590727    -1.542092    -1.292527      78.41
 H       3.072228    -2.430648    -0.958233      25.31
 C       3.226289    -1.331145    -2.797476      96.78
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 O       3.402180    -2.503318    -3.722942     265.98
 H       4.117909    -2.450220    -4.416405      25.69
 H       3.978089    -0.557580    -3.225454      23.26
 H       2.170422    -0.926366    -2.858159      24.69
 C      -0.572825    -0.689567    -0.119646      52.43
 H      -1.221053    -1.511201     0.011024      18.40
 C       0.093507     1.745749    -0.058897      27.28
 H      -0.091027     2.789137     0.104835      15.78
 C       1.500156     1.311719    -0.261643      18.73
 O       2.598064     2.208733    -0.415558     243.27
 C       2.486668     3.582970    -0.232719     119.94
 H       3.376187     4.145679    -0.359136      24.27
 H       1.790842     4.426553    -0.779695      24.47
 H       2.030775     3.708808     0.875897      25.35
 C       1.837810    -0.053295    -0.387908      34.13
 O       3.167148    -0.259903    -0.579006     193.39
 C       0.803251    -0.961474    -0.468253      85.64
 H       1.000081    -1.951043    -0.668418      22.09
 C      -0.912411     0.748564     0.097358      56.95
 C      -2.363234     1.173573     0.390012      70.33
 H      -2.714798     0.083301     0.549592      20.76
 O      -2.279354     2.087195     1.423622     306.59
 H      -2.305278     1.623152     2.266719      24.96
 C      -3.126603     1.646257    -0.739862      83.72
 H      -2.683154     2.532687    -1.088609      24.55
 O      -3.292903     0.417669    -1.602802     224.97
 H      -2.973038     0.754486    -2.640978      19.42
 C      -4.604150     2.174744    -0.131010      88.98
 O      -5.439136     2.661109    -1.303285     259.37
 H      -5.072701     3.780016    -1.519046      25.01
 H      -4.596093     2.921459     0.564868      26.59
 H      -5.327548     1.372210     0.356591      26.54
55
name = lig-etoh-Waterframe_709
 C       5.752165    -1.180689     1.521488      62.56
 H       6.125355    -0.227283     1.198218      24.61
 C       5.286523    -3.442064     0.834665      52.71
 H       5.304320    -4.175928     0.071812      23.78
 C       5.377793    -3.848169     2.189974      10.23
 O       5.060326    -5.147331     2.618178     274.14
 C       4.500612    -6.106379     1.784809     140.06
 H       3.618992    -5.776734     1.182674      24.47
 H       4.176367    -6.942759     2.343400      27.78
 H       5.347252    -6.674902     1.212580      27.82
 C       5.767499    -2.948136     3.246726       7.50
 O       5.979321    -3.197788     4.554798     150.98
 H       5.633740    -4.132485     4.728682      22.43
 C       5.991882    -1.637669     2.812077      55.64
 H       6.655810    -1.057654     3.362455      24.18
 C       5.455772    -2.063763     0.459367       0.79
 C       5.137717    -1.756684    -1.046231      82.11
 H       5.446685    -2.551812    -1.640036      23.86
 O       6.005861    -0.539741    -1.458105     170.16
 H       5.796035     0.336223    -0.927266      23.05
 C       3.625056    -1.583855    -1.324205      74.12
 H       2.949465    -2.281135    -0.843710      22.61
 C       3.297857    -1.383281    -2.845451      94.04
 O       3.392941    -2.496676    -3.776569     277.41
 H       4.083599    -2.253406    -4.442674      24.87
 H       3.789644    -0.296531    -3.016092      22.42
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 H       2.158029    -1.231243    -2.802987      24.56
 C      -0.589154    -0.623909    -0.101657      24.39
 H      -1.352210    -1.396274    -0.197141      18.24
 C       0.115498     1.727239    -0.075686      48.51
 H      -0.128032     2.662060     0.205290      16.25
 C       1.457674     1.368936    -0.252861      14.63
 O       2.584959     2.218840    -0.436424     232.57
 C       2.514672     3.619908    -0.211749      86.21
 H       3.742000     4.157582    -0.210339      20.01
 H       1.766761     4.011256    -0.995390      23.90
 H       2.091008     3.702464     0.799170      25.92
 C       1.830454    -0.082543    -0.383853      15.10
 O       3.194832    -0.285651    -0.590559     168.53
 C       0.745423    -1.034819    -0.479832      94.06
 H       0.945479    -2.003217    -0.716071      21.70
 C      -0.901293     0.664736     0.072256      55.20
 C      -2.282531     1.041620     0.487497      76.14
 H      -2.997896     0.280904     1.077913      19.19
 O      -2.285725     2.163369     1.431396     281.64
 H      -2.652219     1.741963     2.212153      24.00
 C      -3.089719     1.639924    -0.763805      77.72
 H      -2.823444     2.544321    -1.217275      21.69
 O      -3.265001     0.404699    -1.668062     252.81
 H      -2.899932     0.577966    -2.631241      20.99
 C      -4.625480     2.225887    -0.178313      72.23
 O      -5.480592     2.724333    -1.336703     293.20
 H      -5.026148     3.734691    -1.530772      26.94
 H      -4.182068     2.933777     0.530914      25.40
 H      -4.985640     1.286136     0.334737      27.64
55
name = lig-etoh-Waterframe_710
 C       5.872467    -1.186192     1.490371      61.22
 H       5.972715    -0.145786     1.411253      22.22
 C       5.265101    -3.400432     0.841333      76.92
 H       5.009144    -4.022404     0.041870      24.66
 C       5.296887    -3.856814     2.175501      14.98
 O       5.015282    -5.136792     2.616220     241.95
 C       4.485774    -6.192564     1.846782     127.09
 H       3.715342    -5.924145     1.202565      30.95
 H       3.994841    -6.792101     2.499059      28.44
 H       5.227802    -6.613800     1.108589      27.16
 C       5.754594    -2.914371     3.235636       0.91
 O       5.971065    -3.181554     4.548502     185.85
 H       5.653136    -4.018623     4.906129      22.29
 C       5.946619    -1.584302     2.862047      55.68
 H       6.490690    -0.911349     3.578700      24.41
 C       5.500959    -2.063171     0.498764      31.71
 C       5.213808    -1.746340    -1.067670      94.07
 H       5.598006    -2.410236    -1.789005      26.81
 O       5.918296    -0.580348    -1.411836     227.47
 H       5.714782     0.069356    -0.616612      27.95
 C       3.647649    -1.564375    -1.328659      80.86
 H       3.273209    -2.538465    -0.865214      23.09
 C       3.267884    -1.381280    -2.835111      96.21
 O       3.400056    -2.470795    -3.802612     259.24
 H       4.215373    -2.424980    -4.443808      25.20
 H       3.729807    -0.521430    -3.450277      22.44
 H       2.161473    -1.194915    -2.856028      25.68
 C      -0.539842    -0.669599    -0.164300      33.99
 H      -1.489777    -1.282282    -0.198843      16.37
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 C       0.121496     1.671834    -0.036162      59.40
 H      -0.220154     2.629229     0.120352      17.04
 C       1.472329     1.352050    -0.273710      16.50
 O       2.585918     2.152005    -0.465445     219.61
 C       2.453719     3.694942    -0.155571     104.66
 H       3.750597     3.866255    -0.348228      19.84
 H       2.104746     4.012837    -1.036878      25.42
 H       2.236922     4.118349     0.737617      27.79
 C       1.755449    -0.049482    -0.433381      47.52
 O       3.229351    -0.360570    -0.641311     193.54
 C       0.742937    -1.073575    -0.446207      70.92
 H       0.877427    -2.126770    -0.692364      20.14
 C      -0.852900     0.688980     0.089174      60.88
 C      -2.274284     1.040767     0.533355      57.16
 H      -2.817656     0.106081     0.976532      22.06
 O      -2.295393     2.259475     1.469154     251.05
 H      -2.445061     2.034540     2.413887      27.62
 C      -3.202315     1.562714    -0.785000      78.95
 H      -2.405112     2.151393    -1.429599      20.40
 O      -3.256084     0.443042    -1.690652     264.58
 H      -2.904258     0.730616    -2.511275      26.04
 C      -4.530224     2.205350    -0.349599     109.21
 O      -5.473792     2.756206    -1.293366     321.99
 H      -5.286856     3.621225    -1.468472      34.66
 H      -4.318512     3.147752     0.398488      22.85
 H      -5.201408     1.506998     0.172489      27.02
55
name = lig-etoh-Waterframe_711
 C       5.986538    -1.122254     1.524470      34.05
 H       6.029741    -0.114143     1.271372      19.26
 C       5.214615    -3.420321     0.854593      62.50
 H       4.677385    -4.094994     0.196119      19.96
 C       5.251991    -3.823872     2.204580      24.42
 O       5.006947    -5.105463     2.680934     186.88
 C       4.404442    -6.288128     1.810949      93.25
 H       3.692643    -5.787845     1.229948      28.90
 H       4.106612    -6.910862     2.748520      25.08
 H       5.211459    -6.805856     1.300027      26.65
 C       5.688490    -2.905865     3.147952       7.35
 O       5.966343    -3.210138     4.596802     227.90
 H       5.537403    -4.000636     4.886683      24.58
 C       5.971009    -1.530729     2.868079      45.61
 H       5.885712    -0.804316     3.797554      22.35
 C       5.512946    -2.120850     0.414379      10.00
 C       5.258674    -1.709984    -1.003629     104.28
 H       5.565119    -2.673824    -1.612186      26.93
 O       5.872566    -0.560239    -1.376654     232.98
 H       5.706533     0.240729    -0.700855      26.41
 C       3.707299    -1.577680    -1.353117      80.03
 H       3.211288    -2.581121    -1.111090      23.52
 C       3.201875    -1.355998    -2.888850     105.12
 O       3.386970    -2.506328    -3.782830     274.39
 H       4.209625    -2.374523    -4.396581      25.60
 H       3.808674    -0.532113    -3.195328      24.87
 H       2.186120    -1.046131    -2.833830      25.56
 C      -0.568882    -0.693239    -0.220764      57.66
 H      -1.285079    -1.601829    -0.120395      17.16
 C       0.143678     1.686256     0.025655      47.28
 H      -0.088824     2.780504     0.037056      15.97
 C       1.506560     1.248623    -0.315283      12.22
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 O       2.566749     2.159942    -0.429973     195.47
 C       2.487450     3.678058    -0.214354     113.66
 H       3.505882     4.043719    -0.328692      24.13
 H       2.000921     4.362136    -0.923304      25.21
 H       2.060023     4.057639     0.727805      26.22
 C       1.789937    -0.104761    -0.530955      33.60
 O       3.183324    -0.421825    -0.672150     214.00
 C       0.797835    -1.076179    -0.419393      38.20
 H       1.111044    -2.194995    -0.595747      16.74
 C      -0.854076     0.693962     0.136773      43.97
 C      -2.338728     1.153089     0.545838      76.57
 H      -2.585492     0.240512     0.930734      21.78
 O      -2.306731     2.316978     1.480361     283.60
 H      -1.919756     1.846279     2.331798      24.84
 C      -3.182183     1.483752    -0.794071      69.74
 H      -2.396853     2.443111    -1.076424      19.16
 O      -3.307686     0.435499    -1.689422     298.43
 H      -3.084577     0.696159    -2.523650      26.14
 C      -4.470621     2.204450    -0.465107     101.13
 O      -5.489076     2.748242    -1.305618     313.63
 H      -5.188498     3.667327    -1.486217      30.92
 H      -4.201785     3.019354     0.410239      23.42
 H      -5.026305     1.516702     0.142890      27.49
55
name = lig-etoh-Waterframe_712
 C       6.003268    -1.167851     1.456841      66.70
 H       6.308118    -0.224070     1.104784      24.23
 C       5.112633    -3.449943     0.856299      56.14
 H       4.657613    -4.210859     0.140002      22.58
 C       5.240745    -3.826382     2.225474      -4.59
 O       4.995200    -5.132533     2.734498     224.80
 C       4.380407    -6.258266     1.861266     106.88
 H       3.434901    -6.038387     1.230609      25.36
 H       3.850662    -7.173460     2.616756      24.07
 H       5.131383    -6.785834     1.300788      27.95
 C       5.675686    -2.868799     3.253924      -7.48
 O       5.924814    -3.242129     4.563251     311.11
 H       5.455890    -4.047052     4.717364      28.09
 C       5.955702    -1.522227     2.833249      46.20
 H       5.773751    -0.751394     3.689758      21.30
 C       5.567498    -2.099488     0.515739      37.46
 C       5.178831    -1.735691    -0.943884      83.22
 H       5.729032    -2.540913    -1.688210      22.19
 O       5.925741    -0.461343    -1.391244     179.77
 H       5.564902     0.389005    -0.855363      22.85
 C       3.675651    -1.648365    -1.435502      77.89
 H       3.100450    -2.465544    -0.972370      23.10
 C       3.247077    -1.318900    -2.909694     109.02
 O       3.345362    -2.542003    -3.723514     281.12
 H       3.903858    -2.301168    -4.539775      25.97
 H       3.783888    -0.476285    -3.177242      25.61
 H       2.210357    -1.095709    -2.911566      24.95
 C      -0.549874    -0.673757    -0.203204      24.11
 H      -1.266391    -1.538656    -0.032262      18.60
 C       0.246826     1.646380     0.043749      70.24
 H       0.060245     2.811755     0.200988      16.77
 C       1.472460     1.253952    -0.339127      19.53
 O       2.573298     2.223721    -0.400403     203.24
 C       2.502914     3.649169    -0.277727     107.46
 H       3.359632     4.046048    -0.247434      25.87
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 H       1.602709     4.067350    -1.022530      22.89
 H       2.096474     3.527336     0.870476      22.94
 C       1.880267    -0.183658    -0.608090      36.39
 O       3.147434    -0.460499    -0.673561     195.34
 C       0.805084    -1.069571    -0.427529      39.30
 H       1.138059    -2.221320    -0.418305      17.83
 C      -0.911252     0.671385     0.146751      54.20
 C      -2.347052     1.205138     0.518249      85.92
 H      -2.955211     0.529590     1.124786      20.93
 O      -2.306521     2.302805     1.475732     268.68
 H      -1.583811     1.903818     2.122798      26.71
 C      -3.063876     1.585874    -0.776319      85.67
 H      -2.623409     2.353828    -1.458881      22.84
 O      -3.371552     0.377681    -1.668452     208.08
 H      -3.158796     0.610891    -2.603698      22.48
 C      -4.489904     2.165368    -0.367780      87.35
 O      -5.489741     2.738512    -1.388881     249.57
 H      -5.055602     3.727240    -1.665194      27.37
 H      -4.079880     2.973149     0.213265      24.90
 H      -4.917137     1.321986     0.142012      28.26
55
name = lig-etoh-Waterframe_713
 C       5.993387    -1.238710     1.421849      49.64
 H       6.449155    -0.319108     1.054190      23.58
 C       5.044336    -3.428788     0.941351      67.88
 H       4.874376    -4.092887     0.006056      23.89
 C       5.233553    -3.867414     2.247049      -3.58
 O       4.949604    -5.196381     2.755963     269.84
 C       4.359381    -6.205177     1.947013     101.62
 H       3.452295    -5.791830     1.248763      24.61
 H       3.957161    -6.972475     2.801329      23.21
 H       5.083898    -6.507549     1.210582      26.07
 C       5.673785    -2.833392     3.279992       5.53
 O       5.854687    -3.280440     4.529001     264.29
 H       5.482941    -4.140278     4.808469      26.12
 C       5.907310    -1.544731     2.828344      67.56
 H       6.356959    -0.728113     3.414273      25.24
 C       5.493912    -2.174518     0.539416      38.19
 C       5.190493    -1.678654    -0.986738      84.73
 H       5.702455    -2.404624    -1.698568      22.29
 O       5.960592    -0.406443    -1.403691     206.95
 H       5.437241     0.354263    -0.896290      22.70
 C       3.605622    -1.674226    -1.421113      82.00
 H       3.167239    -2.620746    -1.127501      22.77
 C       3.310071    -1.334266    -2.895014      98.46
 O       3.307085    -2.545638    -3.692896     281.52
 H       3.776572    -2.495727    -4.557398      28.30
 H       3.881698    -0.597528    -3.481992      22.98
 H       2.239960    -0.998971    -2.870585      23.70
 C      -0.532634    -0.635267    -0.114818      33.90
 H      -1.372394    -1.303958    -0.043809      17.22
 C       0.195535     1.563619     0.063904     102.32
 H       0.059364     2.671855     0.496881      16.78
 C       1.575916     1.275742    -0.388905       9.06
 O       2.634025     2.168066    -0.434724     234.09
 C       2.364681     3.551719    -0.223490     103.39
 H       3.386444     4.126162    -0.519231      21.95
 H       1.637314     3.994379    -1.148968      23.40
 H       2.106745     4.157986     0.827578      23.01
 C       1.805401    -0.118220    -0.598352      43.29
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 O       3.219322    -0.492574    -0.683600     182.20
 C       0.799186    -1.076904    -0.454451      63.59
 H       0.810324    -2.204002    -0.394764      19.32
 C      -0.872704     0.677119     0.130229      32.54
 C      -2.287263     1.193548     0.475617      52.87
 H      -3.140365     0.310603     0.712012      17.19
 O      -2.264215     2.300732     1.436911     256.94
 H      -1.632200     2.199957     2.266290      25.27
 C      -3.094442     1.694685    -0.883588      80.57
 H      -2.514916     2.180405    -1.533182      24.42
 O      -3.414441     0.336325    -1.589422     196.32
 H      -3.041293     0.620070    -2.539035      21.37
 C      -4.493249     2.179307    -0.287552      94.51
 O      -5.411622     2.680399    -1.452119     224.17
 H      -5.221355     3.808687    -1.561532      24.72
 H      -4.566539     2.940321     0.378883      26.17
 H      -5.211351     1.442192     0.206948      26.37
55
name = lig-etoh-Waterframe_714
 C       5.961202    -1.304630     1.444455      40.29
 H       6.382045    -0.319958     1.110350      22.45
 C       5.014821    -3.457971     0.978619      56.55
 H       4.735545    -4.299943     0.250453      20.43
 C       5.206151    -3.898940     2.320916      21.51
 O       4.941392    -5.160427     2.806927     287.01
 C       4.322877    -6.121526     1.981758     123.56
 H       3.410833    -5.574655     1.603207      26.59
 H       4.111154    -6.912516     2.575182      26.20
 H       5.018428    -6.649646     1.276016      26.28
 C       5.603152    -2.941088     3.190277     -11.90
 O       5.805616    -3.296935     4.574998     187.70
 H       5.347811    -4.202140     4.733593      23.38
 C       5.960693    -1.525280     2.813974      65.25
 H       6.678407    -1.105054     3.442589      26.64
 C       5.357612    -2.159588     0.414780      31.43
 C       5.267677    -1.652855    -1.075399      99.61
 H       5.607178    -2.400538    -1.661957      25.80
 O       5.927195    -0.427244    -1.377521     316.67
 H       5.613253     0.434371    -0.884984      23.72
 C       3.677536    -1.617942    -1.385222      81.52
 H       3.223154    -2.572221    -1.180145      23.75
 C       3.328942    -1.375945    -2.914937      84.38
 O       3.257394    -2.589515    -3.703311     278.32
 H       3.977011    -2.342411    -4.331996      25.40
 H       4.222867    -0.656831    -3.272428      21.78
 H       2.357525    -0.749017    -2.941919      24.96
 C      -0.545043    -0.668287    -0.053938      44.04
 H      -1.289829    -1.393642    -0.042677      18.50
 C       0.261908     1.598565     0.073168      60.30
 H      -0.065235     2.595075     0.501355      15.37
 C       1.553054     1.252953    -0.378603      13.29
 O       2.684071     2.084875    -0.439960     199.12
 C       2.268178     3.586149    -0.243994      75.41
 H       3.345943     4.021122    -0.825538      19.39
 H       1.420456     3.798455    -0.924000      24.92
 H       1.993001     3.937915     0.781087      24.45
 C       1.827362    -0.097563    -0.570822      20.65
 O       3.213730    -0.486722    -0.670607     200.10
 C       0.700260    -1.071667    -0.447917      54.40
 H       1.032767    -2.050042    -0.658271      19.75
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 C      -0.820170     0.720213     0.119979      59.80
 C      -2.236646     1.196563     0.379999      66.89
 H      -2.576859     0.097001     0.776438      19.45
 O      -2.235659     2.310375     1.363341     257.04
 H      -1.903516     1.834856     2.283821      24.05
 C      -3.191326     1.667493    -0.868172      85.26
 H      -2.653658     2.418571    -1.431019      23.78
 O      -3.423631     0.377731    -1.495119     213.66
 H      -3.178228     0.282791    -2.544656      20.56
 C      -4.560507     2.277498    -0.335909      94.81
 O      -5.314098     2.617939    -1.479188     247.66
 H      -5.099850     3.708622    -1.513798      25.35
 H      -4.543224     2.974156     0.549725      26.13
 H      -4.964238     1.203754     0.029725      26.65
55
name = lig-etoh-Waterframe_715
 C       5.883814    -1.326444     1.389458      54.94
 H       6.304269    -0.314725     1.072805      22.23
 C       4.988994    -3.517480     0.899013      49.73
 H       4.463870    -4.296564     0.383776      18.21
 C       5.134432    -3.877784     2.279802       0.32
 O       4.978971    -5.112676     2.897623     281.78
 C       4.255200    -6.073215     2.002142     145.75
 H       3.308606    -5.829337     1.627571      30.11
 H       3.966820    -6.854729     2.576045      28.24
 H       4.874280    -6.361510     1.067791      31.18
 C       5.597900    -2.935367     3.280233       3.01
 O       5.752271    -3.286054     4.577670     219.70
 H       5.289101    -4.206276     4.888511      21.22
 C       6.053340    -1.708689     2.807266      63.16
 H       6.597295    -1.184070     3.569276      24.28
 C       5.293248    -2.128980     0.429401      36.78
 C       5.241723    -1.684039    -1.099983     111.78
 H       5.721502    -2.350283    -1.776637      26.50
 O       5.914896    -0.465330    -1.362069     312.66
 H       5.643215     0.225615    -0.658443      25.52
 C       3.757622    -1.567906    -1.430903      85.95
 H       3.347943    -2.420797    -0.867199      20.94
 C       3.382777    -1.362044    -2.878730      90.26
 O       3.245071    -2.599337    -3.734543     264.09
 H       3.954061    -2.607671    -4.473252      26.03
 H       4.340295    -0.803971    -3.305413      20.72
 H       2.475035    -0.752229    -3.159682      24.41
 C      -0.597742    -0.696363    -0.046624      35.92
 H      -1.344171    -1.439646     0.103941      16.49
 C       0.312887     1.709313     0.077350      55.67
 H       0.167552     2.729957     0.198086      15.68
 C       1.565303     1.219413    -0.310368       5.53
 O       2.664308     2.086597    -0.408904     211.60
 C       2.228054     3.542015    -0.351844      92.79
 H       3.076735     4.416225    -0.558784      21.94
 H       1.378665     3.645504    -0.763229      31.43
 H       2.188433     3.523427     0.613554      29.54
 C       1.822284    -0.204414    -0.542873      26.55
 O       3.151579    -0.431928    -0.625054     215.32
 C       0.779752    -1.049082    -0.464629      60.02
 H       0.952787    -2.023989    -0.767316      19.47
 C      -0.762972     0.731626     0.080317      59.95
 C      -2.195034     1.207452     0.319718      96.78
 H      -2.768656     0.583288     0.920406      20.76
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 O      -2.210284     2.276727     1.305177     243.51
 H      -2.361614     1.673942     2.185405      21.47
 C      -3.192332     1.615241    -0.743991      88.16
 H      -2.850206     2.475346    -1.541183      19.59
 O      -3.454400     0.407842    -1.431818     238.40
 H      -3.166931     0.649941    -2.500509      17.11
 C      -4.573441     2.203270    -0.368871      92.31
 O      -5.252553     2.631343    -1.517338     276.30
 H      -5.111915     3.554174    -1.902430      30.41
 H      -4.250066     3.111269     0.338729      24.60
 H      -5.171566     1.329414     0.138407      27.28
55
name = lig-etoh-Waterframe_716
 C       5.842696    -1.334496     1.418349      46.88
 H       6.235395    -0.322377     1.132313      22.51
 C       4.932567    -3.540127     0.848061      68.63
 H       4.455063    -4.029139     0.070249      21.40
 C       5.084157    -3.804340     2.243270       2.35
 O       4.950586    -5.117246     2.897426     200.43
 C       4.180919    -6.043957     2.039163     107.64
 H       3.262341    -5.573653     1.774443      27.76
 H       4.124390    -7.038023     2.743643      24.13
 H       4.863263    -6.147658     1.125503      26.85
 C       5.592171    -2.955211     3.315111      11.17
 O       5.705266    -3.264247     4.621871     212.51
 H       5.319339    -4.249063     4.915321      17.71
 C       6.160105    -1.835623     2.749377      52.81
 H       6.374703    -0.922363     3.353122      21.89
 C       5.286826    -2.215787     0.471925      20.65
 C       5.182383    -1.712851    -1.040479      84.29
 H       5.681257    -2.545001    -1.744714      23.28
 O       5.934265    -0.481286    -1.336890     273.66
 H       5.635441     0.166311    -0.619269      25.03
 C       3.703343    -1.559250    -1.415214      78.02
 H       3.180154    -2.557514    -1.138222      21.90
 C       3.482575    -1.350930    -2.953341      94.47
 O       3.247839    -2.597897    -3.738052     265.92
 H       3.867480    -2.449156    -4.560402      23.76
 H       4.241278    -0.775028    -3.471316      23.88
 H       2.553554    -0.785043    -2.949916      25.29
 C      -0.517614    -0.625201    -0.102768      35.69
 H      -1.395050    -1.263411     0.148380      16.25
 C       0.299331     1.708685     0.030071      86.31
 H       0.090492     2.678351     0.056530      16.79
 C       1.608601     1.215348    -0.222669      -4.96
 O       2.650189     2.118225    -0.431655     230.56
 C       2.230145     3.467275    -0.362459      97.61
 H       2.934074     4.145403    -0.800580      24.43
 H       1.324236     3.752447    -0.957214      25.58
 H       2.031762     3.758552     0.793144      25.70
 C       1.823637    -0.161763    -0.485927      30.00
 O       3.184244    -0.398873    -0.613837     180.55
 C       0.756655    -1.159636    -0.472171      60.29
 H       0.830558    -2.210168    -0.625076      19.86
 C      -0.771565     0.722563     0.048598      75.09
 C      -2.218382     1.230187     0.391751      69.79
 H      -2.786699     0.319338     0.648266      21.41
 O      -2.173272     2.281314     1.304913     275.45
 H      -2.492705     2.096287     2.302978      25.71
 C      -3.175403     1.599221    -0.706793      74.91
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 H      -2.570567     2.310910    -1.491985      18.14
 O      -3.481983     0.389501    -1.461086     192.25
 H      -3.258741     0.734692    -2.533042      16.95
 C      -4.519382     2.149472    -0.307753     111.30
 O      -5.256216     2.633454    -1.613782     232.76
 H      -4.887131     3.530482    -1.634755      30.66
 H      -4.488308     3.171205     0.286108      25.41
 H      -5.285452     1.805549     0.209133      29.85
55
name = lig-etoh-Waterframe_717
 C       5.853927    -1.407156     1.459536      57.50
 H       6.106745    -0.388075     1.213340      21.68
 C       4.873293    -3.500501     0.857705      61.23
 H       4.592344    -4.235344     0.120636      22.86
 C       5.041715    -3.881028     2.295340      18.87
 O       4.883367    -5.101942     2.827254     279.34
 C       4.153308    -5.994648     2.096973     121.62
 H       3.080049    -5.609265     2.017234      24.74
 H       4.120337    -7.213282     2.586029      23.34
 H       4.551167    -6.300800     1.117166      26.49
 C       5.601607    -3.002180     3.221762     -11.60
 O       5.662591    -3.249400     4.685186     185.93
 H       5.337899    -4.250702     4.806480      17.64
 C       6.210604    -1.745409     2.704936      38.36
 H       6.597618    -0.966664     3.486631      22.74
 C       5.328017    -2.239653     0.463856      42.00
 C       5.137183    -1.742590    -0.931157      81.86
 H       5.477845    -2.664572    -1.656622      22.97
 O       5.939039    -0.534399    -1.287707     252.28
 H       5.672412     0.306898    -0.820479      25.16
 C       3.636110    -1.573929    -1.418685      72.71
 H       2.927123    -2.445810    -1.372669      24.67
 C       3.505024    -1.305131    -3.018356     105.15
 O       3.255290    -2.560334    -3.724856     280.36
 H       3.946403    -2.518608    -4.508332      22.78
 H       4.259961    -0.733392    -3.376808      27.50
 H       2.606230    -0.749213    -3.051557      27.15
 C      -0.459020    -0.586135    -0.171409      48.14
 H      -1.342316    -1.332333    -0.079333      19.75
 C       0.239658     1.623280    -0.045126      77.03
 H      -0.063961     2.594701     0.121025      19.30
 C       1.578557     1.236424    -0.169536       8.83
 O       2.645030     2.119877    -0.458640     190.77
 C       2.242588     3.485841    -0.354923     100.31
 H       3.082427     3.778295    -0.765028      25.09
 H       1.356998     3.618016    -1.266047      23.22
 H       1.871571     4.188322     0.645711      24.59
 C       1.846496    -0.158346    -0.428307       5.24
 O       3.255980    -0.422915    -0.646541     154.52
 C       0.739606    -1.194314    -0.442443      55.78
 H       1.015389    -2.271059    -0.440338      22.16
 C      -0.802155     0.798765     0.040426      38.17
 C      -2.250797     1.130121     0.506333      65.53
 H      -2.486856     0.076000     0.980004      22.04
 O      -2.140648     2.355419     1.356904     260.92
 H      -2.359856     2.016810     2.356182      25.02
 C      -3.157489     1.563661    -0.767134      78.29
 H      -2.646551     2.401806    -1.261848      23.28
 O      -3.487536     0.362918    -1.530566     228.44
 H      -3.438222     0.407293    -2.620083      20.52
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 C      -4.544157     2.271059    -0.295900      88.96
 O      -5.215244     2.626716    -1.637045     233.42
 H      -5.115589     3.571905    -1.680621      31.89
 H      -4.294135     3.165598     0.281747      27.53
 H      -5.110809     1.455849     0.267205      28.94
55
name = lig-etoh-Waterframe_718
 C       5.926498    -1.369276     1.408407      47.76
 H       6.099255    -0.400197     1.039409      25.03
 C       4.853415    -3.526090     0.966272      80.93
 H       4.610731    -4.419280     0.337041      24.03
 C       5.037875    -3.879031     2.256619       3.42
 O       4.836276    -5.136542     2.802683     268.75
 C       4.026588    -6.071113     2.074557     135.60
 H       2.872690    -5.895278     2.089592      26.18
 H       4.144502    -6.934638     2.867276      26.43
 H       4.281074    -6.122571     1.056719      29.88
 C       5.687712    -2.945234     3.231472      -9.28
 O       5.627622    -3.231242     4.622260      61.32
 H       5.357480    -4.135474     4.989905      15.84
 C       6.150633    -1.751340     2.837741      54.11
 H       6.920665    -1.207228     3.507592      21.65
 C       5.325340    -2.246187     0.494823      41.45
 C       5.078591    -1.778905    -0.927668      91.83
 H       5.630238    -2.461809    -1.601048      24.66
 O       5.934216    -0.637881    -1.247166     234.44
 H       5.508487     0.179337    -0.902504      27.49
 C       3.612570    -1.565512    -1.474531      91.54
 H       3.052361    -2.392788    -1.050751      24.26
 C       3.466247    -1.228677    -2.989252     106.20
 O       3.282149    -2.507480    -3.713539     289.96
 H       3.926344    -2.577963    -4.441863      27.53
 H       4.406885    -0.804610    -3.293218      25.56
 H       2.649243    -0.584485    -3.330231      25.07
 C      -0.542523    -0.626106    -0.223770      37.31
 H      -1.355593    -1.423922    -0.259819      20.06
 C       0.213278     1.689586    -0.077435     127.60
 H       0.110872     2.777705     0.217811      13.64
 C       1.562782     1.171100    -0.223388      11.37
 O       2.595921     2.077720    -0.397388     163.71
 C       2.291451     3.595312    -0.482943      70.14
 H       3.286880     4.205467    -0.614404      24.82
 H       1.417970     3.770700    -1.347028      23.24
 H       2.006250     3.742386     0.656064      26.42
 C       1.899232    -0.206051    -0.394111      29.57
 O       3.241207    -0.436239    -0.671380     212.83
 C       0.881984    -1.059375    -0.386502      61.94
 H       0.964253    -2.209330    -0.385046      20.49
 C      -0.869547     0.690418     0.032128      43.72
 C      -2.224426     1.066389     0.538500      82.10
 H      -2.778730     0.566321     1.399591      20.24
 O      -2.142603     2.378751     1.421518     209.20
 H      -1.981293     1.918220     2.385078      23.88
 C      -3.185823     1.528479    -0.763709      82.42
 H      -2.597156     2.128583    -1.334667      27.63
 O      -3.488387     0.331797    -1.572135     257.39
 H      -3.295338     0.758681    -2.514012      22.06
 C      -4.524611     2.340727    -0.377705     105.35
 O      -5.159015     2.650670    -1.579628     302.51
 H      -5.319263     3.518068    -1.696490      33.67
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 H      -4.307920     3.092683     0.294442      29.40
 H      -5.061914     1.365499     0.163876      27.26
55
name = lig-etoh-Waterframe_719
 C       6.007058    -1.336531     1.426150      47.40
 H       6.423609    -0.422252     1.073178      25.05
 C       4.870392    -3.551780     0.993255      56.87
 H       4.363300    -4.174526     0.173541      17.93
 C       5.098475    -3.832376     2.352011      18.24
 O       4.783533    -5.167037     2.792950     223.01
 C       3.855381    -6.178224     2.094286     119.00
 H       2.829482    -5.769911     2.211813      25.49
 H       4.122037    -7.036929     2.479268      27.48
 H       4.227232    -6.354121     1.080965      27.45
 C       5.667183    -3.006564     3.295671       6.32
 O       5.624455    -3.204066     4.563531     158.22
 H       5.304669    -4.103353     4.711929      18.91
 C       6.130954    -1.702914     2.833399      47.87
 H       6.801154    -1.148312     3.526613      24.07
 C       5.261898    -2.245024     0.567084      18.80
 C       5.108254    -1.839634    -1.033777      98.92
 H       5.411464    -2.655591    -1.570052      27.62
 O       5.918273    -0.712974    -1.219633     259.54
 H       5.450598     0.071581    -0.891032      28.13
 C       3.605169    -1.567066    -1.449968      87.13
 H       3.110849    -2.505125    -1.233977      23.86
 C       3.458368    -1.209897    -2.959422      94.96
 O       3.293750    -2.458690    -3.689000     271.63
 H       3.900307    -2.249343    -4.466230      24.38
 H       4.522086    -0.771561    -3.244960      23.21
 H       2.661296    -0.380433    -3.154412      23.77
 C      -0.538408    -0.727036    -0.272137      32.00
 H      -1.317132    -1.494039    -0.241129      20.68
 C       0.219795     1.650769    -0.057162      66.82
 H       0.023547     2.819700     0.178752      15.77
 C       1.484844     1.227057    -0.329546      17.04
 O       2.600864     2.090453    -0.353782     186.85
 C       2.339456     3.601237    -0.541736     108.94
 H       3.368512     4.346604    -0.695807      22.58
 H       1.690938     4.006446    -1.258374      28.26
 H       1.876870     3.864480     0.310707      28.52
 C       1.960078    -0.141310    -0.392084      24.83
 O       3.221713    -0.408937    -0.671213     208.14
 C       0.830136    -1.018844    -0.324313      59.56
 H       1.137184    -2.127624    -0.559383      19.07
 C      -0.884835     0.611326     0.055395      48.99
 C      -2.295543     1.189410     0.551251      74.64
 H      -2.875028     0.237753     0.951840      19.86
 O      -2.138522     2.348298     1.458174     276.25
 H      -1.613568     2.032340     2.324410      26.67
 C      -3.162733     1.499967    -0.691117      87.88
 H      -2.476678     2.019771    -1.340650      23.76
 O      -3.488190     0.341119    -1.586898     232.49
 H      -3.247127     0.594056    -2.525216      24.44
 C      -4.419775     2.252928    -0.406253     123.48
 O      -5.150628     2.718008    -1.571468     303.32
 H      -5.089982     3.626155    -1.436579      31.00
 H      -4.323357     3.094268     0.224960      27.14
 H      -5.353650     1.871589     0.151613      25.92
55
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name = lig-etoh-Waterframe_720
 C       6.036920    -1.376657     1.475439      60.40
 H       6.662835    -0.550492     1.136945      23.81
 C       4.903769    -3.457212     0.978791      49.46
 H       4.190948    -4.117701     0.388784      17.62
 C       5.076859    -3.969885     2.366238       8.83
 O       4.727242    -5.229683     2.808591     318.72
 C       3.780827    -6.178798     2.124630     132.98
 H       2.727330    -5.930654     2.267899      27.46
 H       3.883835    -7.150666     2.584586      26.26
 H       3.923041    -6.268482     0.968647      26.60
 C       5.632045    -2.926865     3.229653       2.14
 O       5.635125    -3.233999     4.641206     232.19
 H       5.264384    -4.079221     4.845965      22.62
 C       6.141204    -1.686191     2.765097      78.17
 H       6.417154    -0.980401     3.472655      24.30
 C       5.236821    -2.197487     0.558495      35.86
 C       5.103758    -1.934620    -1.009141      93.42
 H       5.378406    -2.768040    -1.650482      26.01
 O       5.936702    -0.750818    -1.252059     220.63
 H       5.502726    -0.013368    -0.804280      28.17
 C       3.633734    -1.588816    -1.415228      89.48
 H       2.899136    -2.399449    -1.359844      24.42
 C       3.508204    -1.197105    -2.888486      94.05
 O       3.296973    -2.378415    -3.689461     256.89
 H       3.833838    -2.381237    -4.605327      23.34
 H       4.422988    -0.553091    -3.317713      23.59
 H       2.545132    -0.541362    -2.930581      23.69
 C      -0.537633    -0.750546    -0.236919      38.58
 H      -1.207270    -1.559284    -0.178255      20.76
 C       0.119452     1.515872    -0.012710      70.30
 H      -0.264557     2.658695     0.069075      17.57
 C       1.528748     1.325166    -0.409355      12.99
 O       2.623864     2.201378    -0.367723     218.40
 C       2.360734     3.597841    -0.544858     118.18
 H       3.573477     3.744677    -0.653342      20.02
 H       1.910022     3.657005    -1.466199      27.94
 H       1.981619     4.170926     0.197117      28.11
 C       1.788308    -0.031867    -0.418647      18.79
 O       3.258020    -0.382487    -0.648603     145.85
 C       0.836151    -1.094038    -0.344128      47.54
 H       1.157416    -2.144087    -0.573813      17.93
 C      -0.856926     0.656047     0.084451      33.69
 C      -2.329214     1.188016     0.541178      79.52
 H      -2.696448     0.273000     0.964358      19.50
 O      -2.150676     2.288167     1.441321     310.86
 H      -1.613813     1.832336     2.230277      26.88
 C      -3.110806     1.511173    -0.718785      74.37
 H      -2.594893     2.460250    -1.274280      18.23
 O      -3.482376     0.336103    -1.545949     248.62
 H      -3.218161     0.523988    -2.401360      24.83
 C      -4.423631     2.221357    -0.344483      78.56
 O      -5.140173     2.826313    -1.605591     257.02
 H      -4.938659     3.814935    -1.695030      30.47
 H      -3.889805     3.136997     0.127624      23.69
 H      -4.958778     1.515067     0.312153      28.23
55
name = lig-etoh-Waterframe_721
 C       6.037859    -1.397080     1.351392      40.57
 H       6.531678    -0.450975     0.976054      21.29
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 C       4.845592    -3.467563     1.066136      70.13
 H       4.295543    -4.057031     0.309914      23.30
 C       5.050876    -3.990729     2.255644      13.99
 O       4.673798    -5.312216     2.834726     208.38
 C       3.714066    -6.117745     2.156652     113.99
 H       2.710764    -5.799174     2.397149      26.09
 H       3.885521    -7.135746     2.877983      23.11
 H       3.888836    -6.089535     0.985337      25.18
 C       5.554014    -2.983974     3.277395     -22.22
 O       5.665132    -3.229695     4.688425     255.42
 H       5.260423    -4.058570     5.039744      20.08
 C       6.117632    -1.741933     2.827456      51.81
 H       6.320100    -0.962483     3.486259      25.69
 C       5.312588    -2.165218     0.513024      52.66
 C       5.070444    -1.948747    -0.893619      92.01
 H       5.647859    -2.730814    -1.551613      23.82
 O       5.967616    -0.796624    -1.327750     180.35
 H       5.667940    -0.079307    -0.770018      28.66
 C       3.650766    -1.570686    -1.386969      86.04
 H       2.943652    -2.361074    -1.044486      24.75
 C       3.523764    -1.151214    -2.846374     106.11
 O       3.291694    -2.331126    -3.723391     241.20
 H       4.076615    -2.211379    -4.491178      22.20
 H       4.326975    -0.454132    -3.212732      25.68
 H       2.553922    -0.690293    -2.916909      25.75
 C      -0.529948    -0.747081    -0.124263      36.56
 H      -1.311217    -1.449143    -0.051447      19.84
 C       0.159416     1.608531    -0.026229     102.77
 H      -0.256682     2.621446     0.184220      18.98
 C       1.501124     1.370116    -0.380840      -0.16
 O       2.584473     2.239728    -0.349830     245.93
 C       2.470910     3.609613    -0.624052     126.45
 H       3.395500     4.150471    -0.725325      23.14
 H       2.017169     3.704123    -1.740504      23.58
 H       2.024119     4.296591     0.274162      23.67
 C       1.774344    -0.054072    -0.530456      22.72
 O       3.233421    -0.349381    -0.594550     138.15
 C       0.828081    -1.109019    -0.419199      60.76
 H       1.094510    -2.124903    -0.400420      22.67
 C      -0.921270     0.544951     0.090370      55.68
 C      -2.243667     1.051588     0.493879      90.97
 H      -2.834498     0.483301     1.132636      21.40
 O      -2.173597     2.217804     1.402281     245.87
 H      -2.043527     1.782060     2.354050      25.78
 C      -3.150934     1.591930    -0.805438      80.89
 H      -2.416292     2.247145    -1.565516      21.21
 O      -3.436528     0.343744    -1.475692     256.25
 H      -3.264788     0.534238    -2.339124      26.55
 C      -4.401853     2.303214    -0.339092      97.72
 O      -5.104000     2.843490    -1.574917     255.68
 H      -5.100724     3.971457    -1.615969      24.46
 H      -4.180587     3.146388     0.551940      24.99
 H      -5.001933     1.578337     0.154076      30.13
55
name = lig-etoh-Waterframe_722
 C       6.066563    -1.384604     1.387635      56.54
 H       6.326302    -0.333703     1.028574      22.19
 C       4.736626    -3.476996     0.977888      55.56
 H       4.411373    -4.146317     0.210360      23.14
 C       5.031070    -3.985581     2.383025       4.69
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 O       4.688792    -5.279731     2.837948     291.36
 C       3.630189    -6.036218     2.229273     118.39
 H       2.655697    -5.584209     2.378306      25.67
 H       3.807501    -7.246410     2.476820      23.30
 H       3.866198    -6.272076     1.186507      26.47
 C       5.523587    -3.087889     3.360521       6.63
 O       5.688734    -3.209658     4.682167     168.71
 H       5.260914    -4.136175     4.978803      20.75
 C       6.033274    -1.820596     2.796504       7.36
 H       6.495264    -1.174399     3.587768      21.77
 C       5.351380    -2.297173     0.567463      20.84
 C       5.131611    -1.836946    -0.914297      92.17
 H       5.272465    -2.932837    -1.425777      24.04
 O       5.991183    -0.839959    -1.398178     249.80
 H       5.933362    -0.017828    -0.940533      29.24
 C       3.644441    -1.525643    -1.290841      75.37
 H       3.064066    -2.466749    -1.075358      24.79
 C       3.445408    -1.139126    -2.830582     107.56
 O       3.343956    -2.279358    -3.764163     256.20
 H       4.101332    -2.266975    -4.568123      23.09
 H       4.285729    -0.576326    -3.030350      27.30
 H       2.631460    -0.502701    -2.892975      27.58
 C      -0.526413    -0.803968    -0.022283      41.55
 H      -1.282729    -1.578233     0.151287      18.73
 C       0.130607     1.717718    -0.045678      56.31
 H       0.009850     2.674322     0.267138      16.35
 C       1.430656     1.322478    -0.320950       1.09
 O       2.569872     2.204684    -0.313732     190.34
 C       2.562430     3.726345    -0.761163      84.28
 H       3.470773     4.127844    -0.741149      24.87
 H       1.776024     4.143779    -1.628874      22.95
 H       1.739758     4.060162     0.133609      20.90
 C       1.873749    -0.115076    -0.636560      27.99
 O       3.179115    -0.328531    -0.552305     189.13
 C       0.808170    -1.059519    -0.481997      60.10
 H       1.086435    -2.035783    -0.380012      24.27
 C      -0.845759     0.560934     0.086073      35.13
 C      -2.270622     1.016498     0.440767      68.12
 H      -2.986231     0.093270     0.695053      21.36
 O      -2.177376     2.152845     1.384666     268.72
 H      -2.432898     1.853214     2.307700      26.12
 C      -3.097484     1.607539    -0.802203      84.20
 H      -2.458043     2.151433    -1.525868      25.37
 O      -3.414320     0.348077    -1.445387     244.77
 H      -3.418239     0.441572    -2.382856      26.59
 C      -4.409046     2.407298    -0.367155     110.05
 O      -5.070238     2.843042    -1.508771     274.35
 H      -5.207035     3.888632    -1.236861      25.07
 H      -4.468371     3.175427     0.490752      25.57
 H      -5.183234     1.693052    -0.114575      27.02
55
name = lig-etoh-Waterframe_723
 C       6.013192    -1.465058     1.555261      66.86
 H       6.369258    -0.437556     1.326192      24.88
 C       4.726378    -3.556540     0.994648      54.95
 H       4.330474    -4.269836     0.325757      24.96
 C       4.920175    -3.967992     2.433421       4.73
 O       4.729061    -5.232644     2.856700     303.38
 C       3.592445    -5.990047     2.232924     128.58
 H       2.567372    -5.572852     2.415646      26.43
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 H       3.569478    -6.778008     3.043617      25.73
 H       3.678896    -5.979750     1.209461      29.15
 C       5.550026    -3.065837     3.293887      11.09
 O       5.700311    -3.231029     4.703186      54.63
 H       5.355135    -4.191607     5.124263      23.56
 C       5.988407    -1.877611     2.786558      54.62
 H       6.637117    -1.334737     3.586719      19.28
 C       5.360317    -2.337812     0.558555       2.81
 C       5.122840    -1.802019    -0.934459     100.67
 H       5.250966    -2.558217    -1.765045      24.16
 O       6.071620    -0.868339    -1.484663     283.57
 H       5.933491    -0.046436    -1.047720      29.91
 C       3.630123    -1.488933    -1.241495      82.14
 H       3.034535    -2.396581    -0.979816      23.85
 C       3.420535    -1.138602    -2.813161     101.53
 O       3.396607    -2.239330    -3.780507     274.44
 H       4.072116    -2.096192    -4.546681      25.20
 H       4.287149    -0.615897    -3.052926      24.73
 H       2.542676    -0.505031    -2.963703      25.15
 C      -0.463657    -0.758709     0.003968      54.26
 H      -1.074824    -1.648047     0.360569      19.76
 C       0.100291     1.678352    -0.055471      35.76
 H      -0.135014     2.626257     0.201088      15.69
 C       1.484800     1.264834    -0.340523      -0.23
 O       2.575366     2.194383    -0.330453     141.98
 C       2.476512     3.783012    -0.798113      70.05
 H       3.535331     3.862460    -0.752535      23.50
 H       2.149695     3.776744    -1.912267      22.87
 H       2.188867     4.449822     0.158073      21.84
 C       1.764560    -0.037979    -0.622621      44.34
 O       3.189325    -0.358121    -0.539095     188.43
 C       0.830714    -1.079402    -0.494482      50.33
 H       1.154186    -2.095805    -0.621676      21.01
 C      -0.811472     0.686683     0.108350      57.03
 C      -2.320301     1.066983     0.385204      68.14
 H      -2.727958    -0.028488     0.675790      20.92
 O      -2.212888     2.078199     1.383479     309.46
 H      -2.414085     1.628273     2.240528      25.11
 C      -3.020978     1.603492    -0.751672      99.63
 H      -2.534850     2.292855    -1.257531      28.44
 O      -3.445139     0.334000    -1.460678     227.56
 H      -3.421683     0.616096    -2.430937      23.62
 C      -4.432705     2.365104    -0.348986      87.64
 O      -5.084392     2.911519    -1.504478     294.20
 H      -5.142125     3.964205    -1.736268      27.01
 H      -4.114197     3.133768     0.246493      28.25
 H      -4.899583     1.451006     0.241126      28.91
55
name = lig-etoh-Waterframe_724
 C       5.892003    -1.550821     1.505104      39.15
 H       6.468896    -0.666237     1.303204      23.55
 C       4.807158    -3.608453     1.071802      63.33
 H       4.227128    -4.217418     0.410373      19.44
 C       4.822072    -3.905798     2.355585      20.32
 O       4.710854    -5.231993     2.875949     287.20
 C       3.549707    -5.904024     2.334256     130.16
 H       2.711013    -5.150570     2.494286      26.32
 H       3.407236    -6.827203     2.799747      26.59
 H       3.691596    -6.268556     1.280744      29.54
 C       5.526337    -3.103648     3.327222       0.22
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 O       5.719736    -3.265294     4.700744      74.12
 H       5.325713    -4.215241     4.958879      18.59
 C       6.061606    -1.884132     2.965082      34.33
 H       6.580959    -1.100862     3.656655      21.72
 C       5.330488    -2.310161     0.512400      19.67
 C       5.103284    -1.864606    -0.983731      99.00
 H       5.355216    -2.678853    -1.556206      26.59
 O       6.161076    -0.849684    -1.528872     259.92
 H       5.960938    -0.024886    -1.145563      29.27
 C       3.600923    -1.475112    -1.292000      93.74
 H       3.082897    -2.352944    -0.915382      24.32
 C       3.461409    -1.128703    -2.803820      92.58
 O       3.427131    -2.229062    -3.768971     286.27
 H       4.111386    -2.067909    -4.452677      26.08
 H       4.227468    -0.322471    -3.072701      22.98
 H       2.390688    -0.668077    -2.911936      24.04
 C      -0.384018    -0.637839    -0.011338      38.72
 H      -1.162769    -1.382140     0.376476      17.44
 C       0.187981     1.631940    -0.076666      82.60
 H      -0.225291     2.660883    -0.060423      21.06
 C       1.497417     1.392951    -0.374405      12.09
 O       2.562219     2.232487    -0.362327     245.76
 C       2.468452     3.684626    -0.777825     116.42
 H       3.652562     3.894978    -1.025634      20.54
 H       2.042545     3.723440    -1.733465      26.33
 H       2.038799     4.502775    -0.295839      26.77
 C       1.757719    -0.030903    -0.560912      33.03
 O       3.175126    -0.346555    -0.525209     185.57
 C       0.820100    -1.094153    -0.462673      52.93
 H       1.094868    -2.145960    -0.786588      18.70
 C      -0.857771     0.648897     0.109761      60.09
 C      -2.213502     1.051723     0.421158      88.99
 H      -2.873529     0.328884     0.938019      19.85
 O      -2.294733     2.030990     1.448726     282.69
 H      -2.053012     1.559785     2.228484      28.50
 C      -3.123852     1.590306    -0.782584      84.81
 H      -2.433378     2.277566    -1.372982      22.09
 O      -3.467042     0.369875    -1.524734     232.73
 H      -3.344351     0.644362    -2.564648      20.56
 C      -4.323720     2.316659    -0.316225      92.12
 O      -5.140356     2.934127    -1.551192     271.67
 H      -4.764177     3.846461    -1.334849      28.38
 H      -3.961440     3.070978     0.292426      27.27
 H      -5.191186     1.787581     0.370522      25.96
55
name = lig-etoh-Waterframe_725
 C       5.888525    -1.533819     1.538107      45.09
 H       6.302927    -0.706609     1.005946      23.53
 C       4.845164    -3.553106     0.950682      45.78
 H       4.321035    -4.320450     0.318471      19.07
 C       4.865531    -3.914225     2.450227     -17.10
 O       4.667344    -5.232916     2.886307     302.56
 C       3.486566    -5.837171     2.437033     125.37
 H       2.601169    -5.130504     2.305273      26.54
 H       3.248932    -6.668867     3.023460      25.85
 H       3.749393    -6.177932     1.316082      26.76
 C       5.513579    -3.057451     3.434454       4.93
 O       5.716970    -3.366487     4.691002     199.75
 H       5.356661    -4.185225     5.120544      19.90
 C       6.099219    -1.843866     2.929785      54.38
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 H       6.454738    -1.135516     3.710762      24.49
 C       5.241413    -2.339304     0.516096      24.08
 C       5.154179    -1.914462    -1.014428      82.83
 H       5.292263    -2.862602    -1.455735      25.94
 O       6.189806    -0.861671    -1.518142     215.79
 H       5.992061    -0.041558    -1.132340      30.11
 C       3.650991    -1.509422    -1.365593      75.58
 H       3.007323    -2.370828    -1.229504      25.18
 C       3.430678    -1.101309    -2.817859      97.50
 O       3.479621    -2.232492    -3.740688     296.15
 H       4.114959    -2.277481    -4.410109      28.61
 H       4.149075    -0.184639    -3.085190      24.38
 H       2.336010    -0.675341    -2.820696      24.86
 C      -0.469675    -0.668141    -0.005280      35.03
 H      -1.283603    -1.428785     0.073290      18.74
 C       0.154921     1.703713    -0.112224      52.99
 H      -0.056008     2.882942    -0.190589      18.21
 C       1.491494     1.402840    -0.397183       8.92
 O       2.578625     2.317281    -0.374177     262.44
 C       2.474576     3.554491    -0.864249     121.29
 H       3.565968     4.171380    -0.987549      22.21
 H       1.834694     3.606551    -1.654736      29.24
 H       1.897898     4.050722    -0.151521      27.45
 C       1.887690    -0.060222    -0.484278      25.26
 O       3.164089    -0.301251    -0.531717     168.16
 C       0.868897    -1.008188    -0.443436      79.08
 H       0.941967    -2.185463    -0.554532      20.92
 C      -0.766742     0.670962     0.077277      42.66
 C      -2.254193     1.025116     0.501697      62.65
 H      -2.708018     0.062374     0.644881      24.73
 O      -2.348626     2.058947     1.556934     307.75
 H      -1.906604     1.737947     2.299191      30.43
 C      -3.167583     1.497939    -0.827338      71.10
 H      -2.533462     2.223232    -1.638188      20.43
 O      -3.490768     0.413763    -1.605746     218.65
 H      -3.313034     0.568899    -2.716601      19.26
 C      -4.311665     2.364392    -0.317099     100.39
 O      -5.119464     2.906717    -1.502221     232.44
 H      -5.107852     3.952765    -1.503584      27.70
 H      -4.019476     3.240048     0.324977      25.03
 H      -5.158389     1.768882     0.180433      27.16
55
name = lig-etoh-Waterframe_726
 C       5.926389    -1.446683     1.516857      64.77
 H       6.221285    -0.403433     1.303733      24.29
 C       4.798930    -3.611437     0.984831      13.10
 H       4.602508    -4.400966     0.151946      19.19
 C       4.991060    -3.910813     2.458827     -15.36
 O       4.643528    -5.186086     2.934290     212.18
 C       3.377286    -5.814516     2.454639     102.04
 H       2.507854    -5.145391     2.385326      26.76
 H       3.116773    -6.356902     3.374103      24.05
 H       3.536526    -6.296757     1.403385      22.71
 C       5.491135    -3.007972     3.386239       2.23
 O       5.744037    -3.445269     4.760795     210.41
 H       5.252749    -4.318810     5.062753      17.39
 C       6.052836    -1.815549     2.828861      48.73
 H       6.561071    -1.157040     3.460701      26.87
 C       5.228327    -2.292529     0.558401     -15.74
 C       5.185617    -1.911132    -0.985871      76.93
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 H       5.451998    -2.739513    -1.799993      22.90
 O       6.160570    -0.944537    -1.467307     194.59
 H       5.934154    -0.166305    -1.017336      30.22
 C       3.728571    -1.522800    -1.427639      82.80
 H       3.049848    -2.368831    -1.222698      25.97
 C       3.388083    -1.047703    -2.866817     104.44
 O       3.527845    -2.261195    -3.705144     291.11
 H       4.138897    -2.080313    -4.377156      28.92
 H       4.150701    -0.282595    -3.278743      25.79
 H       2.351867    -0.702985    -2.980453      26.16
 C      -0.486644    -0.721940    -0.074838      44.67
 H      -1.203089    -1.520362    -0.102531      22.35
 C       0.174636     1.814732    -0.188700      62.72
 H      -0.277192     2.931780     0.023885      16.43
 C       1.534609     1.319593    -0.390530      15.03
 O       2.649023     2.221926    -0.366987     188.40
 C       2.349290     3.616664    -0.946533      91.05
 H       3.421803     4.066277    -1.085829      24.36
 H       1.856243     3.575651    -2.020161      25.85
 H       1.937190     4.147687     0.000838      24.19
 C       1.889818     0.013813    -0.403648      22.25
 O       3.303815    -0.321721    -0.577885     142.87
 C       0.835271    -0.971067    -0.371381      62.14
 H       1.309746    -2.043940    -0.369965      22.52
 C      -0.813700     0.785827     0.097483      25.32
 C      -2.311028     1.018423     0.483677      75.60
 H      -2.598159     0.020291     0.816219      25.55
 O      -2.395594     2.076435     1.605803     289.38
 H      -2.126060     1.637428     2.408189      29.02
 C      -3.098860     1.507399    -0.812522      59.86
 H      -2.438853     2.332592    -1.373590      23.61
 O      -3.556333     0.366675    -1.674983     220.63
 H      -3.305304     0.828025    -2.661854      20.02
 C      -4.418320     2.426483    -0.365714     108.39
 O      -5.085076     2.890566    -1.451110     274.88
 H      -5.348713     3.787880    -1.613462      30.15
 H      -3.931423     3.265605     0.348303      25.61
 H      -4.823908     1.725415     0.226449      31.96
55
name = lig-etoh-Waterframe_727
 C       5.893394    -1.354325     1.412132      37.38
 H       6.218589    -0.301811     1.336426      22.30
 C       4.828194    -3.589588     1.099665      69.39
 H       4.624611    -4.430412     0.358559      22.52
 C       5.029663    -3.969206     2.336899       6.76
 O       4.607380    -5.134326     2.977921     227.36
 C       3.277630    -5.749909     2.509252     105.36
 H       2.666138    -4.903158     2.383353      27.70
 H       2.984617    -6.627672     3.286485      23.60
 H       3.474338    -6.424183     1.729674      25.44
 C       5.534770    -3.023178     3.380703     -17.08
 O       5.786390    -3.417314     4.738183     163.34
 H       5.245108    -4.305780     4.943309      19.94
 C       6.011276    -1.791183     2.847104      28.41
 H       6.633696    -1.171654     3.392644      23.15
 C       5.274391    -2.270297     0.566843       3.50
 C       5.167931    -1.916322    -0.997399      76.68
 H       5.470804    -3.001130    -1.537032      23.96
 O       6.133740    -0.995077    -1.377351     202.97
 H       6.031050    -0.167023    -0.976609      29.46
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 C       3.721234    -1.455022    -1.445048      91.71
 H       3.195809    -2.394602    -1.112571      26.01
 C       3.410511    -1.066526    -2.935041     114.41
 O       3.574609    -2.291900    -3.696407     302.02
 H       4.042620    -2.085723    -4.495743      29.80
 H       4.055179    -0.269972    -3.255831      27.42
 H       2.449871    -0.684075    -2.968102      27.47
 C      -0.477623    -0.570612    -0.156586      45.21
 H      -1.169431    -1.354233    -0.016461      22.04
 C       0.158237     1.767013    -0.200333     103.62
 H       0.042550     2.891148     0.023915      18.57
 C       1.571209     1.408789    -0.342186       5.82
 O       2.692764     2.145127    -0.412740     131.93
 C       2.282722     3.650874    -0.950608      79.08
 H       3.197486     3.935565    -1.211480      26.25
 H       1.630680     3.565643    -2.040554      24.47
 H       1.649210     4.605713    -0.513072      23.41
 C       1.891939    -0.025829    -0.385177       3.99
 O       3.421093    -0.350730    -0.604634     149.56
 C       0.906325    -0.986748    -0.269491      52.28
 H       1.215017    -2.042797    -0.369843      21.62
 C      -0.863142     0.771013     0.076215      19.49
 C      -2.305615     1.062488     0.455057      90.09
 H      -2.898114     0.300799     1.005514      20.49
 O      -2.446066     2.063009     1.577725     265.09
 H      -2.567008     1.455968     2.377844      23.68
 C      -3.105780     1.603694    -0.742270      70.77
 H      -2.348762     2.022055    -1.305675      25.56
 O      -3.587674     0.376396    -1.677211     163.81
 H      -3.443665     0.529632    -2.691352      24.62
 C      -4.362260     2.402886    -0.333037     103.06
 O      -5.132224     2.867881    -1.496492     275.59
 H      -5.066948     3.757318    -1.273057      29.84
 H      -4.064106     3.367871     0.336800      24.19
 H      -5.088375     1.837872     0.357462      28.33
55
name = lig-etoh-Waterframe_728
 C       5.827534    -1.345919     1.475364      63.21
 H       6.158620    -0.492944     0.865849      23.35
 C       4.903952    -3.497998     1.028896      43.14
 H       4.338335    -4.202649     0.427622      23.32
 C       5.036845    -3.985453     2.455338     -16.67
 O       4.539716    -5.155741     3.007092     404.91
 C       3.281901    -5.678628     2.579425     107.15
 H       2.519708    -4.959538     2.292886      30.45
 H       2.767901    -6.300002     3.495353      23.93
 H       3.476247    -6.031180     1.643753      27.62
 C       5.637936    -3.052591     3.334305      -1.65
 O       5.819981    -3.333104     4.627217     136.99
 H       5.383692    -4.199248     5.032987      19.38
 C       6.000211    -1.750151     2.842819      65.87
 H       6.469360    -1.142689     3.644088      21.10
 C       5.296200    -2.268642     0.521842      12.54
 C       5.111856    -1.970921    -0.961167      86.51
 H       5.281014    -2.967821    -1.470670      23.43
 O       6.178139    -1.001246    -1.317282     186.45
 H       5.953242    -0.206404    -0.883923      31.89
 C       3.703888    -1.448533    -1.422411      85.47
 H       2.926464    -2.259532    -1.287601      26.14
 C       3.473233    -1.116006    -2.944767     110.81
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 O       3.606936    -2.320110    -3.729427     301.17
 H       4.060204    -2.313240    -4.617513      26.59
 H       4.103603    -0.357789    -3.224948      27.97
 H       2.439202    -0.784729    -3.004555      26.20
 C      -0.427904    -0.497923    -0.177599      56.01
 H      -1.214277    -1.194079     0.046558      21.16
 C       0.216306     1.712938    -0.139020      63.78
 H       0.002454     2.723510    -0.091587      20.46
 C       1.545652     1.344905    -0.279512       5.38
 O       2.654828     2.265586    -0.485610     163.89
 C       2.271698     3.647632    -1.041858      84.42
 H       3.125104     4.081583    -1.306434      26.34
 H       1.584540     3.153609    -1.845614      24.36
 H       1.697486     4.189219    -0.127556      24.10
 C       2.005907    -0.052287    -0.412370      10.32
 O       3.398324    -0.317810    -0.582925     180.79
 C       0.956296    -1.001647    -0.212778      60.87
 H       0.892311    -2.007178    -0.305642      23.51
 C      -0.849266     0.772335     0.015789      25.88
 C      -2.346426     1.123721     0.484539      70.44
 H      -2.814491     0.026039     0.512777      21.15
 O      -2.481458     2.061258     1.510901     283.39
 H      -2.633090     1.626649     2.446734      25.00
 C      -3.149002     1.614804    -0.768181      89.40
 H      -2.669202     2.217569    -1.457028      26.46
 O      -3.599953     0.420447    -1.584064     205.05
 H      -3.267349     0.752164    -2.430502      25.30
 C      -4.309516     2.377309    -0.279192      92.72
 O      -5.171075     2.870170    -1.523443     223.95
 H      -5.103405     3.806933    -1.667719      32.12
 H      -4.023171     3.298130     0.211796      26.50
 H      -5.180171     1.786793     0.310962      27.34
55
name = lig-etoh-Waterframe_729
 C       5.783441    -1.377497     1.523286      62.83
 H       6.216177    -0.348316     1.307269      23.26
 C       4.906331    -3.557853     1.033358      60.90
 H       4.248300    -3.972392     0.339399      21.86
 C       5.005447    -3.914233     2.450242     -15.27
 O       4.514973    -5.159343     3.058435     254.21
 C       3.244590    -5.572090     2.578369     112.15
 H       2.501925    -4.715851     2.531256      28.35
 H       2.883980    -6.292226     3.410895      24.77
 H       3.268244    -6.256543     1.626244      26.45
 C       5.728457    -3.051023     3.242544       4.26
 O       5.877316    -3.242840     4.596120     163.49
 H       5.417068    -4.153036     4.807107      19.09
 C       6.013167    -1.710883     2.825652      32.66
 H       6.211860    -0.912335     3.651949      20.16
 C       5.283891    -2.291557     0.558034      10.10
 C       5.079377    -1.990207    -0.935283      86.18
 H       5.284416    -2.687196    -1.609326      26.42
 O       6.206398    -1.015397    -1.289466     167.20
 H       5.915659    -0.203592    -0.922711      31.69
 C       3.674709    -1.505443    -1.399021      78.20
 H       2.884393    -2.232801    -1.145713      25.29
 C       3.554083    -1.148881    -2.929988      99.04
 O       3.619009    -2.385949    -3.774572     265.60
 H       4.326897    -2.108103    -4.515155      22.56
 H       4.268678    -0.425381    -3.278377      26.37
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 H       2.462976    -0.760606    -3.119004      24.32
 C      -0.372626    -0.582401    -0.118987      38.94
 H      -1.090464    -1.438031    -0.092680      20.66
 C       0.259100     1.738542    -0.050897      59.26
 H      -0.014673     2.690959    -0.101188      20.77
 C       1.643610     1.264583    -0.282222       2.36
 O       2.603505     2.374375    -0.533068     230.37
 C       2.209740     3.534798    -1.082743     119.21
 H       3.057257     4.281199    -1.459779      24.34
 H       1.534413     3.697033    -1.893706      27.52
 H       1.842803     4.080699    -0.234698      27.10
 C       2.042830    -0.047800    -0.404492      30.75
 O       3.327935    -0.262610    -0.562758     178.23
 C       0.934646    -0.985383    -0.233857      46.49
 H       1.124760    -2.015266    -0.213743      22.32
 C      -0.815328     0.865812    -0.009288      90.29
 C      -2.320403     1.111682     0.370236      61.57
 H      -2.693126     0.052785     0.740483      22.67
 O      -2.519560     2.072215     1.470151     238.90
 H      -2.186013     1.570940     2.375445      25.14
 C      -3.192085     1.607268    -0.818688      96.20
 H      -2.742556     2.455632    -1.443233      23.16
 O      -3.570924     0.494782    -1.478042     272.25
 H      -3.306853     0.535252    -2.387330      25.59
 C      -4.421831     2.459391    -0.320063      98.09
 O      -5.180788     2.866194    -1.511516     306.24
 H      -5.102136     3.742994    -1.818998      33.78
 H      -4.030482     3.153650     0.267907      30.27
 H      -4.916934     1.660020     0.388963      28.98
55
name = lig-etoh-Waterframe_730
 C       5.798413    -1.341632     1.495883      59.66
 H       5.839857    -0.231217     1.350638      24.52
 C       4.824484    -3.640823     1.054952      88.68
 H       4.347322    -4.377197     0.423724      25.06
 C       4.966721    -3.933263     2.359186     -28.38
 O       4.558312    -5.076854     3.065317     223.46
 C       3.155094    -5.510766     2.605233      99.94
 H       2.562223    -4.545520     2.592385      27.54
 H       2.862044    -6.192855     3.289771      26.99
 H       3.169344    -6.141387     1.518870      25.89
 C       5.783552    -2.976032     3.255542       6.37
 O       5.935595    -3.201451     4.599352      96.04
 H       5.507120    -4.094534     4.869183      21.37
 C       6.008281    -1.721310     2.837288      47.82
 H       6.274204    -0.832209     3.547018      18.23
 C       5.263878    -2.326427     0.616027      14.43
 C       5.122617    -1.941410    -0.931699      92.72
 H       5.359860    -2.844731    -1.488807      26.16
 O       6.172212    -1.021376    -1.271552     175.09
 H       6.064325    -0.135630    -0.988800      30.35
 C       3.659289    -1.508663    -1.349638      91.46
 H       3.112159    -2.384567    -1.038383      27.18
 C       3.594855    -1.217291    -2.913379      92.70
 O       3.636277    -2.409027    -3.787119     239.14
 H       4.382372    -2.381253    -4.649254      21.21
 H       4.499468    -0.531550    -3.130843      25.18
 H       2.642787    -0.525477    -3.111281      25.05
 C      -0.400344    -0.599686    -0.039211      46.51
 H      -1.129726    -1.462738    -0.118095      21.68
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 C       0.326732     1.767004    -0.000080      45.41
 H       0.250880     2.849014     0.061602      19.38
 C       1.660843     1.407329    -0.319547       8.33
 O       2.609355     2.292496    -0.563772     195.61
 C       2.077921     3.645893    -1.117629      91.78
 H       3.306718     3.935449    -1.467488      21.24
 H       1.375643     3.609921    -1.896658      28.06
 H       1.759108     4.379883    -0.509034      28.16
 C       1.922628    -0.003459    -0.356495      16.74
 O       3.353435    -0.285921    -0.598058     155.22
 C       0.975595    -0.983578    -0.280578      67.84
 H       1.403514    -2.018681    -0.184597      22.99
 C      -0.749298     0.767526     0.003603      42.44
 C      -2.249368     1.130309     0.278186      78.58
 H      -2.734143     0.306585     0.701423      24.79
 O      -2.517362     2.066217     1.446722     211.59
 H      -1.878498     1.637160     2.198799      25.99
 C      -3.205740     1.751761    -0.792036      76.91
 H      -2.336886     2.188522    -1.519262      21.17
 O      -3.568920     0.468933    -1.466425     219.73
 H      -3.406397     0.467012    -2.381439      27.85
 C      -4.497890     2.486657    -0.358066     116.19
 O      -5.204504     2.872005    -1.486822     311.70
 H      -4.984145     3.764907    -1.418462      31.18
 H      -4.280689     3.347903     0.283387      27.36
 H      -5.271678     1.933722     0.192447      28.37
55
name = lig-etoh-Waterframe_731
 C       5.759765    -1.343645     1.454750      65.13
 H       5.582984    -0.467800     0.863736      23.48
 C       4.751741    -3.643672     1.008524      27.19
 H       4.575347    -4.562865     0.375435      21.39
 C       5.063353    -3.909340     2.457526       3.22
 O       4.549757    -5.015612     3.025546     245.49
 C       3.137962    -5.444363     2.654444      93.45
 H       2.392050    -4.606282     2.590879      29.10
 H       2.739733    -6.056078     3.323375      26.37
 H       3.214873    -5.617098     1.532178      22.70
 C       5.699556    -3.009553     3.281241      -3.23
 O       5.996980    -3.207637     4.631626     203.00
 H       5.582239    -4.047951     5.013002      24.73
 C       6.027532    -1.641307     2.807221      31.33
 H       6.516621    -1.060391     3.637001      19.71
 C       5.221482    -2.333813     0.588802       7.97
 C       5.166335    -1.911940    -0.860721      96.50
 H       5.387477    -2.978848    -1.396198      24.33
 O       6.152552    -0.996592    -1.290512     183.21
 H       5.915263    -0.182588    -0.856239      30.87
 C       3.716310    -1.531691    -1.320125      84.82
 H       3.072968    -2.361205    -1.073742      25.70
 C       3.658646    -1.261605    -2.893036      94.33
 O       3.625133    -2.428307    -3.759142     255.65
 H       4.203883    -2.204778    -4.673943      23.88
 H       4.691143    -0.729619    -3.034838      23.45
 H       2.799467    -0.619937    -3.185787      25.36
 C      -0.388025    -0.637804    -0.018017      30.36
 H      -1.322915    -1.250512     0.113377      20.50
 C       0.321007     1.774051     0.020287      42.21
 H      -0.040481     2.856172     0.358032      19.57
 C       1.575665     1.454552    -0.321890      20.47
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 O       2.631377     2.283482    -0.609293     174.51
 C       2.059449     3.749038    -1.181765      64.71
 H       3.063409     4.145907    -1.804329      21.52
 H       1.454105     3.168664    -1.811625      25.90
 H       1.747293     4.416658    -0.334058      24.74
 C       1.946824     0.061888    -0.373066      14.36
 O       3.334342    -0.325547    -0.642517     173.47
 C       0.975014    -0.973047    -0.268745      71.27
 H       1.200068    -2.138404    -0.344841      21.13
 C      -0.698670     0.721395     0.062154      45.22
 C      -2.234863     1.188530     0.321151      71.71
 H      -2.693965     0.232303     0.302879      23.73
 O      -2.437806     2.070774     1.407416     253.21
 H      -1.990996     1.790841     2.352986      25.61
 C      -3.108427     1.766953    -0.790231      66.25
 H      -2.772876     2.593314    -1.624018      22.49
 O      -3.600749     0.432399    -1.484306     185.72
 H      -3.399994     0.758996    -2.316815      25.75
 C      -4.511905     2.472143    -0.309890      89.93
 O      -5.252546     2.966864    -1.525346     225.41
 H      -5.329883     3.925334    -1.732810      28.81
 H      -4.399232     3.502313     0.294211      24.71
 H      -5.083284     1.761857     0.212982      29.63
55
name = lig-etoh-Waterframe_732
 C       5.668622    -1.372635     1.430145      37.81
 H       6.013367    -0.346753     1.197368      19.36
 C       4.825002    -3.575001     1.082125      66.88
 H       4.569329    -4.307820     0.232898      21.30
 C       5.067146    -3.870317     2.416224       7.02
 O       4.488540    -5.043569     3.039949     243.59
 C       3.164228    -5.293201     2.648014     117.27
 H       2.553114    -4.436258     2.917248      28.86
 H       2.902589    -6.254278     3.248565      22.21
 H       3.062433    -5.812125     1.743768      24.16
 C       5.659980    -2.910856     3.337650       2.20
 O       6.051015    -3.232466     4.666855     200.97
 H       5.571949    -4.049211     4.979988      24.73
 C       6.037773    -1.652781     2.780864      32.21
 H       6.584391    -0.964556     3.383059      25.32
 C       5.162480    -2.387394     0.575531      37.48
 C       5.139212    -1.991308    -0.836251      90.37
 H       5.471578    -2.811886    -1.677486      23.45
 O       6.138469    -0.924823    -1.301959     118.49
 H       5.913186    -0.095850    -0.868158      26.11
 C       3.745402    -1.588165    -1.356808      80.02
 H       3.003711    -2.344652    -1.076655      24.02
 C       3.759604    -1.275642    -2.862157     108.06
 O       3.582679    -2.446772    -3.716043     290.88
 H       4.230812    -2.301839    -4.464303      25.36
 H       4.667490    -0.717139    -3.209978      24.56
 H       2.978841    -0.636427    -3.023985      27.31
 C      -0.378743    -0.611224    -0.013336      50.82
 H      -1.048778    -1.467754     0.196792      22.23
 C       0.161936     1.767479     0.065878      63.67
 H      -0.267725     2.896701     0.327047      16.48
 C       1.637342     1.400093    -0.330145      -3.44
 O       2.658165     2.396558    -0.655454     184.49
 C       2.127779     3.694700    -1.258982      80.04
 H       2.627826     4.379293    -1.809074      26.41
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 H       1.090437     3.604498    -1.914830      24.35
 H       1.675418     4.280733    -0.296612      24.30
 C       1.996413    -0.000129    -0.457735      22.14
 O       3.288770    -0.300785    -0.662551     171.41
 C       0.937934    -0.959374    -0.232431      51.94
 H       1.194237    -2.077633    -0.518230      20.60
 C      -0.726636     0.795492     0.154346      38.96
 C      -2.179894     1.184108     0.362161      72.52
 H      -2.754379     0.145072     0.609784      21.25
 O      -2.337869     2.114667     1.413084     236.54
 H      -2.324367     1.506572     2.330452      23.51
 C      -3.142714     1.752766    -0.837746      82.70
 H      -2.757802     2.469959    -1.553501      24.49
 O      -3.590771     0.507247    -1.517598     199.56
 H      -3.470540     0.523827    -2.483042      24.39
 C      -4.486933     2.511676    -0.309001      76.48
 O      -5.311403     3.020673    -1.571525     216.49
 H      -5.304223     4.085785    -1.671276      24.92
 H      -4.147551     3.253912     0.599256      24.27
 H      -4.963364     1.682621     0.169449      29.86
55
name = lig-etoh-Waterframe_733
 C       5.650714    -1.358165     1.485526      53.66
 H       6.230207    -0.486687     1.138792      20.68
 C       4.908585    -3.594634     1.117877      64.11
 H       4.291800    -4.373963     0.550749      21.99
 C       4.996306    -3.871281     2.484410     -12.44
 O       4.526586    -5.038715     3.042997     239.61
 C       3.137433    -5.243032     2.665535      95.30
 H       2.517382    -4.392459     2.951867      28.67
 H       2.857651    -6.159920     3.489996      22.04
 H       2.884479    -5.442433     1.632160      26.83
 C       5.663990    -2.853807     3.406009      16.48
 O       6.072764    -3.251207     4.660230     193.18
 H       5.561884    -4.041240     4.918344      21.89
 C       6.019612    -1.694358     2.768168      74.40
 H       6.490789    -0.880986     3.163482      27.92
 C       5.192460    -2.263524     0.574217      -0.81
 C       5.119163    -2.009604    -0.964248      86.71
 H       5.457494    -2.948331    -1.482675      24.91
 O       6.096649    -0.870320    -1.272931     119.67
 H       5.892757    -0.008532    -0.885229      27.88
 C       3.736507    -1.593192    -1.392255      81.76
 H       3.041927    -2.457403    -1.200013      26.13
 C       3.803602    -1.250828    -2.866023     109.26
 O       3.549309    -2.463222    -3.674389     312.86
 H       4.161093    -2.539929    -4.327590      29.44
 H       4.738243    -0.787092    -3.099229      26.42
 H       2.991122    -0.564286    -2.977524      27.31
 C      -0.380573    -0.548861     0.022660      47.36
 H      -1.010197    -1.413416     0.116808      22.46
 C       0.264631     1.786051     0.049635      65.90
 H      -0.009503     2.930176     0.020113      19.38
 C       1.612770     1.419135    -0.334640     -19.26
 O       2.643425     2.491115    -0.728547     162.37
 C       2.074274     3.629630    -1.265109     100.90
 H       2.895585     4.121864    -1.714728      25.44
 H       1.088700     3.600904    -1.995193      23.90
 H       1.929781     4.400307    -0.314307      23.72
 C       1.941737    -0.005745    -0.517338      14.24
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 O       3.327911    -0.298603    -0.699130     124.42
 C       0.959243    -0.942351    -0.256356      56.43
 H       1.152722    -2.043093    -0.340677      22.32
 C      -0.839313     0.746545     0.208434      42.95
 C      -2.246837     1.140487     0.373216      76.80
 H      -2.806370     0.319083     0.991602      20.29
 O      -2.241882     2.177141     1.489168     195.84
 H      -2.512780     1.587472     2.351476      23.26
 C      -3.194363     1.727937    -0.901590      89.77
 H      -2.447761     2.149979    -1.423726      25.55
 O      -3.591247     0.592015    -1.552336     268.79
 H      -3.192394     0.611623    -2.511178      23.58
 C      -4.428720     2.492352    -0.377626     101.22
 O      -5.318577     3.037751    -1.517384     271.80
 H      -5.064694     4.047892    -1.458207      27.08
 H      -4.201620     3.341319     0.350493      24.94
 H      -5.301497     1.875360     0.008954      25.19
55
name = lig-etoh-Waterframe_734
 C       5.733544    -1.295450     1.468490      67.44
 H       5.973381    -0.383095     0.947566      27.39
 C       4.917042    -3.574662     1.130749      40.29
 H       4.395775    -4.377050     0.604185      24.94
 C       4.993074    -3.777966     2.597700       1.42
 O       4.580885    -5.034459     3.029451     235.76
 C       3.065656    -5.229063     2.748511      72.22
 H       2.554121    -4.300549     3.044156      30.09
 H       2.484654    -6.167726     3.302883      22.74
 H       2.994437    -5.223281     1.633957      28.04
 C       5.639369    -2.956530     3.406450      21.82
 O       6.075970    -3.256971     4.661175     201.08
 H       5.623491    -4.019534     5.042569      25.64
 C       6.013980    -1.649136     2.848254      50.33
 H       6.541575    -1.010781     3.559653      20.78
 C       5.209005    -2.260448     0.545657     -21.07
 C       5.153496    -1.931474    -0.958228      89.90
 H       5.433847    -2.762578    -1.447762      26.51
 O       6.051158    -0.864653    -1.263152     170.35
 H       5.589664    -0.153173    -0.777572      30.59
 C       3.709091    -1.552775    -1.434797      81.39
 H       2.975329    -2.387324    -1.219099      26.42
 C       3.771931    -1.224569    -2.923991     100.27
 O       3.517380    -2.469990    -3.634208     291.13
 H       4.134135    -2.384043    -4.376706      26.15
 H       4.753955    -0.898047    -3.084464      27.10
 H       3.004121    -0.423793    -3.344634      24.43
 C      -0.400740    -0.564294     0.060931      45.46
 H      -1.249705    -1.205065     0.114836      21.87
 C       0.340629     1.753796    -0.010247      71.05
 H       0.190404     2.793115    -0.039008      23.31
 C       1.600408     1.466571    -0.379150      16.21
 O       2.556907     2.389066    -0.753478     189.74
 C       2.052197     3.725312    -1.260404      91.45
 H       3.068209     3.844360    -1.912058      22.32
 H       1.331146     3.307545    -1.945266      26.93
 H       1.755712     4.532877    -0.559327      26.13
 C       1.956856     0.067553    -0.536413       6.22
 O       3.364860    -0.324785    -0.740128     129.03
 C       0.962008    -0.931767    -0.299569      59.18
 H       1.195800    -1.931340    -0.167233      25.66
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 C      -0.787344     0.779611     0.172346      31.82
 C      -2.413608     1.173321     0.507961      54.51
 H      -2.950378     0.206585     0.619046      22.77
 O      -2.168004     2.242662     1.546028     249.77
 H      -2.364273     1.925404     2.540523      24.70
 C      -3.151217     1.701713    -0.815909      80.76
 H      -2.392891     2.425677    -1.411602      22.37
 O      -3.615182     0.582631    -1.644115     253.75
 H      -3.081804     0.797600    -2.537130      22.13
 C      -4.444451     2.509207    -0.492995     104.41
 O      -5.267193     3.042975    -1.426976     319.24
 H      -5.263262     4.026050    -1.800484      28.83
 H      -4.127775     3.294989     0.079574      27.71
 H      -4.992535     1.718157     0.273428      27.41
55
name = lig-etoh-Waterframe_735
 C       5.834069    -1.269012     1.484934      13.45
 H       5.900834    -0.196387     1.407558      26.69
 C       4.879313    -3.483236     1.172813      87.27
 H       4.739506    -4.228943     0.459237      27.77
 C       4.944836    -3.795972     2.496126       1.86
 O       4.563346    -5.079051     3.042921     211.77
 C       3.045885    -5.163382     2.808961     103.37
 H       2.611991    -4.290106     3.302964      28.88
 H       2.843807    -6.151077     3.163865      25.66
 H       2.885281    -5.397007     1.684911      26.72
 C       5.696403    -2.902975     3.405789       7.62
 O       6.077448    -3.257753     4.703337     165.89
 H       5.574610    -3.992390     5.115249      25.24
 C       5.999480    -1.610745     2.910399       5.64
 H       6.522185    -1.006150     3.760561      15.86
 C       5.241037    -2.325204     0.600134      15.77
 C       5.138947    -1.909825    -0.894355      87.29
 H       5.443331    -2.658319    -1.592670      27.72
 O       6.001999    -0.833614    -1.253240     118.18
 H       5.711829     0.055830    -0.903503      25.97
 C       3.668882    -1.477170    -1.475906      88.51
 H       2.965323    -2.288984    -1.195465      27.79
 C       3.723422    -1.212340    -2.998732      95.11
 O       3.494011    -2.466872    -3.647530     270.09
 H       4.033478    -2.378935    -4.566074      24.04
 H       4.722256    -0.885770    -3.284620      26.25
 H       2.999183    -0.297348    -3.366649      24.19
 C      -0.415462    -0.562110     0.052492      53.88
 H      -1.133952    -1.383855     0.212604      21.40
 C       0.230682     1.769158    -0.053982      50.36
 H      -0.042455     2.700077     0.128041      22.77
 C       1.634119     1.374163    -0.461282      11.67
 O       2.513483     2.321675    -0.734924     189.89
 C       2.091999     3.714402    -1.337312      96.77
 H       2.849407     4.448498    -2.061157      23.22
 H       1.282098     3.649617    -1.948145      29.16
 H       1.726482     4.364189    -0.673124      28.85
 C       2.008491     0.047630    -0.532726      32.32
 O       3.340990    -0.294285    -0.747630     179.56
 C       0.936039    -0.899521    -0.302847      52.90
 H       1.305123    -1.847990    -0.254647      26.92
 C      -0.741452     0.842942     0.121548      35.63
 C      -2.390147     1.243869     0.585454      67.60
 H      -2.923284     0.396159     0.962325      24.36
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 O      -2.161161     2.285516     1.566721     285.04
 H      -2.186844     1.778576     2.470720      25.47
 C      -3.116890     1.737137    -0.736362      72.80
 H      -2.502710     2.527018    -1.470674      21.46
 O      -3.595041     0.567801    -1.677976     180.79
 H      -3.359049     0.545831    -2.704748      21.13
 C      -4.369405     2.554778    -0.413761     103.11
 O      -5.300651     3.009628    -1.462932     288.10
 H      -5.081311     4.057112    -1.477186      27.61
 H      -3.983914     3.286098     0.225664      27.78
 H      -5.034515     1.857526     0.229698      28.31
55
name = lig-etoh-Waterframe_736
 C       5.870493    -1.300931     1.619235      89.51
 H       6.026802    -0.254575     1.267698      27.69
 C       4.820894    -3.493525     1.123546       8.84
 H       4.635814    -4.288866     0.431461      20.74
 C       4.993533    -3.850024     2.529869     -28.39
 O       4.511779    -5.072342     3.017172     288.02
 C       3.120801    -5.189881     2.863252     113.13
 H       2.490421    -4.446542     3.411885      29.24
 H       2.917922    -5.976712     3.395479      24.66
 H       2.661140    -4.990051     1.830500      25.13
 C       5.696338    -2.892526     3.394675       4.07
 O       6.075656    -3.225070     4.715784     201.02
 H       5.453299    -3.957085     5.048329      24.75
 C       6.011019    -1.611340     2.927026      70.67
 H       6.376549    -0.656331     3.489770      19.85
 C       5.353312    -2.134959     0.668412      -7.99
 C       5.055111    -1.887290    -0.877339      76.68
 H       5.449526    -2.850466    -1.504748      21.84
 O       6.002110    -0.770031    -1.246875     147.27
 H       5.797556     0.150035    -0.895733      26.63
 C       3.673851    -1.443032    -1.466079      79.26
 H       2.944096    -2.225648    -1.367914      26.68
 C       3.704791    -1.180169    -3.041059      90.59
 O       3.434731    -2.459332    -3.714002     257.08
 H       4.177822    -2.579047    -4.543551      21.64
 H       4.699220    -0.722597    -3.335266      23.81
 H       2.800736    -0.535196    -3.196141      25.91
 C      -0.376140    -0.537985     0.000176      47.23
 H      -0.975916    -1.425922     0.336267      21.76
 C       0.201091     1.792194    -0.125625      56.09
 H      -0.033563     2.798662     0.149004      18.90
 C       1.469528     1.348044    -0.506181     -13.95
 O       2.588840     2.415688    -0.781561     160.30
 C       2.060198     3.676067    -1.403719     106.27
 H       3.137864     4.088125    -1.707638      21.69
 H       1.213119     3.604567    -2.061163      27.20
 H       1.915784     4.123428    -0.442642      24.66
 C       1.961377    -0.026086    -0.520464      26.25
 O       3.306583    -0.219283    -0.739049     174.28
 C       0.941041    -0.898216    -0.275345      65.03
 H       1.076018    -1.987053    -0.393634      22.40
 C      -0.860114     0.773366     0.121590      54.51
 C      -2.184714     1.294134     0.546967      84.14
 H      -2.690887     0.582073     1.148629      22.29
 O      -2.199925     2.325776     1.584118     260.34
 H      -2.041110     1.781594     2.385081      27.04
 C      -3.140988     1.769929    -0.797544      74.09
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 H      -2.254281     2.240984    -1.314809      23.11
 O      -3.573055     0.567662    -1.570236     253.36
 H      -3.142013     0.952250    -2.419252      22.33
 C      -4.345650     2.557277    -0.246195     102.23
 O      -5.286919     2.980900    -1.491784     234.52
 H      -5.312649     4.057976    -1.547419      26.84
 H      -4.126024     3.559998     0.348094      24.85
 H      -5.040214     2.061902     0.280299      29.38
55
name = lig-etoh-Waterframe_737
 C       5.870587    -1.234838     1.624775      37.75
 H       6.385928    -0.322072     1.190664      18.11
 C       4.873532    -3.429304     1.119756      49.87
 H       4.226938    -4.108441     0.484275      21.35
 C       5.081609    -3.819992     2.503371      20.41
 O       4.533848    -5.031701     2.982042     299.86
 C       3.086697    -5.203854     2.962128      94.15
 H       2.777990    -4.373604     3.652683      25.48
 H       2.714487    -6.215281     3.271595      21.95
 H       2.748123    -5.141690     1.895875      27.17
 C       5.665200    -2.939397     3.434530      -0.40
 O       6.059195    -3.159630     4.679253     245.57
 H       5.587858    -3.961416     5.250848      13.78
 C       6.049735    -1.608075     2.988273      26.34
 H       6.342647    -0.855563     3.804868      27.99
 C       5.291714    -2.155709     0.668444       8.47
 C       5.067987    -1.759528    -0.835157      94.00
 H       5.397327    -2.837237    -1.314510      23.21
 O       6.029244    -0.722650    -1.267104     171.87
 H       5.564626    -0.002008    -0.717510      27.37
 C       3.696435    -1.442078    -1.448239      79.49
 H       2.936205    -2.166565    -1.276251      25.42
 C       3.645309    -1.166120    -3.008358      97.55
 O       3.397230    -2.447601    -3.777082     272.53
 H       4.317093    -2.378938    -4.394163      20.05
 H       4.528819    -0.563813    -3.432711      24.29
 H       2.824616    -0.611560    -3.213481      27.86
 C      -0.411331    -0.545020    -0.005465      43.92
 H      -1.185004    -1.321227     0.269010      21.46
 C       0.140279     1.747962    -0.187580      67.93
 H       0.069525     2.927398    -0.112404      18.45
 C       1.459158     1.455288    -0.552706      -0.69
 O       2.573157     2.390540    -0.846166     189.02
 C       2.112573     3.620470    -1.341027     110.29
 H       2.926658     3.975979    -1.866042      25.45
 H       1.384793     3.438048    -2.251046      26.14
 H       1.693297     4.553995    -0.550656      24.09
 C       1.875919     0.050274    -0.529526       9.15
 O       3.264279    -0.163513    -0.745409     125.27
 C       0.941098    -1.008949    -0.273044      57.08
 H       1.016436    -2.178364    -0.358836      20.54
 C      -0.817557     0.782157     0.102760      36.84
 C      -2.141391     1.283064     0.512838      66.46
 H      -2.702464     0.260859     0.670297      22.43
 O      -2.205437     2.383534     1.575054     272.20
 H      -2.016043     2.040562     2.421793      29.92
 C      -3.102636     1.752162    -0.726234      87.51
 H      -2.666558     2.411184    -1.411322      25.96
 O      -3.516870     0.639185    -1.407027     251.89
 H      -3.347073     0.562839    -2.453929      21.44
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 C      -4.409880     2.617662    -0.217511      84.07
 O      -5.225763     2.941522    -1.463606     261.72
 H      -5.374304     3.921565    -1.665191      29.11
 H      -4.035109     3.679357     0.338164      24.52
 H      -4.847659     1.950437     0.496893      30.25
55
name = lig-etoh-Waterframe_738
 C       5.893590    -1.201395     1.601559       8.57
 H       6.421898    -0.239618     1.383462      22.45
 C       4.903816    -3.370136     1.175748      75.98
 H       4.100915    -3.906328     0.539060      22.03
 C       5.092547    -3.799832     2.442896      28.35
 O       4.625940    -5.033473     2.954781     269.41
 C       3.056468    -5.178993     3.034706      72.36
 H       2.555311    -4.463586     3.769522      25.94
 H       2.998064    -6.385502     3.296837      21.26
 H       2.632034    -5.014755     2.065985      29.30
 C       5.665726    -2.888937     3.398640      -2.90
 O       6.056578    -3.116854     4.723509     151.40
 H       5.538133    -3.961242     5.138555      21.09
 C       6.053569    -1.623903     3.007332      39.20
 H       6.521775    -1.196818     3.859262      19.76
 C       5.201885    -2.128159     0.664044       2.74
 C       5.149413    -1.710753    -0.814255      87.58
 H       5.455965    -2.498234    -1.537784      26.11
 O       6.016145    -0.676099    -1.250431     135.60
 H       5.873056     0.280854    -0.851239      24.40
 C       3.674718    -1.388924    -1.407938      84.68
 H       3.108864    -2.260703    -1.039876      25.20
 C       3.531155    -1.178587    -2.955895     102.64
 O       3.429944    -2.380913    -3.797690     289.48
 H       4.127941    -2.514387    -4.533253      25.55
 H       4.490346    -0.667871    -3.308037      24.46
 H       2.716419    -0.532046    -3.094647      27.05
 C      -0.454367    -0.622589     0.022526      45.15
 H      -1.343482    -1.275911     0.100557      19.15
 C       0.201677     1.821276    -0.279314      61.10
 H      -0.462412     2.880260    -0.342658      15.84
 C       1.536701     1.465259    -0.575164      28.85
 O       2.490430     2.293317    -0.859893     218.43
 C       2.184748     3.644197    -1.375232      99.65
 H       2.889543     4.165515    -1.863690      27.24
 H       1.316804     3.386059    -2.178390      25.01
 H       1.508432     4.447437    -0.693534      24.33
 C       1.833421     0.104887    -0.565480      14.12
 O       3.206309    -0.128413    -0.768148     143.93
 C       0.850984    -1.018572    -0.291060      48.71
 H       1.420371    -2.052096    -0.224595      21.69
 C      -0.699911     0.826322     0.074936      48.38
 C      -2.263576     1.275852     0.485401      56.78
 H      -2.879733     0.328734     0.930089      20.55
 O      -2.194545     2.382238     1.502501     280.37
 H      -2.122661     1.951341     2.303736      29.16
 C      -3.062764     1.892578    -0.632152      97.98
 H      -2.726400     2.591323    -1.352018      25.09
 O      -3.504691     0.616431    -1.261202     226.39
 H      -3.341065     0.658011    -2.321796      21.74
 C      -4.417032     2.657045    -0.263077      88.31
 O      -5.164398     2.870375    -1.399443     326.34
 H      -5.126305     3.827951    -1.404153      29.92
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 H      -4.029857     3.646510     0.276536      25.16
 H      -5.073812     2.046856     0.564545      27.76
55
name = lig-etoh-Waterframe_739
 C       5.916332    -1.220622     1.639573      79.33
 H       6.125432    -0.222047     1.275191      31.58
 C       4.806202    -3.338462     1.140914      -6.97
 H       4.376929    -4.183484     0.469300      20.41
 C       5.074954    -3.789217     2.525263       7.49
 O       4.666899    -5.041937     2.928090     235.89
 C       3.138255    -5.168643     3.060985      81.85
 H       2.704569    -4.644451     3.932538      26.73
 H       3.045252    -6.307828     3.526327      21.56
 H       2.585935    -4.899088     2.218060      30.37
 C       5.696016    -2.869587     3.390236       4.63
 O       6.036356    -3.099834     4.744949     195.69
 H       5.553228    -3.865081     5.171115      23.40
 C       6.069655    -1.598722     2.916924      79.51
 H       6.703403    -0.965049     3.427708      19.37
 C       5.254500    -1.932521     0.696954     -29.58
 C       5.142220    -1.654318    -0.878959      80.03
 H       5.494232    -2.455705    -1.389441      24.76
 O       6.059878    -0.588516    -1.230208     146.38
 H       5.920637     0.360312    -0.790320      24.50
 C       3.646018    -1.364028    -1.316926      86.47
 H       3.056651    -2.284086    -0.979714      26.24
 C       3.483895    -1.187744    -2.915411     100.97
 O       3.419782    -2.333109    -3.773746     283.79
 H       4.229538    -2.162820    -4.287367      24.20
 H       4.358733    -0.555662    -3.118092      26.44
 H       2.505847    -0.557773    -3.066082      25.32
 C      -0.487994    -0.605519     0.039159      44.46
 H      -1.250009    -1.371506     0.154731      20.24
 C       0.194589     1.877391    -0.349760      86.18
 H      -0.161113     3.019824    -0.516886      19.16
 C       1.464306     1.429262    -0.574537      -0.43
 O       2.545918     2.319352    -0.890037     194.05
 C       2.124589     3.643827    -1.454728     101.01
 H       3.219689     4.061922    -1.608372      24.76
 H       1.417846     3.595954    -2.350982      25.51
 H       1.887540     3.999130    -0.521325      26.47
 C       1.788906     0.015046    -0.588800      30.98
 O       3.167986    -0.132207    -0.795057     156.13
 C       0.866480    -0.894676    -0.320710      71.77
 H       1.203933    -1.980203    -0.178797      24.90
 C      -0.771681     0.784486     0.064762      41.76
 C      -2.263988     1.347562     0.500341      83.79
 H      -2.847864     0.581852     1.050417      23.38
 O      -2.170397     2.343569     1.445155     290.55
 H      -2.229656     1.904171     2.233978      29.08
 C      -3.131279     1.967435    -0.590819      89.10
 H      -2.247702     2.450907    -1.179203      24.60
 O      -3.510165     0.582311    -1.180635     222.19
 H      -3.200424     0.833598    -2.124833      24.68
 C      -4.336755     2.653023    -0.177954     116.77
 O      -5.139068     2.853567    -1.393288     315.07
 H      -5.288848     3.756425    -1.641141      33.57
 H      -4.218848     3.566259     0.189053      28.63
 H      -5.142413     2.120098     0.544712      27.05
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name = lig-etoh-Waterframe_740
 C       5.901567    -1.121929     1.561000      41.90
 H       6.216101    -0.112149     1.380233      20.74
 C       4.772455    -3.239859     1.142716      55.78
 H       4.678867    -4.006096     0.387592      21.28
 C       5.013665    -3.701089     2.494038     -15.55
 O       4.660352    -5.057825     2.909106     273.17
 C       3.281885    -5.185899     3.155654     112.28
 H       3.160177    -4.496972     3.939649      26.64
 H       2.962826    -6.267636     3.145099      24.75
 H       2.727382    -4.960149     2.232451      28.59
 C       5.743948    -2.854900     3.463991       9.57
 O       6.015013    -3.078272     4.734790     135.94
 H       5.605139    -3.809552     5.169415      22.84
 C       6.167741    -1.564852     2.910841      11.07
 H       6.691891    -0.802172     3.494648      22.69
 C       5.216214    -2.014053     0.654766      -7.76
 C       5.104155    -1.547998    -0.850840      64.87
 H       5.405192    -2.499553    -1.260199      26.58
 O       6.118681    -0.489094    -1.234697     156.26
 H       5.652921     0.215689    -0.600126      24.85
 C       3.626369    -1.408640    -1.307955      95.39
 H       2.949237    -2.220238    -0.893653      26.45
 C       3.446562    -1.134434    -2.812305      98.27
 O       3.441450    -2.288596    -3.722886     280.95
 H       4.242989    -2.389575    -4.288314      25.66
 H       4.096981    -0.405202    -3.188201      28.21
 H       2.343274    -0.637917    -3.021959      25.78
 C      -0.493519    -0.478489     0.029581      48.36
 H      -1.062531    -1.302716     0.407438      24.29
 C       0.075521     1.798453    -0.364320      70.48
 H       0.094385     2.819745    -0.388057      19.68
 C       1.441459     1.434532    -0.619798      -0.76
 O       2.584427     2.308021    -0.963885     187.76
 C       2.145209     3.615150    -1.427993     108.89
 H       3.291031     4.155110    -1.769798      23.23
 H       1.595709     3.790865    -2.285769      29.25
 H       1.732970     4.265497    -0.717373      29.37
 C       1.836423     0.072456    -0.613861      16.05
 O       3.151099    -0.156102    -0.791642     145.76
 C       0.822608    -0.923986    -0.305446      61.01
 H       0.936849    -1.977953    -0.347393      24.35
 C      -0.948351     0.850118     0.027960      40.95
 C      -2.218844     1.345182     0.540685      99.29
 H      -2.703124     0.473484     0.753157      26.90
 O      -2.104366     2.387758     1.511761     304.43
 H      -2.151911     2.047158     2.358332      31.04
 C      -3.092160     1.817553    -0.560310      80.51
 H      -2.598501     2.588485    -1.443217      23.42
 O      -3.510899     0.616066    -1.185744     232.27
 H      -3.354908     0.422526    -2.142671      26.27
 C      -4.366184     2.737549    -0.111787      96.88
 O      -5.152084     2.843849    -1.443785     295.33
 H      -5.302492     3.778546    -1.524331      31.23
 H      -4.129416     3.623433     0.363816      28.92
 H      -4.674854     1.960392     0.605145      30.76
55
name = lig-etoh-Waterframe_741
 C       5.869570    -1.079047     1.549129      19.39
 H       6.319682    -0.183639     1.166089      16.34
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 C       4.800354    -3.218393     1.164634      70.17
 H       4.423526    -3.901031     0.469547      25.17
 C       4.988892    -3.604815     2.494114      18.96
 O       4.750948    -5.030945     2.844809     232.79
 C       3.356805    -5.197217     3.197390     109.69
 H       2.926058    -4.668968     4.097718      25.73
 H       3.172212    -6.174601     3.419320      26.30
 H       2.734088    -4.623917     2.393147      27.10
 C       5.736096    -2.778590     3.373066      -7.82
 O       6.013188    -3.068961     4.774812     149.00
 H       5.558211    -3.886791     5.077247      20.69
 C       6.250028    -1.533759     2.892419      16.35
 H       6.597698    -0.971628     3.844286      24.53
 C       5.215325    -1.972319     0.626083      20.30
 C       5.105753    -1.561220    -0.798658      75.19
 H       5.483685    -2.355819    -1.666825      23.37
 O       6.058923    -0.436898    -1.195233     116.99
 H       5.980303     0.558624    -0.774874      20.19
 C       3.623338    -1.402936    -1.335974      83.85
 H       3.158864    -2.341111    -0.987260      27.96
 C       3.384147    -1.094483    -2.803968     109.51
 O       3.478382    -2.275057    -3.640828     285.46
 H       4.228507    -2.311520    -4.272159      26.57
 H       4.020946    -0.283430    -3.083358      27.08
 H       2.268594    -0.809206    -2.732712      26.58
 C      -0.501487    -0.412911     0.037902      43.55
 H      -1.215961    -1.042451     0.552898      22.76
 C       0.065167     1.765600    -0.384673      72.33
 H      -0.320907     2.677218    -0.209644      24.51
 C       1.434526     1.432477    -0.689078      15.35
 O       2.508755     2.280209    -1.034239     191.87
 C       2.250139     3.661975    -1.397698     113.65
 H       3.207328     4.269030    -1.805400      23.74
 H       1.633287     3.381124    -2.253559      26.33
 H       1.543265     4.374346    -0.838148      25.99
 C       1.811518     0.096435    -0.608854      13.76
 O       3.176303    -0.155850    -0.744961     137.47
 C       0.767553    -0.910711    -0.306252      61.61
 H       0.962111    -1.895195    -0.403092      26.13
 C      -0.933110     0.935439    -0.034529      45.12
 C      -2.234051     1.312626     0.601190      73.11
 H      -2.730355     0.444036     1.086063      24.83
 O      -2.031064     2.459093     1.631889     252.98
 H      -1.970360     1.927218     2.436223      28.39
 C      -3.098079     1.802173    -0.647857      77.47
 H      -2.617796     2.444454    -1.507816      24.65
 O      -3.562978     0.589745    -1.218539     230.52
 H      -3.279900     0.680126    -2.179899      24.99
 C      -4.375040     2.682518    -0.144742      96.40
 O      -5.155716     2.864623    -1.410158     293.55
 H      -5.310600     3.788504    -1.389182      31.00
 H      -3.973836     3.713479     0.355386      25.48
 H      -5.073439     2.252521     0.559536      29.55
55
name = lig-etoh-Waterframe_742
 C       5.913569    -1.089541     1.601798      87.19
 H       6.313435    -0.247500     1.068194      22.45
 C       4.807162    -3.225696     1.130724      35.94
 H       4.097576    -3.897697     0.690373      23.22
 C       5.030644    -3.596178     2.502324     -17.27
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 O       4.849399    -4.926449     2.793396     216.81
 C       3.369885    -5.168833     3.246004      97.37
 H       3.209786    -4.802661     4.330528      22.45
 H       3.341560    -6.214078     3.260694      24.02
 H       2.564407    -4.873409     2.428078      27.26
 C       5.729971    -2.712684     3.358620       9.47
 O       5.999704    -3.049858     4.731793     175.80
 H       5.504278    -3.893018     5.049939      20.15
 C       6.225137    -1.513514     2.864972      71.17
 H       6.832034    -0.770664     3.564291      26.84
 C       5.257843    -1.883538     0.689674     -25.31
 C       5.131420    -1.535254    -0.875285      84.96
 H       5.708392    -2.432260    -1.497761      21.32
 O       5.985650    -0.423536    -1.170066     179.03
 H       5.650726     0.495150    -0.670247      22.83
 C       3.679678    -1.356317    -1.314071      96.61
 H       3.123510    -2.244653    -1.097900      27.46
 C       3.316078    -1.099205    -2.811186     112.48
 O       3.516176    -2.281561    -3.570696     301.17
 H       4.198250    -2.032839    -4.181870      27.18
 H       3.917841    -0.196873    -3.142324      25.68
 H       2.327898    -0.814034    -2.932429      26.78
 C      -0.564414    -0.447693     0.073204      51.93
 H      -1.345259    -1.169302     0.380780      21.15
 C       0.128762     1.925396    -0.433619      72.82
 H      -0.250114     3.004372    -0.342613      22.46
 C       1.393576     1.469412    -0.750684       7.00
 O       2.459205     2.269396    -1.037092     176.46
 C       2.249231     3.702756    -1.488115     107.61
 H       3.198956     4.019944    -1.523432      27.47
 H       1.636787     3.653968    -2.513850      24.66
 H       1.767643     4.073720    -0.437265      23.06
 C       1.742957     0.033089    -0.596664      21.79
 O       3.171385    -0.159853    -0.653282     154.31
 C       0.768966    -0.831503    -0.325894      75.77
 H       1.041758    -1.850160    -0.200718      26.10
 C      -0.825578     0.862738    -0.012740      32.57
 C      -2.252263     1.410888     0.617791      65.22
 H      -2.787378     0.629835     1.314625      22.77
 O      -1.972458     2.465371     1.702207     235.89
 H      -1.866639     1.877874     2.531817      26.53
 C      -3.197178     1.840012    -0.610575     102.72
 H      -2.506891     2.297391    -1.117026      28.96
 O      -3.613417     0.540924    -1.299678     223.29
 H      -3.376438     0.709257    -2.251191      25.26
 C      -4.371491     2.594202    -0.233109     120.42
 O      -5.165662     2.928529    -1.352538     301.44
 H      -5.339528     3.830191    -1.512699      32.99
 H      -3.914412     3.731996     0.072805      24.18
 H      -5.077257     2.333111     0.523603      28.66
55
name = lig-etoh-Waterframe_743
 C       5.999001    -1.079275     1.551131      28.27
 H       6.469659    -0.132747     1.380199      26.06
 C       4.795896    -3.142779     1.143189      69.40
 H       4.161789    -3.786020     0.442267      22.15
 C       5.131900    -3.554426     2.415266      30.36
 O       4.843397    -4.846369     2.800397     280.64
 C       3.450035    -5.216661     3.270438      83.07
 H       3.413160    -4.655779     4.261524      21.54
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 H       3.455383    -6.326926     3.128180      20.62
 H       2.644596    -4.767023     2.612056      29.25
 C       5.730975    -2.702009     3.432618       3.50
 O       5.985869    -3.021000     4.654769     134.16
 H       5.469683    -3.873250     5.002708      23.83
 C       6.204209    -1.444687     2.914538      22.20
 H       7.009185    -0.783597     3.365028      17.82
 C       5.217344    -1.947103     0.681905      16.31
 C       5.187001    -1.524001    -0.884019     104.75
 H       5.486523    -2.465880    -1.282552      27.07
 O       5.926059    -0.380140    -1.171019     232.43
 H       5.383221     0.245419    -0.599062      26.52
 C       3.662250    -1.306538    -1.320865      83.46
 H       3.110680    -2.158364    -0.920896      24.25
 C       3.285678    -1.067312    -2.797099     104.44
 O       3.566961    -2.300570    -3.538754     299.37
 H       4.196066    -2.369561    -4.296425      27.74
 H       3.897159    -0.270929    -3.369108      24.67
 H       2.285358    -0.803072    -2.892665      26.06
 C      -0.570681    -0.524177     0.058237      40.70
 H      -1.299666    -1.364453     0.214223      19.52
 C       0.100504     1.992595    -0.443099      55.99
 H       0.177131     3.196852    -0.656497      17.19
 C       1.371492     1.474671    -0.782566      15.36
 O       2.471870     2.284799    -1.077674     205.79
 C       2.230429     3.645693    -1.503477     132.55
 H       3.193314     3.961855    -1.537309      27.25
 H       1.722569     4.254645    -2.298156      25.86
 H       1.807651     4.394602    -0.649118      24.63
 C       1.758979     0.122855    -0.615954      17.73
 O       3.115916    -0.172785    -0.533922     172.37
 C       0.736643    -0.892158    -0.284089      55.90
 H       1.090193    -1.961326    -0.010051      20.93
 C      -0.852713     0.975221     0.090134      34.71
 C      -2.210989     1.486984     0.643715      78.02
 H      -2.738226     0.461653     0.974089      22.79
 O      -1.924440     2.447180     1.685067     266.97
 H      -2.052146     1.866430     2.582091      23.02
 C      -3.205089     1.759451    -0.534827      77.81
 H      -2.634426     2.432749    -1.271758      23.18
 O      -3.613205     0.548599    -1.356198     221.48
 H      -3.503459     0.620401    -2.306794      24.43
 C      -4.410481     2.685755    -0.267376      97.43
 O      -5.238078     2.980619    -1.386289     333.49
 H      -5.150233     3.969856    -1.361520      28.37
 H      -3.884699     3.503354     0.298616      26.86
 H      -4.746089     2.018857     0.633522      28.62
55
name = lig-etoh-Waterframe_744
 C       6.049967    -1.116809     1.529431      62.94
 H       6.531002    -0.254573     0.999750      25.50
 C       4.753520    -3.084127     1.126405      21.11
 H       4.466532    -3.897183     0.327604      20.30
 C       5.187505    -3.517518     2.414335      14.69
 O       4.831645    -4.838533     2.821281     292.02
 C       3.564292    -5.200881     3.247075      92.11
 H       3.209642    -4.980131     4.280949      22.84
 H       3.443183    -6.349717     3.484833      20.44
 H       2.858403    -4.737016     2.652674      30.22
 C       5.731165    -2.630066     3.322974     -17.40
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 O       5.987545    -3.033605     4.695409     132.06
 H       5.459335    -3.944681     4.912858      21.04
 C       6.214561    -1.387919     2.923196      74.87
 H       6.803646    -0.956189     3.689670      23.17
 C       5.269961    -1.836580     0.609556      22.22
 C       5.112032    -1.573020    -0.829241     100.20
 H       5.483534    -2.214663    -1.530098      26.64
 O       5.887729    -0.329914    -1.181468     199.41
 H       5.735048     0.498053    -0.732107      26.18
 C       3.605944    -1.278318    -1.290258      70.98
 H       3.116245    -2.278963    -1.040680      24.15
 C       3.337058    -1.060355    -2.840382      96.34
 O       3.573992    -2.368985    -3.508324     258.78
 H       4.325299    -2.187454    -4.230086      23.28
 H       3.926097    -0.131302    -3.181233      24.65
 H       2.200378    -0.898767    -2.820728      24.13
 C      -0.537206    -0.426131     0.008567      46.69
 H      -1.358506    -1.113020     0.341312      20.38
 C       0.078854     1.901338    -0.430133      63.08
 H      -0.365711     3.037839    -0.492976      19.99
 C       1.373205     1.465529    -0.789657      16.83
 O       2.463513     2.322805    -1.173114     182.84
 C       2.281949     3.717030    -1.429372     104.37
 H       3.364351     4.156095    -1.819146      23.51
 H       1.586334     3.444499    -2.367479      22.80
 H       1.867695     4.239333    -0.608012      26.58
 C       1.709096     0.118979    -0.586604      22.28
 O       3.084319    -0.170957    -0.430720     149.82
 C       0.768810    -0.898499    -0.220571      43.37
 H       1.080682    -2.061382    -0.173596      19.59
 C      -0.866554     1.074782     0.125780      41.60
 C      -2.177166     1.403787     0.610714      84.56
 H      -2.564528     0.554526     1.210342      21.92
 O      -1.928804     2.423830     1.648542     243.60
 H      -2.238511     1.887835     2.540103      23.64
 C      -3.149043     1.791597    -0.647715      49.08
 H      -2.665798     2.425306    -1.617710      21.42
 O      -3.580116     0.572436    -1.326808     236.19
 H      -3.344308     0.866752    -2.176478      25.93
 C      -4.399813     2.681415    -0.153840      96.00
 O      -5.298628     3.048976    -1.398363     250.10
 H      -5.362746     4.120069    -1.539196      27.23
 H      -4.209374     3.551883     0.296644      26.49
 H      -5.372050     2.160347     0.408693      24.28
55
name = lig-etoh-Waterframe_745
 C       6.118483    -1.056277     1.493473      72.17
 H       6.715231    -0.230274     0.988884      24.86
 C       4.802762    -3.061231     1.090590      51.19
 H       4.385538    -3.930024     0.479939      22.69
 C       5.086548    -3.526534     2.388706     -32.23
 O       4.931975    -4.841161     2.840614     333.48
 C       3.542966    -5.181436     3.278414      97.52
 H       3.374093    -4.706317     4.228400      23.37
 H       3.628653    -6.346167     3.030320      20.48
 H       2.848295    -5.015429     2.506061      29.03
 C       5.757426    -2.620024     3.339184     -32.46
 O       5.978051    -3.030681     4.689439     196.50
 H       5.470567    -3.960939     4.883106      20.50
 C       6.236285    -1.364024     2.883501      76.53
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 H       6.570870    -0.707442     3.613160      24.64
 C       5.313782    -1.841160     0.634472       9.48
 C       5.013229    -1.435413    -0.855802      97.45
 H       5.510651    -2.192411    -1.574559      23.65
 O       5.899560    -0.306769    -1.238963     181.25
 H       5.657003     0.422517    -0.654761      28.01
 C       3.561611    -1.298103    -1.223874      85.56
 H       2.896160    -2.207004    -1.112950      25.29
 C       3.379125    -1.094946    -2.786239      92.04
 O       3.588248    -2.380630    -3.487044     256.33
 H       4.387586    -2.249449    -4.211910      22.42
 H       3.981020    -0.292035    -3.227311      25.46
 H       2.244733    -0.778750    -3.116418      23.99
 C      -0.521428    -0.289206     0.026884      64.22
 H      -1.307287    -0.934719     0.416659      20.56
 C       0.064936     1.901208    -0.426984      79.26
 H      -0.338790     2.935074    -0.408685      20.28
 C       1.393862     1.514467    -0.779508      -0.97
 O       2.495657     2.276334    -1.209592     204.17
 C       2.258563     3.744143    -1.448926      95.51
 H       3.346106     4.280881    -1.904295      22.17
 H       1.394691     3.865406    -2.253197      24.77
 H       1.954778     4.197512    -0.621073      28.41
 C       1.716539     0.062547    -0.511996      25.41
 O       3.076230    -0.198610    -0.392347     188.85
 C       0.747418    -0.819831    -0.194022      64.29
 H       0.937102    -1.965212    -0.268840      21.38
 C      -0.790846     0.911973     0.060829      31.47
 C      -2.200410     1.359208     0.566093      66.66
 H      -2.713102     0.548657     0.973978      22.83
 O      -1.988016     2.420992     1.601482     251.16
 H      -2.166893     1.975162     2.586297      24.46
 C      -3.182699     1.893766    -0.688341      63.02
 H      -2.387529     2.570537    -1.234916      20.79
 O      -3.514271     0.618681    -1.294932     259.03
 H      -3.375650     0.549143    -2.234576      26.71
 C      -4.486784     2.674833    -0.152593      90.62
 O      -5.319613     3.087253    -1.393620     266.69
 H      -5.325570     4.212807    -1.417274      25.51
 H      -4.254555     3.568014     0.379240      25.27
 H      -5.225265     1.985044     0.490445      26.01
55
name = lig-etoh-Waterframe_746
 C       6.169769    -0.993458     1.458732      46.98
 H       6.676760    -0.011441     1.309383      23.78
 C       4.865295    -3.125984     1.088526      91.22
 H       4.187529    -3.550509     0.378587      23.05
 C       5.050994    -3.468234     2.438287       7.26
 O       5.014911    -4.826707     2.845908     155.05
 C       3.546587    -5.216288     3.216396      93.90
 H       3.299916    -4.685477     4.112038      25.87
 H       3.589471    -6.328857     3.509855      22.74
 H       2.768176    -4.819599     2.437621      27.88
 C       5.751547    -2.664333     3.366988      14.78
 O       5.962920    -2.998721     4.636565     138.14
 H       5.547659    -3.945667     4.930094      22.74
 C       6.249435    -1.366941     2.843990      24.99
 H       6.619651    -0.491935     3.362624      20.46
 C       5.343757    -1.845464     0.624781     -46.90
 C       5.056192    -1.347103    -0.895518      84.11
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 H       5.227538    -2.462582    -1.341241      24.56
 O       5.894534    -0.308112    -1.311256     250.42
 H       5.603636     0.482230    -0.767451      27.29
 C       3.497831    -1.304982    -1.212400      87.16
 H       3.073094    -2.227680    -0.754819      24.69
 C       3.401779    -1.113634    -2.761433     101.95
 O       3.603298    -2.367785    -3.458365     281.52
 H       4.318427    -2.407517    -4.244048      25.26
 H       4.203260    -0.538432    -3.079720      25.86
 H       2.362893    -0.637649    -2.998515      25.19
 C      -0.546158    -0.493764     0.112665      32.84
 H      -1.272382    -1.262738     0.367255      20.22
 C       0.143536     1.989283    -0.453881      45.37
 H       0.039449     2.978350    -0.519910      21.08
 C       1.424108     1.489768    -0.719049      15.85
 O       2.525255     2.250130    -1.233304     177.28
 C       2.175937     3.740402    -1.498991     110.29
 H       3.260802     4.088523    -1.832339      23.29
 H       1.493281     4.242002    -2.000642      28.95
 H       2.119339     4.244080    -0.497584      26.05
 C       1.773561     0.176083    -0.451899      29.10
 O       3.076736    -0.236662    -0.404210     206.38
 C       0.741698    -0.809811    -0.211886      73.00
 H       0.886821    -1.874738    -0.043437      21.81
 C      -0.892974     1.025391    -0.005491      40.80
 C      -2.258922     1.396011     0.509522      84.46
 H      -2.784116     0.516581     0.757732      25.65
 O      -2.078274     2.417516     1.535469     237.58
 H      -1.985542     1.756012     2.414389      22.75
 C      -3.185430     1.980015    -0.583445      89.89
 H      -2.736869     2.667215    -1.235727      26.14
 O      -3.447016     0.667844    -1.294101     219.16
 H      -3.323853     0.648547    -2.250612      25.19
 C      -4.564969     2.651441    -0.255894     106.96
 O      -5.316164     3.094747    -1.343942     326.26
 H      -5.200471     4.131449    -1.317280      27.33
 H      -4.149933     3.449645     0.536321      26.06
 H      -4.843907     1.931405     0.346948      33.12
55
name = lig-etoh-Waterframe_747
 C       6.140207    -1.014736     1.492767      86.37
 H       6.332503    -0.029067     1.095543      29.02
 C       4.912447    -3.068532     1.061024      52.64
 H       4.241382    -3.664544     0.504157      23.41
 C       5.105193    -3.471911     2.467712     -25.79
 O       4.977311    -4.824727     2.862332     213.38
 C       3.617781    -5.228921     3.181493     110.52
 H       3.223124    -4.645303     4.039528      26.15
 H       3.434517    -6.198203     3.505213      24.04
 H       2.894587    -4.986956     2.228621      26.87
 C       5.757560    -2.572001     3.305638      11.76
 O       5.966111    -2.964299     4.639566     141.73
 H       5.609426    -3.929367     4.887279      21.35
 C       6.252805    -1.387766     2.811127      64.92
 H       6.860960    -0.849396     3.652173      18.90
 C       5.402068    -1.779317     0.572643     -35.30
 C       5.086299    -1.473583    -0.839057      64.06
 H       5.548107    -2.127640    -1.722396      23.08
 O       5.879678    -0.331115    -1.402454     213.92
 H       5.804207     0.569586    -1.009489      28.29
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 C       3.556002    -1.332282    -1.194735      83.90
 H       3.176278    -2.319767    -0.909579      25.82
 C       3.434186    -1.113790    -2.740356     111.15
 O       3.573980    -2.395558    -3.428542     305.42
 H       4.210601    -2.078949    -4.150812      25.23
 H       4.236071    -0.408049    -2.849974      24.89
 H       2.567728    -0.615020    -3.021013      27.60
 C      -0.620731    -0.495326     0.147845      36.40
 H      -1.285632    -1.326921     0.301431      20.97
 C       0.139050     1.980719    -0.441079      52.16
 H       0.006021     2.973070    -0.601855      21.01
 C       1.500126     1.509631    -0.674662       7.90
 O       2.475146     2.297225    -1.279917     203.49
 C       2.227064     3.719757    -1.447317     102.59
 H       3.014914     4.019408    -1.996371      26.48
 H       1.327515     3.765219    -2.058946      25.89
 H       2.240745     4.173006    -0.296266      23.64
 C       1.748261     0.159130    -0.390935      26.13
 O       3.092317    -0.203130    -0.424961     194.13
 C       0.789115    -0.841215    -0.180574      52.18
 H       1.292807    -1.713117    -0.020521      22.68
 C      -0.929013     1.067304    -0.078934      16.61
 C      -2.323174     1.516943     0.436545      81.27
 H      -2.749607     0.572917     0.951262      22.68
 O      -2.186453     2.386065     1.513900     232.21
 H      -1.865560     1.834692     2.369077      25.55
 C      -3.203424     2.027497    -0.620710     106.50
 H      -2.776559     2.646224    -1.323304      27.03
 O      -3.401741     0.720709    -1.328721     244.41
 H      -3.190875     1.113605    -2.164900      25.52
 C      -4.509642     2.575206    -0.226469     101.65
 O      -5.323259     3.094734    -1.305716     293.62
 H      -5.332322     4.029811    -1.430121      32.11
 H      -4.532824     3.581126     0.496392      23.00
 H      -5.309296     1.827393     0.207572      26.57
55
name = lig-etoh-Waterframe_748
 C       6.065419    -0.975497     1.471073      44.97
 H       6.460646    -0.038769     1.112841      20.74
 C       4.938201    -3.018264     1.101719      73.71
 H       4.622525    -3.840106     0.479831      22.02
 C       5.173306    -3.480736     2.345616       3.20
 O       4.929601    -4.816350     2.881572     260.30
 C       3.610839    -5.203727     3.146179     111.85
 H       3.147575    -4.455644     3.860622      22.52
 H       3.739018    -6.220915     3.280615      22.27
 H       3.047168    -5.289684     2.154224      27.11
 C       5.748661    -2.587296     3.325099     -11.19
 O       5.987944    -2.895293     4.641271     128.78
 H       5.644649    -3.866993     4.763972      18.92
 C       6.309111    -1.369142     2.860537      13.31
 H       7.075075    -0.890016     3.640493      24.43
 C       5.424233    -1.849388     0.580715      30.69
 C       5.159266    -1.519326    -0.902388      79.78
 H       5.497976    -2.434388    -1.426021      25.75
 O       5.884538    -0.350230    -1.491193     239.92
 H       5.588317     0.371056    -0.848675      24.88
 C       3.650836    -1.391261    -1.185000      83.65
 H       2.969463    -2.211898    -1.048743      26.55
 C       3.461090    -1.085128    -2.671327     101.86
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 O       3.545520    -2.373734    -3.413293     296.44
 H       4.129205    -2.444136    -4.214974      27.19
 H       4.270475    -0.405587    -3.138005      23.77
 H       2.540569    -0.688957    -2.922433      26.99
 C      -0.561690    -0.322589     0.064635      30.86
 H      -1.415354    -0.931411     0.322744      20.44
 C       0.116711     1.899096    -0.426098      77.34
 H      -0.375339     2.930701    -0.578532      20.31
 C       1.454223     1.572361    -0.636589      -5.03
 O       2.463555     2.295360    -1.295615     230.73
 C       2.272562     3.679236    -1.403576     119.23
 H       2.858232     4.145149    -2.070196      27.24
 H       1.129994     3.683268    -1.900627      24.56
 H       2.098498     4.443725    -0.449345      26.49
 C       1.757130     0.105167    -0.378482      13.90
 O       3.140210    -0.167017    -0.446413     159.00
 C       0.746023    -0.828302    -0.056970      41.59
 H       1.110642    -1.825768     0.002688      20.97
 C      -0.887407     0.937643    -0.093881      46.83
 C      -2.294096     1.553652     0.434328      52.73
 H      -2.956356     0.554149     0.690660      22.13
 O      -2.278443     2.439335     1.561328     234.62
 H      -1.932200     1.831524     2.346695      25.36
 C      -3.240131     2.018525    -0.726504      90.95
 H      -2.619907     2.843404    -1.270315      23.56
 O      -3.376316     0.810812    -1.425241     236.84
 H      -3.351194     0.738205    -2.443070      22.76
 C      -4.585474     2.587691    -0.131850      68.82
 O      -5.355962     3.077745    -1.346059     278.34
 H      -5.218524     3.998609    -1.284577      30.53
 H      -4.379495     3.278540     0.795865      24.64
 H      -5.339784     1.602120     0.275935      26.20
55
name = lig-etoh-Waterframe_749
 C       6.052614    -0.919152     1.521275      34.95
 H       6.647014    -0.081180     1.211073      18.39
 C       4.943582    -3.129292     1.048854      41.91
 H       4.770666    -3.808105     0.181911      20.50
 C       5.242828    -3.493335     2.409960      29.45
 O       4.969165    -4.743911     2.853619     241.67
 C       3.536786    -5.222967     3.049425      96.38
 H       2.875069    -4.697102     3.830972      23.97
 H       3.748512    -6.151239     3.708310      21.97
 H       2.970426    -5.231225     2.182959      28.08
 C       5.787698    -2.594482     3.327797      21.56
 O       5.996835    -2.859774     4.637064     200.21
 H       5.749658    -3.765015     5.004664      18.38
 C       6.338362    -1.354981     2.842760      23.10
 H       6.953980    -0.555344     3.351546      28.81
 C       5.444932    -1.829219     0.594495     -11.74
 C       5.229224    -1.583204    -0.962014     100.08
 H       5.396046    -2.479624    -1.373175      28.02
 O       5.870244    -0.407691    -1.511084     252.81
 H       5.606046     0.403443    -0.921777      24.27
 C       3.686154    -1.373441    -1.222362      66.29
 H       3.132307    -2.239971    -0.791132      25.01
 C       3.481427    -1.082640    -2.707404      92.55
 O       3.483751    -2.374495    -3.396163     282.49
 H       4.217068    -2.262065    -4.072621      25.82
 H       4.277036    -0.338737    -3.211852      22.20
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 H       2.409368    -0.688781    -2.659125      24.95
 C      -0.536283    -0.340018     0.019088      38.99
 H      -1.347898    -0.994423     0.405162      20.45
 C       0.066440     1.892459    -0.436558      50.87
 H      -0.287690     3.079903    -0.565277      18.27
 C       1.400746     1.481579    -0.612567      14.20
 O       2.493805     2.249584    -1.239772     138.05
 C       2.158419     3.713992    -1.423731     107.63
 H       3.063853     4.111550    -2.104589      24.39
 H       1.170286     4.226517    -1.850209      24.33
 H       2.434307     4.097963    -0.419731      26.68
 C       1.805342     0.145410    -0.398554      17.72
 O       3.198927    -0.160432    -0.467638     132.50
 C       0.775970    -0.794997     0.036012      60.53
 H       0.529292    -1.901111     0.175482      20.20
 C      -0.902197     1.046056    -0.038292      32.10
 C      -2.287920     1.468636     0.394598      70.55
 H      -2.827777     0.537118     0.779067      20.73
 O      -2.333861     2.492528     1.605576     228.06
 H      -2.201409     1.884043     2.420749      25.22
 C      -3.215592     2.058615    -0.751658      68.51
 H      -2.910303     3.047479    -1.414523      21.50
 O      -3.392586     0.849478    -1.563721     220.01
 H      -3.427556     0.932652    -2.623780      20.99
 C      -4.669656     2.540941    -0.135636      90.30
 O      -5.378412     3.077842    -1.324159     307.61
 H      -5.264682     4.034795    -1.375019      32.24
 H      -4.455288     3.200897     0.578557      29.05
 H      -4.968991     1.561950     0.403847      29.40
55
name = lig-etoh-Waterframe_750
 C       6.079172    -0.932347     1.516806      98.17
 H       6.447714     0.008684     1.108719      24.79
 C       5.068315    -3.147396     0.980473      33.85
 H       4.559860    -3.987822     0.356739      20.64
 C       5.240914    -3.469885     2.405887     -32.43
 O       4.961276    -4.750474     2.865249     252.52
 C       3.496334    -5.235008     3.013313      94.38
 H       3.006646    -4.408941     3.585862      25.95
 H       3.445129    -6.342796     3.580764      22.31
 H       3.066823    -5.448138     2.092268      29.07
 C       5.889365    -2.535673     3.317177       4.52
 O       6.016073    -2.840793     4.686747     153.27
 H       5.676796    -3.719712     4.950388      22.61
 C       6.313172    -1.318580     2.801754      88.91
 H       6.679099    -0.682689     3.574381      25.27
 C       5.434361    -1.830026     0.588958      -3.10
 C       5.209813    -1.582001    -0.910751      95.00
 H       5.634766    -2.308074    -1.698288      24.49
 O       5.903430    -0.490466    -1.512164     205.00
 H       5.725600     0.421062    -1.040227      26.89
 C       3.716078    -1.321186    -1.225410      83.12
 H       3.228991    -2.297342    -0.890916      24.15
 C       3.406171    -1.121680    -2.720004      95.77
 O       3.426329    -2.363184    -3.411634     290.33
 H       4.152004    -2.309708    -4.092907      25.92
 H       4.162416    -0.316977    -3.053284      23.06
 H       2.361008    -0.530498    -2.948322      23.36
 C      -0.581294    -0.353740     0.078124      50.54
 H      -1.198757    -1.261936     0.322968      20.72
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 C       0.083025     1.998974    -0.463190      47.92
 H       0.105412     3.206136    -0.592350      16.41
 C       1.431776     1.406304    -0.669189       2.71
 O       2.423517     2.228476    -1.174143     143.90
 C       2.163556     3.768557    -1.389994      95.48
 H       3.131634     3.902683    -2.181087      22.84
 H       1.167438     3.920931    -1.820449      24.72
 H       2.388855     4.112362    -0.495573      28.65
 C       1.857396     0.079217    -0.375879      21.83
 O       3.249727    -0.151709    -0.483621     181.53
 C       0.789987    -0.757532     0.047739      50.32
 H       1.241785    -1.902339     0.308195      19.51
 C      -0.951805     1.126175     0.037525      33.24
 C      -2.350147     1.473880     0.397395      90.51
 H      -2.742492     0.611586     0.766174      24.33
 O      -2.366201     2.481286     1.594596     257.50
 H      -2.466715     1.947129     2.404911      25.99
 C      -3.256392     2.075148    -0.719917      74.60
 H      -2.727038     2.890717    -1.365910      22.63
 O      -3.439875     0.890488    -1.702833     227.10
 H      -3.197807     1.445451    -2.519405      22.05
 C      -4.614011     2.488938    -0.223816     126.99
 O      -5.426512     3.046287    -1.258912     298.54
 H      -5.349434     4.033213    -1.305482      31.94
 H      -4.621507     3.317950     0.420478      26.77
 H      -5.264397     1.780889     0.088107      31.16
55
name = lig-etoh-Waterframe_751
 C       6.080842    -0.959302     1.378719      39.24
 H       6.132864     0.118095     1.116532      27.27
 C       5.201546    -3.147159     1.053520      78.82
 H       4.548431    -3.853715     0.428826      23.72
 C       5.246082    -3.423861     2.350998      -7.27
 O       4.914561    -4.829738     2.913764     153.29
 C       3.503099    -5.194095     2.956523     107.84
 H       2.897497    -4.365430     3.284733      29.31
 H       3.509022    -6.216291     3.574941      23.29
 H       3.192471    -5.419201     1.893489      27.21
 C       5.918866    -2.591246     3.311044       3.00
 O       6.035450    -2.811564     4.692758     144.10
 H       5.647393    -3.657573     4.793942      23.54
 C       6.291046    -1.261309     2.872246      20.17
 H       6.609694    -0.635083     3.625975      17.65
 C       5.451562    -1.880324     0.539115      13.84
 C       5.167177    -1.506670    -0.905445      97.77
 H       5.503814    -2.661331    -1.413547      23.66
 O       6.012291    -0.502909    -1.501440     184.64
 H       5.730382     0.382434    -1.016299      26.76
 C       3.669785    -1.339930    -1.224084      87.27
 H       3.000631    -2.189469    -0.946171      26.22
 C       3.331764    -1.085466    -2.719225     102.46
 O       3.374316    -2.370795    -3.462128     290.21
 H       4.050668    -2.424192    -4.153118      28.33
 H       4.108713    -0.577530    -3.176541      27.37
 H       2.256996    -0.684445    -2.918372      25.35
 C      -0.562853    -0.281531     0.191450      47.92
 H      -1.448657    -0.964349     0.329210      21.28
 C       0.175912     1.977123    -0.440074      77.73
 H      -0.084029     3.057157    -0.470595      22.33
 C       1.400225     1.442415    -0.730916      15.12
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 O       2.380911     2.269246    -1.136269     207.19
 C       2.235292     3.678529    -1.345811     121.34
 H       2.910357     4.142618    -2.217217      24.97
 H       1.326747     3.768323    -1.803438      27.79
 H       2.134803     4.486949    -0.558471      25.94
 C       1.853037     0.079415    -0.363099      18.91
 O       3.272378    -0.153727    -0.474126     163.98
 C       0.851498    -0.760690     0.025028      63.55
 H       1.332740    -1.781387     0.385886      23.04
 C      -0.896567     1.062298     0.045410      36.03
 C      -2.442235     1.542469     0.483187      80.05
 H      -2.957444     0.641851     0.694536      26.37
 O      -2.400351     2.438658     1.541284     304.72
 H      -2.466200     1.883847     2.299185      27.58
 C      -3.261441     1.986458    -0.723487     111.72
 H      -2.682528     2.796935    -0.995441      26.15
 O      -3.488320     1.013684    -1.755661     267.34
 H      -3.199514     1.075475    -2.782274      22.65
 C      -4.614030     2.510161    -0.285140      91.50
 O      -5.510591     3.043355    -1.270031     287.56
 H      -5.317166     4.042292    -1.236094      29.69
 H      -4.419916     3.159517     0.805176      24.14
 H      -5.163227     1.630015     0.116597      28.92
55
name = lig-etoh-Waterframe_752
 C       6.067119    -0.952411     1.436616      56.26
 H       6.132402     0.107384     1.064468      28.07
 C       5.213265    -3.178511     1.040513      40.82
 H       4.833796    -3.901083     0.296099      25.69
 C       5.304158    -3.536721     2.483684     -20.25
 O       4.909733    -4.814791     2.945366     273.92
 C       3.517089    -5.143489     2.845184     122.01
 H       2.773344    -4.524447     3.273955      30.20
 H       3.352916    -5.855512     3.600021      26.98
 H       3.151886    -5.449080     1.757092      28.02
 C       5.922618    -2.553784     3.318197      20.55
 O       6.032222    -2.817621     4.626158     146.32
 H       5.795756    -3.628189     5.064866      23.35
 C       6.231970    -1.263164     2.802660      66.12
 H       6.625101    -0.447646     3.350001      18.40
 C       5.533832    -1.860785     0.508306      -0.73
 C       5.137402    -1.549625    -0.940857      80.29
 H       5.285383    -2.569567    -1.573401      22.84
 O       6.101285    -0.499084    -1.466915     171.16
 H       5.834424     0.426192    -1.072013      26.86
 C       3.575099    -1.337912    -1.244934      76.21
 H       3.092915    -2.213786    -0.800905      27.23
 C       3.309740    -1.095629    -2.774866     118.22
 O       3.296827    -2.406894    -3.501763     291.48
 H       4.082187    -2.236353    -4.040291      26.13
 H       3.913740    -0.366498    -3.195242      28.40
 H       2.359137    -0.665016    -2.688894      28.14
 C      -0.467786    -0.263440     0.291994      34.52
 H      -1.308267    -0.891965     0.637036      20.90
 C       0.098070     1.890962    -0.345372      73.62
 H      -0.141450     2.844532    -0.467729      23.76
 C       1.410924     1.491778    -0.729876      12.90
 O       2.488070     2.337271    -1.112510     192.97
 C       2.191848     3.647086    -1.394995     107.81
 H       3.104496     3.932123    -1.872093      24.58
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 H       1.312063     3.801426    -1.941908      26.45
 H       2.189565     4.355095    -0.247226      23.03
 C       1.836911     0.199309    -0.413185      16.13
 O       3.221203    -0.140766    -0.442912     123.65
 C       0.846498    -0.792694     0.052442      53.38
 H       0.751267    -1.770140     0.325521      24.50
 C      -0.857065     1.035697     0.038994      31.61
 C      -2.432220     1.435700     0.478827      56.89
 H      -2.973355     0.445770     0.943640      22.29
 O      -2.444080     2.418613     1.529026     269.18
 H      -2.207477     1.997384     2.308064      30.44
 C      -3.222495     2.040301    -0.812608     101.63
 H      -2.760980     2.906255    -1.206131      24.48
 O      -3.542946     1.079933    -1.755237     269.98
 H      -3.176728     1.151352    -2.736169      24.03
 C      -4.692016     2.465331    -0.243648      73.05
 O      -5.558836     3.096992    -1.261004     254.11
 H      -5.361633     4.108870    -1.466467      29.38
 H      -4.379098     3.320050     0.660599      22.57
 H      -4.976953     1.417535     0.176984      27.32
55
name = lig-etoh-Waterframe_753
 C       6.005524    -0.909711     1.448235      46.98
 H       6.451788     0.077500     1.186116      15.86
 C       5.212098    -3.212982     1.051069      24.88
 H       5.058735    -4.020543     0.406825      15.79
 C       5.382134    -3.579677     2.440756      30.09
 O       4.933492    -4.759940     2.980298     201.84
 C       3.462552    -5.118646     2.781146      96.78
 H       2.993451    -4.121285     2.985836      23.99
 H       3.314711    -5.953045     3.318645      26.89
 H       3.284802    -5.566535     1.700558      24.36
 C       5.858130    -2.563106     3.303775       9.56
 O       6.061101    -2.791124     4.635540     143.47
 H       5.806162    -3.752384     4.929355      17.55
 C       6.196832    -1.278311     2.741102      49.12
 H       6.623071    -0.509298     3.465527      27.88
 C       5.564562    -1.936933     0.532249       8.55
 C       5.153175    -1.593749    -0.995253      87.77
 H       5.436966    -2.189012    -1.695869      28.36
 O       6.123273    -0.524513    -1.438622     151.80
 H       5.831964     0.382685    -1.035397      25.63
 C       3.599541    -1.289113    -1.229767      76.13
 H       3.096882    -2.205561    -0.921867      28.81
 C       3.230872    -1.133666    -2.761550     108.05
 O       3.252417    -2.374372    -3.526036     266.63
 H       4.037940    -2.532218    -4.171462      24.80
 H       3.883716    -0.314565    -3.181693      27.66
 H       2.251544    -0.794855    -2.898428      29.17
 C      -0.422826    -0.335244     0.390800      48.79
 H      -0.877816    -1.132023     0.933388      23.34
 C       0.061371     1.957265    -0.337974      54.60
 H      -0.201431     2.911182    -0.521874      23.03
 C       1.479776     1.538949    -0.659837     -14.60
 O       2.568992     2.302069    -1.080801     175.09
 C       2.195954     3.744709    -1.419659     100.85
 H       3.054844     4.126782    -1.739570      26.32
 H       1.328127     3.865289    -2.101095      25.90
 H       1.980424     4.085767    -0.285359      25.22
 C       1.795835     0.161141    -0.428347      13.55
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 O       3.136240    -0.120957    -0.443663     147.51
 C       0.809951    -0.744916     0.076015      64.09
 H       1.046134    -1.747772     0.095127      26.63
 C      -0.965975     0.983065     0.121360      39.45
 C      -2.325155     1.335857     0.380212      68.43
 H      -2.849419     0.283333     0.749871      22.70
 O      -2.476934     2.408134     1.537054     171.80
 H      -1.998055     2.095862     2.231695      29.74
 C      -3.264130     2.147595    -0.803062      70.32
 H      -2.701271     2.986996    -1.416009      23.00
 O      -3.586640     1.065566    -1.776932     230.84
 H      -3.230695     1.479170    -2.637055      25.10
 C      -4.661864     2.489420    -0.223387      99.35
 O      -5.583998     3.127818    -1.220943     230.14
 H      -5.144211     4.096138    -1.221954      28.14
 H      -4.806672     3.204682     0.568821      25.77
 H      -5.472839     1.723017     0.063675      25.61
55
name = lig-etoh-Waterframe_754
 C       5.953722    -0.931000     1.362475      -1.05
 H       6.442361    -0.046507     0.902948      12.83
 C       5.249100    -3.270965     1.040677      83.77
 H       4.935476    -4.047578     0.406558      21.71
 C       5.418927    -3.531145     2.344949      39.21
 O       4.951699    -4.767254     3.012120     146.10
 C       3.487573    -5.074908     2.693849      97.63
 H       2.791396    -4.101718     2.721764      25.93
 H       3.139904    -5.843296     3.433800      26.11
 H       3.459226    -5.300400     1.632160      27.07
 C       5.809258    -2.564012     3.279907       7.69
 O       6.093818    -2.754999     4.653409     123.80
 H       5.732007    -3.733883     4.862097      15.89
 C       6.175553    -1.316409     2.818663      -0.64
 H       6.599847    -0.634363     3.694393      25.65
 C       5.513024    -1.993800     0.500915       0.31
 C       5.231327    -1.567301    -0.993684      91.94
 H       5.427902    -2.460581    -1.635378      26.10
 O       6.086110    -0.532810    -1.410609     159.78
 H       5.849662     0.354147    -0.940947      23.21
 C       3.648515    -1.278655    -1.233417      76.45
 H       3.104298    -2.168492    -0.873262      28.20
 C       3.162616    -1.123669    -2.745886      90.46
 O       3.229997    -2.366013    -3.531024     228.14
 H       4.132369    -2.282174    -4.144580      22.16
 H       3.958356    -0.463253    -3.331111      24.54
 H       2.081389    -0.833661    -2.872146      26.30
 C      -0.517492    -0.393679     0.511757      35.66
 H      -1.151167    -1.107708     1.010786      22.41
 C       0.105643     1.978799    -0.378685      85.15
 H      -0.334510     3.012550    -0.559558      20.57
 C       1.434492     1.566655    -0.540711       1.00
 O       2.573037     2.290064    -1.080828     155.10
 C       2.247135     3.796331    -1.344051     109.92
 H       3.011790     4.467239    -1.727008      26.16
 H       1.402125     3.663246    -2.185141      25.81
 H       1.743328     4.332774    -0.699327      31.95
 C       1.740701     0.166986    -0.420868      17.02
 O       3.117646    -0.139660    -0.484565     150.51
 C       0.896805    -0.733847     0.048770      56.80
 H       1.493475    -1.698472     0.141360      25.80
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 C      -0.873096     0.937490     0.176821      41.73
 C      -2.369195     1.399719     0.333193      81.12
 H      -3.000281     0.509319     0.381480      25.62
 O      -2.483847     2.350885     1.504154     264.77
 H      -1.997043     1.988507     2.171406      30.70
 C      -3.330710     2.078058    -0.733133      78.41
 H      -2.739415     3.088534    -1.074809      23.32
 O      -3.594318     1.083453    -1.799818     224.61
 H      -3.548016     1.296885    -2.794612      24.27
 C      -4.732706     2.585786    -0.193175     103.50
 O      -5.548704     3.180383    -1.187076     278.67
 H      -5.427066     4.258503    -1.337899      26.65
 H      -4.564191     3.025258     0.677356      29.43
 H      -5.075788     1.509390     0.105498      28.19
55
name = lig-etoh-Waterframe_755
 C       5.963566    -1.069466     1.406761      85.62
 H       6.125800    -0.140212     0.905641      30.23
 C       5.264128    -3.326623     0.912398      36.74
 H       4.713334    -4.062143     0.287702      25.40
 C       5.376879    -3.579377     2.410887     -22.59
 O       4.944627    -4.760091     3.001473     246.65
 C       3.566222    -4.991419     2.581179     112.12
 H       2.852120    -4.123097     2.794551      27.55
 H       3.056187    -5.727362     3.414424      25.46
 H       3.484920    -5.487204     1.677227      28.63
 C       5.838747    -2.533842     3.315887      13.21
 O       6.086787    -2.740171     4.598900     158.52
 H       5.877444    -3.569199     5.210273      20.12
 C       6.136617    -1.262070     2.757275      75.17
 H       6.564411    -0.455957     3.483240      20.67
 C       5.454808    -1.954559     0.465465     -18.68
 C       5.224706    -1.570919    -0.950034      60.51
 H       5.357867    -2.674201    -1.581973      20.79
 O       6.058183    -0.512226    -1.410561     204.48
 H       5.770007     0.341263    -0.921373      26.92
 C       3.633702    -1.315749    -1.273423      69.95
 H       3.266391    -2.258790    -0.803687      27.42
 C       3.167549    -1.121755    -2.754107      97.53
 O       3.250112    -2.371761    -3.514179     230.73
 H       4.165670    -2.202368    -4.093334      21.70
 H       3.669541    -0.168128    -3.253656      25.21
 H       2.135356    -0.618649    -2.522379      25.64
 C      -0.478619    -0.407554     0.530169      35.36
 H      -1.392695    -0.953136     0.801427      21.46
 C       0.085130     1.891421    -0.355112      65.61
 H      -0.280284     3.039869    -0.620219      20.33
 C       1.441185     1.616358    -0.508584      18.60
 O       2.515651     2.367800    -1.037946     184.46
 C       2.231974     3.775350    -1.318537      94.08
 H       3.369115     4.211910    -1.546817      23.13
 H       1.671311     3.642536    -2.411034      23.61
 H       1.682705     4.321981    -0.586764      27.69
 C       1.784851     0.247481    -0.403710       4.92
 O       3.166445    -0.139020    -0.536602     109.61
 C       0.832367    -0.805804     0.117318      39.75
 H       1.174229    -1.890671     0.544654      23.82
 C      -0.772453     0.968123     0.162174      12.65
 C      -2.496550     1.461336     0.348734      77.22
 H      -2.923486     0.559893     0.650718      25.15
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 O      -2.474877     2.267974     1.455258     286.68
 H      -2.199638     1.781402     2.190810      30.41
 C      -3.331675     2.071498    -0.755040      90.01
 H      -2.876824     2.998489    -1.202987      24.50
 O      -3.591137     1.092917    -1.794140     232.94
 H      -3.596041     1.534546    -2.709559      24.32
 C      -4.736636     2.581238    -0.124101      88.50
 O      -5.529166     3.231190    -1.166269     274.07
 H      -5.287469     4.287138    -1.175844      26.75
 H      -4.389771     3.231761     0.759596      24.47
 H      -5.303001     1.669698     0.112115      28.16
55
name = lig-etoh-Waterframe_756
 C       5.962666    -1.098937     1.380660      48.44
 H       5.983020    -0.077699     1.238874      29.33
 C       5.236982    -3.332593     0.934631      72.91
 H       4.801953    -4.116085     0.203057      24.99
 C       5.350998    -3.548828     2.367429      12.35
 O       4.924388    -4.753532     2.965664     209.33
 C       3.581048    -4.973527     2.550958     116.92
 H       3.194401    -3.983234     2.426151      29.14
 H       3.274965    -5.838122     3.295711      25.79
 H       3.492981    -5.470771     1.597245      28.12
 C       5.863063    -2.564886     3.249489      17.84
 O       6.096765    -2.693673     4.621411     127.75
 H       5.815767    -3.693573     4.754587      22.05
 C       6.115725    -1.239761     2.739129      42.92
 H       6.450102    -0.289946     3.175455      19.08
 C       5.411889    -2.054114     0.495848      13.49
 C       5.100143    -1.588047    -0.956508      72.63
 H       5.629419    -2.289196    -1.787292      22.07
 O       6.034974    -0.485388    -1.428382     174.09
 H       5.707823     0.390529    -1.045629      26.98
 C       3.637923    -1.366485    -1.285080      82.59
 H       2.990979    -2.245790    -0.981078      27.00
 C       3.182323    -1.090209    -2.696649      98.57
 O       3.301686    -2.324288    -3.489132     242.69
 H       4.127597    -2.496916    -4.105688      24.59
 H       3.704735    -0.268568    -3.178391      27.44
 H       2.020675    -1.100699    -2.760260      26.47
 C      -0.434046    -0.296372     0.433825      49.72
 H      -1.140553    -1.157890     0.690036      22.93
 C       0.084193     1.889889    -0.324336      71.06
 H      -0.352281     2.990538    -0.665463      21.37
 C       1.511138     1.557709    -0.544598       1.98
 O       2.429894     2.440030    -0.940819     225.41
 C       2.253687     3.733722    -1.373997     101.80
 H       3.402474     4.130583    -1.179659      22.88
 H       1.843464     4.157140    -2.369833      24.90
 H       1.719166     4.255416    -0.407937      25.27
 C       1.833255     0.143523    -0.298434      -3.71
 O       3.224662    -0.105575    -0.574424     122.62
 C       0.801204    -0.797146     0.238410      52.52
 H       1.029897    -1.966018     0.380332      23.98
 C      -0.910354     0.977271     0.131937      33.15
 C      -2.460996     1.366089     0.367770      65.46
 H      -2.917263     0.324820     0.677028      23.99
 O      -2.472239     2.262308     1.490484     244.19
 H      -2.416715     1.721441     2.267954      27.84
 C      -3.364880     2.116419    -0.798031      88.71
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 H      -2.882292     2.877081    -1.272511      25.34
 O      -3.584118     1.097307    -1.782843     255.00
 H      -3.543937     1.672699    -2.608650      25.14
 C      -4.691022     2.548523    -0.097685     112.69
 O      -5.506812     3.269073    -1.127057     310.45
 H      -5.133898     4.177091    -1.237069      31.38
 H      -4.718090     3.471757     0.730601      22.94
 H      -5.420550     2.005591     0.349822      27.89
55
name = lig-etoh-Waterframe_757
 C       5.891517    -1.027805     1.308945      66.23
 H       5.918905    -0.090803     0.778596      28.79
 C       5.166158    -3.361050     1.016347      69.28
 H       4.999741    -4.289430     0.353837      23.01
 C       5.381383    -3.521012     2.322953      18.92
 O       4.959692    -4.739923     2.923701     208.53
 C       3.560815    -5.029981     2.508356     115.55
 H       2.916330    -4.178247     2.457583      29.24
 H       2.919920    -5.490432     3.262708      27.77
 H       3.645773    -5.406243     1.430834      26.00
 C       5.908428    -2.524437     3.212405      19.70
 O       6.081845    -2.684690     4.584866      59.48
 H       5.906768    -3.641368     5.031316      23.88
 C       6.117722    -1.281742     2.716142      55.56
 H       6.326534    -0.593937     3.470737      20.34
 C       5.415118    -2.068750     0.456225     -27.25
 C       5.098909    -1.598991    -1.034380      78.42
 H       5.217769    -2.472959    -1.647234      24.96
 O       5.960875    -0.454394    -1.423772     165.98
 H       5.717608     0.437634    -1.073935      28.25
 C       3.573562    -1.359304    -1.253737      89.16
 H       2.941936    -2.189524    -0.841506      26.41
 C       3.192241    -1.129405    -2.721566     114.81
 O       3.365107    -2.326357    -3.490204     285.57
 H       4.286784    -2.164983    -3.867958      24.98
 H       3.680565    -0.322468    -3.094290      28.62
 H       2.105847    -0.856225    -2.716360      27.33
 C      -0.519177    -0.262759     0.348628      38.70
 H      -1.147952    -1.112555     0.762141      23.30
 C       0.103132     1.911588    -0.325795      60.72
 H      -0.110052     2.959403    -0.628474      22.49
 C       1.370706     1.410452    -0.526526       2.86
 O       2.411952     2.394583    -0.876293     153.84
 C       2.314850     3.840340    -1.293056      93.05
 H       3.291964     4.387499    -1.315997      23.63
 H       1.964898     3.824056    -2.326894      26.20
 H       1.470810     4.542969    -0.695548      24.16
 C       1.907532     0.068231    -0.192429      24.63
 O       3.250993    -0.098587    -0.575615     150.69
 C       0.957668    -0.716115     0.275891      64.66
 H       1.030242    -1.809078     0.238528      25.73
 C      -1.031535     1.013549     0.058812      41.57
 C      -2.380400     1.278252     0.371954      80.89
 H      -3.124165     0.350967     0.348586      24.99
 O      -2.485306     2.272005     1.567040     187.08
 H      -2.376710     1.827742     2.465346      26.36
 C      -3.357814     2.064101    -0.698839      83.61
 H      -2.831189     2.968522    -1.006563      24.45
 O      -3.586551     1.116044    -1.795764     236.44
 H      -3.636075     1.279147    -2.777703      24.47
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 C      -4.713795     2.654499    -0.113199      89.35
 O      -5.496199     3.257812    -1.113854     330.28
 H      -5.252142     4.144993    -1.267424      32.79
 H      -4.124956     3.292476     0.763042      23.04
 H      -5.127620     1.687503     0.406896      27.53
55
name = lig-etoh-Waterframe_758
 C       5.787321    -0.978963     1.264845      48.96
 H       6.114284    -0.031773     0.772458      18.46
 C       5.140441    -3.324399     0.959521      20.63
 H       4.906062    -4.280200     0.440785      20.20
 C       5.420965    -3.561048     2.407571      40.33
 O       4.961877    -4.746603     2.908866     176.18
 C       3.512628    -5.049895     2.463077      94.26
 H       2.955029    -4.097803     2.388043      27.54
 H       3.161545    -5.742246     3.171911      27.70
 H       3.497134    -5.841203     1.552875      25.20
 C       5.913772    -2.567883     3.219645      10.80
 O       6.074569    -2.677190     4.548376     175.30
 H       5.863144    -3.553473     4.984770      21.31
 C       6.132147    -1.231823     2.623974      37.24
 H       6.349672    -0.610534     3.425504      28.33
 C       5.426279    -2.014280     0.387354      20.99
 C       5.103228    -1.640694    -1.047576     103.77
 H       5.289322    -2.412126    -1.669928      28.35
 O       5.874146    -0.471658    -1.448896     223.78
 H       5.451221     0.263741    -0.987877      27.18
 C       3.522566    -1.319143    -1.203722      84.61
 H       3.141289    -2.166837    -0.655516      29.41
 C       3.155242    -1.136354    -2.730383     112.84
 O       3.450848    -2.335652    -3.504562     296.31
 H       4.294090    -2.314720    -4.029288      27.16
 H       3.805617    -0.346588    -3.092954      26.90
 H       2.222079    -0.689884    -2.777935      28.81
 C      -0.500986    -0.325555     0.299109      41.33
 H      -1.341782    -0.912657     0.679767      23.45
 C       0.019160     1.909670    -0.348825      72.34
 H       0.038590     2.872237    -0.511808      24.63
 C       1.339776     1.422275    -0.492834       5.97
 O       2.430468     2.319874    -0.803472     106.96
 C       2.294959     3.908662    -1.265257      98.19
 H       3.223490     4.216579    -1.111926      24.66
 H       2.094035     3.612614    -2.146591      27.70
 H       1.476444     4.514051    -0.767685      25.36
 C       1.977043     0.197415    -0.183069      25.95
 O       3.247221    -0.106637    -0.536397     175.35
 C       0.910050    -0.718846     0.288752      44.44
 H       1.163243    -1.689111     0.486920      26.72
 C      -0.927189     0.985959    -0.017005      22.76
 C      -2.521736     1.340872     0.381093      66.76
 H      -2.784132     0.299861     0.803262      24.83
 O      -2.496890     2.237088     1.618077     199.15
 H      -2.092411     1.664929     2.422904      25.73
 C      -3.291628     2.052256    -0.665385      93.64
 H      -2.628544     2.987730    -1.038761      22.87
 O      -3.599008     1.089912    -1.776680     228.62
 H      -3.484943     1.552292    -2.664327      25.53
 C      -4.600234     2.675347    -0.093131      85.40
 O      -5.515141     3.224904    -1.101104     286.28
 H      -5.299703     4.190662    -1.129019      29.87
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 H      -4.408852     3.426997     0.714536      25.03
 H      -5.336568     1.719356     0.264409      25.48
55
name = lig-etoh-Waterframe_759
 C       5.767795    -0.964285     1.274885      24.59
 H       6.102788     0.046147     0.947002      19.03
 C       5.197892    -3.243445     0.958563      75.89
 H       4.727800    -3.893968     0.266804      25.68
 C       5.400006    -3.583739     2.308381      22.95
 O       4.906960    -4.812965     2.908221     181.26
 C       3.518813    -5.144517     2.481823     102.66
 H       3.011886    -4.165924     2.196945      27.51
 H       3.288006    -5.707126     3.362449      26.62
 H       3.501642    -5.686768     1.445086      26.22
 C       5.908486    -2.527843     3.175231       5.94
 O       6.086574    -2.661368     4.565063     142.09
 H       5.817764    -3.533694     4.761831      21.81
 C       6.110224    -1.246520     2.577342      49.40
 H       6.507028    -0.260601     2.961682      26.68
 C       5.388050    -2.029851     0.372977      21.13
 C       5.065378    -1.652994    -1.057900     107.18
 H       5.478236    -2.360175    -1.820266      24.15
 O       5.788816    -0.507755    -1.494075     247.67
 H       5.471687     0.313922    -1.098570      26.46
 C       3.542175    -1.360234    -1.193890      72.94
 H       2.901078    -2.142338    -0.802749      27.34
 C       3.185851    -1.115160    -2.716315      93.98
 O       3.478253    -2.362375    -3.502956     278.31
 H       4.253514    -2.254030    -4.069969      26.96
 H       3.993585    -0.323968    -3.058672      23.24
 H       2.162238    -1.010262    -3.047310      25.91
 C      -0.450857    -0.384437     0.276171      48.97
 H      -1.108822    -1.183306     0.542046      23.88
 C       0.028762     1.927852    -0.404202      76.74
 H      -0.359002     2.908818    -0.444670      23.19
 C       1.464557     1.585221    -0.465722      16.11
 O       2.454893     2.351681    -0.732562     207.03
 C       2.262105     3.800964    -1.240500     117.32
 H       3.141292     4.188448    -0.927823      27.09
 H       2.115545     3.958740    -2.395945      25.56
 H       1.536980     4.306163    -0.708257      29.30
 C       1.794394     0.235905    -0.173136       2.37
 O       3.253214    -0.077536    -0.455272      99.55
 C       0.859716    -0.741507     0.258288      63.04
 H       1.183407    -1.575116     0.763870      25.46
 C      -0.951009     0.930242    -0.021999      27.87
 C      -2.485827     1.377969     0.490511      70.04
 H      -3.034662     0.449638     0.758059      26.30
 O      -2.491152     2.185530     1.630099     220.45
 H      -1.916323     1.566764     2.311251      25.00
 C      -3.269751     2.071081    -0.695203      91.03
 H      -2.493739     2.784072    -1.239821      23.68
 O      -3.593042     1.094903    -1.721353     244.64
 H      -3.390427     1.702192    -2.475654      25.85
 C      -4.572247     2.649221    -0.098186     103.33
 O      -5.517520     3.207533    -1.085925     303.27
 H      -5.250178     4.236299    -1.284235      27.59
 H      -4.517911     3.327669     0.576423      27.46
 H      -5.175897     1.886823     0.549874      26.78
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name = lig-etoh-Waterframe_760
 C       5.803248    -1.003555     1.223327      81.44
 H       5.783623    -0.001138     0.739900      26.77
 C       5.200464    -3.268837     0.905344      67.18
 H       4.683151    -3.945727     0.289947      29.15
 C       5.368494    -3.563287     2.263346     -28.05
 O       4.889052    -4.836125     2.871353     237.15
 C       3.565491    -5.228204     2.506068     116.54
 H       2.827670    -4.360195     2.444611      27.82
 H       2.816964    -5.646665     3.262267      26.85
 H       3.644724    -5.851544     1.645368      28.91
 C       5.882260    -2.492895     3.154107      -1.09
 O       6.095539    -2.656542     4.529970     139.36
 H       5.869035    -3.484409     4.961958      24.20
 C       6.092684    -1.240820     2.573093      50.29
 H       6.695668    -0.434165     3.268386      16.23
 C       5.373974    -1.932037     0.405377      16.64
 C       5.014046    -1.646365    -1.063583      86.13
 H       5.185836    -2.684476    -1.726367      22.39
 O       5.745945    -0.510545    -1.565500     222.78
 H       5.581128     0.330364    -1.146215      27.78
 C       3.491480    -1.380478    -1.238040      57.73
 H       2.786931    -2.168293    -0.926881      28.04
 C       3.270707    -1.151776    -2.733050      96.46
 O       3.475020    -2.386448    -3.475526     274.99
 H       4.350305    -2.255831    -3.958607      24.45
 H       3.733681    -0.111628    -3.140999      24.17
 H       2.103169    -0.839588    -2.786817      26.44
 C      -0.537710    -0.432448     0.272738      28.62
 H      -1.093212    -1.298426     0.526260      23.34
 C       0.044295     1.925739    -0.415440      71.99
 H      -0.525008     2.923588    -0.581468      20.99
 C       1.378384     1.651661    -0.416304       4.37
 O       2.563631     2.512570    -0.732230     181.58
 C       2.245283     3.681888    -1.181884     119.08
 H       3.083167     4.458950    -0.940479      25.56
 H       2.079122     3.956220    -2.461132      23.69
 H       1.395306     4.001984    -0.689642      29.00
 C       1.739868     0.224293    -0.214224      -1.96
 O       3.190402    -0.065611    -0.352141      43.66
 C       0.897303    -0.747055     0.223245      53.36
 H       1.223468    -1.713215     0.691431      25.78
 C      -0.983992     0.883687     0.029631      41.11
 C      -2.381576     1.319270     0.477408      84.24
 H      -3.042255     0.530296     0.434488      28.00
 O      -2.435264     2.164643     1.646409     233.61
 H      -2.025371     1.814425     2.626081      23.58
 C      -3.243701     2.080134    -0.667620      93.36
 H      -2.766208     2.967316    -1.072888      25.31
 O      -3.571666     1.117652    -1.669308     248.78
 H      -3.554920     1.214424    -2.645373      25.63
 C      -4.598593     2.675000    -0.103695      96.84
 O      -5.513183     3.176164    -1.082896     286.96
 H      -5.140870     4.189769    -1.319264      26.95
 H      -4.093117     3.445598     0.585665      24.91
 H      -4.928852     1.860987     0.351167      30.62
55
name = lig-etoh-Waterframe_761
 C       5.878678    -0.909921     1.232930      39.52
 H       5.869564     0.166582     0.947092      27.22
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 C       5.146222    -3.313163     0.847301      68.98
 H       4.838188    -4.207891     0.305312      26.44
 C       5.310087    -3.540070     2.298025      14.21
 O       4.927575    -4.801617     2.844055     211.76
 C       3.517253    -5.284335     2.521331     102.09
 H       3.007801    -4.387279     2.126966      29.22
 H       3.289455    -6.053020     3.435726      23.63
 H       3.539842    -5.951411     1.754718      28.85
 C       5.815762    -2.562286     3.142855      18.49
 O       6.110950    -2.642750     4.473391     178.49
 H       5.787838    -3.515460     4.879527      23.18
 C       6.125251    -1.230449     2.613251      -5.32
 H       6.494554    -0.581733     3.554550      19.87
 C       5.327948    -1.996878     0.355909      -3.84
 C       4.924968    -1.614071    -1.000171      81.01
 H       5.201262    -2.582864    -1.676945      22.86
 O       5.745290    -0.538535    -1.674005     177.73
 H       5.466091     0.188577    -1.131854      30.03
 C       3.462683    -1.320692    -1.248635      59.63
 H       2.931716    -2.219071    -0.849967      27.73
 C       3.222148    -1.126657    -2.746890      97.26
 O       3.463755    -2.374855    -3.435801     278.94
 H       4.292968    -2.412872    -4.030744      26.13
 H       3.930279    -0.385711    -3.255815      23.90
 H       2.062818    -0.856436    -2.775959      26.67
 C      -0.562057    -0.485095     0.284623      36.13
 H      -1.426631    -1.084506     0.600027      22.70
 C      -0.077513     1.888830    -0.355686      64.33
 H      -0.175014     3.008790    -0.802569      19.34
 C       1.375776     1.593302    -0.406376       1.93
 O       2.624585     2.466625    -0.685487     118.36
 C       2.163524     3.853640    -1.203099      78.45
 H       3.014162     4.724728    -0.950136      23.31
 H       2.011752     3.309758    -2.226082      23.47
 H       1.162616     4.132947    -0.828091      26.06
 C       1.843770     0.282911    -0.263359      12.38
 O       3.088606    -0.115943    -0.302534     128.64
 C       0.820606    -0.744734     0.199245      31.28
 H       1.304728    -1.842564     0.175713      25.18
 C      -0.928625     0.877231     0.079779      35.29
 C      -2.348591     1.281481     0.370587      63.98
 H      -2.806778     0.233113     0.693413      23.95
 O      -2.361284     2.182996     1.655197     142.85
 H      -2.217236     1.463856     2.485742      22.76
 C      -3.214648     2.163737    -0.677125      97.98
 H      -2.710051     2.986319    -1.049257      26.39
 O      -3.557870     1.067576    -1.624260     225.42
 H      -3.413412     1.335457    -2.572436      26.23
 C      -4.544468     2.672532    -0.090470      83.22
 O      -5.488238     3.149845    -1.083303     247.13
 H      -5.356262     4.232467    -1.247405      26.51
 H      -4.263044     3.666535     0.795941      22.44
 H      -5.181101     1.958073     0.426312      27.22
55
name = lig-etoh-Waterframe_762
 C       5.905726    -0.913974     1.330853      30.68
 H       6.141166     0.089007     0.924202      20.32
 C       5.099817    -3.320453     0.898591      70.29
 H       4.995143    -4.141323     0.112983      25.36
 C       5.217011    -3.564034     2.253813      16.80
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 O       4.970295    -4.771946     2.821960     204.07
 C       3.553990    -5.361924     2.517228      92.89
 H       2.778172    -4.589058     2.396176      29.05
 H       3.364874    -5.689802     3.623667      24.38
 H       3.619638    -6.017146     1.630756      26.32
 C       5.784658    -2.538017     3.099167       7.58
 O       6.111616    -2.674756     4.451261     156.49
 H       5.700310    -3.575203     4.802650      18.25
 C       6.126258    -1.280680     2.621802      83.66
 H       6.302033    -0.405424     3.234029      32.10
 C       5.338711    -2.005261     0.401247     -42.48
 C       4.921296    -1.584090    -1.047017      83.92
 H       5.033706    -2.413274    -1.707770      25.30
 O       5.735244    -0.588529    -1.730696     202.35
 H       5.653594     0.343144    -1.435197      27.82
 C       3.444014    -1.253069    -1.190171      86.03
 H       2.852644    -2.174571    -0.899252      29.10
 C       3.135249    -1.076370    -2.773464     104.90
 O       3.412768    -2.398147    -3.392097     294.13
 H       4.145744    -2.066252    -4.035256      24.10
 H       3.852067    -0.395572    -3.065911      26.97
 H       2.197580    -0.822034    -3.200146      27.65
 C      -0.531837    -0.448604     0.314804      43.39
 H      -1.304820    -1.244679     0.598080      22.92
 C       0.029939     1.867842    -0.324058      68.12
 H      -0.619202     2.873088    -0.574461      20.84
 C       1.459592     1.567067    -0.431094      14.37
 O       2.512586     2.412773    -0.588632     135.60
 C       2.061320     3.923943    -1.277704      71.32
 H       3.032362     4.666882    -1.179567      23.37
 H       1.971274     3.941571    -2.341093      26.87
 H       1.141723     4.421516    -0.776432      25.89
 C       1.714562     0.205912    -0.215457      28.13
 O       3.105454    -0.208248    -0.323771     164.07
 C       0.786940    -0.727051     0.089262      62.88
 H       1.041611    -1.888211    -0.018272      25.10
 C      -0.923348     0.921567     0.084438      32.15
 C      -2.367207     1.342599     0.369054      67.66
 H      -3.075519     0.369336     0.710287      24.41
 O      -2.288327     2.159779     1.607978     169.54
 H      -2.136695     1.464708     2.402103      25.00
 C      -3.192782     2.117534    -0.646148      99.00
 H      -2.505593     2.784058    -1.213722      26.08
 O      -3.536829     1.036150    -1.614654     228.77
 H      -3.314418     1.535456    -2.418449      27.84
 C      -4.520302     2.705111    -0.043594      82.48
 O      -5.459018     3.146881    -1.106465     245.81
 H      -5.374718     4.215809    -1.112889      26.74
 H      -4.469055     3.622224     0.769794      23.69
 H      -5.093800     1.865733     0.655617      25.98
55
name = lig-etoh-Waterframe_763
 C       5.864084    -1.040721     1.263252      88.55
 H       6.247720    -0.136550     0.833836      27.21
 C       5.076575    -3.234858     0.877521      44.10
 H       4.774470    -4.059822     0.112706      26.01
 C       5.195125    -3.527589     2.245538      -6.04
 O       4.955085    -4.804440     2.805454     335.96
 C       3.642814    -5.374972     2.592460     118.22
 H       2.838142    -4.663125     2.469077      30.18
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 H       3.253433    -6.013972     3.384269      27.10
 H       3.703290    -6.245629     1.778770      26.46
 C       5.759385    -2.536424     3.115186      -7.13
 O       6.081777    -2.753165     4.433467     172.52
 H       5.750494    -3.650104     4.935176      19.11
 C       6.110543    -1.253990     2.635484      95.36
 H       6.453697    -0.561463     3.291807      31.50
 C       5.383676    -1.899401     0.455862      26.98
 C       4.964939    -1.586766    -1.100538      73.92
 H       5.020172    -2.426666    -1.620180      27.06
 O       5.767969    -0.629555    -1.778352     241.72
 H       5.636187     0.313359    -1.447191      27.89
 C       3.346632    -1.271974    -1.204603      86.36
 H       2.833521    -2.212162    -0.912797      30.19
 C       3.073636    -1.026620    -2.768724     105.03
 O       3.367070    -2.376751    -3.361025     273.20
 H       4.130115    -2.391084    -4.090569      25.38
 H       3.727638    -0.300685    -3.088400      28.13
 H       2.148755    -0.616365    -3.006823      29.00
 C      -0.568880    -0.350547     0.334839      55.10
 H      -1.115118    -1.317335     0.530944      22.89
 C       0.125749     1.871308    -0.299332      64.86
 H      -0.168577     2.954035    -0.325061      23.40
 C       1.404379     1.540754    -0.424219      17.68
 O       2.350047     2.510366    -0.569302     185.83
 C       2.040420     3.934372    -1.321169      90.21
 H       3.006463     4.265762    -0.967975      25.17
 H       1.900085     3.862851    -2.310070      28.81
 H       1.236100     4.330266    -0.586517      24.35
 C       1.729758     0.120569    -0.204520      16.27
 O       3.111120    -0.220964    -0.329283     154.76
 C       0.722492    -0.836677    -0.022753      56.44
 H       1.005696    -1.922980     0.124116      25.61
 C      -0.951765     0.906051     0.071521      33.46
 C      -2.379650     1.394717     0.480693      94.74
 H      -3.043556     0.493463     0.455664      27.53
 O      -2.230459     2.151072     1.574897     282.31
 H      -1.874941     1.712271     2.401033      28.96
 C      -3.179117     2.036293    -0.622463      84.63
 H      -2.635405     2.935097    -1.195819      24.88
 O      -3.512366     1.043901    -1.621258     223.87
 H      -3.503009     1.257929    -2.564924      26.55
 C      -4.531438     2.748764    -0.018351      94.17
 O      -5.414777     3.145709    -1.106810     301.27
 H      -5.234594     4.148747    -1.187476      29.32
 H      -4.088807     3.442350     0.512886      28.48
 H      -4.884250     1.730746     0.469508      27.23
55
name = lig-etoh-Waterframe_764
 C       5.939281    -0.956473     1.266565      35.65
 H       6.209281    -0.018159     0.850760      29.57
 C       5.031648    -3.155203     0.861030      80.59
 H       4.459686    -3.918673     0.258266      27.53
 C       5.205492    -3.489591     2.245229      14.76
 O       4.945825    -4.834732     2.812239     199.19
 C       3.676729    -5.444275     2.669947     125.16
 H       3.048766    -4.663041     2.282964      28.30
 H       3.569945    -6.073745     3.471735      27.72
 H       3.761360    -6.012696     1.573257      26.75
 C       5.732817    -2.561491     3.175519       3.00
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 O       6.050533    -2.839177     4.456410     133.59
 H       5.706896    -3.842866     4.692255      19.42
 C       6.080963    -1.257490     2.660456      43.39
 H       6.686858    -0.727052     3.315070      19.31
 C       5.300966    -1.954313     0.268298       1.97
 C       4.959894    -1.629365    -1.089249      74.91
 H       5.242322    -2.608266    -1.588846      22.81
 O       5.820717    -0.651089    -1.819126     207.35
 H       5.564524     0.177383    -1.282388      27.59
 C       3.378444    -1.366300    -1.293571      65.51
 H       2.822817    -2.212563    -0.919395      29.18
 C       3.058496    -1.004945    -2.727756     105.57
 O       3.278588    -2.329660    -3.345413     247.36
 H       4.178934    -2.237337    -3.917719      23.33
 H       3.795819    -0.293570    -3.236223      25.18
 H       1.941186    -0.809330    -2.726393      26.76
 C      -0.585962    -0.434409     0.285475      24.04
 H      -1.555101    -0.866698     0.646117      21.28
 C      -0.007962     1.894559    -0.228610      54.14
 H       0.095706     2.852074    -0.258322      23.07
 C       1.357278     1.437000    -0.390541      -2.23
 O       2.258352     2.633818    -0.604013     206.09
 C       2.079745     3.825841    -1.219429     126.69
 H       2.911810     4.418278    -1.119645      26.98
 H       1.866234     3.541187    -2.163583      29.26
 H       1.193870     4.551207    -0.877924      25.62
 C       1.797330     0.101101    -0.259537      30.49
 O       3.085371    -0.176536    -0.320832     142.71
 C       0.704740    -0.908259    -0.055250      58.84
 H       0.916496    -1.883631     0.184376      27.48
 C      -0.968109     0.982926     0.048133      25.11
 C      -2.340023     1.302446     0.476952      82.15
 H      -2.735432     0.441732     0.887148      27.30
 O      -2.201293     2.244230     1.644146     233.33
 H      -1.788833     1.682884     2.282472      30.67
 C      -3.213827     2.106926    -0.690954      78.86
 H      -2.577351     3.020093    -1.080128      24.22
 O      -3.496375     1.007548    -1.612242     221.63
 H      -3.539325     1.377360    -2.511807      26.10
 C      -4.452921     2.666418    -0.079495     117.49
 O      -5.359052     3.172159    -1.084230     328.94
 H      -5.198841     4.076374    -1.294755      33.83
 H      -4.121497     3.458112     0.582412      27.60
 H      -5.219133     2.228094     0.593876      27.14
55
name = lig-etoh-Waterframe_765
 C       5.965785    -0.914612     1.243210      44.06
 H       6.249999     0.089287     1.013353      31.23
 C       4.919641    -3.181980     0.892079      62.17
 H       4.393482    -3.907296     0.310984      26.42
 C       5.195095    -3.510181     2.258436      18.96
 O       5.019667    -4.784764     2.822303     210.71
 C       3.687983    -5.489480     2.606811     111.00
 H       2.739990    -4.834340     2.796125      24.54
 H       3.503863    -5.976103     3.559283      27.67
 H       3.687283    -6.184628     1.745071      27.85
 C       5.720829    -2.566322     3.170082      10.10
 O       6.014385    -2.923975     4.485898     126.67
 H       5.738655    -3.894674     4.789703      20.72
 C       6.078821    -1.300609     2.621910       9.69
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 H       6.713429    -0.582078     3.222949      15.88
 C       5.319088    -1.887146     0.322400     -25.18
 C       4.944570    -1.703975    -1.193844      68.21
 H       5.159587    -2.701679    -1.918050      20.92
 O       5.823407    -0.673238    -1.798673     161.60
 H       5.846340     0.286097    -1.447597      27.43
 C       3.516709    -1.372967    -1.296850      84.37
 H       2.877086    -2.195613    -1.030458      28.48
 C       3.031509    -1.059561    -2.673338      93.03
 O       3.195045    -2.282255    -3.375467     250.18
 H       4.110202    -2.150807    -3.894299      23.03
 H       3.578986    -0.064289    -3.160906      25.16
 H       1.872634    -0.769858    -2.819063      25.87
 C      -0.629675    -0.437775     0.156966      42.95
 H      -1.355432    -1.175165     0.611789      24.51
 C      -0.014029     1.928937    -0.188845      52.87
 H      -0.439938     2.921660    -0.201301      21.50
 C       1.291841     1.499580    -0.390902       1.48
 O       2.252487     2.543961    -0.514301     182.44
 C       2.039903     3.814139    -1.224759     124.40
 H       2.902212     4.429297    -1.322057      27.41
 H       1.859096     3.661793    -2.424217      26.11
 H       1.193161     4.408244    -0.966492      28.06
 C       1.689843     0.095960    -0.319405      -8.17
 O       3.136389    -0.196363    -0.364394      81.64
 C       0.710428    -0.894971    -0.001685      52.06
 H       0.955458    -1.867474     0.106100      25.76
 C      -0.982706     0.918116     0.066326      41.76
 C      -2.343152     1.334900     0.470168      79.04
 H      -2.902695     0.490093     0.955401      25.83
 O      -2.185279     2.345023     1.696711     204.07
 H      -1.965001     1.856335     2.443892      29.12
 C      -3.193745     2.044532    -0.646787     100.43
 H      -2.571965     2.731362    -1.178437      26.22
 O      -3.477193     0.992508    -1.623008     232.23
 H      -3.508133     1.433948    -2.481782      26.18
 C      -4.452068     2.681215    -0.081638      98.46
 O      -5.328216     3.214783    -1.115239     315.10
 H      -5.145751     4.115575    -1.119432      32.20
 H      -4.193224     3.687040     0.651990      23.23
 H      -4.944815     1.941892     0.558206      29.01
55
name = lig-etoh-Waterframe_766
 C       5.923773    -0.976981     1.225943      69.16
 H       6.307849    -0.028598     0.851707      18.12
 C       4.845729    -3.156341     0.942494      60.31
 H       4.503693    -3.862263     0.266686      24.69
 C       5.157676    -3.524577     2.241244      20.13
 O       5.027927    -4.766042     2.807537     263.41
 C       3.693950    -5.494340     2.640397     103.54
 H       2.762232    -4.764029     2.678887      24.58
 H       3.759717    -6.345595     3.480806      24.13
 H       3.639031    -6.046117     1.781564      29.02
 C       5.742680    -2.583524     3.151336      -0.21
 O       5.987665    -2.944962     4.482081     201.44
 H       5.684360    -3.803228     4.808330      19.51
 C       6.128656    -1.326112     2.575494      24.41
 H       6.430587    -0.465339     3.363772      26.38
 C       5.338579    -1.898555     0.450752      26.78
 C       5.029792    -1.670042    -1.228660      80.81
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 H       5.101004    -2.674640    -1.890263      23.45
 O       5.847412    -0.711912    -1.809111     199.11
 H       5.606693     0.131033    -1.227428      23.74
 C       3.496986    -1.303927    -1.239273      82.09
 H       3.113899    -2.291910    -0.863827      27.02
 C       2.971695    -1.056289    -2.668849      93.45
 O       3.160251    -2.251815    -3.462357     267.10
 H       3.921998    -2.325148    -4.144042      25.82
 H       3.582941    -0.156300    -3.123345      25.21
 H       1.845984    -0.793948    -2.509052      25.55
 C      -0.651297    -0.500203     0.065888      63.11
 H      -1.176286    -1.400985     0.243357      25.78
 C      -0.065797     1.910553    -0.165879      59.16
 H      -0.627142     2.939711    -0.172388      20.46
 C       1.265874     1.621454    -0.405294       6.72
 O       2.318119     2.420683    -0.415583     141.78
 C       1.964700     3.821192    -1.326069      69.97
 H       2.962944     4.198374    -0.977504      23.77
 H       1.782804     3.420571    -2.527075      22.48
 H       1.226398     4.169863    -0.744582      25.97
 C       1.646783     0.120434    -0.359762     -16.43
 O       3.141814    -0.226029    -0.431367     128.20
 C       0.730159    -0.817070     0.030730      56.67
 H       1.022039    -1.871286     0.042912      24.18
 C      -1.005367     0.834808     0.105727      26.22
 C      -2.386300     1.437937     0.586821      80.98
 H      -3.161470     0.507352     0.679289      23.07
 O      -2.186793     2.416170     1.680105     270.55
 H      -2.179761     1.925789     2.454804      29.82
 C      -3.110425     1.976802    -0.608409      93.46
 H      -2.560256     2.689592    -1.103793      26.92
 O      -3.471978     0.979200    -1.620974     223.61
 H      -3.441876     1.304130    -2.526314      25.42
 C      -4.501971     2.729777    -0.049559      85.15
 O      -5.304204     3.239324    -1.152364     292.08
 H      -5.312298     4.249078    -1.083707      28.10
 H      -3.912548     3.536144     0.711355      22.65
 H      -4.858089     1.832011     0.327806      30.33
55
name = lig-etoh-Waterframe_767
 C       5.927348    -1.025316     1.266284      36.44
 H       6.311297    -0.166185     0.675316      17.09
 C       4.818067    -3.136832     0.950551      69.98
 H       4.495906    -3.881371     0.257818      24.92
 C       5.134078    -3.507055     2.267808      28.61
 O       4.961804    -4.818216     2.787847     273.67
 C       3.745312    -5.495198     2.671042     115.29
 H       2.915793    -4.729183     2.798750      26.94
 H       3.788335    -6.410724     3.452950      24.19
 H       3.710148    -5.742431     1.642302      28.92
 C       5.780473    -2.603205     3.117934      19.66
 O       5.971312    -2.892919     4.440447     186.95
 H       5.625388    -3.756895     4.584278      19.92
 C       6.163434    -1.337423     2.637043      35.07
 H       6.407697    -0.492071     3.438815      27.35
 C       5.282172    -1.996074     0.354912      16.44
 C       5.060296    -1.644900    -1.085684      95.63
 H       5.255151    -2.568923    -1.565374      24.76
 O       5.897455    -0.693343    -1.808995     205.86
 H       5.648960     0.238805    -1.351014      22.92
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 C       3.455891    -1.330498    -1.240441      68.04
 H       2.984932    -2.239807    -0.742676      24.50
 C       2.958515    -1.060842    -2.671405     106.27
 O       3.112882    -2.251916    -3.551555     276.18
 H       3.859267    -1.920111    -4.130391      24.90
 H       3.432347    -0.251912    -3.117156      27.02
 H       1.916242    -0.922797    -2.657524      26.71
 C      -0.644582    -0.602903     0.040546      41.23
 H      -1.503131    -1.207183     0.055211      23.56
 C      -0.177589     1.833472    -0.143487      55.38
 H      -0.191844     3.018476    -0.089001      19.29
 C       1.280039     1.512552    -0.377039      12.71
 O       2.395220     2.428659    -0.419118     151.61
 C       1.969041     3.691393    -1.285200      82.51
 H       2.816931     4.606221    -1.276026      23.06
 H       1.660920     3.398129    -2.436589      23.48
 H       1.099836     4.177761    -0.873458      24.71
 C       1.716867     0.240179    -0.368214      28.33
 O       3.061498    -0.164668    -0.455704     158.45
 C       0.756836    -0.780800    -0.024631      45.30
 H       1.119573    -1.904430     0.099502      21.82
 C      -1.081822     0.848509     0.169938      10.92
 C      -2.407610     1.408654     0.643262      84.44
 H      -2.987191     0.630552     1.309390      21.51
 O      -2.219146     2.443156     1.633197     257.00
 H      -2.141161     1.923310     2.412964      28.61
 C      -3.131866     2.083728    -0.648737      80.20
 H      -2.457670     2.882743    -1.061017      25.34
 O      -3.457611     0.948927    -1.570260     253.62
 H      -3.206438     1.253425    -2.440097      27.00
 C      -4.433541     2.696876    -0.097122     112.55
 O      -5.279514     3.246311    -1.155668     277.85
 H      -5.309731     4.325194    -1.172824      26.58
 H      -4.406106     3.412752     0.744202      25.92
 H      -5.315683     2.145586     0.469688      25.36
55
name = lig-etoh-Waterframe_768
 C       5.940004    -1.114544     1.256255      58.33
 H       6.298370    -0.087255     0.989344      26.76
 C       4.803596    -3.233623     0.915334      48.56
 H       4.232217    -4.048367     0.388926      21.54
 C       5.104386    -3.525079     2.275886       9.07
 O       4.976697    -4.821304     2.802822     297.59
 C       3.720227    -5.471189     2.640971     122.11
 H       2.948631    -5.009966     3.134628      30.62
 H       3.619836    -6.408268     3.276986      25.49
 H       3.460925    -5.910481     1.531934      26.90
 C       5.806753    -2.593110     3.107242       0.24
 O       5.959966    -2.846245     4.413763     141.78
 H       5.703467    -3.748656     4.676328      26.22
 C       6.157122    -1.318391     2.647383      49.85
 H       6.721913    -0.641870     3.315413      17.56
 C       5.314250    -1.938248     0.393140      50.90
 C       4.985119    -1.639190    -1.016023      92.20
 H       5.190714    -2.446221    -1.559390      26.87
 O       5.930410    -0.643841    -1.749878     156.99
 H       5.879896     0.374603    -1.636352      25.06
 C       3.438678    -1.385048    -1.256757      67.25
 H       2.769883    -2.200809    -0.912889      23.03
 C       2.927408    -1.113668    -2.702725     112.26
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 O       3.101565    -2.213841    -3.607568     284.32
 H       3.919977    -2.140452    -4.183063      25.57
 H       3.357784    -0.253267    -3.028093      28.19
 H       1.932972    -0.856862    -2.706067      26.75
 C      -0.664536    -0.511586     0.065833      34.42
 H      -1.383790    -1.373520     0.173493      23.60
 C      -0.048798     1.778952    -0.125139      82.12
 H      -0.485175     2.835158     0.154522      18.19
 C       1.259565     1.492255    -0.328393       6.78
 O       2.386644     2.532028    -0.496056     201.73
 C       1.980281     3.570874    -1.215208     121.03
 H       2.792425     4.373465    -1.536122      24.15
 H       1.801762     3.191066    -2.123860      29.00
 H       0.965609     4.063834    -0.940806      24.84
 C       1.740619     0.157309    -0.322654      21.59
 O       3.027269    -0.054978    -0.463627     129.34
 C       0.722546    -0.821626    -0.125857      58.84
 H       1.234716    -1.895407     0.023572      20.56
 C      -1.096768     0.804960     0.194585      60.31
 C      -2.443716     1.370427     0.645999      74.41
 H      -3.130103     0.584592     1.026556      22.26
 O      -2.246133     2.473177     1.611692     277.02
 H      -1.854352     2.131825     2.445644      29.31
 C      -3.226651     2.096857    -0.578671      81.87
 H      -2.497930     2.859770    -1.127850      23.27
 O      -3.405175     0.974743    -1.505150     246.49
 H      -3.048767     1.049031    -2.378242      25.79
 C      -4.494458     2.710892    -0.134837      96.25
 O      -5.273239     3.252126    -1.197499     286.64
 H      -4.984335     4.281097    -1.051937      25.86
 H      -4.174325     3.468590     0.450473      26.23
 H      -5.021079     1.667376     0.422973      25.56
55
name = lig-etoh-Waterframe_769
 C       6.010163    -1.071326     1.294591      53.60
 H       6.212614    -0.090382     0.776929      26.89
 C       4.842943    -3.278936     0.919402      68.86
 H       4.150849    -3.912708     0.244886      20.31
 C       5.105567    -3.550440     2.223806      19.77
 O       4.998953    -4.809272     2.829052     190.67
 C       3.618858    -5.517001     2.652405     103.43
 H       2.879339    -4.893834     3.071285      28.78
 H       3.961876    -6.396063     3.023740      24.86
 H       3.256603    -5.678512     1.438085      25.37
 C       5.772215    -2.591582     3.104953       6.92
 O       5.971019    -2.829378     4.462118     143.92
 H       5.730776    -3.764130     4.765034      23.47
 C       6.172893    -1.354882     2.615396      72.48
 H       6.827347    -0.756605     3.098658      21.16
 C       5.265958    -2.005502     0.482968       9.90
 C       4.906145    -1.562351    -1.083413      74.01
 H       5.098020    -2.489263    -1.742867      23.15
 O       5.936034    -0.632684    -1.674467     178.53
 H       5.534318     0.210820    -1.224514      27.07
 C       3.402264    -1.347440    -1.260713      81.97
 H       2.989001    -2.234412    -0.761375      23.23
 C       2.927270    -1.106032    -2.741452     103.46
 O       3.109056    -2.198094    -3.640177     279.94
 H       3.978967    -2.179278    -4.065266      26.31
 H       3.542689    -0.193179    -3.098394      24.84
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 H       1.824333    -0.947108    -2.595024      25.16
 C      -0.663564    -0.497932     0.111322      48.80
 H      -1.177364    -1.437613     0.517437      21.03
 C      -0.021200     1.775201    -0.021235      53.55
 H      -0.379201     2.833784     0.045225      21.06
 C       1.358142     1.559339    -0.286959      -4.68
 O       2.331996     2.483394    -0.458160     230.94
 C       1.917679     3.577272    -1.352350     114.42
 H       2.804171     4.109203    -1.144458      25.60
 H       1.655341     3.180676    -2.300299      27.48
 H       1.083805     4.160393    -0.721738      23.69
 C       1.645121     0.071467    -0.263828      10.42
 O       3.094641    -0.045250    -0.513760     120.60
 C       0.685280    -0.882363    -0.213840      78.66
 H       0.759341    -2.018687    -0.200222      22.40
 C      -1.027397     0.823925     0.174297      38.45
 C      -2.488461     1.395339     0.611463      78.28
 H      -3.098907     0.588644     0.763122      27.30
 O      -2.272005     2.486345     1.604140     260.83
 H      -1.688205     2.048246     2.317522      28.38
 C      -3.190445     2.006134    -0.547303      97.52
 H      -2.603763     2.904467    -1.007339      24.40
 O      -3.375711     0.980400    -1.449431     283.34
 H      -2.966458     1.160941    -2.281754      27.11
 C      -4.557015     2.688880    -0.130259     101.80
 O      -5.271199     3.253068    -1.251113     274.96
 H      -5.421714     4.308869    -1.267638      26.96
 H      -4.190651     3.388752     0.576728      27.65
 H      -5.143669     1.852498     0.371435      29.01
55
name = lig-etoh-Waterframe_770
 C       5.980642    -1.065114     1.209000      43.44
 H       6.423292    -0.199681     0.643236      18.76
 C       4.867862    -3.242950     0.894526      57.95
 H       4.382161    -3.979016     0.143385      21.26
 C       5.173389    -3.592390     2.288649      19.02
 O       4.938896    -4.825539     2.830314     288.76
 C       3.605498    -5.529507     2.647804     111.63
 H       2.806233    -4.993202     3.282521      24.54
 H       3.737258    -6.520365     2.984598      25.02
 H       3.443150    -5.394692     1.545507      25.97
 C       5.707389    -2.636847     3.137589       1.01
 O       5.983147    -2.834780     4.505871     191.20
 H       5.640929    -3.806107     4.677428      18.14
 C       6.264661    -1.380122     2.610155      30.78
 H       6.755189    -0.788283     3.307118      28.85
 C       5.211401    -1.992743     0.416208      19.08
 C       4.928165    -1.593465    -1.110247      78.44
 H       5.070635    -2.660480    -1.744379      22.87
 O       5.845493    -0.608409    -1.549567     168.53
 H       5.741750     0.288124    -1.045290      23.17
 C       3.422324    -1.234375    -1.257345     102.09
 H       2.970674    -2.080925    -0.746005      23.93
 C       2.943390    -1.074430    -2.724725      86.17
 O       3.115950    -2.209663    -3.631480     272.06
 H       3.943698    -2.056511    -4.113387      25.69
 H       3.440034    -0.057486    -3.255724      23.60
 H       1.764617    -0.852954    -2.849302      24.14
 C      -0.641019    -0.576189     0.181618      30.97
 H      -1.547575    -1.125594     0.574445      19.36
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 C       0.007531     1.884526     0.065081      45.36
 H      -0.156576     2.887195    -0.069262      22.31
 C       1.332736     1.423277    -0.184314      23.31
 O       2.286245     2.392116    -0.411154     140.88
 C       1.890309     3.635846    -1.416426      87.75
 H       2.744551     4.237097    -1.507089      26.02
 H       1.482259     3.493856    -2.606722      23.29
 H       1.048946     4.334941    -0.999047      24.42
 C       1.713806     0.155656    -0.284881      17.82
 O       3.085495    -0.126575    -0.575302     173.00
 C       0.597534    -0.974242    -0.249261      54.85
 H       0.821536    -1.985708    -0.477692      23.31
 C      -1.020229     0.894558     0.198649      17.53
 C      -2.404569     1.424937     0.598880      83.41
 H      -2.943760     0.589268     1.162973      23.81
 O      -2.302730     2.442627     1.599476     206.53
 H      -1.799335     1.941551     2.380562      26.71
 C      -3.178587     2.042560    -0.559122      92.07
 H      -2.545286     2.816934    -0.952453      25.96
 O      -3.367371     0.925326    -1.445271     270.29
 H      -3.148208     1.134565    -2.364114      25.43
 C      -4.587521     2.670077    -0.112029     106.47
 O      -5.290029     3.234199    -1.319036     272.80
 H      -5.404770     4.199055    -0.957453      25.71
 H      -4.668414     3.411298     0.794171      25.59
 H      -5.368535     2.151403     0.271829      29.12
55
name = lig-etoh-Waterframe_771
 C       5.953112    -1.116271     1.184898      46.92
 H       6.566698    -0.291246     0.885559      20.46
 C       4.900975    -3.231747     0.945243      51.88
 H       4.630735    -4.137686     0.346994      22.59
 C       5.178496    -3.606636     2.266421      -3.82
 O       4.870124    -4.909328     2.859936     225.41
 C       3.631802    -5.475711     2.629820     132.84
 H       2.827108    -5.096698     3.421155      23.54
 H       3.540572    -6.608039     2.835772      24.99
 H       3.243834    -5.432733     1.710558      27.76
 C       5.751099    -2.590093     3.192966      -1.51
 O       5.960898    -2.877043     4.498732     169.92
 H       5.657854    -3.803809     4.927373      19.28
 C       6.283541    -1.447731     2.539997      45.97
 H       6.667691    -0.712786     3.316478      24.18
 C       5.217414    -1.920763     0.320103      45.41
 C       4.940810    -1.647916    -1.044339      95.26
 H       5.242764    -2.472385    -1.860639      23.33
 O       5.777863    -0.573062    -1.465723     214.34
 H       5.662116     0.307774    -0.966501      23.50
 C       3.439619    -1.276245    -1.330665      89.88
 H       2.792142    -2.111498    -1.076782      25.42
 C       2.933407    -1.025676    -2.781290      93.32
 O       3.118313    -2.218908    -3.568350     269.89
 H       3.918862    -2.235161    -4.203319      25.22
 H       3.509228    -0.085438    -3.178319      24.34
 H       1.792641    -0.745535    -2.662157      24.55
 C      -0.716631    -0.477517     0.249871      40.05
 H      -1.527209    -1.241885     0.179727      19.64
 C       0.004063     1.902850     0.113232      54.83
 H      -0.158474     2.895065     0.095642      22.23
 C       1.248939     1.398728    -0.098862      -6.39
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 O       2.275265     2.432161    -0.457237     115.61
 C       1.883824     3.682806    -1.425900      82.09
 H       2.794056     4.164855    -1.727078      25.23
 H       1.538015     2.914162    -2.435982      21.49
 H       1.090895     4.256217    -1.005471      25.23
 C       1.701518    -0.009931    -0.349883      11.32
 O       3.027834    -0.097335    -0.567902     168.34
 C       0.652552    -0.957489    -0.241990      61.99
 H       0.952636    -1.887045    -0.505188      23.21
 C      -0.953518     0.928857     0.269411      46.22
 C      -2.311872     1.412498     0.648613      69.70
 H      -2.998400     0.450835     1.053356      24.42
 O      -2.307770     2.423856     1.638747     218.53
 H      -2.055601     2.022006     2.609376      25.27
 C      -3.236566     2.072595    -0.544595      86.29
 H      -2.691533     2.790320    -1.056866      26.77
 O      -3.378537     0.871582    -1.433921     208.35
 H      -3.352723     0.963210    -2.405347      22.82
 C      -4.661182     2.649405    -0.136813      67.31
 O      -5.281519     3.231567    -1.334195     230.11
 H      -5.295234     4.265309    -1.303929      27.77
 H      -4.391371     3.634783     0.566339      22.25
 H      -5.284850     1.553519     0.211497      25.58
55
name = lig-etoh-Waterframe_772
 C       5.998404    -1.143190     1.221452      55.93
 H       6.336657    -0.234342     0.809370      24.93
 C       4.940317    -3.252985     0.969901      71.87
 H       4.567474    -3.992977     0.315014      23.05
 C       5.161070    -3.570186     2.308718       7.37
 O       4.898105    -4.940480     2.862099     229.22
 C       3.515567    -5.477439     2.628531      99.37
 H       2.854028    -4.910205     3.394818      24.09
 H       3.911615    -6.591144     2.752446      22.91
 H       3.040977    -5.267269     1.694950      28.24
 C       5.793853    -2.673167     3.162340      19.90
 O       5.943642    -2.896819     4.521122      74.77
 H       5.603675    -3.908783     4.677424      19.19
 C       6.227352    -1.506675     2.536938      56.40
 H       6.856798    -0.577594     2.929700      22.50
 C       5.245189    -2.029468     0.424474      17.58
 C       4.908838    -1.605928    -1.095956      99.29
 H       5.191007    -2.453965    -1.632654      28.33
 O       5.763522    -0.514074    -1.441673     257.93
 H       5.289967     0.207707    -1.025748      27.92
 C       3.400476    -1.391059    -1.424028      68.65
 H       2.873046    -2.318889    -1.064732      23.06
 C       2.994207    -0.958739    -2.830108     114.75
 O       3.084506    -2.249991    -3.507022     262.39
 H       4.057858    -2.176586    -3.938763      24.67
 H       3.539086    -0.243792    -3.308166      26.34
 H       1.951369    -0.783515    -2.771130      26.20
 C      -0.656324    -0.406058     0.183902      51.19
 H      -1.431838    -1.150136     0.088617      21.32
 C       0.029460     1.876160     0.160094      93.79
 H      -0.294734     2.875619     0.399503      19.54
 C       1.343570     1.498269    -0.153119      -1.61
 O       2.273571     2.501521    -0.506549     225.16
 C       1.877227     3.526863    -1.407222     107.47
 H       2.858412     4.081791    -1.554397      25.35
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 H       1.321048     3.060386    -2.320515      25.31
 H       1.245965     4.225326    -1.041824      27.99
 C       1.603053     0.009883    -0.341354      21.09
 O       2.996058    -0.093398    -0.560392     114.94
 C       0.621112    -0.926026    -0.167232      53.38
 H       0.622821    -1.957248    -0.277900      20.94
 C      -0.989844     0.891455     0.393586      38.17
 C      -2.386372     1.414644     0.674681      75.82
 H      -2.983486     0.426658     0.794186      23.07
 O      -2.307504     2.446473     1.736284     231.32
 H      -2.181909     1.868995     2.673558      23.09
 C      -3.252497     2.008127    -0.562493      89.16
 H      -2.809651     2.851670    -1.138056      25.89
 O      -3.427269     0.824727    -1.369460     231.04
 H      -3.106130     1.108175    -2.275493      22.72
 C      -4.636296     2.631899    -0.235243      85.43
 O      -5.280480     3.207882    -1.344838     284.23
 H      -5.151680     4.203906    -1.291544      28.69
 H      -4.497745     3.286282     0.745795      24.66
 H      -5.257240     1.692768     0.434669      26.32
55
name = lig-etoh-Waterframe_773
 C       6.005153    -1.178154     1.219570      62.55
 H       6.139664    -0.220243     0.806131      25.23
 C       4.925202    -3.357424     0.958730      64.64
 H       4.335083    -3.958457     0.369116      21.68
 C       5.124742    -3.652645     2.366937      20.00
 O       4.939243    -4.891392     2.806493     184.77
 C       3.451476    -5.459637     2.654922      85.12
 H       2.817531    -5.207027     3.497424      25.93
 H       3.371293    -6.643202     2.809488      22.23
 H       3.192007    -5.145755     1.555326      24.72
 C       5.840470    -2.743386     3.167555      -5.64
 O       5.923669    -2.932043     4.517476     166.29
 H       5.645042    -3.935860     4.763254      21.01
 C       6.243938    -1.447648     2.576214      44.02
 H       6.976587    -0.936165     3.373606      20.98
 C       5.266716    -2.083263     0.467264      30.81
 C       4.897502    -1.616273    -1.107385      95.93
 H       5.190665    -2.416103    -1.664282      27.87
 O       5.735897    -0.481288    -1.453778     245.73
 H       5.489556     0.434904    -1.274715      25.68
 C       3.384326    -1.366615    -1.398452      74.55
 H       2.793181    -2.278506    -1.056321      22.28
 C       3.031464    -0.989376    -2.853266     113.89
 O       3.082111    -2.288114    -3.493780     264.01
 H       3.999542    -2.507893    -4.025505      24.88
 H       3.649937    -0.294920    -3.288842      27.60
 H       2.113224    -0.557920    -3.006713      27.61
 C      -0.692316    -0.433354     0.097357      37.51
 H      -1.495009    -1.068670     0.320478      22.37
 C       0.052006     1.849663     0.257883      52.59
 H      -0.168043     2.962414     0.522375      19.55
 C       1.353516     1.558583    -0.251179      31.94
 O       2.313754     2.492435    -0.499964     256.82
 C       1.847596     3.425338    -1.422406     125.62
 H       2.822945     3.954415    -1.852571      24.50
 H       1.442743     3.231333    -2.243414      30.42
 H       1.232642     4.190884    -0.893099      25.40
 C       1.673029     0.250184    -0.309154      10.94
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 O       2.956447    -0.197621    -0.581389     138.57
 C       0.561252    -0.916796    -0.078504      49.47
 H       0.732095    -2.045056    -0.094028      18.12
 C      -1.013717     0.949678     0.459573      31.67
 C      -2.509498     1.447037     0.691249      90.71
 H      -3.108858     0.758085     1.141381      24.60
 O      -2.345111     2.426630     1.834868     224.51
 H      -2.004477     1.791497     2.686942      23.78
 C      -3.233958     1.952240    -0.560770      85.81
 H      -2.503830     2.677815    -1.151434      23.86
 O      -3.472335     0.795232    -1.343158     245.58
 H      -2.853858     0.735212    -2.164495      23.60
 C      -4.584267     2.563346    -0.183905     122.95
 O      -5.272333     3.183596    -1.347204     263.04
 H      -5.268052     4.103118    -1.107247      29.17
 H      -4.545099     3.306182     0.508550      28.44
 H      -5.359276     1.984916    -0.045275      29.83
55
name = lig-etoh-Waterframe_774
 C       5.987161    -1.177686     1.270276      35.92
 H       6.283886    -0.203052     0.884161      25.57
 C       4.870660    -3.421950     0.970064      57.82
 H       4.257443    -4.118857     0.480917      21.40
 C       5.134175    -3.681130     2.273104       6.93
 O       4.880645    -4.975442     2.807289     252.96
 C       3.467189    -5.441262     2.700418      96.52
 H       2.938116    -4.923477     3.418022      27.84
 H       3.440646    -6.513288     2.613273      23.80
 H       2.941223    -5.071140     1.629358      24.52
 C       5.849637    -2.717842     3.152981       0.55
 O       5.924950    -2.981659     4.525563      63.96
 H       5.726143    -3.898809     4.922916      19.64
 C       6.297894    -1.499691     2.696032      61.21
 H       6.798420    -0.812426     3.429665      21.48
 C       5.250268    -2.103540     0.383177      21.77
 C       4.903653    -1.614256    -1.012728     104.87
 H       5.213231    -2.323622    -1.875007      26.01
 O       5.737924    -0.502344    -1.520878     181.10
 H       5.509892     0.374798    -1.069272      27.01
 C       3.330364    -1.288326    -1.323280      95.52
 H       2.724460    -2.207855    -1.161656      24.80
 C       3.100055    -1.067690    -2.879195      95.56
 O       3.080475    -2.368961    -3.531376     253.90
 H       3.941867    -2.312703    -4.201844      23.30
 H       4.065564    -0.452191    -3.170072      22.87
 H       2.113929    -0.533896    -3.022495      25.43
 C      -0.856082    -0.423149     0.125592      36.14
 H      -1.551529    -1.214020     0.354647      21.12
 C       0.032515     1.900235     0.367940      48.93
 H      -0.028976     3.072709     0.569219      20.11
 C       1.272155     1.551594    -0.260868      -4.68
 O       2.383091     2.447427    -0.485430     163.80
 C       1.863090     3.496429    -1.487140      74.35
 H       2.771172     4.036327    -1.961746      23.61
 H       1.226007     2.806676    -2.332785      22.91
 H       1.146849     4.240660    -0.856740      21.98
 C       1.668508     0.145466    -0.297681      21.38
 O       2.961547    -0.241974    -0.567919     198.39
 C       0.665760    -0.746650    -0.041420      42.58
 H       1.161486    -1.847135    -0.054765      18.73
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 C      -1.033776     0.972904     0.410914      25.83
 C      -2.509184     1.462125     0.837400      76.18
 H      -3.167893     0.668432     1.177172      24.86
 O      -2.408074     2.418230     1.901923     256.67
 H      -1.795621     1.911430     2.637932      24.98
 C      -3.193461     1.920626    -0.526391      76.50
 H      -2.488063     2.677380    -1.089720      23.96
 O      -3.510090     0.736980    -1.343152     217.73
 H      -2.850018     0.485619    -2.092630      23.81
 C      -4.589237     2.546378    -0.175320     101.92
 O      -5.236649     3.195474    -1.346427     260.88
 H      -5.391752     4.101592    -1.292576      30.33
 H      -4.393595     3.244250     0.554275      27.86
 H      -5.148550     1.610726     0.156721      28.39
55
name = lig-etoh-Waterframe_775
 C       5.947920    -1.240666     1.358255      42.56
 H       6.447022    -0.314138     0.950679      22.29
 C       4.811812    -3.351118     0.892855      70.00
 H       4.386471    -4.184552     0.311299      23.64
 C       5.215510    -3.682687     2.252295      -4.43
 O       4.812348    -5.065192     2.806593     227.40
 C       3.479339    -5.378815     2.712113     117.87
 H       2.954832    -4.943357     3.556720      24.85
 H       3.539876    -6.386198     2.839349      20.25
 H       2.891276    -5.038427     1.772334      24.04
 C       5.783411    -2.805246     3.188472      13.44
 O       5.946353    -3.019990     4.538690     252.23
 H       5.710749    -3.950059     4.618049      22.22
 C       6.303270    -1.537853     2.684878      52.67
 H       6.597759    -0.719534     3.201912      25.34
 C       5.270514    -2.096635     0.416511      23.55
 C       4.887620    -1.604850    -1.009143      89.11
 H       5.023394    -2.653282    -1.685335      21.27
 O       5.743696    -0.529947    -1.563028     243.76
 H       5.505920     0.194273    -0.907525      25.37
 C       3.327601    -1.362027    -1.329606      74.12
 H       2.795756    -2.227801    -0.969896      21.67
 C       3.209084    -1.137816    -2.845747      81.80
 O       3.101722    -2.439154    -3.591149     253.28
 H       3.889353    -2.406099    -4.306029      23.47
 H       4.165386    -0.541663    -3.391197      20.30
 H       2.205872    -0.527043    -3.121900      22.52
 C      -0.764714    -0.374073     0.202657      30.04
 H      -1.534633    -1.201920     0.201991      20.01
 C       0.068090     1.963224     0.376164      49.56
 H      -0.293703     3.007976     0.731910      21.14
 C       1.283097     1.516244    -0.172249      -4.50
 O       2.376530     2.436090    -0.510295     158.89
 C       1.890358     3.521825    -1.520343      68.93
 H       2.720973     4.028765    -1.995609      23.32
 H       1.088206     2.761153    -2.284142      20.75
 H       1.151173     4.392106    -1.120029      22.00
 C       1.625350     0.122525    -0.323551      23.37
 O       2.975312    -0.156028    -0.484698     156.71
 C       0.564519    -0.694763     0.000382      43.81
 H       0.810181    -1.858505     0.032126      18.91
 C      -1.136958     0.944710     0.401213      45.29
 C      -2.435767     1.414578     0.922391      72.15
 H      -2.971594     0.377908     1.047826      23.92
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 O      -2.465004     2.438987     1.950723     257.25
 H      -1.902263     2.101172     2.763293      26.63
 C      -3.197485     1.913270    -0.489255      81.31
 H      -2.623969     2.621131    -1.086944      25.42
 O      -3.526402     0.683679    -1.292346     206.91
 H      -2.910070     0.798925    -2.138637      22.43
 C      -4.570447     2.559418    -0.211217      95.89
 O      -5.205818     3.169691    -1.331443     281.12
 H      -5.114113     4.119426    -1.110566      27.04
 H      -4.455352     3.230569     0.757621      24.63
 H      -5.080913     1.631194     0.483409      26.22
55
name = lig-etoh-Waterframe_776
 C       5.947141    -1.282775     1.354186      70.86
 H       6.335672    -0.288485     0.962587      21.74
 C       4.845938    -3.285579     0.912533      63.29
 H       4.462555    -4.003706     0.131611      22.30
 C       5.207959    -3.774574     2.249597       2.09
 O       4.867827    -5.016152     2.748389     326.30
 C       3.389699    -5.352450     2.770630     108.28
 H       2.824701    -4.999244     3.710504      23.28
 H       3.215563    -6.439969     2.917781      23.65
 H       3.026726    -5.140345     1.828606      27.27
 C       5.768512    -2.827366     3.217882       7.27
 O       5.955158    -3.100532     4.528946     201.17
 H       5.746478    -3.989520     4.879744      22.20
 C       6.212860    -1.611183     2.654478      68.28
 H       6.642624    -0.941602     3.299773      25.90
 C       5.252148    -2.049912     0.472858      37.16
 C       4.871185    -1.653721    -1.033210      88.87
 H       5.262127    -2.603623    -1.653840      21.90
 O       5.723497    -0.606227    -1.554583     229.31
 H       5.669274     0.360743    -1.243149      22.88
 C       3.421180    -1.423824    -1.294215      66.78
 H       2.782513    -2.196953    -0.909872      22.22
 C       3.262527    -1.215098    -2.869013      88.65
 O       3.147081    -2.491480    -3.627243     276.77
 H       3.953993    -2.597752    -4.233218      25.38
 H       4.201022    -0.564780    -3.190251      21.12
 H       2.333198    -0.549925    -3.084251      24.26
 C      -0.726169    -0.303224     0.288699      32.40
 H      -1.560177    -1.110225     0.252147      19.30
 C      -0.028604     1.907353     0.338319      72.93
 H      -0.100194     2.966516     0.595292      20.27
 C       1.353384     1.579151    -0.074833      20.48
 O       2.299946     2.473941    -0.553077     217.49
 C       1.876913     3.466299    -1.524520     109.08
 H       2.748127     3.721801    -1.939239      27.36
 H       1.355219     3.196933    -2.525417      24.70
 H       1.414294     4.276728    -0.983618      25.81
 C       1.593937     0.233432    -0.312241       1.30
 O       2.977820    -0.096862    -0.441820      61.64
 C       0.503717    -0.862379     0.004716      44.48
 H       0.424186    -1.959407    -0.015440      19.11
 C      -1.007390     1.047599     0.473746      33.46
 C      -2.442397     1.365174     0.845485      75.48
 H      -3.072249     0.567152     1.431736      21.56
 O      -2.514071     2.445525     1.972760     226.82
 H      -2.195588     1.982017     2.802210      26.61
 C      -3.248655     1.885390    -0.428720      90.01
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 H      -2.594667     2.448524    -0.970584      26.04
 O      -3.481322     0.679369    -1.219811     217.58
 H      -3.353969     0.875942    -2.252616      22.05
 C      -4.526883     2.528115    -0.089881     109.99
 O      -5.175737     3.143758    -1.295664     249.43
 H      -5.041802     4.160856    -1.269767      27.54
 H      -4.475078     3.565002     0.524283      22.38
 H      -5.498985     1.969331    -0.059845      23.54
55
name = lig-etoh-Waterframe_777
 C       5.984772    -1.190518     1.297642      32.97
 H       6.242124    -0.133936     1.039798      25.09
 C       4.921478    -3.328417     1.007153      64.08
 H       4.310940    -4.026856     0.304370      21.51
 C       5.151535    -3.760606     2.242066      41.78
 O       4.878371    -5.015348     2.698619     152.11
 C       3.320568    -5.362691     2.837791      79.15
 H       2.923441    -4.518756     3.554208      22.77
 H       3.297151    -6.552392     2.824412      22.51
 H       2.874196    -5.027835     1.980189      27.80
 C       5.742607    -2.923033     3.164201       7.01
 O       5.971909    -3.159208     4.539502     157.07
 H       5.789980    -4.161764     4.841300      20.76
 C       6.134550    -1.663955     2.723485      44.90
 H       6.840965    -1.135240     3.434834      21.84
 C       5.183713    -2.010611     0.447572      42.17
 C       4.955919    -1.697225    -0.963687     112.35
 H       5.177014    -2.449473    -1.616345      27.85
 O       5.747715    -0.673297    -1.565050     207.64
 H       5.310728     0.224157    -1.315485      25.07
 C       3.437224    -1.409208    -1.270614      67.91
 H       2.798065    -2.241801    -0.949579      23.62
 C       3.281891    -1.262478    -2.870798     110.32
 O       3.222206    -2.529564    -3.621142     297.36
 H       4.026362    -2.467014    -4.140324      27.09
 H       4.137478    -0.800738    -3.170668      25.34
 H       2.367880    -0.781207    -3.047414      26.84
 C      -0.750015    -0.333756     0.352426      43.83
 H      -1.719934    -0.872310     0.626448      21.02
 C       0.071942     2.040423     0.278566      94.98
 H      -0.192086     3.046089     0.354966      21.54
 C       1.295811     1.603835    -0.037417      11.35
 O       2.223908     2.496101    -0.571941     235.82
 C       1.908668     3.464254    -1.550962     118.08
 H       2.932463     3.796987    -1.803335      26.02
 H       1.301502     3.103523    -2.211401      30.73
 H       1.531662     4.285844    -1.096316      28.04
 C       1.572348     0.120030    -0.216596       4.81
 O       2.985139    -0.103508    -0.478507     111.96
 C       0.583747    -0.871178    -0.034901      31.76
 H       0.906807    -1.835916    -0.242429      19.29
 C      -0.990190     1.035996     0.598065      28.26
 C      -2.496416     1.430337     0.855940      76.35
 H      -3.008589     0.417668     1.142440      23.57
 O      -2.556236     2.428731     1.944091     271.14
 H      -2.402057     1.830326     2.657054      27.30
 C      -3.250039     1.806273    -0.352688      84.22
 H      -2.653887     2.609574    -0.834615      25.60
 O      -3.446481     0.661714    -1.162600     232.37
 H      -3.484754     0.981775    -2.159918      21.50
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 C      -4.632312     2.615542    -0.031709      87.62
 O      -5.130423     3.135538    -1.322769     276.47
 H      -5.125965     4.178878    -1.420286      25.86
 H      -4.284694     3.219027     0.934040      24.70
 H      -5.210553     1.819995     0.526836      29.27
55
name = lig-etoh-Waterframe_778
 C       5.959822    -1.141994     1.392247      61.46
 H       6.327513    -0.179479     1.053475      27.22
 C       4.908902    -3.332422     0.923991      58.33
 H       4.292134    -4.173266     0.436753      21.71
 C       5.096185    -3.760174     2.301975       6.93
 O       4.780175    -5.116558     2.661925     192.82
 C       3.358804    -5.282683     2.823927     123.43
 H       3.021579    -4.814800     3.837748      24.96
 H       3.222832    -6.381381     3.340325      23.15
 H       2.714024    -5.085083     1.929170      26.19
 C       5.768453    -2.937752     3.214300       3.30
 O       5.988775    -3.201136     4.504259     127.53
 H       5.835398    -4.219402     4.676126      22.42
 C       6.132572    -1.623124     2.682588      41.62
 H       6.822613    -1.017235     3.481832      20.62
 C       5.229543    -2.021927     0.537117      41.83
 C       4.949709    -1.738356    -0.960479      92.96
 H       5.047432    -2.651255    -1.394844      28.09
 O       5.790657    -0.690973    -1.562927     201.94
 H       5.405005     0.219439    -1.251931      26.64
 C       3.407022    -1.377351    -1.272319      84.22
 H       2.879697    -2.284543    -0.863427      24.44
 C       3.265947    -1.282829    -2.832070     115.21
 O       3.325587    -2.569107    -3.581954     305.59
 H       4.017506    -2.571524    -4.208302      28.83
 H       3.953310    -0.677715    -3.258522      27.63
 H       2.394323    -0.789547    -3.086474      28.17
 C      -0.715181    -0.373565     0.438223      47.79
 H      -1.389458    -1.212537     0.683551      21.72
 C       0.049056     2.164386     0.295584      26.17
 H      -0.214990     3.134638     0.089417      20.26
 C       1.274721     1.531739    -0.115028     -13.51
 O       2.235194     2.451243    -0.527239     186.01
 C       1.940229     3.523259    -1.553926      90.90
 H       2.966800     3.876725    -2.201665      22.63
 H       1.256168     3.003446    -2.238235      26.75
 H       1.367032     4.444105    -1.250777      24.72
 C       1.643413     0.089824    -0.113109      15.65
 O       2.975811    -0.173396    -0.572473     163.31
 C       0.613684    -0.784717    -0.052104      61.07
 H       0.929601    -1.732312    -0.285382      23.04
 C      -1.012731     1.000108     0.660272       9.70
 C      -2.463017     1.423210     0.928774      88.79
 H      -2.957384     0.513671     1.069562      26.71
 O      -2.613594     2.379629     1.913561     301.11
 H      -2.335105     2.088323     2.737023      30.59
 C      -3.295698     1.887560    -0.325289      65.28
 H      -2.731133     2.680976    -1.031577      22.76
 O      -3.437443     0.633766    -1.118244     215.24
 H      -3.214500     0.918440    -2.108992      21.88
 C      -4.651710     2.605850     0.044984     101.49
 O      -5.104688     3.105659    -1.312829     260.93
 H      -5.050653     4.095304    -1.028483      25.27
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 H      -4.482228     3.542285     0.624119      26.14
 H      -5.310567     1.930949     0.565726      29.38
55
name = lig-etoh-Waterframe_779
 C       5.873340    -1.165565     1.477204      43.91
 H       6.350861    -0.313293     1.085982      19.14
 C       4.857323    -3.362304     0.959022      50.35
 H       4.521610    -3.893384     0.047850      21.25
 C       5.069624    -3.788672     2.288992       0.87
 O       4.687025    -5.174426     2.603844     253.67
 C       3.353556    -5.260959     2.937651     110.45
 H       3.009731    -4.528233     3.671041      25.29
 H       3.159951    -6.339860     3.139945      22.55
 H       2.654102    -5.206831     1.965099      26.54
 C       5.779850    -2.848538     3.189529      12.84
 O       6.036450    -3.224248     4.483921     190.79
 H       5.771152    -4.103522     4.926441      20.93
 C       6.206945    -1.597233     2.749251      46.37
 H       6.629330    -0.735107     3.461311      23.83
 C       5.292476    -2.054011     0.559853       7.21
 C       4.874981    -1.699385    -0.941869      76.68
 H       5.226954    -2.677211    -1.529059      22.82
 O       5.819977    -0.722569    -1.543190     161.95
 H       5.821553     0.230610    -1.147447      25.56
 C       3.404367    -1.428473    -1.274609      88.78
 H       2.755346    -2.276699    -0.911752      24.15
 C       3.223518    -1.275670    -2.839027      91.43
 O       3.412124    -2.610063    -3.507613     276.89
 H       4.187124    -2.561944    -4.091417      26.14
 H       3.993825    -0.427039    -3.156152      23.68
 H       2.133975    -0.954826    -3.027436      25.65
 C      -0.602063    -0.373744     0.520106      39.48
 H      -1.202198    -1.210468     0.648991      21.82
 C      -0.071689     1.977056     0.328559      62.39
 H      -0.181061     3.006618     0.078141      22.18
 C       1.265817     1.560580    -0.185633      -5.44
 O       2.332425     2.446408    -0.510792     167.03
 C       1.912874     3.511411    -1.572273      74.88
 H       3.024642     3.718816    -2.127743      21.70
 H       1.239807     3.048030    -2.540560      22.72
 H       1.438396     4.459026    -0.980290      22.10
 C       1.745435     0.205053    -0.111396      15.18
 O       2.967103    -0.212843    -0.665951     150.54
 C       0.596340    -0.754552    -0.002734      49.15
 H       0.507502    -1.824657    -0.145951      22.64
 C      -0.972687     1.060028     0.630801      37.84
 C      -2.438014     1.343802     0.937368      86.07
 H      -3.047905     0.565603     1.285858      25.26
 O      -2.678297     2.386345     1.958900     273.66
 H      -2.092697     2.210884     2.624866      32.06
 C      -3.294928     1.961465    -0.308141      63.27
 H      -2.695973     2.667570    -1.041892      22.42
 O      -3.458392     0.648807    -1.076658     222.12
 H      -2.945440     0.598498    -1.976524      23.58
 C      -4.622961     2.593416     0.057988     124.41
 O      -5.112784     3.058980    -1.245440     272.90
 H      -5.181618     4.092841    -1.458528      28.26
 H      -4.539490     3.470021     0.506992      28.22
 H      -5.516383     2.103477     0.297105      27.39
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name = lig-etoh-Waterframe_780
 C       5.831708    -1.192483     1.470001      33.25
 H       6.115822    -0.230687     1.152852      20.39
 C       4.845158    -3.334694     0.984790      57.79
 H       4.538277    -4.095574     0.261665      22.18
 C       5.083622    -3.811696     2.241881      26.56
 O       4.702223    -5.131916     2.542558     270.96
 C       3.209852    -5.290556     3.027594      81.36
 H       3.012819    -4.478499     3.601054      26.12
 H       3.121191    -6.234837     3.387604      22.35
 H       2.646279    -4.970083     2.066628      25.56
 C       5.738493    -2.900420     3.182419      -8.76
 O       6.105666    -3.204307     4.499449     212.89
 H       5.691113    -4.111046     4.630521      21.81
 C       6.239811    -1.558241     2.855764      30.78
 H       6.640680    -0.891589     3.654397      22.82
 C       5.257116    -2.084571     0.521748      41.71
 C       4.905942    -1.658907    -0.878037      86.84
 H       5.097050    -2.565500    -1.744087      21.10
 O       5.830712    -0.735723    -1.514057     148.43
 H       5.826049     0.102276    -0.912053      24.33
 C       3.362892    -1.501816    -1.298338      75.93
 H       2.739155    -2.339845    -0.966405      25.51
 C       3.163481    -1.312345    -2.825492      85.41
 O       3.494516    -2.608104    -3.426668     260.37
 H       4.380492    -2.530852    -3.911981      24.27
 H       3.954057    -0.419666    -3.268793      22.19
 H       1.989163    -1.130255    -3.021648      25.01
 C      -0.566813    -0.299835     0.601043      43.32
 H      -1.411889    -0.877541     0.801407      20.72
 C       0.020486     1.852951     0.236779      59.53
 H      -0.462645     2.926232     0.430710      22.29
 C       1.330067     1.579067    -0.177474      13.09
 O       2.360598     2.489634    -0.555797     217.56
 C       1.960929     3.438481    -1.556184     103.52
 H       2.877104     3.883502    -1.880705      24.32
 H       1.036526     3.058417    -2.279459      23.54
 H       1.552748     4.382424    -0.954274      23.18
 C       1.691879     0.194977    -0.237597       9.72
 O       2.976312    -0.144092    -0.719186      99.18
 C       0.699977    -0.723118     0.091633      67.23
 H       0.977982    -1.867825    -0.058042      24.30
 C      -1.050497     0.948723     0.635678      51.31
 C      -2.504803     1.384628     0.933882      74.41
 H      -2.934158     0.323466     1.187796      24.30
 O      -2.691045     2.415110     2.030283     277.82
 H      -2.036082     2.146627     2.588371      32.05
 C      -3.210681     1.859573    -0.282378      99.54
 H      -2.655247     2.682445    -0.711282      25.82
 O      -3.510624     0.681060    -1.033163     251.14
 H      -2.892612     0.722547    -1.854221      24.82
 C      -4.624786     2.658263    -0.011062      92.32
 O      -5.175282     3.007325    -1.272679     299.67
 H      -5.008284     4.082531    -1.301109      25.42
 H      -4.379488     3.247257     0.949029      24.78
 H      -5.231219     1.802078     0.581367      26.88
55
name = lig-etoh-Waterframe_781
 C       5.863052    -1.188553     1.514248      59.54
 H       5.833812    -0.152527     1.213996      27.59
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 C       4.843248    -3.363455     0.927195      43.19
 H       4.336991    -4.150398     0.491198      20.57
 C       5.125282    -3.784740     2.283614      10.01
 O       4.698120    -5.086536     2.529907     266.85
 C       3.156866    -5.235596     3.044943      90.70
 H       3.037092    -4.610065     3.954698      24.00
 H       3.053976    -6.116069     3.596034      23.46
 H       2.430140    -5.241724     2.207936      27.95
 C       5.775202    -2.922348     3.234434      10.24
 O       6.131128    -3.227618     4.483908     167.68
 H       5.945977    -4.171962     4.867153      23.65
 C       6.121328    -1.616124     2.799896      66.87
 H       6.634714    -1.143060     3.514635      22.03
 C       5.193262    -2.048329     0.536007       7.99
 C       4.921802    -1.703160    -0.941843      90.63
 H       5.120715    -2.777223    -1.296901      21.50
 O       5.809807    -0.699860    -1.445417     171.09
 H       5.690511     0.224559    -0.987907      24.02
 C       3.358342    -1.429037    -1.288249      84.74
 H       2.862205    -2.249846    -0.795980      24.91
 C       3.126350    -1.402593    -2.790757     105.10
 O       3.565288    -2.602876    -3.365724     264.34
 H       4.369525    -2.520364    -4.065387      22.50
 H       3.619601    -0.463902    -3.304265      24.19
 H       2.055426    -1.132432    -3.098309      25.01
 C      -0.612722    -0.404683     0.670296      30.45
 H      -1.215118    -1.325304     1.010520      22.00
 C       0.066383     1.898612     0.170711      56.29
 H      -0.065873     3.102074     0.428288      19.70
 C       1.401037     1.565074    -0.157909      13.02
 O       2.347554     2.484698    -0.583343     232.56
 C       1.983554     3.480619    -1.490791     128.92
 H       2.706528     3.754334    -2.094742      29.49
 H       1.349757     2.980371    -2.230765      27.42
 H       1.416286     4.248195    -1.082456      28.43
 C       1.651507     0.164450    -0.408839      14.63
 O       2.964299    -0.069003    -0.754844     130.97
 C       0.799432    -0.743585     0.213964      42.59
 H       1.262414    -1.863062     0.260245      20.62
 C      -1.027387     0.968188     0.617271      17.61
 C      -2.526769     1.411719     1.011844      68.55
 H      -3.174293     0.400390     1.268020      23.14
 O      -2.646500     2.395930     2.067262     266.93
 H      -2.250673     2.051226     2.836271      29.82
 C      -3.215164     1.862072    -0.265048     102.86
 H      -2.492585     2.355122    -0.830482      26.62
 O      -3.544373     0.706176    -1.040557     222.17
 H      -3.147044     0.790452    -1.980896      24.83
 C      -4.553834     2.556047    -0.012062      72.02
 O      -5.233982     3.008887    -1.270174     243.24
 H      -5.146080     4.060652    -1.258282      26.29
 H      -4.474203     3.684276     0.714393      21.40
 H      -5.229244     1.629704     0.435554      25.62
55
name = lig-etoh-Waterframe_782
 C       5.800304    -1.182906     1.463403      49.57
 H       5.990087    -0.099118     1.370520      23.74
 C       4.865236    -3.378613     0.977667      53.57
 H       4.273255    -3.857277     0.246741      21.11
 C       5.122036    -3.748257     2.280382      20.40
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 O       4.617707    -5.079014     2.582226     155.36
 C       3.238618    -5.191997     3.094741      75.51
 H       2.963263    -4.256315     3.846857      24.81
 H       3.314931    -6.315943     3.400562      20.36
 H       2.511484    -5.128299     2.310678      29.16
 C       5.804829    -2.986635     3.218084      17.07
 O       6.169717    -3.278315     4.528859     173.30
 H       5.877376    -4.234071     4.871468      24.65
 C       6.027074    -1.690018     2.768284      55.67
 H       6.582367    -1.023773     3.328706      22.28
 C       5.133115    -2.014680     0.579636      17.62
 C       4.890875    -1.729973    -0.946762     103.97
 H       5.256317    -2.462274    -1.556339      24.49
 O       5.793956    -0.661015    -1.397411     189.22
 H       5.347881     0.239775    -1.197836      24.45
 C       3.413424    -1.320231    -1.241887      95.61
 H       2.796699    -2.020369    -0.682754      23.79
 C       3.081978    -1.410652    -2.790568     111.47
 O       3.623277    -2.651425    -3.351157     257.11
 H       4.204590    -2.332663    -4.188861      23.56
 H       3.600379    -0.631696    -3.118310      27.28
 H       2.055227    -1.481468    -2.892240      25.99
 C      -0.517142    -0.533090     0.676433      30.66
 H      -1.035047    -1.462417     1.250051      20.80
 C       0.048787     1.968424     0.205854      56.92
 H       0.008092     3.104439     0.127670      19.74
 C       1.348328     1.520710    -0.215432       9.29
 O       2.381203     2.443770    -0.546073     187.20
 C       1.918527     3.533639    -1.526886     100.46
 H       2.957334     3.817552    -2.109990      23.76
 H       1.368906     3.078143    -2.207547      29.13
 H       1.444473     4.354627    -1.112322      26.33
 C       1.648465     0.181167    -0.455444      19.32
 O       2.985395    -0.049909    -0.816240     173.18
 C       0.771754    -0.789184     0.332769      40.64
 H       1.044189    -1.851689     0.651128      19.81
 C      -0.929889     1.007296     0.606558       7.53
 C      -2.471457     1.377103     1.084234      69.59
 H      -3.097923     0.543637     1.497385      22.59
 O      -2.576054     2.372519     2.094879     263.55
 H      -2.485728     1.821499     2.886042      27.24
 C      -3.212381     1.933378    -0.302822      82.28
 H      -2.556614     2.505945    -0.974352      24.80
 O      -3.572985     0.673757    -1.082105     181.21
 H      -3.446731     0.899330    -2.058468      25.12
 C      -4.539754     2.510164    -0.045855     111.33
 O      -5.272492     3.007524    -1.243813     270.47
 H      -5.285672     4.010984    -1.254349      29.15
 H      -4.516915     3.542623     0.610403      23.86
 H      -5.313721     1.936903     0.436213      28.38
55
name = lig-etoh-Waterframe_783
 C       5.691463    -1.192131     1.465196      47.67
 H       6.160737    -0.208074     1.131602      22.05
 C       4.852730    -3.278741     0.991394      61.12
 H       4.390338    -4.032796     0.257750      21.76
 C       5.041574    -3.868731     2.272698       7.42
 O       4.593918    -5.062430     2.650764     336.07
 C       3.333819    -5.152650     3.101544     103.89
 H       3.024241    -4.366442     4.007121      24.70
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 H       3.132610    -6.229565     3.686386      20.67
 H       2.713281    -4.973959     2.273229      30.16
 C       5.825098    -3.031531     3.227702     -14.33
 O       6.193136    -3.353566     4.551108     181.48
 H       5.692166    -4.215855     4.750000      22.94
 C       6.034870    -1.671622     2.759717      37.51
 H       6.473715    -0.909737     3.524019      20.68
 C       5.096692    -2.042397     0.526129      42.96
 C       4.883766    -1.645903    -0.905435     111.80
 H       4.963995    -2.426354    -1.597922      24.12
 O       5.772877    -0.609672    -1.370275     238.90
 H       5.400606     0.319352    -1.183840      23.47
 C       3.413653    -1.351671    -1.231768      86.84
 H       2.762520    -2.092016    -0.718407      23.53
 C       3.074592    -1.445814    -2.746870     104.58
 O       3.644115    -2.673492    -3.364119     250.77
 H       4.308119    -2.553532    -4.210006      23.32
 H       3.375261    -0.583689    -3.304877      25.04
 H       2.004104    -1.471063    -2.816547      25.23
 C      -0.454018    -0.413141     0.707500      47.53
 H      -1.256112    -1.005469     1.297692      20.09
 C       0.019631     1.957636     0.248224      26.21
 H      -0.438221     2.856440     0.165479      18.21
 C       1.275761     1.516613    -0.324079       1.66
 O       2.358416     2.440056    -0.532441     189.39
 C       1.912198     3.524230    -1.576723      90.23
 H       3.065236     4.103939    -1.777479      20.43
 H       1.163294     3.203943    -2.327569      24.57
 H       1.505864     4.394102    -0.956287      23.23
 C       1.633831     0.120398    -0.324153       5.48
 O       3.018242     0.000855    -0.864649     153.25
 C       0.841886    -0.844905     0.340749      59.64
 H       1.227831    -1.784160     0.570351      21.14
 C      -0.882622     0.922033     0.655249      59.43
 C      -2.367039     1.372091     0.997046      66.30
 H      -2.759270     0.441079     1.141959      25.06
 O      -2.492573     2.358898     2.123155     262.52
 H      -2.324975     1.830530     2.980145      25.92
 C      -3.202225     1.872784    -0.332876      74.92
 H      -2.677599     2.806481    -0.794538      21.55
 O      -3.572498     0.654446    -1.121471     227.03
 H      -3.445720     0.933728    -2.070856      22.68
 C      -4.636654     2.620523    -0.030552     111.42
 O      -5.301159     2.994904    -1.242099     345.25
 H      -5.184716     3.937487    -1.163202      30.95
 H      -4.326700     3.208663     0.645582      32.27
 H      -5.086227     1.893886     0.515210      32.81
55
name = lig-etoh-Waterframe_784
 C       5.653266    -1.191369     1.515514      55.65
 H       5.979276    -0.220716     1.022969      20.83
 C       4.744525    -3.368123     0.980905      37.83
 H       4.470827    -4.289703     0.288922      19.33
 C       5.080184    -3.796120     2.313476       7.20
 O       4.700169    -5.134625     2.709038     233.49
 C       3.245065    -5.113414     3.178280      88.40
 H       3.263459    -4.403903     3.960352      24.08
 H       2.991509    -6.180415     3.615643      21.50
 H       2.490775    -4.980710     2.389731      27.00
 C       5.785076    -3.016718     3.201221       5.62
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 O       6.178160    -3.429969     4.493159     235.22
 H       5.889739    -4.290518     4.927741      23.76
 C       6.062557    -1.665393     2.782240      38.98
 H       6.466026    -0.967603     3.701706      20.52
 C       5.120900    -2.016100     0.502043       5.98
 C       4.852576    -1.554311    -0.912146      96.58
 H       5.095630    -2.638087    -1.368164      19.14
 O       5.767054    -0.558642    -1.369363     237.16
 H       5.614393     0.300042    -0.891995      24.26
 C       3.376858    -1.379606    -1.254605      78.24
 H       2.892024    -2.229476    -0.702744      22.96
 C       3.091686    -1.502379    -2.756668      96.62
 O       3.612905    -2.679895    -3.380624     249.45
 H       4.381203    -2.366721    -4.017932      22.70
 H       3.276065    -0.501620    -3.422195      22.28
 H       1.920722    -1.586119    -2.831516      23.86
 C      -0.446679    -0.323292     0.811532      36.10
 H      -1.131796    -1.099624     1.099128      18.76
 C       0.004403     1.883639     0.218964      55.11
 H      -0.385545     2.822249     0.251685      22.07
 C       1.217108     1.558252    -0.344027      15.25
 O       2.245629     2.449273    -0.611351     218.26
 C       1.969944     3.553430    -1.478530      97.78
 H       2.899780     3.942938    -2.134508      21.59
 H       1.416288     3.177878    -2.513506      22.88
 H       1.222012     4.241636    -0.868844      21.89
 C       1.729610     0.143695    -0.202441       2.90
 O       2.963391     0.020332    -0.861086     125.82
 C       0.930405    -0.879533     0.309701      61.13
 H       1.274748    -1.825214     0.377787      23.21
 C      -0.874996     0.962688     0.677857      47.60
 C      -2.284503     1.343111     0.859933      79.65
 H      -2.839719     0.433822     1.084646      24.33
 O      -2.411953     2.306256     2.092369     193.40
 H      -1.815994     1.805910     2.842657      25.05
 C      -3.250809     1.845863    -0.314517      77.14
 H      -2.525397     2.403361    -1.070541      21.39
 O      -3.518027     0.694916    -1.154695     229.83
 H      -3.147114     0.779751    -2.059567      23.61
 C      -4.636276     2.607103     0.051323      89.53
 O      -5.311739     3.014978    -1.211148     311.23
 H      -5.296870     3.952589    -1.386137      30.22
 H      -4.417651     3.574420     0.679039      23.84
 H      -5.319838     1.776964     0.499839      26.52
55
name = lig-etoh-Waterframe_785
 C       5.678624    -1.184384     1.541722      41.58
 H       5.774924    -0.078101     1.544271      19.89
 C       4.707314    -3.437131     0.980740      50.50
 H       4.293965    -4.170545     0.194321      20.23
 C       5.086317    -3.782065     2.264611       5.69
 O       4.748857    -5.185071     2.750558     207.48
 C       3.202907    -5.105657     3.269665      77.05
 H       3.138986    -4.419560     3.966873      24.28
 H       3.111780    -6.089450     3.554733      22.39
 H       2.495148    -4.727299     2.425930      25.13
 C       5.763247    -2.960403     3.244731      18.58
 O       6.173455    -3.457955     4.412004      99.02
 H       5.893925    -4.423254     4.464198      25.87
 C       6.062933    -1.677673     2.844076      33.79
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 H       6.660781    -0.907097     3.526506      22.03
 C       5.086254    -2.084976     0.611979       9.23
 C       4.857911    -1.570810    -0.901081      73.07
 H       5.377433    -2.334320    -1.693152      21.07
 O       5.779965    -0.527862    -1.389091     167.02
 H       5.618429     0.289585    -0.878664      23.99
 C       3.375000    -1.353174    -1.278052      85.81
 H       2.780599    -2.083816    -0.689400      23.24
 C       3.011012    -1.524042    -2.806611      90.13
 O       3.578282    -2.670915    -3.409273     252.86
 H       4.377012    -2.459287    -3.990603      25.14
 H       3.588524    -0.522442    -3.225705      21.64
 H       1.844443    -1.704020    -2.857187      23.95
 C      -0.335201    -0.469386     0.867519      31.13
 H      -0.967244    -1.247486     1.027580      19.52
 C       0.015840     1.956036     0.126858      45.64
 H      -0.003410     3.084375     0.149025      19.26
 C       1.269332     1.514576    -0.269532      25.50
 O       2.173583     2.446429    -0.707132     218.97
 C       1.952258     3.579551    -1.472431     119.04
 H       2.864280     3.986213    -1.566275      24.90
 H       1.352021     3.088260    -2.380572      23.39
 H       1.367868     4.527556    -1.124967      24.25
 C       1.793264     0.244962    -0.160838      30.90
 O       2.904597    -0.036279    -0.848035     175.74
 C       0.886317    -0.776472     0.343253      62.15
 H       1.015195    -1.848180     0.304707      22.20
 C      -0.905257     0.970570     0.662478      23.72
 C      -2.375811     1.310330     0.854253      83.41
 H      -2.942661     0.407015     1.358585      21.80
 O      -2.315655     2.229840     1.999278     159.90
 H      -1.624601     1.677798     2.635161      24.85
 C      -3.211522     1.877377    -0.348002      80.54
 H      -2.729117     2.690937    -0.988544      22.04
 O      -3.478984     0.701892    -1.176111     265.02
 H      -2.877815     0.803348    -1.918493      26.12
 C      -4.567520     2.563045     0.077912      91.92
 O      -5.315806     2.996255    -1.175189     279.71
 H      -5.249515     4.017412    -1.166644      26.58
 H      -4.692747     3.659524     0.744831      21.23
 H      -5.483896     2.002353     0.641256      23.96
55
name = lig-etoh-Waterframe_786
 C       5.690137    -1.220891     1.624631      45.71
 H       5.669207    -0.157889     1.376564      21.47
 C       4.747415    -3.401551     0.978013      49.90
 H       4.139048    -4.004847     0.288460      20.07
 C       5.054373    -3.920939     2.264346       4.69
 O       4.682726    -5.109348     2.778893     350.74
 C       3.288501    -5.109881     3.318207      88.50
 H       3.116806    -4.530756     4.269580      21.82
 H       2.984044    -6.030837     3.585312      22.52
 H       2.708166    -4.766633     2.347225      25.88
 C       5.741938    -2.947126     3.209339     -13.73
 O       6.184861    -3.491926     4.358727     141.45
 H       5.840474    -4.446141     4.412085      21.90
 C       6.066727    -1.614513     2.867641      74.90
 H       6.706225    -1.028416     3.512820      23.09
 C       5.036616    -2.081629     0.642861      16.02
 C       4.930954    -1.622414    -0.904201      72.43
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 H       4.916187    -2.570259    -1.531684      22.71
 O       5.791020    -0.520209    -1.384562     241.01
 H       5.470460     0.377643    -1.121169      23.63
 C       3.332403    -1.371245    -1.265327      89.22
 H       2.763181    -2.133394    -0.730570      23.33
 C       2.972655    -1.487322    -2.803007     105.85
 O       3.543129    -2.696767    -3.453852     285.45
 H       4.229388    -2.494479    -4.087486      27.37
 H       3.248895    -0.574297    -3.408633      24.07
 H       1.912523    -1.314374    -3.036730      24.91
 C      -0.391052    -0.428526     0.857256      24.96
 H      -0.971581    -1.239965     1.204516      17.65
 C      -0.006493     1.959577     0.100406      95.04
 H      -0.304415     3.145316    -0.070091      16.83
 C       1.338978     1.565043    -0.181163       3.09
 O       2.209807     2.425556    -0.740158     205.37
 C       1.884044     3.655976    -1.545860     118.20
 H       2.851845     4.021322    -1.510597      25.67
 H       1.523237     3.593759    -2.554968      26.49
 H       1.321861     4.342528    -0.950055      25.64
 C       1.740200     0.189981    -0.135651      24.78
 O       2.943322    -0.077274    -0.872091     206.35
 C       0.913145    -0.681880     0.382407      63.80
 H       1.199594    -1.800412     0.208991      19.68
 C      -0.880253     0.852367     0.584921      49.51
 C      -2.459507     1.278879     0.928178      56.55
 H      -3.059814     0.243347     1.061702      20.75
 O      -2.229682     2.203164     1.914911     201.70
 H      -1.823664     1.685561     2.812345      23.63
 C      -3.195083     1.933339    -0.330013      89.45
 H      -2.694917     2.754170    -0.670454      24.92
 O      -3.432735     0.720225    -1.190171     242.59
 H      -2.944917     0.754917    -2.015785      24.98
 C      -4.618039     2.567380     0.059304      87.11
 O      -5.293174     2.956534    -1.119932     330.69
 H      -5.312076     4.030775    -1.107836      26.13
 H      -3.986227     3.259926     0.807486      25.16
 H      -4.966110     1.674045     0.697715      28.07
55
name = lig-etoh-Waterframe_787
 C       5.627725    -1.193096     1.571503      46.18
 H       5.977969    -0.297366     1.089717      23.15
 C       4.758484    -3.395185     0.999806      44.02
 H       4.221077    -3.986096     0.339923      20.13
 C       5.062887    -3.851499     2.281654      39.81
 O       4.600497    -5.076221     2.818264     308.07
 C       3.359018    -5.128159     3.329876      88.82
 H       3.342738    -4.402862     4.371960      18.92
 H       3.074449    -6.193132     3.457615      20.42
 H       2.500912    -4.675741     2.676456      26.43
 C       5.728142    -3.040006     3.117565      -2.44
 O       6.212738    -3.513046     4.338856     219.48
 H       5.880981    -4.369706     4.815968      21.51
 C       6.071600    -1.629138     2.916413      63.68
 H       6.547545    -1.099816     3.619173      22.52
 C       5.065157    -1.994855     0.618496       1.82
 C       4.866827    -1.661230    -0.884596      90.01
 H       5.308928    -2.523711    -1.314812      22.78
 O       5.789380    -0.601439    -1.375872     216.12
 H       5.301861     0.220198    -1.115136      25.58
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 C       3.325431    -1.425019    -1.276613      82.27
 H       2.844611    -2.256177    -0.791968      23.38
 C       2.977878    -1.417432    -2.848541     110.08
 O       3.458151    -2.702939    -3.489606     288.36
 H       4.116626    -2.415785    -4.073655      28.40
 H       3.427262    -0.641231    -3.296869      25.70
 H       1.934036    -1.519751    -2.847384      25.54
 C      -0.474965    -0.369232     0.817749      42.56
 H      -1.091163    -1.119773     1.397784      19.87
 C      -0.029928     1.826232     0.114762      81.70
 H      -0.761434     2.709492    -0.202000      16.04
 C       1.303947     1.669837    -0.139246       4.73
 O       2.310803     2.448757    -0.816841     186.64
 C       1.863870     3.735530    -1.525937      91.06
 H       2.945574     4.381073    -1.809219      22.55
 H       1.551472     3.494898    -2.478287      26.41
 H       1.149417     4.114321    -0.888765      26.31
 C       1.772585     0.220851    -0.189025      -2.53
 O       2.965253    -0.061811    -0.861761     174.39
 C       0.924658    -0.774991     0.444987      36.65
 H       1.392221    -1.884419     0.466105      18.33
 C      -0.964604     0.856873     0.480271      30.35
 C      -2.392888     1.200769     0.859461      74.32
 H      -3.065764     0.413407     1.264572      23.07
 O      -2.197180     2.233395     1.934883     189.84
 H      -2.123612     1.665701     2.876090      23.62
 C      -3.191682     1.906951    -0.296778     105.80
 H      -2.451043     2.486683    -0.811362      24.50
 O      -3.369947     0.770739    -1.206285     250.52
 H      -3.125362     0.940617    -2.112471      25.86
 C      -4.490998     2.477932     0.089876     118.22
 O      -5.285143     2.936348    -1.036593     295.85
 H      -5.424624     3.961654    -1.192318      28.71
 H      -4.454357     3.353230     0.710426      26.07
 H      -5.207213     1.766524     0.510762      27.78
55
name = lig-etoh-Waterframe_788
 C       5.667035    -1.097954     1.553751      47.55
 H       6.214319    -0.198827     1.349366      21.75
 C       4.730346    -3.328960     0.972589      68.08
 H       4.375596    -4.053537     0.335171      22.35
 C       4.998774    -3.784836     2.250651      -6.69
 O       4.641416    -5.071601     2.753531     289.41
 C       3.268592    -5.109465     3.396942      86.53
 H       3.344512    -4.681899     4.541017      20.57
 H       3.222301    -6.270034     3.604175      21.82
 H       2.499330    -4.644590     2.856741      31.44
 C       5.830720    -3.028390     3.210637       2.47
 O       6.262913    -3.500566     4.360341     162.37
 H       5.771329    -4.430896     4.518258      20.38
 C       5.993415    -1.723765     2.826403      44.65
 H       6.375367    -1.134010     3.594501      22.19
 C       5.057970    -2.041093     0.597041      22.77
 C       4.832569    -1.693622    -0.872395     110.11
 H       5.241103    -2.493928    -1.423709      24.22
 O       5.735291    -0.698907    -1.356060     199.30
 H       5.619370     0.254217    -0.997625      23.61
 C       3.386653    -1.474488    -1.334907      72.08
 H       2.674003    -2.137365    -0.826591      23.81
 C       3.016603    -1.445406    -2.838467     108.10
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 O       3.353879    -2.658621    -3.526620     297.02
 H       4.150612    -2.576126    -4.054015      28.30
 H       3.475536    -0.562428    -3.222301      24.81
 H       1.899982    -1.391179    -2.860229      25.41
 C      -0.410482    -0.471110     0.768485      26.45
 H      -1.192914    -1.129141     1.350788      19.06
 C      -0.120186     1.805638     0.046677      79.04
 H      -0.322453     2.863420    -0.221533      19.42
 C       1.367474     1.617957    -0.224050      -2.86
 O       2.373791     2.516164    -0.882968     178.06
 C       1.870789     3.722051    -1.487178      96.72
 H       2.721835     4.710189    -1.506957      22.05
 H       1.323924     3.309612    -2.272518      26.08
 H       1.082519     4.318925    -0.976099      25.25
 C       1.734797     0.261739    -0.180907       8.85
 O       2.969512    -0.043756    -0.820233     116.77
 C       0.895897    -0.786463     0.479302      57.66
 H       1.135502    -1.816063     0.910381      20.29
 C      -1.025350     0.805400     0.427103      18.93
 C      -2.336881     1.238573     0.844373      94.54
 H      -2.752939     0.406144     1.286729      24.08
 O      -2.216351     2.263193     1.976433     171.38
 H      -2.068444     1.638148     2.844689      23.77
 C      -3.084335     1.796742    -0.304006      91.94
 H      -2.523774     2.734700    -0.894485      22.29
 O      -3.342919     0.788408    -1.239229     263.29
 H      -3.215939     1.180815    -2.080176      24.90
 C      -4.476851     2.477949     0.157786     106.08
 O      -5.306762     2.908639    -1.028608     292.64
 H      -5.094212     3.889287    -0.844778      27.44
 H      -4.594427     3.201624     0.853785      28.30
 H      -5.068037     1.698634     0.579346      29.77
55
name = lig-etoh-Waterframe_789
 C       5.721323    -1.150030     1.536333      58.73
 H       5.891559    -0.066729     1.438782      20.30
 C       4.682985    -3.305410     0.972656      36.08
 H       4.357733    -3.993870     0.203352      21.16
 C       4.994073    -3.763230     2.337147       0.76
 O       4.658405    -5.058127     2.645060     231.17
 C       3.246853    -5.131258     3.506441      58.26
 H       3.286813    -4.692741     4.453956      23.65
 H       2.862872    -6.265786     3.547055      22.37
 H       2.618716    -4.721815     2.848851      32.90
 C       5.813108    -3.026113     3.175021       1.86
 O       6.314701    -3.501791     4.419666     191.95
 H       6.038548    -4.502600     4.564724      27.19
 C       5.963794    -1.681010     2.747674      56.26
 H       6.455960    -0.949084     3.496779      22.35
 C       5.074104    -1.980402     0.575383      22.19
 C       4.844451    -1.739000    -0.899023     105.38
 H       4.852481    -2.702483    -1.481588      24.07
 O       5.711290    -0.737831    -1.363279     229.34
 H       5.624975     0.107283    -0.771044      24.42
 C       3.361258    -1.447096    -1.308130      73.85
 H       2.694165    -2.204142    -0.796611      22.88
 C       3.052676    -1.445362    -2.806116     102.39
 O       3.258814    -2.642440    -3.578400     269.30
 H       4.119959    -2.464276    -4.094494      25.26
 H       3.523498    -0.514818    -3.410692      22.88
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 H       1.976445    -1.071998    -2.971838      24.44
 C      -0.444968    -0.511064     0.719186      42.47
 H      -0.921947    -1.498011     1.114949      19.56
 C      -0.017681     1.879588    -0.113325      67.44
 H      -0.340359     2.858774    -0.024594      19.10
 C       1.343668     1.538550    -0.366646     -14.06
 O       2.367951     2.536683    -0.854302     179.01
 C       1.780251     3.717883    -1.440648      92.26
 H       2.813521     4.183436    -1.834522      22.46
 H       1.392880     3.649144    -2.514549      24.78
 H       1.118418     4.233787    -0.633252      23.08
 C       1.746238     0.167879    -0.163336      14.38
 O       2.980113    -0.057248    -0.774757     152.99
 C       0.903337    -0.726440     0.488727      62.40
 H       1.420695    -1.626741     0.746236      20.67
 C      -0.873641     0.750444     0.407103      48.56
 C      -2.309587     1.285244     0.943975      77.85
 H      -2.894881     0.381453     1.141976      26.10
 O      -2.257239     2.263061     1.994786     255.29
 H      -1.800193     1.756407     2.770601      25.59
 C      -3.088123     1.846167    -0.307848      78.97
 H      -2.436090     2.825570    -0.665803      23.61
 O      -3.336503     0.777697    -1.278218     230.87
 H      -3.153382     0.952692    -2.204812      23.87
 C      -4.542072     2.396981     0.211419      93.31
 O      -5.281167     2.899709    -0.990800     261.60
 H      -5.300263     3.921690    -1.163626      27.55
 H      -4.116779     3.126731     0.981130      25.87
 H      -4.845216     1.478566     0.657735      29.92
55
name = lig-etoh-Waterframe_790
 C       5.706569    -1.185683     1.447727      36.65
 H       5.597994    -0.091414     1.209336      20.61
 C       4.693648    -3.255384     1.061672      54.54
 H       4.152829    -3.968410     0.336948      21.48
 C       4.970669    -3.785019     2.301248      12.86
 O       4.593072    -5.110344     2.609464     248.61
 C       3.294692    -5.146555     3.503676      77.35
 H       3.441644    -4.669217     4.345394      25.36
 H       3.055390    -6.273144     3.537682      22.28
 H       2.600024    -4.537518     2.899604      30.62
 C       5.779999    -3.001149     3.188183     -10.95
 O       6.355846    -3.467204     4.420820     170.55
 H       6.026575    -4.328940     4.801670      25.56
 C       6.041613    -1.610599     2.824182      32.71
 H       6.660315    -0.845557     3.550155      19.09
 C       5.059885    -2.019393     0.546937      29.77
 C       4.789401    -1.759146    -0.934872      95.86
 H       5.270424    -2.742129    -1.451739      22.46
 O       5.732027    -0.749459    -1.412386     154.46
 H       5.426154     0.060705    -0.841908      25.96
 C       3.303990    -1.383913    -1.217169      90.25
 H       2.767426    -2.266487    -0.792688      23.09
 C       3.039961    -1.324237    -2.839298      83.76
 O       3.187222    -2.648370    -3.620059     222.45
 H       3.953149    -2.393189    -4.320367      23.78
 H       3.987484    -0.679916    -3.211047      20.69
 H       1.918515    -1.127737    -2.864061      23.75
 C      -0.434078    -0.539015     0.664485      44.63
 H      -1.180688    -1.325801     0.963979      20.71
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 C       0.068769     1.840557    -0.186328      70.85
 H      -0.415761     2.711338    -0.091551      21.43
 C       1.340991     1.522306    -0.540421      18.68
 O       2.270691     2.445153    -0.797135     197.81
 C       1.789120     3.725420    -1.422447      98.71
 H       2.585488     4.228106    -1.617856      26.56
 H       0.991673     3.435538    -2.339079      23.94
 H       1.310407     4.416994    -0.610051      25.02
 C       1.794725     0.167311    -0.220066      19.75
 O       3.023623    -0.127979    -0.726913     214.59
 C       1.026003    -0.754858     0.456635      53.23
 H       1.455259    -1.677344     0.486083      21.79
 C      -0.810280     0.874971     0.442291      27.45
 C      -2.261187     1.251696     0.919700      66.11
 H      -2.969118     0.399971     1.356693      22.39
 O      -2.279719     2.242104     2.012953     235.51
 H      -1.705027     1.907555     2.740546      27.44
 C      -3.153374     1.940697    -0.289467      86.57
 H      -2.590965     2.652806    -0.850374      25.60
 O      -3.324458     0.774479    -1.281153     216.52
 H      -2.814881     0.862004    -2.115298      25.40
 C      -4.478920     2.313037     0.176769      94.89
 O      -5.267135     2.864328    -0.919905     249.27
 H      -5.333344     3.894272    -0.822323      26.10
 H      -4.355231     3.295147     1.029266      23.05
 H      -5.304141     1.610447     0.617656      25.17
55
name = lig-etoh-Waterframe_791
 C       5.671575    -1.165053     1.472529      30.02
 H       5.987134    -0.140797     1.068874      20.46
 C       4.649049    -3.300710     1.083352      53.43
 H       3.903019    -4.022158     0.538960      19.94
 C       4.988009    -3.824784     2.314394       0.54
 O       4.502771    -5.160100     2.602691     313.77
 C       3.407024    -5.129738     3.404768     103.37
 H       3.654282    -4.763837     4.462595      20.76
 H       3.180051    -6.150772     3.680395      19.61
 H       2.384974    -4.572391     3.034675      28.49
 C       5.796299    -2.917920     3.274353      -2.88
 O       6.369840    -3.398253     4.384841     148.63
 H       5.831817    -4.171154     4.574667      30.14
 C       6.102436    -1.602864     2.812534      33.35
 H       6.707234    -0.953360     3.606225      21.41
 C       5.047259    -2.085551     0.545470      27.48
 C       4.805198    -1.752452    -0.940688      85.78
 H       5.075440    -2.695826    -1.635291      22.15
 O       5.724195    -0.732336    -1.457288     179.65
 H       5.597772     0.283940    -1.322925      23.04
 C       3.313897    -1.475370    -1.268792      84.50
 H       2.567929    -2.118969    -0.798923      23.21
 C       3.047923    -1.288909    -2.826880      95.34
 O       3.119197    -2.603401    -3.629177     249.87
 H       3.927999    -2.551485    -4.355071      23.46
 H       3.744676    -0.455392    -3.173816      24.08
 H       2.148062    -0.722330    -3.141480      25.37
 C      -0.310251    -0.428464     0.593698      43.44
 H      -1.095055    -1.010550     0.926414      22.07
 C      -0.024244     1.776135    -0.159121      63.77
 H      -0.142340     2.844306    -0.463579      18.14
 C       1.332161     1.430317    -0.617180      20.37
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 O       2.237365     2.427806    -0.806375     209.54
 C       1.803038     3.710199    -1.356199     107.04
 H       2.581989     4.262445    -1.808757      24.62
 H       0.871705     3.371668    -2.029346      25.37
 H       1.313956     4.359375    -0.640040      26.48
 C       1.813840     0.210447    -0.311509      16.17
 O       3.122320    -0.161230    -0.656791     169.82
 C       1.012807    -0.838117     0.374278      51.92
 H       1.225974    -1.869736     0.496014      20.05
 C      -0.827149     0.878292     0.499395      35.86
 C      -2.240755     1.286115     0.841157      72.36
 H      -2.555776     0.185225     1.195629      22.11
 O      -2.275822     2.238985     2.019596     240.48
 H      -1.829331     1.751395     2.717130      26.94
 C      -3.123643     1.842409    -0.294381     102.16
 H      -2.840333     2.701336    -0.757899      27.43
 O      -3.312133     0.788966    -1.242910     283.75
 H      -2.624995     1.009564    -1.888817      26.85
 C      -4.523678     2.353582     0.164321      91.99
 O      -5.284948     2.854894    -0.876357     282.93
 H      -5.284112     3.852029    -0.676170      25.69
 H      -4.527310     3.079436     1.124055      24.80
 H      -5.027412     1.328832     0.701905      26.02
55
name = lig-etoh-Waterframe_792
 C       5.688012    -1.180962     1.508183      50.80
 H       6.323688    -0.352623     1.138281      18.74
 C       4.560000    -3.416881     1.088236      15.32
 H       3.889130    -4.029560     0.393758      18.96
 C       5.057011    -3.793521     2.398518       4.44
 O       4.523611    -5.146773     2.535147     224.53
 C       3.406531    -5.151694     3.456919      50.84
 H       3.619833    -4.477665     4.516785      18.68
 H       3.096459    -6.111108     3.606553      21.97
 H       2.507028    -4.567347     2.797969      25.28
 C       5.760466    -2.892483     3.201660      36.77
 O       6.355026    -3.352982     4.390385     160.64
 H       6.116728    -4.270852     4.614490      30.29
 C       6.099961    -1.625495     2.735169      46.20
 H       6.691676    -0.957332     3.335571      25.36
 C       5.063927    -2.059237     0.590254     -18.87
 C       4.832567    -1.745300    -0.955712      89.48
 H       5.041317    -2.628937    -1.519468      24.53
 O       5.726122    -0.726897    -1.521171     202.71
 H       5.291530     0.202576    -1.316237      23.49
 C       3.330591    -1.523213    -1.374675      64.31
 H       2.685331    -2.305161    -0.970725      24.99
 C       3.071786    -1.260513    -2.861381     113.77
 O       3.058288    -2.506750    -3.610241     277.91
 H       4.060368    -2.418793    -4.015394      22.20
 H       3.863440    -0.726566    -3.240569      25.76
 H       2.098739    -0.815245    -2.977304      26.53
 C      -0.275786    -0.347285     0.617257      32.25
 H      -0.724747    -1.180611     1.051022      21.59
 C      -0.001027     1.787927    -0.200278      54.19
 H      -0.476280     2.905047    -0.490055      17.54
 C       1.217646     1.387632    -0.562287      -0.65
 O       2.295940     2.464177    -0.862530     201.93
 C       1.742807     3.680206    -1.290961     114.28
 H       2.621444     3.973775    -2.191829      22.11
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 H       1.050161     3.695859    -2.070384      28.18
 H       1.564476     4.297042    -0.461282      27.46
 C       1.857126     0.021220    -0.360036      12.61
 O       3.213064    -0.148174    -0.591776     136.97
 C       0.951621    -0.825713     0.194502      71.74
 H       1.209849    -1.876563     0.529231      21.38
 C      -0.831405     0.920208     0.464455      61.87
 C      -2.220879     1.291218     0.861511      90.89
 H      -2.858914     0.416916     1.043955      24.47
 O      -2.260622     2.202268     1.995578     287.49
 H      -2.103740     1.657699     2.703900      28.51
 C      -3.104208     1.797957    -0.262882      87.95
 H      -2.539190     2.746475    -0.661629      24.19
 O      -3.286333     0.798345    -1.214000     289.92
 H      -2.794321     0.831683    -2.065086      26.04
 C      -4.568343     2.279942     0.286400      97.06
 O      -5.339132     2.878591    -0.859960     310.72
 H      -5.372066     3.832390    -1.094704      28.80
 H      -4.335743     2.895438     1.013468      29.19
 H      -4.980400     1.289528     0.459679      29.23
55
name = lig-etoh-Waterframe_793
 C       5.760200    -1.224594     1.414981      45.45
 H       6.119866    -0.273634     1.036140      23.95
 C       4.597746    -3.306392     1.081818      63.12
 H       4.137593    -4.104586     0.510434      21.28
 C       4.975308    -3.810034     2.285683      27.49
 O       4.636376    -5.116258     2.533785     331.78
 C       3.339426    -5.134741     3.486891      67.92
 H       3.585307    -4.502667     4.500640      20.48
 H       3.123568    -6.130352     3.683349      21.44
 H       2.595460    -4.612494     2.870281      30.77
 C       5.766602    -2.978832     3.184168      -6.05
 O       6.324670    -3.312954     4.412240     146.30
 H       6.319090    -4.286127     4.502338      31.81
 C       6.092950    -1.643498     2.731865      57.54
 H       6.734280    -1.082627     3.252016      22.53
 C       4.991387    -2.114685     0.600395      30.78
 C       4.879241    -1.806620    -0.983060      97.89
 H       5.347259    -2.632725    -1.311509      26.12
 O       5.691350    -0.728705    -1.562024     190.97
 H       5.305049     0.119063    -1.096548      24.38
 C       3.448593    -1.472424    -1.389613      75.88
 H       2.846768    -2.321018    -1.064330      24.56
 C       3.090465    -1.215858    -2.888285     109.77
 O       3.038665    -2.430108    -3.591195     285.37
 H       3.931679    -2.660544    -4.101505      25.94
 H       3.855085    -0.597672    -3.272722      24.60
 H       2.094507    -0.816498    -2.828565      26.52
 C      -0.348272    -0.389794     0.695955      35.80
 H      -0.906990    -1.118761     1.373071      18.93
 C      -0.011836     1.862716    -0.267433      59.21
 H      -0.512871     3.005331    -0.359374      18.50
 C       1.391353     1.404104    -0.520172       5.92
 O       2.283330     2.363769    -0.920378     175.04
 C       1.745959     3.701128    -1.325926     103.85
 H       2.751646     4.319950    -1.815787      22.27
 H       0.783743     3.641212    -1.713695      26.21
 H       1.783884     4.433995    -0.505159      25.81
 C       1.858211     0.056944    -0.420402      24.04
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 O       3.214582    -0.200182    -0.582752     170.56
 C       0.915289    -0.863033     0.055152      62.20
 H       1.278920    -1.938136     0.379415      19.97
 C      -0.847203     0.901367     0.411346      32.27
 C      -2.288515     1.229296     0.931140      88.19
 H      -2.768703     0.385253     1.309482      24.13
 O      -2.242491     2.164787     1.986267     275.54
 H      -2.147447     1.728398     2.771279      29.81
 C      -3.108226     1.909809    -0.236616      76.85
 H      -2.466114     2.757225    -0.850583      22.18
 O      -3.265323     0.748992    -1.218085     212.45
 H      -3.075279     1.027301    -2.184583      24.70
 C      -4.543213     2.215984     0.277223     106.12
 O      -5.406548     2.853873    -0.827311     286.30
 H      -5.048567     3.757918    -0.805422      29.97
 H      -4.482363     2.824323     1.161396      28.02
 H      -5.236949     1.530658     0.529976      28.87
55
name = lig-etoh-Waterframe_794
 C       5.810474    -1.278576     1.328075      44.35
 H       5.885723    -0.281015     0.994995      23.20
 C       4.605698    -3.279795     1.012484      46.44
 H       4.204439    -3.952142     0.328044      21.82
 C       4.950549    -3.799485     2.277085      14.02
 O       4.690701    -5.124909     2.625364     243.63
 C       3.362293    -5.100856     3.448703      95.95
 H       3.576371    -4.653029     4.378442      24.85
 H       3.201014    -6.181268     3.735676      22.57
 H       2.602276    -4.720189     2.989892      35.13
 C       5.787319    -3.011881     3.148974      -6.49
 O       6.282562    -3.312665     4.418443     176.63
 H       6.139705    -4.300265     4.550266      26.52
 C       6.098003    -1.695859     2.712337      49.77
 H       6.731827    -1.194754     3.386274      21.88
 C       4.987816    -2.001689     0.490306      42.00
 C       4.962278    -1.863605    -0.991132     104.38
 H       5.333309    -2.795493    -1.552422      25.25
 O       5.665350    -0.722943    -1.548564     209.44
 H       5.701425     0.178618    -1.066663      25.17
 C       3.546379    -1.448259    -1.375244      85.46
 H       2.793502    -2.169702    -1.016303      21.98
 C       3.146532    -1.135749    -2.857397      80.20
 O       3.016061    -2.436242    -3.605594     291.52
 H       3.883771    -2.388553    -4.172930      25.24
 H       3.625870    -0.211614    -3.387111      22.10
 H       2.118985    -0.675390    -2.933921      24.74
 C      -0.351497    -0.480875     0.680893      25.72
 H      -1.150156    -0.968559     1.385963      18.61
 C       0.023487     1.794902    -0.262630      66.54
 H      -0.076052     2.891601    -0.334481      19.71
 C       1.424765     1.508639    -0.484688      17.16
 O       2.320868     2.324773    -1.027202     188.36
 C       1.841605     3.752771    -1.287998      97.18
 H       2.413410     4.139689    -2.169606      23.99
 H       0.834471     3.596249    -1.730130      25.58
 H       1.594257     4.171906    -0.226058      24.95
 C       1.793190     0.150318    -0.447781       4.07
 O       3.173630    -0.284989    -0.616765     166.17
 C       0.810281    -0.889271     0.070950      48.71
 H       1.224438    -1.972043     0.012501      18.44
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 C      -0.861478     0.854477     0.371854      30.84
 C      -2.309243     1.195478     0.937125      72.13
 H      -2.667415     0.199625     1.228047      23.41
 O      -2.229970     2.180391     2.035158     249.07
 H      -1.872952     1.686661     2.770883      27.47
 C      -3.168966     1.853522    -0.235320      84.98
 H      -2.811810     2.890530    -0.634072      23.61
 O      -3.237968     0.731714    -1.223534     217.47
 H      -3.284052     1.269980    -2.085089      24.04
 C      -4.569991     2.227679     0.202797      87.86
 O      -5.418188     2.818915    -0.748199     257.35
 H      -5.269751     3.814615    -0.786804      27.57
 H      -4.679878     3.002290     1.206649      23.79
 H      -4.949860     1.175110     0.615127      26.55
55
name = lig-etoh-Waterframe_795
 C       5.840767    -1.243258     1.360438      71.92
 H       6.249370    -0.252916     1.205151      23.63
 C       4.597169    -3.326945     0.918838      36.53
 H       4.061116    -3.897618     0.237331      22.59
 C       4.993458    -3.767381     2.282127     -16.04
 O       4.663025    -5.124823     2.736023     267.61
 C       3.479947    -5.120148     3.425345     103.91
 H       3.531355    -4.582480     4.276903      27.45
 H       3.168122    -6.291906     3.567752      22.45
 H       2.701851    -4.666873     2.810776      31.60
 C       5.791909    -2.978683     3.106129      17.76
 O       6.218899    -3.364739     4.395463     109.02
 H       5.899968    -4.254334     4.769195      26.60
 C       6.126258    -1.736401     2.608968      51.91
 H       6.627453    -1.003750     3.357783      20.50
 C       5.075870    -2.013156     0.433036      -6.97
 C       4.977809    -1.771719    -1.052369      97.71
 H       5.180823    -2.743526    -1.763476      24.58
 O       5.754420    -0.709860    -1.554220     141.98
 H       5.616060     0.019264    -0.841855      26.38
 C       3.458670    -1.463102    -1.410751      75.60
 H       2.884203    -2.422302    -1.202806      22.83
 C       3.135018    -1.082139    -2.843552      86.25
 O       3.040414    -2.396199    -3.630913     275.94
 H       3.850842    -2.438787    -4.157553      27.67
 H       3.998904    -0.473773    -3.426312      21.07
 H       2.043334    -0.810279    -2.668154      24.76
 C      -0.443295    -0.473253     0.602641      41.13
 H      -0.920156    -1.462509     1.023733      20.39
 C       0.066825     1.729105    -0.180834      70.85
 H      -0.358150     2.617484    -0.266735      22.87
 C       1.364216     1.467099    -0.478243     -17.63
 O       2.419069     2.410872    -1.169509     134.09
 C       1.879037     3.693962    -1.265393     118.51
 H       2.493807     4.189093    -1.858927      28.00
 H       0.906025     3.742143    -1.909222      26.37
 H       1.937457     4.362006    -0.262512      26.66
 C       1.709692     0.048250    -0.403085       3.57
 O       3.099518    -0.272015    -0.622505     140.63
 C       0.839355    -0.846244     0.080850      56.03
 H       0.969208    -1.934157    -0.016884      22.18
 C      -0.851157     0.815492     0.378525      46.52
 C      -2.243067     1.241348     0.874523      79.71
 H      -2.889616     0.296520     1.182374      25.70
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 O      -2.222553     2.165893     2.083664     214.24
 H      -1.643359     1.636991     2.719485      26.67
 C      -3.215593     1.765962    -0.207311     107.33
 H      -2.638683     2.547461    -0.568207      27.41
 O      -3.218044     0.785062    -1.226226     227.79
 H      -3.320406     1.034387    -2.212587      24.11
 C      -4.651064     2.199786     0.264891      87.00
 O      -5.458783     2.777867    -0.727014     271.61
 H      -5.532433     3.748032    -0.832195      27.63
 H      -4.248089     2.937045     1.202249      23.73
 H      -5.092442     1.063155     0.443052      26.05
55
name = lig-etoh-Waterframe_796
 C       5.853637    -1.190652     1.341600      19.89
 H       6.493790    -0.318825     1.042433      15.87
 C       4.660730    -3.325898     0.906683      78.92
 H       3.981103    -3.999295     0.411950      23.53
 C       5.000882    -3.809209     2.180349      25.36
 O       4.736035    -5.065839     2.763189     251.16
 C       3.464649    -5.149292     3.428775      85.40
 H       3.389161    -4.618897     4.450961      22.48
 H       3.147234    -6.308538     3.637850      21.53
 H       2.670686    -4.628459     2.630811      25.94
 C       5.778740    -3.001736     3.114028       3.48
 O       6.146126    -3.387276     4.356996     156.21
 H       5.819847    -4.375333     4.438179      17.42
 C       6.198300    -1.704597     2.603303      19.66
 H       6.716757    -0.870597     3.336469      23.90
 C       5.200839    -2.154547     0.432639       5.14
 C       4.872817    -1.662051    -1.158896      75.23
 H       5.337262    -2.621310    -1.654992      23.27
 O       5.889704    -0.663563    -1.541095     153.89
 H       5.619966     0.209586    -1.053071      24.92
 C       3.381419    -1.476876    -1.432619      79.39
 H       2.838894    -2.423578    -1.161326      26.69
 C       3.099054    -1.168646    -2.876203     114.61
 O       3.059742    -2.335194    -3.640806     301.74
 H       3.906520    -2.450369    -4.118551      25.88
 H       3.924930    -0.369141    -3.142100      25.53
 H       2.225973    -0.449479    -3.081449      26.30
 C      -0.479073    -0.562013     0.471965      45.74
 H      -1.244407    -1.367733     0.725274      21.70
 C       0.028862     1.779513    -0.081802      40.03
 H      -0.463637     2.660899    -0.306408      22.72
 C       1.440311     1.375803    -0.567532     -30.94
 O       2.411824     2.369343    -1.223218     144.35
 C       1.951407     3.745020    -1.309777     104.36
 H       2.830960     4.339467    -1.672101      24.73
 H       0.837305     3.842679    -1.596968      23.90
 H       1.837293     4.187167    -0.255451      26.19
 C       1.783454     0.035725    -0.374681      44.34
 O       3.008791    -0.251572    -0.618603     151.33
 C       0.798648    -0.899750     0.117050      63.21
 H       1.117336    -1.898813     0.196079      26.62
 C      -0.896341     0.789954     0.449067      29.24
 C      -2.252999     1.256534     0.881712      85.29
 H      -2.630752     0.258427     1.377641      25.14
 O      -2.199488     2.129752     2.058530     184.87
 H      -1.778636     1.533949     2.881715      24.14
 C      -3.181003     1.799841    -0.245779      92.69
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 H      -2.767185     2.689589    -0.683689      26.86
 O      -3.226185     0.762581    -1.241358     235.76
 H      -3.144777     1.181102    -2.188515      24.73
 C      -4.627892     2.114295     0.355736     106.20
 O      -5.545406     2.731137    -0.746747     277.59
 H      -5.286692     3.654393    -0.673384      29.21
 H      -4.643146     2.678218     1.261781      28.43
 H      -5.434296     1.550465     0.788306      26.80
55
name = lig-etoh-Waterframe_797
 C       5.906189    -1.273549     1.266775      18.38
 H       6.174558    -0.336478     0.663698      17.06
 C       4.723693    -3.390196     0.923533       0.77
 H       4.045028    -3.986482     0.222269      18.37
 C       5.088328    -3.805812     2.199217      54.29
 O       4.821147    -5.031614     2.746880     299.32
 C       3.362791    -5.165337     3.427843      73.70
 H       3.475699    -4.646864     4.521504      21.43
 H       3.327005    -6.255346     3.550118      22.96
 H       2.384992    -4.771531     2.768407      23.49
 C       5.776324    -2.936272     3.026431      -2.54
 O       6.058804    -3.418874     4.313169      57.41
 H       6.116062    -4.461895     4.431822      21.38
 C       6.236091    -1.661055     2.666118      43.70
 H       6.969792    -1.139654     3.432925      22.50
 C       5.282899    -2.122985     0.357398      -8.56
 C       4.898615    -1.665555    -1.126572      67.70
 H       5.087396    -2.421300    -1.879820      25.19
 O       5.958870    -0.591649    -1.513841     115.69
 H       5.755020     0.387468    -1.499319      23.01
 C       3.323378    -1.435692    -1.407055      87.99
 H       2.769069    -2.233762    -0.925467      26.71
 C       3.074468    -1.122168    -2.934144     106.16
 O       3.052719    -2.330285    -3.670630     297.46
 H       3.973027    -2.358806    -4.250313      21.94
 H       3.935862    -0.594647    -3.185202      28.12
 H       2.178492    -0.572185    -3.253211      26.06
 C      -0.570487    -0.633481     0.358710      31.32
 H      -1.393696    -1.193831     0.607997      23.72
 C       0.073064     1.778444    -0.039412      66.62
 H      -0.087117     2.928772    -0.222075      22.56
 C       1.357133     1.444742    -0.629613       4.74
 O       2.327382     2.225163    -1.228038     145.93
 C       2.004036     3.810145    -1.231031      82.17
 H       2.843843     4.321431    -2.075736      21.77
 H       1.177120     3.976181    -1.975068      23.80
 H       1.896151     3.947435    -0.257449      26.52
 C       1.730166     0.083716    -0.328526       2.52
 O       3.076216    -0.304790    -0.647117     154.48
 C       0.815875    -0.998617     0.140075      47.90
 H       1.242284    -1.902356     0.387851      24.19
 C      -0.847007     0.831239     0.446396      25.83
 C      -2.276566     1.197899     0.966832      76.42
 H      -2.863737     0.270549     1.107989      25.67
 O      -2.174401     2.120588     2.019585     234.79
 H      -2.036636     1.428639     2.881815      23.85
 C      -3.201575     1.816099    -0.223482      66.46
 H      -3.088133     2.908977    -0.631167      24.52
 O      -3.244954     0.731332    -1.260259     230.22
 H      -3.014742     1.195249    -2.157308      24.47
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 C      -4.698137     2.086729     0.400356      90.58
 O      -5.564536     2.679514    -0.698040     275.71
 H      -5.418048     3.631807    -0.952395      28.80
 H      -4.603792     2.886259     1.028629      27.81
 H      -5.000458     1.091481     0.757376      28.08
55
name = lig-etoh-Waterframe_798
 C       6.013245    -1.341081     1.222145      22.20
 H       6.154939    -0.235732     1.013466      26.28
 C       4.820160    -3.394456     0.837496      68.20
 H       4.274328    -4.174319     0.154977      23.86
 C       5.139808    -3.775459     2.170764       8.45
 O       4.778032    -5.038914     2.729080     238.43
 C       3.373002    -5.210055     3.418234      90.55
 H       3.464643    -4.605930     4.415729      22.00
 H       3.327190    -6.172118     3.519101      24.79
 H       2.645940    -4.739517     2.714978      29.36
 C       5.846850    -2.884752     3.045760      -0.61
 O       6.003735    -3.402184     4.287010     129.05
 H       6.031326    -4.440389     4.392708      20.86
 C       6.243752    -1.621279     2.605396      51.14
 H       6.939494    -1.115481     3.244467      16.10
 C       5.244474    -2.155809     0.318266       8.49
 C       4.993114    -1.682256    -1.088302      67.40
 H       5.156969    -2.384220    -1.798698      26.84
 O       5.972204    -0.560239    -1.510544     138.11
 H       5.401772     0.252715    -1.462150      26.39
 C       3.341665    -1.377424    -1.384644      70.88
 H       2.832730    -2.319352    -1.171251      28.16
 C       3.082360    -1.065762    -2.968152     101.75
 O       3.026977    -2.383803    -3.720409     262.21
 H       3.884900    -2.515683    -4.388542      23.58
 H       3.856073    -0.518611    -3.373905      27.70
 H       2.113600    -0.641738    -2.918041      28.60
 C      -0.598618    -0.563422     0.297809      48.95
 H      -1.213180    -1.318213     0.571384      25.01
 C       0.133403     1.832802    -0.048894      73.00
 H      -0.213166     2.966778     0.324180      21.77
 C       1.260758     1.412154    -0.602724      24.58
 O       2.217092     2.164360    -1.242022     152.77
 C       2.056290     3.730393    -1.237590      90.53
 H       3.259674     4.146564    -1.551625      21.98
 H       1.178896     3.968937    -1.820854      25.48
 H       2.037315     4.280587    -0.329857      26.03
 C       1.650978     0.027451    -0.315183       6.94
 O       3.112634    -0.247986    -0.610222     148.15
 C       0.832039    -0.970283     0.127241      64.03
 H       1.132898    -1.971284     0.381947      24.65
 C      -0.819835     0.782762     0.385282      35.51
 C      -2.293270     1.178141     0.894837      85.66
 H      -2.821607     0.329035     1.208577      26.65
 O      -2.181942     2.104604     2.027830     235.77
 H      -1.881822     1.621573     2.968299      25.72
 C      -3.290956     1.807477    -0.158778      76.21
 H      -2.625746     2.701424    -0.654855      24.32
 O      -3.267919     0.757598    -1.235420     201.62
 H      -3.089593     0.986539    -2.232641      24.55
 C      -4.724799     2.109817     0.335757      99.59
 O      -5.587284     2.561910    -0.625838     281.33
 H      -5.430777     3.558328    -0.773813      28.14
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 H      -4.426695     2.874159     1.251199      24.74
 H      -4.976903     1.041422     0.589700      27.93
55
name = lig-etoh-Waterframe_799
 C       6.054359    -1.315807     1.204715      61.21
 H       6.470781    -0.335048     0.920736      27.48
 C       4.927782    -3.438779     0.766905      69.99
 H       4.486466    -4.292928     0.126659      27.91
 C       5.132075    -3.743636     2.116462     -20.43
 O       4.695095    -5.035801     2.684093     215.68
 C       3.482569    -5.188928     3.355566     111.08
 H       3.350897    -4.730841     4.326748      24.50
 H       3.215208    -6.207785     3.551096      23.84
 H       2.766231    -4.850606     2.754587      34.87
 C       5.865753    -2.947668     3.046474       7.78
 O       6.002615    -3.335440     4.337020      98.76
 H       5.678060    -4.290083     4.314175      18.33
 C       6.283441    -1.634856     2.523974      73.07
 H       6.696806    -0.849306     2.988786      20.20
 C       5.263896    -2.146331     0.342388       3.23
 C       5.047295    -1.682455    -1.136146      92.20
 H       5.422456    -2.597398    -1.665630      24.12
 O       5.894661    -0.579471    -1.498771     195.79
 H       5.485059     0.254963    -1.133728      26.57
 C       3.539533    -1.354278    -1.459723      62.01
 H       2.890322    -2.234382    -1.232896      26.65
 C       3.110554    -1.109725    -2.957382      99.10
 O       2.974366    -2.411810    -3.737941     267.91
 H       3.927718    -2.342461    -4.145169      24.06
 H       3.586822    -0.225704    -3.512627      25.24
 H       2.103497    -0.655972    -2.944390      27.72
 C      -0.491464    -0.540933     0.288591      46.25
 H      -1.227130    -1.296709     0.594996      23.92
 C      -0.005216     1.839503     0.042024      54.79
 H      -0.186829     3.000843     0.378364      20.86
 C       1.281815     1.325695    -0.549523      -7.60
 O       2.138644     2.198295    -1.242881     195.05
 C       2.150485     3.584041    -1.224138     114.38
 H       3.145136     3.796693    -1.613722      25.26
 H       1.399992     3.973709    -1.855274      26.94
 H       1.911098     4.124443    -0.140549      24.46
 C       1.723100    -0.018113    -0.391268      30.10
 O       3.038659    -0.143517    -0.521759     134.68
 C       0.751192    -0.912835     0.104912      62.99
 H       1.037583    -2.008128     0.192382      24.88
 C      -0.923748     0.831052     0.308892      35.49
 C      -2.290277     1.166791     0.853781      94.45
 H      -2.528914     0.224008     1.304379      27.14
 O      -2.199182     2.115008     2.039480     206.65
 H      -1.700517     1.415850     2.687276      26.53
 C      -3.229122     1.780603    -0.204235     100.76
 H      -2.695300     2.745346    -0.541751      25.94
 O      -3.324018     0.761692    -1.186446     236.50
 H      -3.270669     1.273920    -2.090692      25.12
 C      -4.617734     2.068014     0.334812     108.12
 O      -5.652020     2.504999    -0.593312     247.44
 H      -5.486601     3.513078    -0.665584      28.79
 H      -4.863702     2.532463     1.446175      25.57
 H      -5.292587     1.288016     0.752015      26.73
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name = lig-etoh-Waterframe_800
 C       6.035933    -1.269861     1.150417      53.85
 H       6.525698    -0.536039     0.588434      23.00
 C       5.015130    -3.476976     0.747472      59.53
 H       4.586312    -4.155180    -0.020351      27.90
 C       5.107648    -3.781455     2.129970      -4.54
 O       4.707303    -5.010625     2.582860     205.29
 C       3.469424    -5.142827     3.304410     103.46
 H       3.549798    -4.667931     4.234562      24.97
 H       3.419592    -6.414722     3.450205      20.28
 H       2.592690    -4.837219     2.769277      29.83
 C       5.848285    -2.924787     2.989854       3.23
 O       6.007073    -3.258951     4.387412     153.99
 H       5.740878    -4.158167     4.724940      20.54
 C       6.334525    -1.707360     2.517354      79.01
 H       6.603464    -0.952997     3.243635      26.58
 C       5.341772    -2.102612     0.313868       1.80
 C       5.078202    -1.683905    -1.150343      98.00
 H       5.441410    -2.579086    -1.937856      23.31
 O       5.821248    -0.577943    -1.498880     197.20
 H       5.801845     0.179105    -0.931018      27.65
 C       3.690761    -1.354048    -1.544918      61.12
 H       3.087240    -2.102186    -0.976448      26.35
 C       3.074241    -1.137108    -2.941722      91.13
 O       2.989322    -2.364464    -3.711632     259.32
 H       3.785220    -2.669903    -4.223089      27.63
 H       3.788026    -0.423811    -3.632378      24.09
 H       1.961857    -0.916807    -2.813436      27.36
 C      -0.553410    -0.483091     0.335236      32.44
 H      -1.397721    -1.264850     0.639676      21.89
 C      -0.011895     1.788081     0.061081      79.72
 H      -0.183109     2.853165     0.018414      25.48
 C       1.218937     1.386327    -0.458721       7.01
 O       2.097492     2.126314    -1.228670     192.24
 C       2.193920     3.532817    -1.207813     117.84
 H       3.068929     3.806032    -1.549138      27.95
 H       1.626833     4.038906    -1.975337      26.15
 H       2.094554     3.733566     0.000793      24.73
 C       1.713267     0.050414    -0.453674       4.94
 O       3.083599    -0.141200    -0.496747      38.39
 C       0.812280    -0.950170     0.023677      40.96
 H       1.003084    -2.110408     0.109786      24.61
 C      -1.013811     0.882008     0.269590      42.37
 C      -2.288784     1.172774     0.912375      89.17
 H      -2.899768     0.171013     1.101290      27.29
 O      -2.199828     2.081445     2.011036     232.78
 H      -1.725427     1.591106     2.805379      27.49
 C      -3.176245     1.761496    -0.176254     101.86
 H      -2.968269     2.661135    -0.580572      29.15
 O      -3.383152     0.769049    -1.198877     215.33
 H      -3.501524     1.241044    -2.118604      25.02
 C      -4.665144     1.961821     0.465245      66.93
 O      -5.690114     2.525300    -0.580413     203.37
 H      -5.597721     3.498710    -0.869411      30.04
 H      -4.456602     2.868171     1.080033      25.00
 H      -4.762974     0.810260     0.617741      26.91
55
name = lig-etoh-Waterframe_801
 C       6.062870    -1.256720     1.161290      31.75
 H       6.518052    -0.328557     0.895302      20.18
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 C       5.062469    -3.409695     0.733929     103.86
 H       4.637815    -4.128787     0.098909      28.28
 C       5.126717    -3.790003     2.082026      26.46
 O       4.729051    -5.022673     2.461814     250.08
 C       3.429610    -5.130344     3.282201      87.20
 H       3.617884    -4.611900     4.210031      22.76
 H       3.464378    -6.410024     3.493975      20.09
 H       2.515116    -4.701793     2.645025      27.19
 C       5.801228    -2.932454     3.026956     -17.59
 O       6.009545    -3.137915     4.394292      57.99
 H       6.118785    -4.103138     4.585449      21.35
 C       6.344439    -1.703594     2.497383      21.98
 H       6.947464    -1.253432     3.426624      23.45
 C       5.397220    -2.192926     0.244544       6.68
 C       5.123520    -1.671440    -1.170296      91.42
 H       5.373887    -2.470164    -1.997868      25.03
 O       5.878688    -0.502883    -1.553292     187.81
 H       5.600883     0.110823    -0.888214      29.65
 C       3.604578    -1.386496    -1.475117      54.97
 H       3.079667    -2.356145    -1.181037      26.84
 C       3.097103    -1.184190    -2.952164     105.00
 O       3.004937    -2.380670    -3.689813     265.49
 H       3.891504    -2.449884    -4.142770      26.44
 H       3.674520    -0.268251    -3.471733      25.57
 H       2.086116    -0.716207    -2.722007      27.55
 C      -0.599897    -0.488072     0.350865      52.96
 H      -1.313649    -1.373515     0.709400      21.82
 C       0.002539     1.858478    -0.008690      80.37
 H      -0.304487     2.751313    -0.217680      27.08
 C       1.229631     1.425761    -0.439192       8.40
 O       2.099204     2.038846    -1.247946     189.75
 C       2.233255     3.532019    -1.161193     106.81
 H       3.393542     3.797573    -1.358510      23.26
 H       1.348239     4.044795    -1.665901      24.36
 H       2.093762     4.130313    -0.214625      25.78
 C       1.658415     0.036211    -0.406628      -2.45
 O       3.199622    -0.178638    -0.550294      26.62
 C       0.776151    -0.932779    -0.066979      49.95
 H       1.153862    -2.016284     0.076786      27.22
 C      -0.985005     0.776176     0.339678      32.07
 C      -2.362158     1.186972     0.920382      84.10
 H      -2.940989     0.198066     1.266040      26.64
 O      -2.199941     2.052960     2.007679     246.59
 H      -1.889589     1.603786     2.826544      28.54
 C      -3.305572     1.810506    -0.160762      96.20
 H      -2.835637     2.674290    -0.595375      27.39
 O      -3.417471     0.760904    -1.240258     190.72
 H      -3.547411     1.137950    -2.205314      24.83
 C      -4.662921     1.966452     0.461657      90.29
 O      -5.694923     2.489298    -0.532498     253.94
 H      -5.168269     3.357547    -0.629353      29.24
 H      -4.519794     2.561558     1.350425      27.78
 H      -5.082169     0.941465     0.940847      26.81
55
name = lig-etoh-Waterframe_802
 C       6.114817    -1.294033     1.223148      23.26
 H       6.319721    -0.220442     1.084935      26.51
 C       5.042612    -3.408638     0.704385      50.70
 H       4.643582    -4.172133     0.155906      22.10
 C       5.202230    -3.731565     2.082464      36.75
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 O       4.678396    -5.086890     2.372186     240.24
 C       3.486935    -5.127467     3.240444      87.77
 H       3.468255    -4.556669     4.209410      23.11
 H       3.085723    -6.126742     3.507702      22.70
 H       2.548451    -4.724532     2.554871      28.03
 C       5.771379    -2.893659     3.024767      16.43
 O       6.013719    -3.054484     4.375421     152.19
 H       6.228292    -3.991802     4.495495      23.86
 C       6.308637    -1.725634     2.516245      20.81
 H       7.239283    -1.059406     2.898927      20.45
 C       5.525606    -2.118402     0.201700     -33.05
 C       5.130731    -1.656086    -1.252372      65.37
 H       5.449941    -2.425851    -1.869994      25.74
 O       5.955266    -0.422199    -1.588081     169.79
 H       5.536522     0.383365    -1.284122      27.72
 C       3.476693    -1.432599    -1.349719      83.28
 H       2.923686    -2.351169    -1.136131      28.65
 C       3.116909    -1.127500    -2.877969     103.47
 O       3.055482    -2.419902    -3.690855     269.50
 H       3.900636    -2.435809    -4.169498      26.59
 H       3.731166    -0.422285    -3.387906      29.13
 H       2.085078    -0.756812    -2.992459      28.61
 C      -0.542423    -0.654253     0.339330      58.10
 H      -1.282491    -1.414983     0.742510      24.18
 C      -0.090472     1.854552    -0.081132      50.13
 H      -0.453337     2.837041    -0.285049      24.34
 C       1.292169     1.358213    -0.476221     -27.62
 O       2.180384     2.109333    -1.268990     152.06
 C       2.238381     3.559940    -1.085309     100.16
 H       3.287353     3.818232    -1.885483      21.88
 H       1.479212     3.936779    -1.903428      23.49
 H       2.162047     3.790795    -0.096446      27.78
 C       1.735334     0.011922    -0.321263      12.01
 O       3.199324    -0.268547    -0.646421     104.35
 C       0.681056    -0.926497    -0.094497      53.00
 H       1.021485    -1.958707    -0.022217      28.53
 C      -0.933362     0.820281     0.443678      -3.66
 C      -2.405673     1.137802     0.878882      85.24
 H      -2.749908     0.189108     1.298002      27.37
 O      -2.214283     2.075878     2.046731     233.56
 H      -1.970885     1.430577     2.637381      30.62
 C      -3.417949     1.776997    -0.206389      85.28
 H      -2.899608     2.810654    -0.478445      25.42
 O      -3.438335     0.764395    -1.255973     227.18
 H      -3.348877     1.254154    -2.168878      24.07
 C      -4.752701     2.000585     0.486791     113.06
 O      -5.627260     2.465053    -0.423823     281.31
 H      -5.463027     3.410925    -0.868231      27.87
 H      -4.805173     2.511431     1.413224      28.52
 H      -5.306108     1.099257     0.786513      27.60
55
name = lig-etoh-Waterframe_803
 C       6.111945    -1.289936     1.176875      61.04
 H       6.402337    -0.253671     0.799603      18.09
 C       5.076582    -3.358208     0.686066      12.62
 H       4.639781    -4.046928     0.010774      19.93
 C       5.183166    -3.787119     2.052954      18.17
 O       4.637855    -5.103340     2.322443     277.03
 C       3.475793    -5.097522     3.168167     113.27
 H       3.727921    -4.455904     4.088924      20.76
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 H       3.321127    -6.013351     3.371853      22.86
 H       2.664814    -4.584282     2.559713      29.92
 C       5.805553    -2.830995     3.044370       1.78
 O       6.020793    -3.041486     4.367532     102.40
 H       5.872610    -3.931383     4.737564      24.86
 C       6.340111    -1.670890     2.503018      61.89
 H       6.932979    -1.016192     3.286878      28.66
 C       5.573674    -2.065978     0.199562      30.70
 C       5.135390    -1.588267    -1.244071      79.08
 H       5.395251    -2.266500    -1.975271      26.38
 O       5.981410    -0.395563    -1.630405     178.67
 H       5.569407     0.454768    -1.561456      26.08
 C       3.458606    -1.492558    -1.381778      90.69
 H       2.993689    -2.261786    -0.799569      28.60
 C       3.103080    -1.148294    -2.841724     106.37
 O       3.141659    -2.432310    -3.676786     296.28
 H       3.864077    -2.612308    -4.261501      28.45
 H       3.887498    -0.618586    -3.131481      29.91
 H       2.112264    -0.774746    -2.975138      27.93
 C      -0.588562    -0.603710     0.381137      29.67
 H      -1.193908    -1.433764     0.625853      24.61
 C      -0.067892     1.693340    -0.164618      51.79
 H      -0.366801     2.865488    -0.201276      22.49
 C       1.308684     1.349926    -0.542977     -11.01
 O       2.276627     2.172504    -1.252801     173.36
 C       2.224152     3.560988    -1.145032     117.98
 H       3.291837     4.053605    -1.467087      23.43
 H       1.296841     4.158410    -1.522228      24.62
 H       2.323024     3.798237    -0.129918      27.98
 C       1.813970     0.017152    -0.291322      20.37
 O       3.067329    -0.309362    -0.661547     151.85
 C       0.773819    -1.031006    -0.084420      25.26
 H       0.847731    -2.052294    -0.214837      25.01
 C      -0.934099     0.796187     0.464879      34.69
 C      -2.365200     1.121316     0.866901      95.04
 H      -2.874552     0.255196     1.099468      28.08
 O      -2.255127     2.067597     2.072160     244.11
 H      -1.935301     1.619271     2.797875      30.73
 C      -3.378841     1.671006    -0.133217      77.48
 H      -3.285216     2.756405    -0.622558      23.46
 O      -3.471063     0.808043    -1.262056     250.12
 H      -3.200790     1.160117    -2.197282      23.27
 C      -4.852127     1.965164     0.574247      98.09
 O      -5.688899     2.513696    -0.430763     270.82
 H      -5.550296     3.515503    -0.774437      26.64
 H      -4.543777     2.783331     1.363661      24.69
 H      -5.046176     0.977585     0.694670      28.93
55
name = lig-etoh-Waterframe_804
 C       6.148238    -1.164361     1.104761       4.57
 H       6.702193    -0.237660     0.719609      18.42
 C       5.130178    -3.312455     0.682381      80.22
 H       4.620406    -3.954417    -0.091390      23.18
 C       5.164086    -3.794595     2.003092      41.30
 O       4.663461    -5.060024     2.253595     252.93
 C       3.458217    -5.020931     3.100764     112.19
 H       3.725286    -4.531438     4.091392      22.02
 H       3.357214    -6.094697     3.379482      20.99
 H       2.594982    -4.615435     2.721478      31.44
 C       5.823276    -2.894186     2.985490     -17.97
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 O       6.013808    -3.058869     4.397828     189.99
 H       5.589074    -3.912236     4.578881      20.45
 C       6.366972    -1.573281     2.522272      19.81
 H       6.503556    -0.975064     3.352709      23.21
 C       5.502454    -2.106415     0.185587      15.57
 C       5.139078    -1.510748    -1.187874      80.57
 H       5.335536    -2.310324    -2.015136      23.91
 O       5.960017    -0.412646    -1.686052     210.59
 H       5.537815     0.383561    -1.309253      27.17
 C       3.525138    -1.508370    -1.395283      65.74
 H       3.232728    -2.516826    -1.001585      27.44
 C       3.135828    -1.303793    -2.872995     115.82
 O       3.205411    -2.452715    -3.648993     310.95
 H       4.008337    -2.285962    -4.153490      26.42
 H       3.838077    -0.451622    -3.132079      24.93
 H       2.239958    -0.687364    -2.909265      27.50
 C      -0.507914    -0.576275     0.395859      44.55
 H      -1.263052    -1.228930     0.609228      23.94
 C       0.068464     1.587422    -0.231949      66.94
 H      -0.314716     2.788946    -0.256013      21.52
 C       1.329256     1.346976    -0.598535       0.41
 O       2.330744     2.157488    -1.222542     225.76
 C       2.222918     3.665455    -1.112093     109.57
 H       2.996085     4.009812    -1.589903      25.96
 H       1.250514     3.984689    -1.424458      26.01
 H       2.228235     4.030967     0.038591      25.66
 C       1.706829    -0.068515    -0.341576       8.64
 O       3.006058    -0.274017    -0.638661     124.70
 C       0.811795    -1.029362    -0.008080      74.47
 H       1.032208    -2.021385    -0.255934      25.22
 C      -0.958593     0.693335     0.393049      44.81
 C      -2.307131     1.138720     0.947001      88.34
 H      -2.777122     0.167402     1.242495      25.11
 O      -2.320079     2.037011     2.061867     272.47
 H      -1.899733     1.630445     2.788160      29.35
 C      -3.372265     1.711524    -0.097937      85.14
 H      -2.920789     2.697352    -0.460745      23.91
 O      -3.520567     0.800193    -1.239764     236.22
 H      -3.156491     1.212964    -2.114526      24.43
 C      -4.799959     1.917884     0.560410      76.91
 O      -5.820465     2.563915    -0.458301     254.13
 H      -5.273356     3.386555    -0.402113      28.34
 H      -4.627292     2.566027     1.644645      23.82
 H      -5.340335     1.021576     1.164550      24.63
55
name = lig-etoh-Waterframe_805
 C       6.207040    -1.112970     1.140916      79.76
 H       6.610065    -0.137517     0.783741      26.32
 C       5.112936    -3.332572     0.633991      50.07
 H       4.584971    -4.140182    -0.029637      24.07
 C       5.236322    -3.698653     1.987942     -14.92
 O       4.671544    -5.000570     2.191709     164.05
 C       3.479104    -4.992943     3.089274      88.74
 H       3.575177    -4.472530     4.047201      22.62
 H       3.035629    -6.196572     3.331536      21.78
 H       2.665335    -4.584602     2.564921      31.66
 C       5.870134    -2.880953     2.910132       6.91
 O       5.956799    -3.085328     4.340980      92.88
 H       5.937950    -4.104310     4.692571      22.74
 C       6.267032    -1.557596     2.468595      62.15
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 H       6.539810    -0.812681     3.093551      22.70
 C       5.512953    -1.957914     0.229055     -42.95
 C       5.120722    -1.547687    -1.200710      89.69
 H       5.494433    -2.519011    -1.843198      21.75
 O       5.875259    -0.418745    -1.703762     191.22
 H       5.849046     0.333181    -1.067698      28.56
 C       3.631700    -1.447557    -1.366695      82.15
 H       3.183729    -2.477584    -1.129635      26.98
 C       3.182620    -1.317885    -2.846854      88.37
 O       3.286551    -2.505564    -3.659409     258.72
 H       4.106593    -2.510150    -4.259929      25.38
 H       3.792888    -0.512129    -3.557328      22.10
 H       2.032796    -1.135704    -2.876026      25.29
 C      -0.480453    -0.697976     0.420720      49.62
 H      -1.158203    -1.430771     0.781935      21.15
 C       0.041101     1.642439    -0.223117      65.37
 H      -0.253672     2.743508    -0.491396      18.83
 C       1.405733     1.256547    -0.629393       7.38
 O       2.354313     2.152165    -1.155737     190.14
 C       2.163210     3.715250    -1.051869      87.15
 H       2.811482     4.062251    -1.782661      25.95
 H       1.324176     3.852864    -1.611144      27.86
 H       2.317065     3.992229     0.145707      25.21
 C       1.646732    -0.060144    -0.486869      32.28
 O       3.058359    -0.306290    -0.639778     166.27
 C       0.773876    -1.036114     0.077918      36.03
 H       1.182296    -2.073950     0.147093      23.00
 C      -0.858556     0.730239     0.253614      46.08
 C      -2.324042     1.086296     0.988179      54.58
 H      -2.596693     0.043428     1.497668      22.93
 O      -2.354726     2.024330     2.064863     255.01
 H      -1.878014     1.495100     2.750842      26.67
 C      -3.373799     1.742728    -0.074923     101.15
 H      -2.919431     2.648430    -0.261041      26.15
 O      -3.554492     0.802644    -1.165962     246.05
 H      -3.239673     1.197348    -2.066641      24.14
 C      -4.773703     1.899189     0.546681      80.91
 O      -5.849335     2.574157    -0.375861     240.37
 H      -5.641937     3.491013    -0.743200      31.58
 H      -4.777911     2.723827     1.316819      25.56
 H      -5.479195     0.895762     0.855752      24.51
55
name = lig-etoh-Waterframe_806
 C       6.180777    -1.117928     1.149055      66.11
 H       6.369843    -0.077000     1.054079      26.45
 C       5.126634    -3.211950     0.603268      66.48
 H       4.655937    -3.986734    -0.134011      23.21
 C       5.282153    -3.668222     1.913686      -4.67
 O       4.686622    -4.946862     2.194879     143.16
 C       3.458791    -4.962518     3.050808      87.65
 H       3.666942    -4.453225     3.955907      24.15
 H       3.278354    -6.233861     3.143916      21.59
 H       2.763540    -4.409015     2.364173      27.80
 C       5.917428    -2.795394     2.940946       8.66
 O       5.894388    -3.098691     4.226823     146.97
 H       6.217316    -4.035543     4.444592      24.99
 C       6.194883    -1.540662     2.468993      45.36
 H       6.829444    -0.941362     3.176961      18.44
 C       5.514242    -1.906754     0.245449      30.50
 C       5.176767    -1.605266    -1.181369      99.22
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 H       5.498933    -2.436211    -1.917698      26.38
 O       5.800846    -0.420118    -1.719948     184.40
 H       5.868851     0.273800    -1.027877      28.40
 C       3.644881    -1.402833    -1.416367      82.01
 H       3.125313    -2.249078    -0.893968      27.70
 C       3.201151    -1.297833    -2.893581      80.19
 O       3.364468    -2.624923    -3.668916     247.17
 H       4.259521    -2.709275    -4.247049      24.04
 H       3.581092    -0.245092    -3.415821      23.88
 H       2.076203    -1.335602    -2.739836      25.40
 C      -0.549452    -0.708806     0.451120      25.06
 H      -1.084309    -1.533789     1.030728      20.02
 C       0.057873     1.745984    -0.268807      54.57
 H      -0.316760     2.697097    -0.385242      20.13
 C       1.345520     1.307328    -0.650569      -2.90
 O       2.376803     2.173760    -1.069064     190.08
 C       2.080370     3.613735    -1.051003      97.76
 H       3.110897     4.170109    -1.628583      21.38
 H       1.068413     3.970600    -1.291592      26.99
 H       2.233612     4.188207    -0.017916      25.83
 C       1.765887    -0.135807    -0.616601       9.65
 O       3.142548    -0.366918    -0.630119     174.51
 C       0.832800    -1.083192     0.100321      26.45
 H       1.188088    -2.066767     0.643861      22.44
 C      -0.865628     0.696056     0.235439      32.56
 C      -2.335956     1.033095     0.932862      60.16
 H      -2.780790    -0.018742     1.229206      23.80
 O      -2.331548     2.003468     2.085327     224.41
 H      -1.930354     1.645383     2.981326      25.65
 C      -3.376915     1.675294    -0.006964     113.21
 H      -3.109117     2.644768    -0.374665      25.67
 O      -3.565914     0.826152    -1.093917     261.95
 H      -3.299759     1.077409    -2.046600      24.12
 C      -4.847790     2.012947     0.500713     108.73
 O      -5.861496     2.533395    -0.302309     289.30
 H      -5.531985     3.423499    -0.654572      32.03
 H      -4.677477     2.463997     1.400514      30.15
 H      -4.973787     0.906598     0.572357      28.71
55
name = lig-etoh-Waterframe_807
 C       6.085842    -1.045383     1.174941      20.35
 H       6.306536    -0.048078     0.923948      27.65
 C       5.146846    -3.138197     0.621542      84.83
 H       4.712936    -3.674451    -0.243125      23.79
 C       5.290019    -3.652165     1.884555      78.10
 O       4.761258    -4.891775     2.212919     322.15
 C       3.496893    -4.905718     2.942816     112.14
 H       3.587403    -4.562518     3.943083      24.63
 H       3.229097    -5.955901     3.100200      24.52
 H       2.455975    -4.457324     2.557407      26.49
 C       5.839220    -2.806410     2.827878     -12.22
 O       5.876875    -3.063296     4.177568     -31.67
 H       5.742466    -4.071447     4.412595      15.31
 C       6.268459    -1.471167     2.553876       8.10
 H       6.876186    -0.910609     3.450016      12.70
 C       5.521582    -1.914399     0.176092      16.68
 C       5.203813    -1.577939    -1.231489      92.95
 H       5.496553    -2.377873    -1.810182      28.21
 O       5.789151    -0.408811    -1.742039     214.65
 H       5.551037     0.347331    -1.120867      27.73
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 C       3.641397    -1.500947    -1.467044      71.03
 H       3.218518    -2.471437    -1.189338      29.74
 C       3.171482    -1.367291    -2.952934     104.97
 O       3.424405    -2.703532    -3.628331     280.77
 H       4.269795    -2.475327    -4.150691      24.07
 H       3.511098    -0.453308    -3.383983      27.78
 H       2.106229    -1.145426    -2.974368      27.65
 C      -0.446976    -0.629134     0.424273      30.03
 H      -1.244862    -1.173245     1.105997      20.79
 C       0.006342     1.706942    -0.286950      59.20
 H      -0.247451     2.644033    -0.186632      22.69
 C       1.317825     1.323285    -0.696322     -20.92
 O       2.356852     2.202571    -0.979399     196.16
 C       2.050391     3.557887    -1.002001      95.04
 H       2.964738     4.127191    -1.845175      21.85
 H       0.985609     3.804281    -1.452304      25.06
 H       2.124889     3.813190    -0.023515      28.69
 C       1.778438    -0.214633    -0.574556      -5.52
 O       3.219852    -0.340601    -0.610745     140.04
 C       0.896502    -1.031298     0.094048      47.39
 H       1.363163    -2.004256     0.550587      24.47
 C      -0.973941     0.651036     0.308395      29.08
 C      -2.337362     1.046119     0.894830      79.73
 H      -2.825121     0.117464     1.116297      24.85
 O      -2.286594     1.963293     2.078758     209.18
 H      -1.871566     1.278867     2.854037      22.80
 C      -3.382325     1.757922    -0.035229      83.76
 H      -2.780057     2.693245    -0.496302      22.79
 O      -3.592994     0.773454    -1.077849     254.81
 H      -3.154756     1.127811    -1.917814      26.25
 C      -4.823478     1.966643     0.586810     106.94
 O      -5.865747     2.531207    -0.285387     300.20
 H      -5.504342     3.434637    -0.328118      31.37
 H      -4.871300     2.283765     1.610267      28.43
 H      -5.297883     1.070574     0.814889      29.15
55
name = lig-etoh-Waterframe_808
 C       6.004104    -0.926138     1.242099      30.52
 H       6.358021    -0.034968     0.787242      19.09
 C       5.127018    -3.177433     0.536308      36.76
 H       4.667274    -3.939412    -0.026068      19.91
 C       5.260990    -3.621084     1.856411      56.24
 O       4.811603    -4.864777     2.229319     233.56
 C       3.502611    -4.891971     2.899513     104.84
 H       3.588434    -4.457125     3.917177      23.67
 H       3.267213    -5.808380     2.925307      25.86
 H       2.721005    -4.294354     2.193908      26.50
 C       5.787932    -2.736537     2.825232      -2.44
 O       5.865175    -3.041237     4.163259     257.78
 H       5.485726    -3.839760     4.555272      20.72
 C       6.336680    -1.441205     2.505667      45.91
 H       6.589437    -0.671040     3.404516      22.83
 C       5.576179    -1.829587     0.208989      -0.38
 C       5.166481    -1.549566    -1.345289      92.92
 H       5.628619    -2.309172    -1.885412      26.37
 O       5.823335    -0.349734    -1.761542     270.70
 H       5.276518     0.468628    -1.491338      24.94
 C       3.639125    -1.608355    -1.513945      66.67
 H       3.218238    -2.543288    -1.156385      28.61
 C       3.134424    -1.457784    -3.000535     112.99
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 O       3.451536    -2.705815    -3.551033     300.62
 H       4.197891    -2.809981    -4.228635      26.59
 H       3.776068    -0.905567    -3.546594      25.99
 H       2.089838    -1.293546    -3.106087      27.90
 C      -0.373485    -0.547954     0.445724      56.11
 H      -0.899644    -1.499551     0.904318      22.16
 C      -0.083763     1.572530    -0.263305      69.06
 H      -0.174100     2.658782    -0.082831      22.00
 C       1.298442     1.196827    -0.696290      13.44
 O       2.320512     2.135259    -0.924850     181.79
 C       2.009184     3.581228    -0.967319     112.89
 H       2.738536     4.075463    -1.618223      25.45
 H       1.053599     3.592411    -1.614443      24.84
 H       1.993548     4.012291    -0.033579      28.15
 C       1.790888    -0.044096    -0.475241      12.99
 O       3.217142    -0.355390    -0.632548     108.01
 C       0.932961    -0.992979     0.109631      43.29
 H       1.255691    -2.049850     0.236338      23.83
 C      -0.958824     0.731930     0.299810      38.38
 C      -2.382922     1.100477     0.897256      83.36
 H      -2.810201     0.228143     1.234545      26.18
 O      -2.209653     1.869819     2.063194     227.08
 H      -1.725639     1.214639     2.855513      21.72
 C      -3.384466     1.800379    -0.084655      71.17
 H      -2.964545     2.888300    -0.476423      22.83
 O      -3.610067     0.731969    -1.091298     255.50
 H      -3.173569     0.891175    -1.997182      25.56
 C      -4.806142     1.837911     0.741965      80.53
 O      -5.821632     2.583091    -0.264390     233.55
 H      -5.801657     3.527302    -0.345234      31.84
 H      -4.827958     2.730079     1.537686      23.45
 H      -5.269689     0.870616     0.862029      27.36
55
name = lig-etoh-Waterframe_809
 C       5.982001    -0.871712     1.178041      31.46
 H       6.275913     0.178120     1.034570      18.90
 C       5.146979    -3.185532     0.487571      64.27
 H       4.805990    -3.881054    -0.213465      21.97
 C       5.245352    -3.533884     1.840061      17.06
 O       4.842661    -4.868159     2.251520     221.88
 C       3.506122    -4.860834     2.826099      91.61
 H       3.443661    -4.328344     3.859613      21.84
 H       3.145488    -5.943832     2.840186      22.65
 H       2.992530    -4.233944     2.104512      30.41
 C       5.794697    -2.627795     2.898215      -6.20
 O       5.854482    -2.978375     4.190409     155.75
 H       5.769602    -3.967128     4.272245      18.82
 C       6.286235    -1.413026     2.445691      47.46
 H       6.578798    -0.699151     3.254246      24.31
 C       5.508005    -1.834500     0.188653       5.23
 C       5.195803    -1.509271    -1.348783      76.97
 H       5.665818    -2.306805    -2.066038      23.18
 O       5.842959    -0.266963    -1.814919     254.87
 H       5.222877     0.522626    -1.609412      25.31
 C       3.584661    -1.581172    -1.539423      68.12
 H       3.222976    -2.410237    -0.933916      28.24
 C       3.182619    -1.520864    -3.024277      94.72
 O       3.428548    -2.847176    -3.506541     286.88
 H       4.265964    -2.661481    -4.098747      24.00
 H       3.822159    -0.604207    -3.550935      23.15
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 H       2.114894    -1.238287    -3.128907      27.12
 C      -0.356566    -0.624134     0.511638      38.37
 H      -1.000653    -1.482167     0.758119      21.54
 C      -0.008504     1.579476    -0.289028      59.40
 H      -0.344581     2.782431    -0.349579      20.52
 C       1.238149     1.219228    -0.627373      32.77
 O       2.289893     2.102661    -0.890577     193.47
 C       1.943857     3.558675    -0.983585     121.14
 H       2.733151     3.935062    -1.349011      27.26
 H       0.990682     3.787171    -1.486744      26.33
 H       1.745064     4.236210    -0.009514      26.00
 C       1.907081    -0.032005    -0.379961      26.33
 O       3.157073    -0.395130    -0.694831     184.55
 C       0.933169    -0.935938     0.108944      55.74
 H       1.063102    -1.963808     0.085376      25.47
 C      -0.967890     0.701744     0.304228      31.89
 C      -2.363253     1.111849     0.886437      81.74
 H      -2.869830     0.093854     1.044709      24.40
 O      -2.126253     1.836622     2.084108     207.36
 H      -1.633362     1.244374     2.873920      22.79
 C      -3.442874     1.712766    -0.058038      93.23
 H      -3.447148     2.704897    -0.497457      24.98
 O      -3.612924     0.731376    -1.098898     255.45
 H      -3.300211     0.906316    -2.020321      25.64
 C      -4.817154     1.920464     0.703802      80.85
 O      -5.785374     2.558640    -0.209598     271.89
 H      -5.411461     3.454150    -0.171751      29.81
 H      -4.406953     2.459028     1.811099      24.46
 H      -4.996673     0.848407     1.060405      27.24
55
name = lig-etoh-Waterframe_810
 C       5.974894    -0.936691     1.051660      34.42
 H       5.973192     0.185019     0.871870      23.37
 C       5.208898    -3.134498     0.520924      67.47
 H       5.028942    -3.740252    -0.345310      26.97
 C       5.260439    -3.480541     1.907767      16.41
 O       4.884892    -4.814375     2.273870     152.83
 C       3.487279    -4.800371     2.718963      84.59
 H       3.409692    -4.401253     3.800930      23.36
 H       2.969947    -5.995266     2.852174      22.10
 H       2.767994    -4.356061     2.160887      32.92
 C       5.772974    -2.610308     2.838352       7.80
 O       5.852264    -2.940449     4.247783     149.57
 H       6.095667    -3.877815     4.321120      26.20
 C       6.182994    -1.301452     2.437762      54.60
 H       6.746487    -0.762389     3.070582      21.96
 C       5.425638    -1.796406     0.084904     -12.89
 C       5.224310    -1.426904    -1.309523      88.11
 H       5.581623    -2.362012    -2.003001      23.80
 O       5.821263    -0.220109    -1.871979     217.57
 H       5.441717     0.590686    -1.305052      25.94
 C       3.578310    -1.475911    -1.502000      82.89
 H       3.190322    -2.482970    -1.157005      27.59
 C       3.204811    -1.538696    -2.980269      77.60
 O       3.426811    -2.986955    -3.519787     236.78
 H       4.296221    -2.955512    -4.101921      24.97
 H       3.778300    -0.570946    -3.593966      22.99
 H       2.087543    -1.326362    -3.132207      26.76
 C      -0.464104    -0.653472     0.548822      25.61
 H      -1.139006    -1.338288     0.868080      20.42
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 C      -0.039239     1.649190    -0.275402      72.07
 H      -0.442600     2.732811    -0.790025      18.35
 C       1.365798     1.286842    -0.519851       2.47
 O       2.244536     2.192636    -0.890144     195.60
 C       1.874614     3.548806    -0.984040      79.95
 H       2.938777     4.045513    -1.414399      22.07
 H       1.175942     3.752319    -1.779767      25.29
 H       1.717664     3.650353     0.255378      22.82
 C       1.856320    -0.134166    -0.302090      24.84
 O       3.150606    -0.383183    -0.786088     221.78
 C       0.925443    -0.987888     0.118436      71.09
 H       1.227191    -1.974664     0.114223      25.09
 C      -0.919558     0.599047     0.300698      45.59
 C      -2.283182     1.042792     0.857909      68.44
 H      -2.827267    -0.009440     1.140699      23.43
 O      -2.078855     1.866572     2.094377     207.66
 H      -1.727167     1.282166     2.713977      28.33
 C      -3.513465     1.657338    -0.050361     100.55
 H      -3.111705     2.513216    -0.511993      26.42
 O      -3.639271     0.706098    -1.102961     269.39
 H      -3.296209     1.175196    -1.851479      26.96
 C      -4.743700     1.928071     0.670442     109.57
 O      -5.724141     2.527500    -0.083504     300.20
 H      -5.403668     3.408480    -0.498374      30.14
 H      -4.611591     2.534151     1.609952      27.07
 H      -5.445963     1.034487     1.044166      24.91
55
name = lig-etoh-Waterframe_811
 C       5.937788    -0.935863     1.018492      66.07
 H       6.143157     0.080262     0.530514      24.26
 C       5.262835    -3.079020     0.539714      63.97
 H       5.025336    -4.063527    -0.000834      23.29
 C       5.276781    -3.488024     1.883767      -0.98
 O       4.869560    -4.704669     2.282403     237.80
 C       3.420407    -4.782901     2.680593      88.32
 H       3.436152    -4.335708     3.677637      24.02
 H       3.384458    -6.036721     2.634883      21.14
 H       2.786961    -4.288849     1.946923      30.04
 C       5.780631    -2.557011     2.885755      -7.26
 O       5.872577    -2.883835     4.237106     148.20
 H       5.884114    -3.811362     4.560761      24.34
 C       6.080671    -1.227187     2.382497      69.86
 H       6.678804    -0.621242     2.949739      22.10
 C       5.436717    -1.779425     0.087775      29.87
 C       5.146877    -1.373609    -1.365098     109.03
 H       5.668295    -2.188257    -1.994993      25.46
 O       5.775901    -0.192190    -1.882650     196.84
 H       5.843028     0.542077    -1.143003      26.39
 C       3.650545    -1.467726    -1.516606      83.49
 H       3.301628    -2.437988    -1.035937      25.98
 C       3.190656    -1.568566    -2.986973      95.25
 O       3.435858    -3.038520    -3.525241     226.63
 H       4.214638    -3.030658    -4.196902      27.37
 H       3.840836    -1.118525    -3.764335      23.10
 H       2.080486    -1.557530    -3.071973      25.98
 C      -0.475619    -0.720100     0.531977      27.30
 H      -1.059058    -1.384353     1.078638      21.49
 C      -0.012254     1.589521    -0.262741      70.88
 H      -0.516503     2.503278    -0.704938      17.90
 C       1.375562     1.290592    -0.363765       7.79
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 O       2.292596     2.230911    -0.955344     214.76
 C       1.870966     3.566149    -0.950546      94.21
 H       2.883480     4.448936    -1.148933      22.05
 H       1.135370     3.707727    -1.715183      27.71
 H       1.272183     4.089875    -0.066192      26.42
 C       1.757297    -0.062018    -0.318997       4.98
 O       3.122796    -0.285037    -0.831222     157.46
 C       0.815887    -1.176245     0.194231      36.40
 H       1.240288    -2.178060     0.333557      21.26
 C      -0.884072     0.671392     0.257809      32.43
 C      -2.280814     0.952828     0.890597      79.98
 H      -2.619702     0.030067     1.466760      23.43
 O      -2.070716     1.913615     2.017780     222.15
 H      -1.704189     1.396253     2.778848      25.25
 C      -3.366794     1.592325    -0.036692      89.00
 H      -2.860667     2.569959    -0.353664      23.30
 O      -3.702368     0.672022    -1.112597     264.45
 H      -3.310344     0.833804    -1.980559      25.87
 C      -4.740678     1.913691     0.768292     101.73
 O      -5.738852     2.570051    -0.042406     316.44
 H      -5.520626     3.327461    -0.663155      30.66
 H      -4.473194     2.517931     1.472627      29.49
 H      -5.143609     0.864148     1.042475      26.19
55
name = lig-etoh-Waterframe_812
 C       5.905594    -0.826214     1.017801      22.91
 H       6.532093     0.084177     0.811035      16.98
 C       5.258838    -3.150386     0.546752      85.71
 H       4.840667    -3.975209    -0.200501      22.91
 C       5.350345    -3.366093     1.912485      18.34
 O       4.826083    -4.641168     2.285369     195.05
 C       3.435241    -4.797399     2.644255      99.64
 H       3.044913    -4.398263     3.538407      25.74
 H       3.138468    -5.842980     2.676751      23.55
 H       2.832969    -4.267114     1.777083      29.26
 C       5.767680    -2.488048     2.900984      34.95
 O       5.904085    -2.803424     4.227669     130.10
 H       5.468381    -3.687671     4.246463      22.26
 C       6.041112    -1.211876     2.383441      21.41
 H       6.348175    -0.337864     3.070450      23.74
 C       5.485376    -1.821506     0.057656     -53.76
 C       5.148329    -1.387761    -1.413397     106.94
 H       5.453369    -2.117833    -2.090394      26.21
 O       5.754011    -0.166373    -1.876151     180.39
 H       5.641937     0.638540    -1.185950      21.28
 C       3.643452    -1.477596    -1.570260      62.39
 H       3.374857    -2.264148    -0.870565      27.51
 C       3.190335    -1.714264    -3.068411     114.40
 O       3.430177    -3.053899    -3.509254     299.09
 H       4.188895    -2.820715    -4.124476      25.52
 H       3.564803    -0.949555    -3.619238      27.28
 H       2.153146    -1.355256    -3.111416      27.18
 C      -0.442117    -0.756538     0.511100      23.93
 H      -1.130574    -1.379066     1.153360      21.02
 C       0.002481     1.548608    -0.244881      65.94
 H      -0.240944     2.493262    -0.380193      20.67
 C       1.371210     1.302046    -0.316648      -3.01
 O       2.346535     2.198652    -0.962578     138.32
 C       1.797792     3.716878    -0.945797      88.06
 H       2.874878     4.268033    -0.959749      24.11
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 H       1.247249     3.791811    -1.876282      26.82
 H       1.278639     3.938571    -0.115446      29.90
 C       1.700010    -0.129591    -0.349017       1.83
 O       3.034893    -0.162952    -0.838243      91.56
 C       0.827196    -1.197819     0.209175      53.03
 H       1.040592    -2.302070     0.506443      22.63
 C      -0.922034     0.589193     0.294922      38.10
 C      -2.253937     0.917445     0.971752      94.42
 H      -2.626474    -0.010446     1.299843      24.98
 O      -2.073739     1.971950     1.925604     233.68
 H      -1.610050     1.498512     2.748078      24.32
 C      -3.232165     1.520961    -0.005649      83.23
 H      -2.989856     2.578477    -0.440692      22.27
 O      -3.774906     0.644604    -1.113477     244.48
 H      -3.188691     0.608778    -1.858759      28.08
 C      -4.662129     1.906546     0.796150      83.01
 O      -5.803653     2.584403    -0.028455     247.00
 H      -5.145183     3.327444    -0.250649      28.84
 H      -4.315415     2.435305     1.768502      25.84
 H      -4.939183     0.985044     1.228061      27.74
55
name = lig-etoh-Waterframe_813
 C       5.926474    -0.809463     1.036939      19.83
 H       6.267412     0.194194     0.732499      20.42
 C       5.240923    -3.111542     0.499974      26.59
 H       4.763627    -3.873205    -0.232337      19.96
 C       5.338475    -3.361451     1.927865       1.43
 O       4.822920    -4.623602     2.337899     238.68
 C       3.389900    -4.778322     2.566918      98.50
 H       3.069530    -4.310886     3.496122      24.06
 H       3.186366    -5.716588     2.614219      24.90
 H       2.692151    -4.396848     1.658622      27.16
 C       5.762444    -2.369818     2.880891       8.00
 O       5.903268    -2.743656     4.208884     148.36
 H       5.473838    -3.628273     4.403510      23.68
 C       6.034556    -1.109787     2.407121      42.35
 H       6.072266    -0.294388     3.323362      19.03
 C       5.574456    -1.815892     0.024342     -32.24
 C       5.198383    -1.426648    -1.422681      87.71
 H       5.509521    -2.137729    -2.102696      24.95
 O       5.751194    -0.146295    -1.861489     224.13
 H       5.120391     0.531263    -1.447880      23.94
 C       3.548999    -1.436771    -1.559649      64.83
 H       3.118688    -2.273597    -1.038037      27.82
 C       3.118425    -1.719529    -3.069554     104.35
 O       3.449300    -3.036968    -3.535296     275.17
 H       4.260118    -3.160610    -4.063345      27.35
 H       3.640912    -0.938224    -3.609419      25.95
 H       2.015484    -1.697781    -3.148078      26.84
 C      -0.459061    -0.760326     0.539064      46.99
 H      -1.155347    -1.614305     0.985159      21.09
 C      -0.027206     1.562806    -0.162436      70.90
 H      -0.314602     2.529956    -0.070655      20.83
 C       1.365153     1.238636    -0.410799     -13.72
 O       2.301650     2.195869    -0.889551     144.40
 C       1.810578     3.741036    -0.959712      99.76
 H       2.631745     4.234095    -0.899971      30.10
 H       1.398880     3.991593    -1.957350      27.03
 H       1.336413     3.749488    -0.077841      30.01
 C       1.738045    -0.204088    -0.364557      26.60
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 O       2.968677    -0.158518    -0.896528     172.62
 C       0.920204    -1.116703     0.173374      63.77
 H       1.259107    -2.244254     0.261762      23.00
 C      -0.915316     0.464434     0.358787      45.49
 C      -2.207886     0.916266     0.951379      93.61
 H      -2.731327     0.141266     1.395163      26.42
 O      -2.064150     2.027536     1.884734     206.19
 H      -1.523538     1.569959     2.740476      22.99
 C      -3.348614     1.509395    -0.032844      89.96
 H      -2.706461     2.284426    -0.583908      23.46
 O      -3.805988     0.624634    -1.064154     279.70
 H      -3.117905     0.724183    -1.701467      29.36
 C      -4.556416     1.855014     0.804521      87.55
 O      -5.730533     2.564444     0.052492     174.36
 H      -5.536226     3.564272    -0.187026      29.37
 H      -4.469153     2.751156     1.729532      23.76
 H      -5.145009     1.060681     1.112433      28.00
55
name = lig-etoh-Waterframe_814
 C       5.975917    -0.817912     1.013207      50.56
 H       5.829741     0.112549     0.570860      23.36
 C       5.236251    -3.020170     0.523271      82.85
 H       4.880028    -3.840822    -0.060738      22.30
 C       5.260030    -3.392160     1.850153     -13.49
 O       4.848964    -4.612412     2.397760     253.03
 C       3.316659    -4.746580     2.488420      86.14
 H       3.160471    -4.137987     3.422547      22.55
 H       3.326754    -5.865126     2.637822      21.90
 H       2.793934    -4.335117     1.569562      29.31
 C       5.735703    -2.386534     2.854619     -39.27
 O       5.879480    -2.668367     4.194841     103.00
 H       5.800016    -3.635788     4.485063      21.58
 C       6.003947    -0.978403     2.437782      20.98
 H       6.268213    -0.082957     3.208304      19.96
 C       5.653204    -1.760066     0.053299      -6.30
 C       5.175209    -1.436316    -1.408127      64.79
 H       5.664567    -2.225249    -2.094961      23.38
 O       5.722752    -0.180558    -1.859756     245.26
 H       5.213645     0.639578    -1.570348      25.65
 C       3.481884    -1.440931    -1.530511      92.15
 H       3.083103    -2.320992    -1.013783      28.78
 C       3.042613    -1.619082    -3.036564      91.36
 O       3.479033    -3.067589    -3.568729     217.62
 H       4.361468    -2.878594    -3.985508      25.88
 H       3.535142    -1.034246    -3.935182      24.96
 H       1.978970    -1.779829    -3.174139      27.99
 C      -0.370366    -0.900792     0.561235      44.65
 H      -1.075013    -1.821551     0.829242      20.03
 C      -0.013924     1.502385    -0.021702      64.94
 H      -0.555529     2.519836     0.080706      18.19
 C       1.217104     1.222288    -0.534760      31.06
 O       2.214817     2.225131    -0.814109     205.35
 C       1.893816     3.616571    -0.937028     113.80
 H       2.725500     4.218296    -0.790805      25.17
 H       1.187391     3.842666    -1.832826      24.92
 H       1.045521     4.047978    -0.100797      23.71
 C       1.778279    -0.053072    -0.406422      23.70
 O       3.031898    -0.283071    -1.034592     205.65
 C       0.938886    -1.112018     0.150411      54.04
 H       1.421584    -2.121019     0.004696      23.57
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 C      -0.880341     0.528710     0.396821      57.68
 C      -2.292716     0.933381     0.915050      88.63
 H      -2.636565     0.158411     1.635396      25.34
 O      -2.022102     2.079511     1.866660     161.86
 H      -1.568740     1.588014     2.771554      23.68
 C      -3.402702     1.506352    -0.057485     102.78
 H      -3.028712     2.458007    -0.490231      26.09
 O      -3.811265     0.577999    -1.013902     282.95
 H      -3.417685     0.678204    -1.900433      27.97
 C      -4.594963     1.931497     0.781531      98.62
 O      -5.636007     2.533463     0.132091     230.10
 H      -5.484777     3.522841    -0.152011      30.97
 H      -4.000336     2.534711     1.763844      25.40
 H      -4.994595     0.924638     1.151580      28.04
55
name = lig-etoh-Waterframe_815
 C       5.988532    -0.740913     1.016009      36.54
 H       6.154541     0.272052     0.754712      24.76
 C       5.236736    -3.028151     0.533010      94.29
 H       4.987741    -3.669947    -0.213675      24.82
 C       5.238836    -3.318948     1.916918       5.54
 O       4.854279    -4.601300     2.404591     248.06
 C       3.359743    -4.713425     2.450930      62.47
 H       2.749851    -4.132595     3.258650      25.43
 H       2.897722    -5.906528     2.707870      21.55
 H       2.960100    -4.437980     1.523402      31.90
 C       5.710675    -2.353720     2.812494      -5.09
 O       5.855558    -2.604790     4.187901     102.46
 H       5.868877    -3.616036     4.210153      23.57
 C       5.969716    -1.018341     2.401500      42.62
 H       6.378472    -0.206369     3.001964      18.77
 C       5.627899    -1.756106     0.065376     -22.51
 C       5.123293    -1.406754    -1.352822      81.77
 H       5.454230    -2.305350    -2.120125      23.54
 O       5.692284    -0.236021    -1.902285     264.96
 H       5.496006     0.517674    -1.266409      27.12
 C       3.529397    -1.576291    -1.596292      74.22
 H       3.237428    -2.444925    -0.956268      26.83
 C       3.006277    -1.666501    -3.066629      90.40
 O       3.506070    -3.040723    -3.578069     241.14
 H       4.315366    -2.757621    -4.079703      26.33
 H       3.240416    -0.602706    -3.668497      23.89
 H       1.919508    -1.443237    -2.998344      26.11
 C      -0.316128    -0.898551     0.528691      27.98
 H      -0.912479    -1.792674     0.836678      19.29
 C      -0.071398     1.487809     0.096829      79.80
 H      -0.314490     2.717888     0.008798      16.93
 C       1.192961     1.297360    -0.604433      36.71
 O       2.132649     2.225922    -0.743947     216.25
 C       1.852037     3.531701    -0.891598      92.56
 H       2.997492     4.112980    -0.957243      21.31
 H       1.537476     3.634479    -2.023759      22.76
 H       1.191910     4.099993     0.078703      21.61
 C       1.759838    -0.009439    -0.483708      12.64
 O       3.071509    -0.284406    -1.112520     163.30
 C       1.023010    -1.097993     0.061599      63.65
 H       1.322577    -2.117309     0.096527      23.25
 C      -0.895362     0.401461     0.484631      39.75
 C      -2.327352     0.994754     0.948017      79.26
 H      -2.807938     0.001825     1.414710      21.79
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 O      -1.978635     2.121908     1.854364     188.11
 H      -1.597810     1.556447     2.720008      23.73
 C      -3.377770     1.550654    -0.062518      92.54
 H      -3.167822     2.452180    -0.554906      25.63
 O      -3.830237     0.481803    -1.013763     259.02
 H      -3.568189     0.812748    -1.912141      25.73
 C      -4.563335     1.909585     0.859548     100.00
 O      -5.623990     2.568398     0.167030     269.87
 H      -4.998637     3.351758    -0.102089      30.94
 H      -4.213202     2.493421     1.610538      29.07
 H      -4.942771     0.957048     1.443067      27.60
55
name = lig-etoh-Waterframe_816
 C       5.965320    -0.672207     1.002526      61.50
 H       6.611911     0.109005     0.784309      21.80
 C       5.257596    -3.042109     0.542157      76.31
 H       4.951837    -3.799766    -0.156684      24.32
 C       5.232669    -3.283176     1.961432     -34.54
 O       4.823898    -4.583630     2.414650     232.62
 C       3.369044    -4.694327     2.407545      81.67
 H       2.935120    -3.914176     3.114732      24.59
 H       3.177336    -5.949009     2.627059      21.17
 H       3.090399    -4.552007     1.434529      32.76
 C       5.676793    -2.284561     2.867589      28.48
 O       5.832872    -2.577860     4.150550     131.63
 H       5.597396    -3.551135     4.400712      21.33
 C       5.999128    -1.069992     2.312013      71.06
 H       6.324573    -0.561765     3.103859      24.02
 C       5.513110    -1.709845     0.077340     -45.08
 C       5.086278    -1.465405    -1.372208      92.20
 H       5.596575    -2.310983    -1.979481      24.82
 O       5.669399    -0.270661    -1.938189     161.83
 H       5.609342     0.426542    -1.250884      28.68
 C       3.609887    -1.641223    -1.631856      62.51
 H       3.190071    -2.506598    -1.058311      26.78
 C       3.004633    -1.734354    -3.038443     113.47
 O       3.488531    -2.918644    -3.611443     283.39
 H       4.225768    -2.963116    -4.241007      29.65
 H       3.545160    -0.867926    -3.515860      23.90
 H       1.886782    -1.903162    -2.937139      25.64
 C      -0.291984    -0.856200     0.483131      27.13
 H      -0.736950    -1.683270     0.897816      22.30
 C      -0.040592     1.495663     0.072485      87.03
 H      -0.587511     2.584414     0.329263      16.04
 C       1.142103     1.258515    -0.497053      30.73
 O       2.146247     2.184197    -0.679539     225.65
 C       1.840735     3.611184    -0.929983      94.85
 H       3.060990     4.050175    -0.898849      20.60
 H       1.331541     3.891851    -1.864209      25.27
 H       1.296747     4.000933    -0.040102      25.24
 C       1.777226    -0.118940    -0.640117      19.97
 O       3.030299    -0.200359    -1.123874     133.82
 C       1.052625    -1.078193    -0.023958      48.76
 H       1.473951    -2.006646     0.112835      24.16
 C      -0.952247     0.364985     0.552439      67.85
 C      -2.249175     0.989751     0.970893      86.86
 H      -3.082468     0.375656     1.558134      17.90
 O      -1.960854     2.106625     1.862264     211.75
 H      -1.520524     1.703370     2.737721      26.98
 C      -3.377593     1.533336    -0.046367      76.33
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 H      -2.940930     2.268395    -0.701875      23.78
 O      -3.830038     0.431625    -0.995633     239.62
 H      -3.436279     0.720336    -1.881766      25.96
 C      -4.528205     1.846436     0.981337      94.24
 O      -5.607719     2.646808     0.187103     273.04
 H      -5.309136     3.456986    -0.406892      28.64
 H      -4.309737     2.575693     1.661096      27.32
 H      -5.134626     0.964005     1.387903      25.74
55
name = lig-etoh-Waterframe_817
 C       5.955731    -0.704123     0.922018      38.74
 H       6.499495     0.080733     0.435329      21.05
 C       5.251028    -2.994886     0.607277      60.70
 H       4.922572    -3.939389     0.034576      20.30
 C       5.228023    -3.315917     1.923297      14.93
 O       4.834293    -4.538603     2.424661     272.93
 C       3.399496    -4.704213     2.334891     104.39
 H       2.953455    -3.993513     3.001833      25.47
 H       3.227726    -5.641836     2.831441      22.65
 H       2.913283    -4.576372     1.323591      27.29
 C       5.586011    -2.342670     2.837873       1.87
 O       5.811587    -2.562395     4.198785     188.44
 H       5.310589    -3.423013     4.445314      24.17
 C       6.089693    -1.042322     2.363993      42.55
 H       6.512387    -0.358378     3.039551      26.16
 C       5.376404    -1.670737     0.088885     -19.68
 C       5.150137    -1.550786    -1.433390     100.00
 H       5.624866    -2.329138    -1.901188      26.09
 O       5.662839    -0.302250    -1.967087     228.14
 H       5.333637     0.518442    -1.558177      26.60
 C       3.577648    -1.580708    -1.583609      76.92
 H       3.174714    -2.359775    -0.911608      24.06
 C       3.091786    -1.752582    -2.995193     119.91
 O       3.459622    -2.919097    -3.693188     290.25
 H       4.337613    -2.635751    -4.162291      24.75
 H       3.164793    -0.960732    -3.644798      25.39
 H       1.965122    -1.821322    -3.036196      24.83
 C      -0.306161    -0.877416     0.477742      37.86
 H      -0.714836    -1.683857     0.944859      22.08
 C      -0.135975     1.443826     0.069192      61.73
 H      -0.308577     2.513182     0.377432      18.16
 C       1.220984     1.148182    -0.393603      10.48
 O       2.194659     2.204400    -0.664352     181.85
 C       1.862756     3.677187    -0.922928     115.71
 H       2.792947     4.326701    -0.983189      25.45
 H       1.194085     3.804209    -1.667800      29.06
 H       1.401622     4.067986    -0.183303      30.73
 C       1.711004    -0.111269    -0.757364      20.31
 O       3.030101    -0.176761    -1.157142     161.20
 C       0.994643    -1.139139    -0.070738      47.05
 H       1.474272    -2.067987     0.083429      20.50
 C      -0.884640     0.465381     0.502058      33.28
 C      -2.264781     0.924796     1.050268      94.53
 H      -2.535227     0.128071     1.766930      21.37
 O      -1.941359     2.109798     1.890186     211.99
 H      -1.507715     1.628200     2.681018      24.33
 C      -3.346448     1.412417     0.006696      78.40
 H      -3.013761     2.408486    -0.529580      21.60
 O      -3.803160     0.437504    -0.937734     265.71
 H      -3.232035     0.420482    -1.791095      25.14
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 C      -4.593516     1.942029     0.902709      76.87
 O      -5.610408     2.681099     0.224460     257.15
 H      -5.127474     3.510691    -0.219470      26.38
 H      -4.007848     2.437292     2.068048      21.73
 H      -5.035489     0.995188     1.204564      25.24
55
name = lig-etoh-Waterframe_818
 C       5.970299    -0.786185     0.931739      39.74
 H       6.037611     0.211506     0.459271      23.74
 C       5.153776    -2.976316     0.588305      51.27
 H       4.954363    -3.761422    -0.276536      20.29
 C       5.241630    -3.307794     1.942278      19.40
 O       4.854823    -4.534539     2.402008     238.52
 C       3.391973    -4.723231     2.334800      96.12
 H       2.845433    -3.969131     2.830053      26.84
 H       3.139816    -5.539313     2.744186      24.70
 H       2.949495    -4.794251     1.186180      24.40
 C       5.617728    -2.254455     2.858508       4.11
 O       5.746093    -2.558474     4.246540     185.56
 H       5.409479    -3.519083     4.456606      24.28
 C       6.139399    -1.039278     2.343810      56.36
 H       6.699595    -0.213419     2.897619      22.59
 C       5.329151    -1.717473     0.080939      13.35
 C       5.160598    -1.531333    -1.421224      99.59
 H       5.487000    -2.336859    -1.990401      24.80
 O       5.683694    -0.336392    -2.018620     242.05
 H       5.002147     0.283875    -1.774674      28.13
 C       3.539489    -1.466264    -1.540234      84.77
 H       3.156981    -2.181980    -0.821506      23.64
 C       3.043738    -1.711600    -3.025809      93.25
 O       3.461440    -2.975818    -3.780182     239.11
 H       4.496630    -2.957749    -4.177920      22.02
 H       3.177194    -0.753486    -3.542348      25.20
 H       1.982316    -1.724943    -2.754227      25.59
 C      -0.335736    -0.902831     0.481979      19.39
 H      -0.950926    -1.663966     1.006883      19.95
 C       0.010290     1.509579     0.005458      69.38
 H      -0.223085     2.456923     0.148756      20.48
 C       1.312758     1.235000    -0.383606       6.56
 O       2.243029     2.260390    -0.657374     188.37
 C       1.840782     3.674060    -0.875016     107.16
 H       2.625864     4.115392    -1.226632      28.52
 H       1.256647     3.584441    -1.792436      26.41
 H       1.386704     4.150706     0.128082      24.60
 C       1.634222    -0.119987    -0.741337      14.63
 O       3.068854    -0.218731    -1.216302     174.99
 C       0.887642    -1.198998    -0.123608      62.44
 H       1.200218    -2.273812    -0.061012      19.35
 C      -0.893597     0.405245     0.448961      23.24
 C      -2.237103     0.844398     1.140357      88.44
 H      -2.543190    -0.056561     1.588060      24.23
 O      -1.926659     2.090849     1.939943     221.96
 H      -1.534987     1.724035     2.741391      26.90
 C      -3.353370     1.356881     0.125690      81.14
 H      -2.782482     2.285197    -0.378259      21.71
 O      -3.762641     0.433012    -0.871811     263.03
 H      -3.023394     0.486056    -1.592531      25.12
 C      -4.622686     1.928144     0.806159      94.97
 O      -5.584815     2.737605     0.268696     271.67
 H      -5.207637     3.662443     0.000681      27.32
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 H      -4.146977     2.515819     1.933587      22.94
 H      -5.148995     1.097480     1.159306      26.29
55
name = lig-etoh-Waterframe_819
 C       5.927734    -0.825007     0.958665      79.60
 H       6.102093     0.272879     0.759115      18.48
 C       5.033787    -3.034971     0.528328      22.65
 H       4.784846    -3.905585    -0.190917      19.22
 C       5.244251    -3.210583     1.950309     -26.43
 O       4.846728    -4.570949     2.384944     204.56
 C       3.364790    -4.749867     2.324199      81.42
 H       2.884620    -3.808523     2.654838      26.42
 H       3.162786    -5.777739     2.819440      23.11
 H       3.271925    -4.908171     1.148335      24.99
 C       5.726918    -2.215121     2.934978      -7.30
 O       5.656400    -2.547271     4.253261      47.44
 H       5.741852    -3.575919     4.249484      18.89
 C       6.165433    -1.040090     2.272887      42.92
 H       6.660843    -0.300734     3.078557      22.73
 C       5.428414    -1.742802     0.066732      37.13
 C       5.047842    -1.475342    -1.388782      97.99
 H       5.369873    -2.439066    -1.996060      23.39
 O       5.700839    -0.368191    -2.062580     218.65
 H       5.201138     0.452022    -1.965026      27.16
 C       3.567351    -1.485278    -1.588424      95.02
 H       3.147221    -2.261856    -0.970492      27.50
 C       2.980460    -1.712488    -3.063125      88.04
 O       3.419570    -2.993893    -3.794303     224.75
 H       4.268438    -2.876341    -4.410965      23.38
 H       3.496724    -0.836286    -3.634251      24.79
 H       1.924338    -1.991635    -3.117054      25.88
 C      -0.434527    -0.888127     0.480384      36.97
 H      -1.074559    -1.781520     0.946940      18.71
 C       0.092302     1.545237    -0.017852      69.39
 H      -0.340163     2.434128    -0.009746      22.87
 C       1.393971     1.344190    -0.462824       1.82
 O       2.309979     2.296770    -0.633822     204.17
 C       1.809778     3.597896    -0.870191      94.19
 H       2.733056     4.035673    -1.212616      24.10
 H       0.860949     3.698020    -1.644249      24.19
 H       1.392858     4.278467     0.245893      22.82
 C       1.703080    -0.159144    -0.638768       3.57
 O       3.005570    -0.199244    -1.228367     154.80
 C       0.817701    -1.215078    -0.210156      61.61
 H       1.071055    -2.326439    -0.468016      23.06
 C      -0.869628     0.415649     0.407688      53.59
 C      -2.176074     0.805566     1.171123      90.93
 H      -2.720188     0.132873     1.760216      26.21
 O      -1.924074     2.003473     2.009671     258.47
 H      -1.549985     1.730138     2.796685      30.70
 C      -3.324668     1.391691     0.218426      94.00
 H      -2.769099     2.127269    -0.340907      24.37
 O      -3.694998     0.402773    -0.815715     257.72
 H      -3.104654     0.573741    -1.660199      25.52
 C      -4.607400     1.845788     0.884738     112.26
 O      -5.590143     2.839789     0.253114     290.15
 H      -5.197851     3.706278    -0.094388      29.47
 H      -4.348879     2.352857     1.582627      31.59
 H      -5.254278     1.064125     1.207277      27.79
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name = lig-etoh-Waterframe_820
 C       5.905146    -0.766561     0.949807      -8.20
 H       6.332899     0.171905     0.381323      15.89
 C       5.019785    -3.039732     0.581540      55.35
 H       4.562253    -3.900321     0.160741      23.03
 C       5.185068    -3.223931     1.922969      16.52
 O       4.858267    -4.542272     2.388773     216.75
 C       3.420533    -4.790866     2.246748      82.68
 H       2.748586    -3.918949     2.645205      25.12
 H       3.081222    -5.698608     3.137792      21.98
 H       2.965451    -5.026780     1.276891      26.81
 C       5.774369    -2.313273     2.861214      19.28
 O       5.605745    -2.536331     4.243037     163.32
 H       5.597317    -3.553478     4.431925      18.96
 C       6.189441    -1.080185     2.393669      43.17
 H       6.552838    -0.082337     2.928233      23.92
 C       5.474310    -1.793235     0.009281       9.91
 C       4.983934    -1.436721    -1.409340      88.52
 H       5.442504    -2.426288    -1.992157      22.65
 O       5.714271    -0.392790    -2.106000     191.34
 H       5.589726     0.510126    -1.757128      25.42
 C       3.471788    -1.565685    -1.689045      83.23
 H       3.136398    -2.386660    -1.035317      27.34
 C       3.016973    -1.787987    -3.150343     110.32
 O       3.358122    -2.997586    -3.775197     272.25
 H       4.156052    -2.728069    -4.285353      25.17
 H       3.204116    -0.888409    -3.926977      24.39
 H       1.923120    -1.520460    -3.233390      25.80
 C      -0.453903    -0.878080     0.383426      36.73
 H      -1.150167    -1.773606     0.788267      19.01
 C       0.018434     1.507562    -0.009577      50.86
 H      -0.392709     2.605764     0.010412      20.12
 C       1.366501     1.225677    -0.485675       0.99
 O       2.376267     2.302844    -0.628596     166.98
 C       1.802481     3.618592    -0.869153      89.20
 H       2.583927     4.462707    -1.288382      22.64
 H       0.759489     3.599257    -1.480092      24.17
 H       1.607426     3.988668     0.254336      24.23
 C       1.779361    -0.102277    -0.513729      25.90
 O       2.913675    -0.194331    -1.215779     128.57
 C       0.793214    -1.150453    -0.303418      56.95
 H       1.033403    -2.223857    -0.676640      24.11
 C      -0.816029     0.505751     0.434897      36.70
 C      -2.163678     0.882897     1.165300      82.01
 H      -2.479219    -0.052611     1.746669      24.06
 O      -1.912145     1.917280     2.095723     280.23
 H      -1.555802     1.409866     2.773190      29.39
 C      -3.266037     1.402760     0.186487      95.63
 H      -3.040969     2.343681    -0.190410      26.64
 O      -3.611394     0.360679    -0.765015     252.77
 H      -3.367540     0.675726    -1.736350      24.70
 C      -4.634635     1.869861     0.991530      71.43
 O      -5.578600     2.882296     0.212948     235.90
 H      -4.898098     3.442205    -0.108563      32.21
 H      -4.267180     2.340340     2.073618      25.80
 H      -5.216321     0.897114     1.182634      26.13
55
name = lig-etoh-Waterframe_821
 C       5.959247    -0.809052     0.939827      38.67
 H       6.366980     0.144819     0.437480      21.93
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 C       5.048051    -2.983711     0.598738      89.93
 H       4.522216    -3.626428    -0.004040      26.99
 C       5.171139    -3.318517     1.946891      27.60
 O       4.830965    -4.506540     2.385270     299.14
 C       3.420013    -4.835217     2.248423     102.33
 H       2.872369    -3.882047     2.564183      30.02
 H       3.296967    -5.785009     3.082528      24.45
 H       3.094117    -5.243498     1.389018      30.81
 C       5.747381    -2.406837     2.838748     -15.71
 O       5.591375    -2.539687     4.208214      54.41
 H       5.270362    -3.403258     4.508006      16.95
 C       6.167578    -1.046524     2.338536      18.54
 H       6.484635    -0.338944     3.179192      19.18
 C       5.411420    -1.768197     0.029384      15.00
 C       5.028306    -1.500166    -1.492098      66.32
 H       5.335030    -2.353814    -2.140537      26.61
 O       5.716246    -0.391474    -2.124131     137.13
 H       5.691676     0.260775    -1.413739      28.74
 C       3.374319    -1.548941    -1.744271      81.35
 H       2.956068    -2.400571    -1.140155      28.67
 C       2.968098    -1.720534    -3.264431     108.14
 O       3.323232    -3.032648    -3.765391     284.95
 H       4.154226    -3.113309    -4.189183      29.87
 H       3.574906    -0.924758    -3.777984      26.69
 H       1.879714    -1.668660    -3.026655      26.98
 C      -0.401588    -0.805153     0.222671      53.36
 H      -1.141172    -1.621703     0.482159      22.13
 C       0.012918     1.504550    -0.032567      59.12
 H      -0.272342     2.727592     0.197094      19.09
 C       1.269760     1.240053    -0.389491      12.77
 O       2.371796     2.247716    -0.668788     161.06
 C       1.789979     3.667310    -0.783093     105.91
 H       2.497127     4.336145    -1.547535      24.01
 H       0.954888     3.479892    -1.419464      28.15
 H       1.587976     4.030309     0.039141      31.70
 C       1.743706    -0.092862    -0.472668      24.05
 O       2.921343    -0.284823    -1.246570     157.69
 C       0.792661    -1.067497    -0.346826      78.60
 H       1.057930    -2.110150    -0.591016      26.22
 C      -0.836231     0.520329     0.505761      44.22
 C      -2.146152     0.954083     1.091247      81.44
 H      -2.530404    -0.152459     1.328301      22.85
 O      -1.892932     1.856691     2.219536     240.06
 H      -1.538452     1.291833     3.012664      23.87
 C      -3.308549     1.447538     0.190931      77.67
 H      -2.945881     2.386476    -0.373144      24.94
 O      -3.524075     0.345001    -0.733861     223.87
 H      -3.476830     0.771188    -1.681703      24.93
 C      -4.664467     1.904498     1.036255      65.51
 O      -5.473621     2.824181     0.229378     207.78
 H      -4.981510     3.567320    -0.122534      30.95
 H      -4.367764     2.315759     2.378884      23.72
 H      -5.351420     0.935875     1.105787      25.86
55
name = lig-etoh-Waterframe_822
 C       6.057177    -0.843856     0.921328      62.93
 H       6.261934     0.221225     0.755942      25.88
 C       5.029522    -2.961268     0.537257      58.24
 H       4.615853    -3.616004    -0.200641      23.26
 C       5.239960    -3.316441     1.914996      21.98
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 O       4.784948    -4.589632     2.409425     264.94
 C       3.408986    -4.910296     2.310875     119.00
 H       2.725565    -4.075991     2.412561      29.35
 H       3.214961    -5.645482     3.017697      26.61
 H       3.346799    -5.287242     1.278539      27.40
 C       5.691445    -2.341638     2.839334      15.93
 O       5.593637    -2.515514     4.171288     133.69
 H       5.396309    -3.469211     4.341475      19.58
 C       6.087316    -1.153115     2.275022      56.44
 H       6.488785    -0.502801     2.989706      21.25
 C       5.333509    -1.690749     0.042587     -10.39
 C       5.036858    -1.630682    -1.569955      77.76
 H       5.380590    -2.445400    -2.061832      27.16
 O       5.693863    -0.389118    -2.085272     155.29
 H       5.626675     0.372750    -1.484521      27.79
 C       3.401999    -1.521250    -1.760813      94.32
 H       2.930082    -2.398146    -1.252249      25.29
 C       2.959894    -1.635731    -3.275858     100.64
 O       3.289828    -3.099323    -3.763325     275.06
 H       4.138684    -3.015026    -4.203143      27.91
 H       3.421414    -0.895963    -3.869231      27.39
 H       1.929236    -1.694168    -3.700748      25.57
 C      -0.489909    -0.714618     0.144039      58.57
 H      -1.086679    -1.548500     0.273723      24.04
 C      -0.005851     1.599876     0.037045      80.70
 H      -0.336885     2.787246     0.266322      18.89
 C       1.376012     1.333584    -0.314520      19.27
 O       2.258113     2.211054    -0.698511     186.95
 C       1.787721     3.611901    -0.789036     108.49
 H       2.744774     4.062580    -1.257441      24.51
 H       0.900940     3.658023    -1.276752      29.13
 H       1.584558     4.307839     0.179588      25.43
 C       1.749814    -0.077510    -0.595270      16.68
 O       2.937624    -0.328411    -1.251529     200.54
 C       0.835953    -1.091028    -0.360371      59.68
 H       1.048841    -2.107489    -0.501574      22.30
 C      -0.845347     0.551440     0.461764      34.66
 C      -2.167068     0.927553     1.084792      89.68
 H      -2.798159     0.147651     1.569241      21.78
 O      -1.901945     1.809353     2.312775     195.00
 H      -1.534986     1.154628     3.165047      20.76
 C      -3.342480     1.546044     0.240649      74.39
 H      -2.977082     2.331497    -0.554172      22.90
 O      -3.470530     0.357793    -0.715095     206.08
 H      -3.405240     0.716894    -1.689019      24.51
 C      -4.638458     1.894347     1.002109     107.22
 O      -5.373807     2.760652     0.256210     271.79
 H      -4.944741     3.605627     0.152818      32.10
 H      -4.438160     2.472023     1.990757      26.44
 H      -5.331679     1.011030     1.200131      27.43
55
name = lig-etoh-Waterframe_823
 C       6.063435    -0.835298     0.870313      59.77
 H       6.251081     0.179097     0.622667      26.54
 C       5.001592    -2.989846     0.514726      44.49
 H       4.703981    -3.928639    -0.073969      20.55
 C       5.233954    -3.342604     1.825329      38.09
 O       4.824668    -4.646409     2.462140     146.61
 C       3.361853    -5.002983     2.313965     105.84
 H       2.685987    -4.192504     2.400112      26.86
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 H       3.093200    -5.632682     2.992063      27.28
 H       3.104031    -5.503190     1.204852      24.96
 C       5.577727    -2.371688     2.802985       6.36
 O       5.605277    -2.482716     4.156264     168.53
 H       5.606688    -3.422002     4.558008      19.54
 C       6.090330    -1.174479     2.257090      54.77
 H       6.489648    -0.426503     2.764767      23.45
 C       5.296119    -1.679129    -0.036398     -13.75
 C       5.002725    -1.595242    -1.531837      93.81
 H       5.508078    -2.412999    -1.996006      25.18
 O       5.668160    -0.427760    -2.049986     208.22
 H       5.202117     0.327527    -1.606744      26.98
 C       3.439266    -1.577418    -1.835963      79.81
 H       3.069865    -2.418470    -1.241083      25.73
 C       2.984034    -1.663297    -3.339054     101.16
 O       3.294814    -3.093198    -3.764354     259.51
 H       4.094641    -2.952265    -4.315067      25.35
 H       3.533942    -0.997159    -3.953988      27.23
 H       1.895597    -1.269400    -3.450618      25.52
 C      -0.519333    -0.752961     0.085828      35.13
 H      -1.245138    -1.388364     0.391707      21.75
 C       0.072444     1.697918     0.164484      57.35
 H      -0.317513     2.700314     0.321158      19.37
 C       1.349963     1.262876    -0.265247      19.59
 O       2.184969     2.286363    -0.730036     157.98
 C       1.833644     3.581065    -0.811290     111.41
 H       2.642211     4.084983    -1.237427      27.41
 H       0.961864     3.880521    -1.427013      26.77
 H       1.849670     4.004703     0.552684      22.58
 C       1.722862    -0.046951    -0.730299      17.31
 O       2.997112    -0.253330    -1.225369     147.09
 C       0.791522    -1.094834    -0.335467      59.37
 H       1.008705    -2.085903    -0.508525      22.41
 C      -0.903841     0.657915     0.366050       2.46
 C      -2.253454     0.947911     1.228832      79.45
 H      -2.571429    -0.044292     1.532262      22.54
 O      -1.939292     1.795610     2.333694     256.73
 H      -1.400346     1.091973     2.993371      22.43
 C      -3.268104     1.550836     0.222336      86.53
 H      -3.113307     2.621573    -0.164796      21.19
 O      -3.469656     0.388530    -0.698804     241.61
 H      -3.202048     0.694417    -1.657153      24.23
 C      -4.539060     1.857642     0.993057     109.46
 O      -5.380340     2.773764     0.214383     282.27
 H      -4.800170     3.533398     0.203908      33.10
 H      -4.197369     2.259576     1.837849      30.17
 H      -4.979847     0.955691     1.309535      29.94
55
name = lig-etoh-Waterframe_824
 C       5.934753    -0.857713     0.789544      53.53
 H       6.363953    -0.053319     0.305090      21.96
 C       4.989163    -3.053984     0.475593      44.62
 H       4.629708    -3.900282    -0.278815      20.72
 C       5.134170    -3.435171     1.867236      43.19
 O       4.851599    -4.671942     2.460664     159.22
 C       3.338285    -5.075660     2.284605      84.76
 H       2.901687    -4.101519     2.420399      24.02
 H       3.190681    -5.836258     3.200353      23.34
 H       3.050290    -5.742132     1.278351      24.01
 C       5.526764    -2.413144     2.764019     -23.27
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 O       5.622489    -2.445903     4.155653     154.29
 H       5.350622    -3.362368     4.622988      18.36
 C       6.128919    -1.105070     2.187311      31.71
 H       6.486440    -0.446029     2.975365      22.17
 C       5.300519    -1.798988    -0.041938      53.29
 C       4.976927    -1.509826    -1.488787      97.24
 H       5.407572    -2.469202    -2.098678      23.12
 O       5.624739    -0.427394    -2.025982     214.79
 H       5.049338     0.368624    -1.831095      25.27
 C       3.485981    -1.591867    -1.876998      69.97
 H       2.977075    -2.351352    -1.320079      27.09
 C       3.058813    -1.703966    -3.373619     111.44
 O       3.287645    -3.023811    -3.787118     269.43
 H       4.092435    -3.146206    -4.378640      25.43
 H       3.797009    -1.062618    -3.905955      25.62
 H       1.999286    -1.515782    -3.162307      25.83
 C      -0.561607    -0.669782     0.096319      46.85
 H      -1.221138    -1.460876     0.419007      22.83
 C       0.086779     1.659920     0.308277      68.24
 H       0.079513     2.607728     0.456653      25.23
 C       1.278989     1.261561    -0.331186      -7.70
 O       2.214727     2.267708    -0.793399     141.97
 C       1.907476     3.694077    -0.767709     112.24
 H       2.638454     4.201701    -1.227365      28.34
 H       0.862125     3.863089    -1.358124      25.50
 H       1.607659     4.080414     0.308131      25.70
 C       1.627605    -0.066046    -0.750801       1.22
 O       3.066302    -0.184483    -1.222978      63.72
 C       0.737961    -1.065358    -0.361396      64.94
 H       0.997871    -2.096594    -0.493175      23.16
 C      -0.929494     0.694510     0.333188      24.50
 C      -2.218821     0.953658     1.254027      84.60
 H      -2.508155    -0.036285     1.468479      25.44
 O      -1.989090     1.816531     2.309645     281.05
 H      -1.598372     1.487432     3.123176      29.21
 C      -3.219657     1.493215     0.246406      98.33
 H      -2.622916     2.298982    -0.187448      24.23
 O      -3.474950     0.471215    -0.711002     285.32
 H      -3.028781     0.683645    -1.613761      25.87
 C      -4.467421     1.823219     0.972752      78.06
 O      -5.398759     2.773289     0.206740     259.47
 H      -5.006382     3.611445    -0.169819      29.76
 H      -3.990565     2.377970     2.140790      23.01
 H      -5.040186     0.962779     1.162952      27.68
55
name = lig-etoh-Waterframe_825
 C       5.841382    -0.873705     0.767060      51.32
 H       6.298605    -0.133223     0.217871      18.31
 C       4.959170    -3.208271     0.479470      54.35
 H       4.505978    -3.852653    -0.356076      23.22
 C       5.038547    -3.450522     1.909231      -6.27
 O       4.813649    -4.739930     2.406578     229.01
 C       3.411578    -5.136947     2.314703      90.84
 H       2.677308    -4.274099     2.320414      27.49
 H       3.163243    -5.842929     3.401833      23.08
 H       3.264887    -5.627926     1.320480      26.30
 C       5.586801    -2.318973     2.717302       1.82
 O       5.617824    -2.413798     4.120539     122.78
 H       5.271513    -3.361125     4.400682      17.03
 C       6.056620    -1.166921     2.125753      50.54
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 H       6.593821    -0.417790     2.908738      22.54
 C       5.298890    -1.939657    -0.004111      13.57
 C       4.962624    -1.581035    -1.497567      81.75
 H       5.419270    -2.463079    -2.200237      22.11
 O       5.601412    -0.348533    -2.036590     162.44
 H       5.186880     0.537065    -1.825368      23.91
 C       3.505529    -1.495009    -1.803339      88.91
 H       2.970796    -2.295965    -1.327519      27.32
 C       3.180285    -1.679536    -3.309739     102.86
 O       3.282459    -3.035333    -3.846843     255.84
 H       4.237409    -2.989544    -4.341742      21.19
 H       3.442990    -0.785249    -4.054829      24.84
 H       2.171909    -1.557547    -3.677174      26.23
 C      -0.586700    -0.601480     0.118109      53.95
 H      -1.258731    -1.492751     0.326651      22.53
 C       0.138291     1.608339     0.359417      60.13
 H       0.081963     2.558005     0.862680      25.96
 C       1.279731     1.345694    -0.485334       3.10
 O       2.273594     2.221317    -0.840800     115.55
 C       1.895107     3.795445    -0.717674      90.45
 H       2.806901     4.284480    -1.113717      24.97
 H       0.894608     3.872990    -1.377993      24.32
 H       1.775867     4.218139     0.113090      28.83
 C       1.659093    -0.040867    -0.739622       1.07
 O       3.010392    -0.180925    -1.241598     110.99
 C       0.668922    -1.030641    -0.427586      69.43
 H       0.888369    -2.150699    -0.390270      26.66
 C      -0.924413     0.661936     0.465472      48.65
 C      -2.106991     0.859285     1.189774     104.90
 H      -2.554096     0.044552     1.738367      25.91
 O      -2.042011     1.919255     2.293185     247.22
 H      -1.829712     1.324209     2.995730      28.60
 C      -3.150917     1.462530     0.263901      91.33
 H      -2.685453     2.253535    -0.298105      25.87
 O      -3.489605     0.524161    -0.765513     277.05
 H      -3.021816     0.782395    -1.640237      27.05
 C      -4.466876     1.925182     0.927510      85.55
 O      -5.413657     2.731029     0.225931     257.95
 H      -4.879709     3.505467    -0.170892      28.82
 H      -4.475657     2.511454     2.150827      22.81
 H      -5.109301     1.039149     1.033165      25.55
55
name = lig-etoh-Waterframe_826
 C       5.796088    -0.971645     0.746918      76.06
 H       6.029408     0.034699     0.411103      25.79
 C       4.912665    -3.324827     0.525144      75.89
 H       4.517490    -4.217781     0.066976      27.33
 C       5.013562    -3.385045     1.874909     -19.48
 O       4.769700    -4.768909     2.382309     227.45
 C       3.458301    -5.201276     2.350692     117.14
 H       2.665997    -4.409580     2.302627      31.18
 H       3.157912    -6.021022     3.222529      24.21
 H       3.335105    -5.800702     1.581993      30.24
 C       5.582196    -2.373590     2.712925      12.43
 O       5.602322    -2.382246     4.038317      36.09
 H       5.590819    -3.332235     4.477227      18.44
 C       5.986504    -1.173598     2.086103      47.82
 H       6.653739    -0.298170     2.620216      20.93
 C       5.278204    -1.993647    -0.049070      10.19
 C       5.011285    -1.624288    -1.510752      70.91
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 H       5.401453    -2.342096    -2.233910      25.29
 O       5.615686    -0.294725    -2.046744     134.73
 H       5.188895     0.322264    -1.352516      28.07
 C       3.418937    -1.415297    -1.733170      84.19
 H       2.980593    -2.263562    -1.180573      27.82
 C       3.147351    -1.579233    -3.321529      74.17
 O       3.354911    -3.040406    -3.903189     219.68
 H       4.350328    -3.091118    -4.398753      21.92
 H       3.980650    -0.938611    -3.900794      22.42
 H       2.029117    -1.327343    -3.306142      26.21
 C      -0.568266    -0.700041     0.099140      46.14
 H      -1.498785    -1.367952     0.295979      22.30
 C       0.224925     1.620246     0.333905      51.29
 H      -0.104539     2.495449     1.089698      22.43
 C       1.295018     1.368744    -0.570427      15.81
 O       2.305356     2.314654    -0.854197     157.16
 C       1.916253     3.771738    -0.731412      88.98
 H       2.878964     4.280870    -1.291000      23.22
 H       1.074752     4.099918    -1.412411      24.56
 H       1.877865     4.092852     0.486641      22.10
 C       1.676658    -0.011473    -0.751069      24.97
 O       2.900277    -0.208310    -1.270620     182.12
 C       0.651353    -0.965660    -0.495034      68.11
 H       0.861652    -2.121653    -0.554420      26.02
 C      -0.729298     0.614604     0.623860      23.66
 C      -2.156075     0.901052     1.252321      80.50
 H      -2.446490    -0.168190     1.660034      25.47
 O      -2.060463     1.980931     2.270751     267.74
 H      -1.805816     1.518876     3.078430      29.40
 C      -3.133259     1.511408     0.205761      74.30
 H      -2.792375     2.519853    -0.087885      27.30
 O      -3.521058     0.534957    -0.844855     252.00
 H      -3.187447     0.882085    -1.747106      26.62
 C      -4.563149     1.976424     0.960106     103.12
 O      -5.415475     2.723542     0.170321     285.30
 H      -4.979500     3.676033     0.043646      27.65
 H      -4.275439     2.355287     1.818265      29.11
 H      -4.912681     0.911833     1.218387      27.34
55
name = lig-etoh-Waterframe_827
 C       5.750695    -1.081462     0.710185      39.74
 H       5.872434    -0.022407     0.331972      23.53
 C       4.892720    -3.285666     0.481970      59.63
 H       4.683166    -4.206365     0.089850      27.82
 C       5.013449    -3.448476     1.902662      12.23
 O       4.800336    -4.703079     2.407486     366.86
 C       3.399588    -5.347364     2.363298     103.38
 H       2.761591    -4.451243     2.379644      31.82
 H       3.412118    -5.780959     3.248179      28.26
 H       3.224690    -6.038249     1.495251      29.13
 C       5.547523    -2.424228     2.683747       7.13
 O       5.604977    -2.384852     4.044272      13.69
 H       5.732924    -3.254533     4.537979      14.05
 C       5.954168    -1.180726     2.086930      41.27
 H       6.371538    -0.364466     2.793587      21.26
 C       5.240777    -2.082474    -0.160476      17.78
 C       5.001818    -1.572625    -1.567611      96.56
 H       5.225071    -2.304714    -2.207489      30.37
 O       5.610557    -0.312893    -1.977331     129.33
 H       5.538743     0.410769    -1.234435      26.33
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 C       3.381666    -1.510025    -1.754678      78.41
 H       2.835455    -2.301918    -1.162367      27.66
 C       3.123433    -1.564741    -3.310394      88.37
 O       3.378211    -2.973050    -3.893821     268.11
 H       4.241754    -2.804715    -4.371491      25.22
 H       3.953750    -0.902574    -3.662181      25.38
 H       2.072010    -1.128048    -3.557808      26.61
 C      -0.558435    -0.711261     0.124554      48.09
 H      -1.287311    -1.600299     0.124126      24.12
 C       0.250236     1.621489     0.330527      47.54
 H       0.249788     2.869467     0.501595      20.91
 C       1.350103     1.411832    -0.522718      12.29
 O       2.292118     2.427965    -0.879353     200.34
 C       2.006743     3.727022    -0.773969     103.45
 H       2.955462     4.436312    -1.152687      22.69
 H       1.105315     4.022273    -1.127429      27.75
 H       1.691627     3.989411     0.573879      21.30
 C       1.579905     0.035647    -0.788644      20.00
 O       2.856603    -0.194553    -1.312258     129.95
 C       0.683891    -1.003639    -0.568412      60.61
 H       1.033763    -1.977129    -1.068947      24.89
 C      -0.585487     0.538701     0.730118      37.24
 C      -2.142871     1.008837     1.297094      71.30
 H      -2.656552    -0.013844     1.641800      25.36
 O      -2.066675     1.996380     2.268999     272.66
 H      -1.631971     1.823401     3.088118      29.86
 C      -3.247373     1.580476     0.175386      70.37
 H      -2.612315     2.434150    -0.268887      25.54
 O      -3.528278     0.581400    -0.908326     220.60
 H      -3.359419     0.905487    -1.851340      26.87
 C      -4.522328     1.898170     0.993160      91.28
 O      -5.436988     2.749523     0.072858     224.18
 H      -5.282670     3.777922     0.215132      27.51
 H      -4.133215     2.468914     1.826219      26.42
 H      -5.279984     1.038604     1.309219      25.81
55
name = lig-etoh-Waterframe_828
 C       5.713811    -1.121094     0.693843      32.34
 H       6.133810    -0.178532     0.140459      19.71
 C       4.886935    -3.286046     0.428149      50.80
 H       4.660960    -4.009481    -0.340273      23.45
 C       5.029460    -3.500567     1.841298      24.30
 O       4.811582    -4.701289     2.465988     246.49
 C       3.398740    -5.414389     2.412646      85.21
 H       2.537906    -4.707862     2.356247      27.16
 H       3.402138    -5.855974     3.310959      26.85
 H       3.306118    -6.116789     1.362209      24.38
 C       5.522502    -2.414485     2.700830       0.30
 O       5.623189    -2.412623     4.108658     154.86
 H       5.458302    -3.320856     4.447704      18.63
 C       5.888946    -1.262157     2.078903      64.12
 H       6.052067    -0.480195     2.725933      21.20
 C       5.247029    -2.082132    -0.197827      32.84
 C       4.876674    -1.545752    -1.618259     100.14
 H       5.288391    -2.217551    -2.395944      25.97
 O       5.620349    -0.376298    -1.900407     157.79
 H       5.548513     0.478689    -1.323046      21.31
 C       3.333350    -1.577828    -1.826930      72.80
 H       2.922205    -2.464233    -1.258176      25.54
 C       3.116864    -1.584198    -3.299245     123.03
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 O       3.320728    -2.836363    -3.831337     295.23
 H       4.192961    -2.976683    -4.288311      26.96
 H       3.647486    -0.820402    -3.681249      28.32
 H       2.251845    -1.282405    -3.873676      26.15
 C      -0.422452    -0.745514     0.134269      37.87
 H      -1.245350    -1.471621     0.366130      23.75
 C       0.295708     1.668004     0.305138      53.02
 H      -0.180939     2.747488     0.499763      20.92
 C       1.406934     1.444819    -0.411806      23.62
 O       2.306790     2.376969    -0.940191     181.81
 C       2.008594     3.821195    -0.716532     120.29
 H       2.898603     4.409143    -1.051895      26.89
 H       1.127052     4.028897    -1.275492      27.68
 H       1.993978     4.159443     0.349769      26.52
 C       1.595911     0.063805    -0.888269       8.05
 O       2.865791    -0.173998    -1.369714      87.34
 C       0.681796    -1.021902    -0.650977      65.10
 H       0.757219    -1.930645    -1.241254      23.44
 C      -0.693397     0.573060     0.799411      35.13
 C      -2.069151     1.019464     1.249909      82.87
 H      -2.612393     0.221642     1.746860      23.77
 O      -2.063378     2.070710     2.297064     259.06
 H      -1.524725     1.505583     2.882095      26.62
 C      -3.274063     1.558410     0.151983      72.14
 H      -3.046031     2.556714    -0.408387      23.70
 O      -3.537905     0.632059    -0.922317     244.58
 H      -3.313798     1.101423    -1.772625      25.83
 C      -4.513521     1.933119     0.909496      78.45
 O      -5.457269     2.736532     0.017023     203.41
 H      -5.164714     3.719114     0.235727      26.93
 H      -4.346593     2.716757     2.006644      22.53
 H      -5.146023     1.038024     1.289447      25.94
55
name = lig-etoh-Waterframe_829
 C       5.757115    -1.073892     0.667934      53.34
 H       6.326201    -0.096858     0.396756      20.76
 C       4.886801    -3.337704     0.358389      66.23
 H       4.370352    -4.181160    -0.264525      23.93
 C       5.057114    -3.498990     1.767255     -37.43
 O       4.745775    -4.767120     2.539217     180.04
 C       3.463612    -5.412328     2.451390     108.54
 H       2.571530    -4.777614     2.338783      28.11
 H       3.269462    -6.276744     3.276268      23.78
 H       3.658625    -6.230881     1.511407      25.55
 C       5.461177    -2.490054     2.741894      -4.08
 O       5.620179    -2.475593     4.116600     162.78
 H       5.299347    -3.272430     4.566370      20.55
 C       5.811515    -1.274636     2.051924      51.27
 H       6.088770    -0.436127     2.521820      23.00
 C       5.226382    -2.028512    -0.181317      13.37
 C       4.815766    -1.611245    -1.601079      87.25
 H       5.279685    -2.330285    -2.456077      23.87
 O       5.636798    -0.397607    -1.876951     154.51
 H       5.045224     0.235429    -1.318996      27.13
 C       3.283739    -1.492350    -1.872908      88.95
 H       2.791354    -2.314773    -1.323418      26.61
 C       3.048448    -1.497385    -3.386147     110.97
 O       3.280646    -2.830696    -3.809503     281.05
 H       4.205882    -2.955738    -4.193061      25.98
 H       3.788170    -0.816663    -3.791891      25.90
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 H       1.965045    -1.338070    -3.313702      26.48
 C      -0.388083    -0.679119     0.254583      43.14
 H      -1.049163    -1.505440     0.443183      20.92
 C       0.143354     1.682397     0.383152      43.06
 H      -0.185308     2.627188     0.689947      20.85
 C       1.463299     1.381809    -0.373186      -9.49
 O       2.338002     2.339113    -0.973900      96.22
 C       2.026975     3.902133    -0.678895     110.74
 H       2.785536     4.210414    -1.206501      28.55
 H       1.142649     4.262516    -1.393542      25.83
 H       1.908560     4.112817     0.204592      31.12
 C       1.668692     0.047709    -0.944187      17.48
 O       2.904043    -0.194013    -1.448103     174.17
 C       0.681427    -0.947880    -0.740644      65.43
 H       0.656364    -1.911004    -1.099206      23.87
 C      -0.692138     0.646727     0.657715      37.38
 C      -2.103550     1.037269     1.166472      84.66
 H      -2.396775     0.095744     1.502655      25.48
 O      -2.006107     2.108148     2.315566     221.83
 H      -1.638447     1.635039     3.136686      26.93
 C      -3.199472     1.574821     0.130921      88.79
 H      -2.907394     2.573198    -0.194177      25.73
 O      -3.556394     0.660825    -0.908485     282.68
 H      -3.228147     1.005174    -1.787655      26.13
 C      -4.618463     2.002532     0.832612      93.73
 O      -5.450657     2.699788     0.002363     238.03
 H      -5.026180     3.655074    -0.208198      27.74
 H      -4.228089     2.624531     1.942700      23.89
 H      -4.933474     1.068880     1.103207      28.66
55
name = lig-etoh-Waterframe_830
 C       5.831080    -1.032634     0.701015      41.88
 H       6.082990    -0.034159     0.274104      22.39
 C       4.888613    -3.329439     0.362889      58.97
 H       4.277397    -4.242556    -0.075576      22.79
 C       5.031520    -3.584739     1.826904       2.78
 O       4.705983    -4.770657     2.607063     174.86
 C       3.539184    -5.495334     2.404711     110.61
 H       2.741971    -4.769393     2.307965      28.75
 H       3.390223    -6.117666     3.545741      22.44
 H       3.459937    -6.061078     1.522466      27.89
 C       5.418389    -2.515381     2.680200       6.27
 O       5.586967    -2.539257     4.066730     181.19
 H       5.506947    -3.374379     4.615045      19.66
 C       5.760014    -1.264427     2.078814      52.00
 H       6.287352    -0.522166     2.731234      23.50
 C       5.149907    -2.063688    -0.182410      10.15
 C       4.879717    -1.692234    -1.586645      97.07
 H       5.054735    -2.689218    -2.224309      23.20
 O       5.577463    -0.417583    -1.872335     201.36
 H       5.096554     0.417263    -1.493204      24.49
 C       3.331364    -1.396984    -1.917721     100.28
 H       2.614916    -2.055665    -1.472781      25.94
 C       2.946143    -1.439287    -3.409571      82.85
 O       3.243875    -2.904561    -3.840871     256.47
 H       4.091513    -2.743596    -4.360451      25.64
 H       3.464628    -0.637259    -4.162235      23.98
 H       1.816147    -1.114695    -3.512949      25.30
 C      -0.353970    -0.626994     0.266569      52.92
 H      -0.944546    -1.443901     0.511794      21.50
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 C       0.223783     1.732906     0.342970      60.20
 H       0.128248     2.631320     0.669613      22.28
 C       1.380820     1.361298    -0.366231       1.73
 O       2.314541     2.376562    -0.931497     133.63
 C       2.075778     3.853413    -0.764016     100.25
 H       3.000759     4.344578    -1.114766      24.76
 H       0.935528     4.157925    -1.174662      23.12
 H       1.923443     4.107796     0.307367      25.44
 C       1.686816     0.055523    -0.895888       8.64
 O       2.952868    -0.148516    -1.515778     193.43
 C       0.626497    -0.856752    -0.697052      72.77
 H       0.869635    -1.833028    -0.966908      23.74
 C      -0.757425     0.689755     0.499296      38.01
 C      -2.150091     1.038460     1.166245      78.07
 H      -2.593180     0.105633     1.546260      23.36
 O      -1.954928     2.078828     2.274940     233.00
 H      -1.838792     1.641235     3.188858      26.06
 C      -3.147104     1.688184     0.155682      84.66
 H      -2.494097     2.388102    -0.304924      24.74
 O      -3.554347     0.676890    -0.897035     277.78
 H      -3.176284     0.761904    -1.798764      27.69
 C      -4.561516     1.978791     0.826571     107.56
 O      -5.477668     2.710312    -0.051656     239.31
 H      -4.909230     3.444918    -0.546561      30.26
 H      -4.469313     2.539738     1.656463      28.78
 H      -5.193261     1.159083     1.008152      27.48
55
name = lig-etoh-Waterframe_831
 C       5.767393    -1.105833     0.716213      60.99
 H       6.091885    -0.199873     0.234811      26.44
 C       4.844583    -3.366738     0.518701      62.62
 H       4.481675    -3.993029    -0.359663      23.83
 C       4.971716    -3.629955     1.886202      59.58
 O       4.764277    -4.734390     2.639569     233.68
 C       3.507623    -5.549747     2.360273     110.84
 H       2.672985    -4.882646     2.356607      29.73
 H       3.438165    -6.182912     3.378154      24.41
 H       3.507270    -6.185009     1.603808      29.18
 C       5.406525    -2.524086     2.627049       3.02
 O       5.546640    -2.575288     3.986029     158.41
 H       5.571345    -3.509754     4.320790      20.42
 C       5.796161    -1.253303     2.114507      41.03
 H       6.250229    -0.651286     3.056913      18.08
 C       5.152485    -2.067460    -0.064980      19.84
 C       4.859125    -1.695182    -1.587786     109.00
 H       5.363010    -2.345524    -2.319285      25.02
 O       5.545328    -0.484586    -1.934458     214.36
 H       5.078736     0.306140    -1.462732      26.73
 C       3.365482    -1.396578    -2.008201      85.69
 H       2.866575    -2.204522    -1.489273      26.28
 C       2.865820    -1.475401    -3.470359      89.34
 O       3.189110    -2.896837    -3.896610     254.26
 H       3.962949    -3.011385    -4.540647      27.52
 H       3.427288    -0.699515    -4.220568      24.05
 H       1.768933    -1.441321    -3.744727      25.39
 C      -0.436316    -0.578443     0.195112      37.21
 H      -1.048496    -1.344637     0.570321      20.72
 C       0.293362     1.765764     0.255317      61.66
 H       0.254403     2.780674     0.558305      21.19
 C       1.410351     1.455294    -0.478325      25.60
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 O       2.286624     2.407960    -0.850929     212.16
 C       2.079794     3.735302    -0.795028      99.79
 H       2.928110     4.485602    -1.280720      23.37
 H       1.129961     4.076842    -1.430148      23.67
 H       2.161852     4.153978     0.478546      21.47
 C       1.687486     0.119179    -0.824812      18.62
 O       2.938406     0.032675    -1.510528     147.05
 C       0.724046    -0.858548    -0.616231      67.42
 H       0.872398    -1.930067    -0.865956      23.52
 C      -0.858711     0.760055     0.474030      31.20
 C      -2.139416     1.048184     1.208452      81.61
 H      -2.748404     0.175570     1.665088      22.37
 O      -1.932629     2.016182     2.203202     263.40
 H      -1.793389     1.328975     2.955945      24.62
 C      -3.139584     1.708549     0.139965      83.82
 H      -2.745760     2.650860    -0.397538      23.88
 O      -3.532447     0.679294    -0.860979     270.30
 H      -3.066159     0.929018    -1.672542      27.47
 C      -4.492287     2.009646     0.788136      88.86
 O      -5.495062     2.740631    -0.136748     211.68
 H      -4.855657     3.465749    -0.554759      30.32
 H      -4.470235     2.526346     1.694228      27.78
 H      -4.988135     0.957395     1.046712      25.99
55
name = lig-etoh-Waterframe_832
 C       5.696802    -1.102900     0.782515      34.58
 H       6.182203    -0.315399     0.341179      21.04
 C       4.765495    -3.373637     0.538352      59.52
 H       4.585966    -4.243466    -0.089408      24.26
 C       4.921724    -3.579849     1.890806      -8.17
 O       4.776902    -4.782519     2.646281     321.69
 C       3.497739    -5.576544     2.389577     111.49
 H       2.577749    -4.971140     2.224277      26.96
 H       3.375517    -6.263536     3.096080      29.12
 H       3.847407    -6.242635     1.481986      28.81
 C       5.427239    -2.481334     2.644536       3.91
 O       5.515931    -2.607158     3.937187     227.82
 H       5.231398    -3.485341     4.373364      14.90
 C       5.859367    -1.314706     2.140611      66.93
 H       6.197191    -0.322789     2.740863      20.82
 C       5.131635    -2.126107     0.012787      26.70
 C       4.851591    -1.639934    -1.628446      98.69
 H       5.260572    -2.386087    -2.219314      26.56
 O       5.562936    -0.503255    -2.000979     197.77
 H       5.166639     0.216528    -1.389480      23.98
 C       3.315814    -1.409265    -2.038461      54.38
 H       2.748676    -2.081518    -1.371412      24.30
 C       2.871194    -1.591270    -3.580925     112.36
 O       3.127774    -2.896920    -3.968124     272.07
 H       4.053083    -2.841076    -4.430150      25.88
 H       3.465595    -0.835565    -4.101070      25.72
 H       1.839626    -1.478442    -3.365351      27.04
 C      -0.556384    -0.495739     0.090748      51.12
 H      -1.191502    -1.364391     0.344002      23.12
 C       0.159483     1.777478     0.196397      62.79
 H      -0.035834     2.938762     0.480673      19.27
 C       1.380701     1.521440    -0.553761      18.60
 O       2.391983     2.388264    -0.812808     196.96
 C       2.066696     3.795273    -0.808865      96.55
 H       2.963585     3.962589    -1.569700      20.97
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 H       1.170360     3.980776    -1.252663      28.02
 H       1.907508     4.337310     0.363165      22.54
 C       1.738969     0.168245    -0.832318      14.50
 O       2.918642     0.117707    -1.504431     114.96
 C       0.826694    -0.896421    -0.480638      60.52
 H       0.956272    -2.007107    -0.802283      20.94
 C      -0.764944     0.810506     0.478863      35.82
 C      -2.155689     1.121898     1.116942      77.57
 H      -2.478931     0.035814     1.398716      22.75
 O      -1.922917     1.952076     2.216672     275.70
 H      -1.382438     1.588269     3.024148      26.86
 C      -3.191787     1.684430     0.111348      90.46
 H      -2.866647     2.731459    -0.268717      23.80
 O      -3.470353     0.693378    -0.833271     274.42
 H      -3.166085     0.936188    -1.721128      26.66
 C      -4.530494     2.067321     0.731509      74.99
 O      -5.436412     2.741059    -0.174402     227.85
 H      -5.082106     3.729483    -0.338488      27.59
 H      -4.265776     2.710589     1.859036      23.01
 H      -4.843196     0.919793     0.971216      25.07
55
name = lig-etoh-Waterframe_833
 C       5.657759    -1.095639     0.788995      44.17
 H       5.983162    -0.213252     0.366932      23.13
 C       4.689715    -3.415861     0.481870      49.89
 H       4.398215    -4.308909     0.062118      23.41
 C       4.892662    -3.531568     1.917055      -7.91
 O       4.722586    -4.818574     2.638626     253.39
 C       3.572382    -5.619952     2.377901     106.55
 H       2.666349    -4.947996     2.121430      26.06
 H       3.382901    -6.228568     3.152522      28.15
 H       3.737232    -6.161520     1.203331      26.41
 C       5.416220    -2.515649     2.707786      -6.37
 O       5.500233    -2.624804     4.049140     186.57
 H       5.033568    -3.463941     4.415376      18.34
 C       5.929934    -1.271419     2.116067      45.63
 H       6.322721    -0.414523     2.776172      19.63
 C       5.062235    -2.110079    -0.103818      11.17
 C       4.809634    -1.669442    -1.619762      90.64
 H       4.967593    -2.605432    -2.139398      25.04
 O       5.612695    -0.465426    -2.037046     164.90
 H       5.417758     0.370094    -1.509622      24.89
 C       3.291717    -1.385874    -1.976469      80.62
 H       2.518551    -1.962778    -1.442046      23.72
 C       2.885255    -1.601274    -3.514900     109.23
 O       3.133012    -2.950873    -4.060122     279.45
 H       4.103813    -2.919178    -4.428696      25.92
 H       3.189112    -0.944908    -4.228606      27.13
 H       1.844824    -1.291249    -3.674710      26.88
 C      -0.467725    -0.514225    -0.049966      42.58
 H      -1.397775    -1.205122     0.027438      21.49
 C       0.113130     1.884629     0.078081      60.65
 H      -0.415579     2.934429     0.466637      18.71
 C       1.268873     1.509213    -0.507044      12.42
 O       2.479684     2.392931    -0.770708     144.52
 C       2.071595     3.869217    -0.871991     122.07
 H       2.818809     4.521442    -1.382515      25.94
 H       1.177227     3.892837    -1.263452      29.78
 H       2.198610     4.361669     0.016472      27.56
 C       1.703047     0.166155    -0.838162       1.79
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 O       2.951050     0.049968    -1.555638     132.39
 C       0.805393    -0.841827    -0.342719      64.66
 H       1.095448    -1.933541    -0.588705      21.37
 C      -0.754097     0.808019     0.445449      29.07
 C      -2.093866     1.120529     1.008269      80.98
 H      -2.549131     0.156432     1.325123      23.23
 O      -1.947920     1.961355     2.294224     217.87
 H      -1.191191     1.374168     2.738104      25.02
 C      -3.218838     1.759996     0.110656      84.03
 H      -2.642501     2.497411    -0.454977      24.49
 O      -3.402074     0.671159    -0.870030     252.03
 H      -3.376118     0.939353    -1.797815      26.74
 C      -4.562796     2.069371     0.734421      99.79
 O      -5.358726     2.758620    -0.180250     263.80
 H      -5.295025     3.756266     0.051592      27.18
 H      -4.401774     2.900995     1.747670      22.56
 H      -5.364437     1.402767     1.083949      24.51
55
name = lig-etoh-Waterframe_834
 C       5.612811    -1.129075     0.671267      42.51
 H       5.752803    -0.166030     0.322362      23.51
 C       4.663539    -3.378063     0.477828      58.96
 H       4.173522    -4.049663    -0.169096      23.58
 C       4.854246    -3.567749     1.891037      -7.54
 O       4.695271    -4.777236     2.615570     273.25
 C       3.603325    -5.623255     2.262171     113.66
 H       2.678157    -4.975992     2.334431      28.35
 H       3.477570    -6.327983     3.215785      25.13
 H       3.662572    -6.472699     1.447792      26.59
 C       5.438389    -2.484310     2.779545     -18.72
 O       5.482162    -2.605964     4.193491      84.45
 H       5.320723    -3.606339     4.517482      15.35
 C       5.923470    -1.318088     2.149903      55.37
 H       6.459681    -0.707677     2.782524      23.01
 C       4.991774    -2.069372    -0.168238      28.36
 C       4.717564    -1.679707    -1.565903      80.04
 H       5.164485    -2.378364    -2.422072      23.89
 O       5.665936    -0.499954    -2.063633     115.71
 H       5.314816     0.241338    -1.494209      28.26
 C       3.249192    -1.339278    -1.935754     101.37
 H       2.784446    -2.217756    -1.400808      25.09
 C       2.881512    -1.535903    -3.468121      88.15
 O       3.189720    -2.998518    -4.087244     222.06
 H       4.008120    -2.994414    -4.713356      25.63
 H       3.518179    -0.877639    -4.078522      25.16
 H       1.783391    -1.652101    -3.658056      25.31
 C      -0.464178    -0.469319    -0.054946      52.06
 H      -1.223961    -1.372592    -0.112303      21.68
 C       0.016108     1.939994     0.023558      42.72
 H      -0.002258     3.107093     0.239932      19.49
 C       1.405585     1.563348    -0.519684      -5.63
 O       2.438898     2.460654    -0.739133     174.29
 C       2.134798     3.911547    -0.912035     111.34
 H       2.670785     4.486581    -1.586114      26.67
 H       1.067224     3.967566    -1.402195      25.61
 H       2.112561     4.220604     0.047655      27.37
 C       1.660192     0.187501    -0.815747      15.34
 O       2.929037    -0.068267    -1.582310     183.05
 C       0.881359    -0.832003    -0.358571      58.53
 H       1.053544    -1.932658    -0.307545      21.06
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 C      -0.796151     0.813100     0.289574      31.81
 C      -2.115736     1.118208     1.029611      85.62
 H      -2.604227     0.254595     1.360233      24.29
 O      -1.963551     1.940871     2.304964     226.99
 H      -1.402675     1.267485     2.935692      23.60
 C      -3.149202     1.745526     0.072670      64.78
 H      -2.989387     2.723901    -0.418086      24.59
 O      -3.362675     0.623766    -0.931982     241.48
 H      -3.521136     1.101360    -1.740925      26.76
 C      -4.597771     2.138018     0.826089      99.92
 O      -5.326880     2.842011    -0.219897     253.69
 H      -5.311685     3.851858    -0.013639      27.63
 H      -4.330413     2.744671     1.621318      27.74
 H      -4.977798     1.241068     1.260569      28.54
55
name = lig-etoh-Waterframe_835
 C       5.604277    -1.159144     0.705155      61.03
 H       6.022482    -0.239846     0.276949      22.50
 C       4.636705    -3.276784     0.489455      66.04
 H       4.111217    -4.050569    -0.154890      22.66
 C       4.862405    -3.547466     1.875056     -32.29
 O       4.697489    -4.722260     2.552484     279.57
 C       3.565424    -5.667538     2.237085     108.18
 H       2.572879    -5.226348     2.041640      28.80
 H       3.626807    -6.409080     3.261683      24.31
 H       3.872989    -6.128191     1.403548      31.14
 C       5.430957    -2.528468     2.823105     -12.68
 O       5.465883    -2.575485     4.253293     105.67
 H       5.751553    -3.476763     4.687662      11.70
 C       5.855928    -1.410777     2.088653      64.20
 H       6.428981    -0.701196     2.508892      25.69
 C       4.948970    -2.068806    -0.083125      29.82
 C       4.729263    -1.618520    -1.654513      89.51
 H       5.046484    -2.631813    -2.315908      22.85
 O       5.650290    -0.577323    -2.034026     182.01
 H       5.410518     0.287159    -1.600253      26.24
 C       3.233219    -1.467138    -1.952844      83.71
 H       2.671282    -2.172469    -1.293137      22.73
 C       2.928221    -1.594767    -3.486672      91.37
 O       3.263212    -2.995156    -4.040681     263.89
 H       4.012261    -2.773826    -4.670422      25.06
 H       3.535055    -0.647497    -3.875189      23.71
 H       1.785135    -1.352933    -3.471467      24.84
 C      -0.441066    -0.481337    -0.013076      35.69
 H      -1.122151    -1.335586     0.343501      20.26
 C       0.158075     1.908347    -0.083538      69.15
 H      -0.145753     2.894618     0.263436      22.03
 C       1.421303     1.636547    -0.519161      26.95
 O       2.401272     2.552945    -0.756057     218.90
 C       2.137289     3.914012    -0.935133      89.44
 H       3.009001     4.054582    -1.569757      22.56
 H       0.942571     4.082602    -1.458408      22.72
 H       2.030624     4.516310     0.180970      23.03
 C       1.775438     0.232269    -0.829235       9.55
 O       2.833690    -0.096320    -1.533457     163.38
 C       0.863055    -0.845032    -0.416628      41.90
 H       1.264323    -1.836368    -0.436169      19.83
 C      -0.902664     0.930252     0.163257      36.43
 C      -2.181705     1.134456     1.086419      85.75
 H      -2.477483     0.127941     1.300845      24.81
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 O      -1.957200     1.886883     2.262100     269.30
 H      -1.917234     1.360931     3.156901      24.96
 C      -3.188104     1.706486     0.071347      75.03
 H      -2.872972     2.682121    -0.378469      24.00
 O      -3.341008     0.641575    -0.962787     239.27
 H      -3.539344     0.993385    -1.823448      26.41
 C      -4.499414     2.185392     0.859548      95.50
 O      -5.327644     2.916453    -0.219452     255.67
 H      -4.997139     3.891053    -0.193213      28.70
 H      -4.279963     2.776561     1.612319      28.21
 H      -4.921830     1.196043     1.055265      27.36
55
name = lig-etoh-Waterframe_836
 C       5.640850    -1.155292     0.780458      55.32
 H       6.333132    -0.355052     0.341253      22.12
 C       4.561247    -3.253432     0.541191      50.32
 H       4.180604    -4.246211     0.028421      22.30
 C       4.884379    -3.473868     1.929237      10.12
 O       4.654105    -4.728863     2.502367     246.36
 C       3.596657    -5.693607     2.195896     115.82
 H       2.641095    -5.291065     1.996156      27.82
 H       3.480074    -6.511686     3.083469      24.30
 H       3.952200    -6.135526     1.311428      27.18
 C       5.396552    -2.602199     2.803417      19.47
 O       5.472888    -2.529612     4.225573     177.45
 H       5.629030    -3.473480     4.623312      17.66
 C       5.829754    -1.432972     2.085271      68.21
 H       6.333231    -0.571791     2.596274      20.74
 C       4.922626    -2.005509    -0.099491      22.82
 C       4.770298    -1.676822    -1.630347     106.49
 H       5.055278    -2.618738    -2.143828      21.89
 O       5.608324    -0.643495    -2.019421     221.59
 H       5.369366     0.216929    -1.602106      24.87
 C       3.241181    -1.577632    -1.968047      77.65
 H       2.615504    -2.317972    -1.444277      21.37
 C       2.951244    -1.657665    -3.441626     106.24
 O       3.326418    -2.898017    -3.954936     290.53
 H       4.174865    -2.912751    -4.481919      26.82
 H       3.486268    -0.896962    -4.195670      22.15
 H       1.929791    -1.368209    -3.809387      24.35
 C      -0.439742    -0.443061     0.082204      27.60
 H      -0.987629    -1.096179     0.664649      17.54
 C       0.130455     1.887857    -0.114869      63.74
 H      -0.052274     2.814479     0.188364      22.79
 C       1.458555     1.570455    -0.565641      17.69
 O       2.400141     2.584144    -0.767326     222.99
 C       2.116167     3.955572    -0.945333     105.83
 H       3.065528     4.447910    -1.473502      23.22
 H       1.253244     4.195565    -1.829765      23.08
 H       2.352720     4.788594    -0.031712      21.37
 C       1.738516     0.225975    -0.776531      30.03
 O       2.857224    -0.089595    -1.541316     150.71
 C       0.820339    -0.740256    -0.485705      60.26
 H       1.081400    -1.743247    -0.600955      21.58
 C      -0.859544     0.910893     0.108551      45.54
 C      -2.164295     1.093227     1.030836      66.43
 H      -2.459779     0.020378     1.318063      22.71
 O      -1.974009     1.876581     2.229583     244.09
 H      -2.092544     1.124874     2.914191      24.49
 C      -3.246913     1.722057     0.087318      97.05
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 H      -2.540052     2.383259    -0.371171      23.55
 O      -3.354366     0.691547    -0.937822     266.17
 H      -3.388431     1.024665    -1.824727      27.22
 C      -4.429028     2.182475     0.723528     104.26
 O      -5.299226     2.992101    -0.149226     272.03
 H      -4.765036     3.799378    -0.274617      30.75
 H      -4.235357     2.850187     1.766956      23.90
 H      -5.320514     1.561627     1.053311      24.23
55
name = lig-etoh-Waterframe_837
 C       5.693653    -1.145371     0.735454      39.81
 H       6.186826    -0.153932     0.355728      22.89
 C       4.514938    -3.216947     0.605856      60.22
 H       4.136738    -4.087264    -0.073098      23.76
 C       4.791927    -3.544659     1.924242      23.94
 O       4.613740    -4.791325     2.520612     254.92
 C       3.641821    -5.700302     2.086916     127.97
 H       2.725022    -5.160392     2.057682      28.27
 H       3.557917    -6.328448     2.906620      26.86
 H       3.818778    -6.569112     1.201522      25.68
 C       5.414153    -2.489627     2.813384      15.80
 O       5.491587    -2.530835     4.150216     109.75
 H       5.213845    -3.418051     4.508847      18.69
 C       5.852555    -1.385104     2.219662      48.63
 H       6.312285    -0.651013     3.086460      19.38
 C       4.919315    -2.007194    -0.067466      44.77
 C       4.754191    -1.843208    -1.513964     111.90
 H       5.227085    -2.510184    -2.050947      28.58
 O       5.577697    -0.667268    -2.036396     158.53
 H       5.171931     0.047245    -1.525704      28.72
 C       3.249039    -1.533333    -1.958236      86.76
 H       2.764732    -2.372641    -1.506630      25.51
 C       2.968427    -1.604890    -3.501723     108.15
 O       3.379609    -2.917895    -3.872042     269.11
 H       4.210364    -2.754421    -4.436320      26.52
 H       3.683024    -0.864011    -3.871580      24.50
 H       1.911259    -1.684426    -3.608210      26.09
 C      -0.421315    -0.418118     0.172888      14.75
 H      -0.928102    -1.184478     0.576700      18.58
 C       0.078388     1.917313    -0.134846      62.26
 H      -0.001430     2.927055     0.023243      19.70
 C       1.420254     1.592782    -0.591505       9.42
 O       2.432099     2.559711    -0.774333     205.96
 C       2.176733     4.091090    -1.021426      83.12
 H       3.084943     4.475490    -1.623640      21.44
 H       1.316485     4.177394    -1.568134      27.11
 H       1.672790     4.209325    -0.002945      21.65
 C       1.742496     0.195810    -0.822205      20.58
 O       2.951070    -0.128018    -1.574565     175.73
 C       0.714262    -0.725230    -0.498426      54.01
 H       0.827188    -1.745433    -0.708612      22.03
 C      -0.816092     0.860311     0.212350      52.06
 C      -2.108758     1.046162     0.913128      78.63
 H      -2.559873     0.036936     1.288452      20.67
 O      -2.004805     1.852911     2.194769     203.97
 H      -1.702367     1.242758     2.986756      23.92
 C      -3.134107     1.679725     0.046637      82.28
 H      -2.830658     2.770507    -0.327366      21.78
 O      -3.415360     0.714692    -0.924699     289.09
 H      -3.243674     1.138664    -1.747135      26.81
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 C      -4.551217     2.241828     0.658215      82.58
 O      -5.252505     3.110882    -0.103768     313.24
 H      -4.885447     3.981504    -0.227227      31.02
 H      -3.881854     2.830430     1.652527      22.26
 H      -5.039986     1.246772     1.132667      25.59
55
name = lig-etoh-Waterframe_838
 C       5.750321    -1.098289     0.816264      49.16
 H       5.870985    -0.117795     0.260390      18.18
 C       4.471352    -3.224379     0.625154      57.35
 H       3.973771    -3.868818    -0.101606      21.19
 C       4.730611    -3.557565     1.960655      20.48
 O       4.638167    -4.838062     2.551616     257.59
 C       3.600319    -5.755804     2.030891     111.62
 H       2.641365    -5.227020     1.738654      26.16
 H       3.471518    -6.354020     2.809823      26.61
 H       4.038958    -6.230820     0.912164      25.34
 C       5.351613    -2.492942     2.750486       3.34
 O       5.502197    -2.579774     4.136167     130.75
 H       5.078693    -3.412854     4.449466      23.61
 C       5.890460    -1.238777     2.200980      57.23
 H       6.430989    -0.440725     2.946558      23.66
 C       4.981831    -2.034717     0.101455      43.23
 C       4.753255    -1.884291    -1.507227      96.87
 H       5.083881    -2.849873    -1.999810      25.63
 O       5.517477    -0.700350    -2.015982     191.12
 H       5.237480     0.134147    -1.628810      29.59
 C       3.276657    -1.500052    -1.933902      93.11
 H       2.512733    -2.040126    -1.391449      22.35
 C       3.011642    -1.548650    -3.449701      96.82
 O       3.443011    -3.000213    -3.838655     260.23
 H       4.120367    -2.877495    -4.625712      25.54
 H       3.352582    -0.701454    -3.961259      26.30
 H       1.947050    -1.285590    -3.583969      26.20
 C      -0.408862    -0.494032     0.245962      26.47
 H      -1.131275    -1.303104     0.382715      15.42
 C       0.106382     1.949046    -0.163335      47.48
 H      -0.418364     2.993321    -0.093078      16.64
 C       1.373983     1.640397    -0.622826      15.16
 O       2.465064     2.537333    -0.822515     187.98
 C       2.124697     4.060791    -1.040760     108.27
 H       3.113013     4.531683    -1.109277      23.08
 H       1.423978     4.109481    -1.749746      27.34
 H       1.885322     4.563926    -0.103770      25.33
 C       1.760067     0.179186    -0.941331       5.38
 O       2.993823    -0.167709    -1.550679     203.59
 C       0.758313    -0.816966    -0.552715      52.72
 H       0.874803    -1.861522    -0.833119      18.33
 C      -0.776667     0.922907     0.392886      56.36
 C      -2.123743     1.070421     0.954919      73.33
 H      -2.507909     0.010442     1.010567      21.09
 O      -2.023040     1.822620     2.165248     247.77
 H      -1.265706     1.434511     2.702920      24.91
 C      -3.141678     1.762435    -0.006811      70.13
 H      -2.751825     2.724276    -0.592750      19.95
 O      -3.482890     0.722279    -0.989331     293.13
 H      -3.263086     0.904652    -1.893821      26.31
 C      -4.446640     2.234611     0.747733      91.92
 O      -5.280437     3.225222    -0.117861     268.69
 H      -4.918687     4.084013     0.070973      29.03
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 H      -4.383003     2.842611     1.708368      23.94
 H      -5.207766     1.348483     0.856499      26.11
55
name = lig-etoh-Waterframe_839
 C       5.727192    -1.016918     0.862719      54.48
 H       6.098278    -0.113810     0.363313      22.19
 C       4.441670    -3.253602     0.635682      65.50
 H       3.855823    -3.883534     0.069739      24.06
 C       4.729523    -3.520899     2.020460       5.43
 O       4.639304    -4.850549     2.580221     346.63
 C       3.583333    -5.763163     1.953803     133.77
 H       2.601278    -5.248348     1.617092      24.24
 H       3.289765    -6.715272     2.530467      24.14
 H       4.199307    -6.158448     1.116256      29.31
 C       5.326583    -2.468551     2.732853      25.41
 O       5.498781    -2.642849     4.124647     197.91
 H       5.335504    -3.573256     4.424134      24.17
 C       5.878108    -1.207515     2.192113      63.83
 H       6.411448    -0.374974     2.712425      17.25
 C       5.028002    -2.052816     0.133437      23.48
 C       4.740236    -1.781364    -1.434239      99.84
 H       4.956708    -2.855551    -2.015899      20.83
 O       5.496009    -0.777964    -2.001036     232.91
 H       5.143044     0.031184    -1.621152      26.56
 C       3.282318    -1.516484    -1.876143      84.62
 H       2.549295    -2.242060    -1.428716      18.82
 C       3.047823    -1.563283    -3.382102      98.20
 O       3.434520    -3.004425    -3.838763     246.70
 H       4.148081    -2.942927    -4.575437      26.77
 H       3.669405    -1.006129    -4.088293      21.81
 H       1.944347    -1.512453    -3.640218      22.71
 C      -0.341768    -0.484658     0.215842      42.01
 H      -1.235999    -1.232972     0.407947      13.79
 C       0.061400     1.923851    -0.117034      85.70
 H      -0.331376     3.115844    -0.250743      17.31
 C       1.443483     1.584072    -0.706319       4.72
 O       2.435580     2.564687    -0.885663     221.70
 C       2.100279     3.948822    -0.978646     124.67
 H       3.078956     4.360913    -1.181090      24.62
 H       1.747087     4.145133    -2.066055      24.23
 H       1.713204     4.545948    -0.229111      27.37
 C       1.680147     0.182061    -1.000127      12.50
 O       2.997518    -0.094313    -1.483616     199.06
 C       0.844671    -0.859018    -0.589136      63.11
 H       0.963674    -1.933550    -0.883112      16.10
 C      -0.637639     0.855976     0.466265      31.67
 C      -2.180585     1.135405     0.976511      60.81
 H      -2.626258     0.193050     1.192031      20.40
 O      -2.043945     1.823591     2.186782     258.93
 H      -1.183430     1.465489     2.520375      21.13
 C      -3.193436     1.856387    -0.075572      77.36
 H      -2.556956     2.505482    -0.619460      21.98
 O      -3.563608     0.727661    -1.047906     286.72
 H      -3.307170     0.976575    -1.937006      25.57
 C      -4.426109     2.295528     0.773483     104.30
 O      -5.298765     3.252838    -0.096111     317.73
 H      -4.939871     4.202271    -0.068734      27.07
 H      -4.338568     2.469757     1.712277      29.46
 H      -5.095721     1.457276     0.752771      27.66
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name = lig-etoh-Waterframe_840
 C       5.642463    -1.006975     0.796864      54.96
 H       6.208371    -0.234192     0.430309      23.96
 C       4.477174    -3.224200     0.691683      63.28
 H       3.966706    -3.916909     0.120318      25.13
 C       4.735843    -3.516799     2.002888       2.50
 O       4.572693    -4.834566     2.620712     231.58
 C       3.650285    -5.747542     1.849464     110.16
 H       2.727624    -5.113322     1.646003      25.39
 H       3.402946    -6.665339     2.701668      23.39
 H       4.000347    -6.159851     1.045389      29.90
 C       5.371082    -2.432218     2.848120      12.89
 O       5.505070    -2.704482     4.125737      98.09
 H       5.737402    -3.634844     4.269212      16.19
 C       5.822284    -1.266065     2.259187      52.99
 H       6.254516    -0.690044     2.964332      21.04
 C       4.999652    -2.023026     0.033813      37.13
 C       4.679268    -1.764838    -1.328890     114.29
 H       5.126178    -2.673670    -1.988346      22.73
 O       5.537392    -0.792328    -1.990983     181.53
 H       5.242732     0.070186    -1.697295      28.42
 C       3.271610    -1.498342    -1.798268      79.69
 H       2.783176    -2.407251    -1.336525      21.96
 C       3.114863    -1.695445    -3.394350      99.04
 O       3.367626    -2.990282    -3.836029     283.11
 H       4.187859    -2.867096    -4.377086      26.25
 H       3.929753    -0.923443    -3.728063      22.27
 H       1.993623    -1.490925    -3.611901      24.55
 C      -0.231145    -0.495856     0.111721      53.13
 H      -0.911610    -1.362831     0.590283      20.45
 C       0.193715     1.835024    -0.114454      88.07
 H      -0.161555     2.998327    -0.019772      18.44
 C       1.349280     1.548077    -0.728109      26.40
 O       2.372655     2.514669    -0.934646     226.32
 C       2.156397     3.892358    -0.994969     100.15
 H       3.150906     4.348753    -1.044256      23.21
 H       1.280235     4.092969    -2.051180      21.18
 H       1.326217     4.025569    -0.239570      21.97
 C       1.693588     0.215361    -1.017439      24.17
 O       2.965045    -0.031632    -1.420461     156.88
 C       0.810800    -0.839964    -0.559696      65.94
 H       1.045459    -1.910395    -0.837229      19.00
 C      -0.669649     0.826308     0.443619      72.18
 C      -2.171601     1.134908     0.917855      75.97
 H      -2.696499     0.262992     1.219291      22.43
 O      -2.060899     1.895028     2.254611     235.15
 H      -1.381101     1.451837     2.842609      23.85
 C      -3.172440     1.835144    -0.100267      81.49
 H      -2.805643     2.687930    -0.579451      24.69
 O      -3.640693     0.779147    -1.062200     280.05
 H      -3.427729     1.151459    -1.917285      26.36
 C      -4.487149     2.369450     0.634128     101.73
 O      -5.300255     3.241579    -0.005903     325.90
 H      -4.875980     4.102737    -0.362642      28.83
 H      -4.005929     2.582459     1.751040      24.11
 H      -4.923454     1.457103     0.708363      29.34
55
name = lig-etoh-Waterframe_841
 C       5.586722    -1.066138     0.867170      58.58
 H       5.889713    -0.218709     0.343599      24.46
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 C       4.532172    -3.174831     0.682333      60.29
 H       4.190434    -3.964921     0.002037      23.66
 C       4.793223    -3.507178     2.043217      27.58
 O       4.498088    -4.767800     2.605431     317.75
 C       3.718484    -5.683182     1.830318     120.68
 H       2.740306    -5.252959     1.614796      25.91
 H       3.471079    -6.490597     2.731146      24.25
 H       4.090425    -6.107679     0.875113      27.77
 C       5.356647    -2.547959     2.840906       8.68
 O       5.553204    -2.763306     4.230235      56.49
 H       5.779565    -3.692261     4.428480      16.17
 C       5.750855    -1.309124     2.262051      71.20
 H       6.224031    -0.682267     2.925006      26.95
 C       4.933318    -1.967394     0.092502      48.67
 C       4.706570    -1.780327    -1.422731      98.47
 H       4.810790    -2.766857    -1.787790      24.91
 O       5.603443    -0.736541    -1.969314     149.16
 H       5.470310     0.163991    -1.716811      28.49
 C       3.256708    -1.507887    -1.748099      92.89
 H       2.496763    -1.955021    -1.100128      19.89
 C       3.145033    -1.698565    -3.290238     107.69
 O       3.320390    -3.012698    -3.865244     276.03
 H       4.112188    -3.138224    -4.425043      27.22
 H       3.786164    -0.855678    -3.811835      24.35
 H       2.269462    -1.186448    -3.682704      26.63
 C      -0.353518    -0.507480     0.163436      54.02
 H      -0.696341    -1.499058     0.590557      19.18
 C       0.169664     1.786226    -0.022578      60.54
 H       0.013147     2.800218     0.294004      23.05
 C       1.345632     1.540735    -0.772983      32.79
 O       2.360426     2.374951    -1.007492     193.33
 C       2.065365     3.833518    -1.034398     105.51
 H       2.826605     4.562162    -0.796951      24.19
 H       1.437730     4.213706    -1.999346      23.70
 H       1.595217     4.161275     0.103926      21.71
 C       1.705493     0.191316    -0.984080      27.42
 O       2.968842    -0.070523    -1.414222     168.68
 C       0.910596    -0.799838    -0.634797      63.38
 H       1.086274    -1.913374    -0.655442      20.17
 C      -0.767562     0.824484     0.321628      51.91
 C      -2.095039     1.129294     0.929435      70.07
 H      -2.537209     0.076680     1.026605      22.99
 O      -2.072402     1.983762     2.280759     201.88
 H      -1.889760     1.281364     2.950366      25.65
 C      -3.173983     1.823031    -0.118478      86.77
 H      -2.773433     2.723729    -0.695365      22.14
 O      -3.687650     0.871961    -1.053783     268.09
 H      -3.528548     0.987312    -2.007945      26.69
 C      -4.412790     2.298773     0.593102      82.15
 O      -5.365433     3.267347     0.016727     230.99
 H      -4.752359     4.091590    -0.159013      29.00
 H      -4.134438     3.223706     1.538462      19.85
 H      -5.147378     1.502969     0.971559      25.27
55
name = lig-etoh-Waterframe_842
 C       5.550069    -1.042952     0.984774      57.78
 H       5.706266     0.002246     0.683863      23.77
 C       4.583014    -3.211766     0.655150      67.99
 H       4.255972    -4.056176    -0.055628      23.07
 C       4.800299    -3.542078     1.994219      32.31
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 O       4.458737    -4.683968     2.578943     213.81
 C       3.700907    -5.637150     1.858371     132.56
 H       2.768827    -5.334352     1.470783      26.94
 H       3.590493    -6.570091     2.321278      27.63
 H       4.571472    -6.029128     1.004466      26.42
 C       5.387866    -2.623097     2.916477       8.69
 O       5.617564    -2.796048     4.313787     132.34
 H       5.500986    -3.738266     4.640404      21.82
 C       5.715047    -1.359410     2.296877      61.41
 H       6.251958    -0.467680     2.771468      26.11
 C       4.854084    -1.965162     0.136412      36.22
 C       4.760262    -1.761844    -1.437143      86.91
 H       5.049177    -2.575804    -1.992439      26.71
 O       5.664999    -0.719515    -1.966937     161.68
 H       5.317966     0.004709    -1.467946      30.78
 C       3.257403    -1.464227    -1.744090      99.11
 H       2.672102    -2.246307    -1.172893      24.68
 C       3.117681    -1.562179    -3.254170      97.21
 O       3.261502    -3.061431    -3.892163     191.78
 H       4.036167    -2.866803    -4.506353      25.01
 H       4.069548    -1.262330    -3.656697      25.48
 H       2.115335    -1.399203    -3.544009      27.00
 C      -0.387892    -0.574010     0.129601      41.41
 H      -1.095256    -1.245754     0.553399      20.59
 C       0.139661     1.839895     0.033533      56.93
 H      -0.026369     2.704796     0.430622      23.45
 C       1.322100     1.485739    -0.748795       8.11
 O       2.404375     2.370452    -1.109707     169.90
 C       1.974391     3.793341    -0.969830     109.72
 H       3.033115     4.155680    -1.204397      23.37
 H       1.395051     3.990832    -1.715193      29.11
 H       1.340892     4.089229     0.004640      24.20
 C       1.750040     0.161041    -0.979098      14.04
 O       3.041513    -0.119273    -1.473428     195.63
 C       0.759747    -0.826206    -0.548669      60.62
 H       1.118731    -1.881811    -0.590244      23.31
 C      -0.840266     0.771363     0.236736      30.82
 C      -2.107092     1.162017     0.970133      73.05
 H      -2.584301     0.142176     1.356815      21.65
 O      -2.074045     1.993239     2.224881     226.72
 H      -2.253035     1.361657     2.926023      26.64
 C      -3.188790     1.840444    -0.138886      74.66
 H      -2.433182     2.601631    -0.646745      22.01
 O      -3.735211     0.906492    -1.059399     280.07
 H      -3.263929     1.018072    -1.938972      26.64
 C      -4.383147     2.359874     0.707187      75.01
 O      -5.424022     3.284804    -0.055113     226.47
 H      -5.123723     4.300862     0.062569      28.15
 H      -3.769612     2.738216     1.662077      23.21
 H      -4.971232     1.455358     1.295223      26.14
55
name = lig-etoh-Waterframe_843
 C       5.422566    -1.011462     1.022014      54.03
 H       5.736374     0.068801     0.907104      22.69
 C       4.615477    -3.300331     0.608438      51.15
 H       4.156321    -4.111731    -0.095456      19.79
 C       4.818897    -3.512635     1.981732       9.75
 O       4.392122    -4.692515     2.635483     191.75
 C       3.742351    -5.676453     1.809415     127.21
 H       2.862434    -5.258136     1.331564      26.23
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 H       3.598372    -6.444160     2.421881      27.94
 H       4.413989    -5.893450     0.790313      26.50
 C       5.457618    -2.597252     3.001132       3.75
 O       5.663203    -2.804403     4.330459      66.46
 H       5.471199    -3.793568     4.545381      19.60
 C       5.754352    -1.408466     2.428338      40.10
 H       6.207011    -0.599816     3.255046      20.24
 C       4.894467    -1.935262     0.099447      36.94
 C       4.823993    -1.750187    -1.377340     103.61
 H       5.246947    -2.607533    -1.939897      25.86
 O       5.662459    -0.688823    -1.919466     163.23
 H       5.541911     0.162658    -1.495215      27.69
 C       3.367792    -1.530141    -1.818000      94.66
 H       2.840870    -2.363752    -1.348353      25.01
 C       3.084837    -1.575282    -3.310487      98.21
 O       3.200852    -3.047974    -3.889806     234.29
 H       3.979252    -2.955122    -4.565606      25.61
 H       3.796706    -0.864509    -3.740084      26.02
 H       2.123859    -1.090230    -3.625424      26.43
 C      -0.544088    -0.558249     0.078932      31.36
 H      -1.223854    -1.319448     0.289922      18.49
 C       0.132801     1.808341    -0.013406      68.20
 H      -0.106208     2.778381     0.311642      20.21
 C       1.363325     1.465524    -0.677381      11.97
 O       2.352252     2.395342    -1.154977     229.64
 C       1.962421     3.729994    -0.967814     114.07
 H       2.874027     4.424268    -1.277096      24.52
 H       1.128164     3.895933    -1.688931      26.07
 H       1.682198     3.928321     0.044578      28.76
 C       1.672140     0.084546    -0.933096      23.73
 O       3.036635    -0.111104    -1.489523     171.95
 C       0.749374    -0.927267    -0.480473      64.15
 H       0.913856    -2.002268    -0.577820      19.16
 C      -0.818795     0.812381     0.272564      55.45
 C      -2.236292     1.141159     0.990911      66.11
 H      -2.763471     0.232195     1.407520      22.78
 O      -2.042562     1.990368     2.127193     263.65
 H      -2.174088     1.515879     2.946340      28.18
 C      -3.198851     1.844484    -0.067298      82.18
 H      -2.714617     2.729909    -0.622742      22.49
 O      -3.755574     0.914765    -1.080699     271.69
 H      -3.170084     0.957131    -1.907562      25.08
 C      -4.358507     2.503920     0.818625      95.13
 O      -5.415708     3.247766    -0.072226     219.97
 H      -5.293572     4.262511     0.197254      28.78
 H      -4.027240     2.997946     1.551370      29.59
 H      -4.917203     1.494687     0.949107      26.91
55
name = lig-etoh-Waterframe_844
 C       5.341298    -1.011138     1.163784      64.70
 H       5.565842    -0.039101     0.565431      23.41
 C       4.671222    -3.266119     0.610854      50.63
 H       4.178129    -4.058135    -0.042368      18.29
 C       4.839393    -3.521128     2.069177       1.07
 O       4.344221    -4.719950     2.685792     207.53
 C       3.778898    -5.702865     1.716772     120.06
 H       2.744031    -5.283630     1.467855      24.30
 H       3.466663    -6.507153     2.433150      24.41
 H       4.388127    -6.111073     0.962845      28.15
 C       5.463818    -2.629495     2.947568      10.32
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 O       5.686686    -2.823735     4.326066     167.41
 H       5.837104    -3.849580     4.584731      19.97
 C       5.800888    -1.346105     2.478549      44.87
 H       6.230962    -0.627551     3.340281      19.44
 C       5.000564    -1.973984     0.156243      17.77
 C       4.896993    -1.696705    -1.373624      96.52
 H       5.227775    -2.801791    -1.675257      21.93
 O       5.676290    -0.628048    -1.870349     213.18
 H       5.570019     0.226793    -1.450919      27.19
 C       3.447233    -1.605408    -1.918510      71.46
 H       2.726782    -2.111624    -1.357250      22.04
 C       3.097592    -1.617602    -3.439073     104.79
 O       3.157132    -2.935205    -3.889838     273.76
 H       3.977066    -3.165058    -4.459773      26.96
 H       3.603970    -0.901603    -4.073248      25.14
 H       1.970208    -1.252042    -3.469517      24.08
 C      -0.646047    -0.523938    -0.002747      59.40
 H      -1.287874    -1.346805     0.105961      19.38
 C       0.148462     1.766487    -0.086592      54.72
 H      -0.102743     2.931649    -0.049927      15.96
 C       1.398677     1.430650    -0.614385      11.37
 O       2.272979     2.348237    -1.162173     208.34
 C       1.960179     3.742156    -0.993399     101.37
 H       2.614165     4.605674    -1.285676      24.73
 H       0.718291     4.093362    -1.417536      21.59
 H       2.012510     3.901617     0.007292      28.65
 C       1.629743    -0.000746    -0.859112       7.36
 O       2.928807    -0.139034    -1.449861     132.57
 C       0.755457    -1.007034    -0.450401      67.55
 H       0.868581    -2.027862    -0.664642      19.18
 C      -0.876056     0.808149     0.388069      25.00
 C      -2.309483     1.109928     0.932530      83.71
 H      -2.747100     0.172149     1.039912      22.69
 O      -2.002270     2.029238     2.055477     272.71
 H      -1.752433     1.472459     2.807570      26.31
 C      -3.240847     1.916272     0.016337      81.57
 H      -2.758486     2.680424    -0.541924      24.05
 O      -3.758321     0.933331    -1.040603     270.52
 H      -3.298965     1.040315    -1.960761      24.77
 C      -4.434432     2.569718     0.759270     117.69
 O      -5.356605     3.194404    -0.033052     269.66
 H      -5.215375     4.239704    -0.000007      27.93
 H      -4.306770     3.366320     1.579592      23.97
 H      -5.030315     1.852042     1.327760      27.92
55
name = lig-etoh-Waterframe_845
 C       5.363200    -0.987963     1.212487      63.16
 H       5.477049     0.136850     0.918969      23.54
 C       4.737400    -3.241002     0.757569      57.98
 H       4.417337    -3.957300     0.019536      23.63
 C       4.811607    -3.607533     2.082787      27.01
 O       4.332650    -4.752711     2.663517     313.86
 C       3.748474    -5.721261     1.748052     121.90
 H       2.821920    -5.340259     1.103995      24.36
 H       3.506517    -6.779093     2.332632      23.11
 H       4.464361    -6.018491     1.103152      29.00
 C       5.485637    -2.648122     2.939750      -0.29
 O       5.718541    -2.853174     4.294722     116.51
 H       5.769636    -3.888911     4.537772      16.80
 C       5.798543    -1.283001     2.465390      57.05
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 H       6.273942    -0.475557     3.004201      19.80
 C       5.068359    -1.998239     0.275490      35.24
 C       4.912562    -1.693434    -1.332447      86.16
 H       5.522355    -2.448787    -2.018243      20.24
 O       5.733564    -0.553660    -1.840198     200.28
 H       5.276057     0.093901    -1.320253      25.78
 C       3.429214    -1.524674    -1.946874      67.29
 H       2.895338    -2.431093    -1.550138      22.49
 C       3.073969    -1.574820    -3.500674     101.81
 O       3.149976    -2.917423    -3.944591     236.55
 H       4.075841    -2.921136    -4.391824      25.03
 H       3.728753    -1.014605    -4.205224      23.38
 H       1.977908    -1.545520    -3.404913      24.33
 C      -0.591105    -0.559685    -0.064763      43.86
 H      -1.485449    -1.185149     0.100642      18.60
 C       0.099596     1.738096    -0.094529      56.69
 H      -0.221053     2.947136    -0.208410      15.51
 C       1.331094     1.336045    -0.570328      11.78
 O       2.234246     2.310277    -1.198918     149.63
 C       1.917029     3.810427    -0.946126      87.19
 H       2.579286     4.002999    -1.736647      24.46
 H       0.658788     4.031382    -1.228205      20.79
 H       2.040559     4.043604     0.199265      25.07
 C       1.694241    -0.052146    -0.781061      10.16
 O       2.836883    -0.224980    -1.421612     178.56
 C       0.630015    -0.990791    -0.439789      54.31
 H       0.821193    -1.974321    -0.709859      19.79
 C      -0.916494     0.750304     0.361374      38.07
 C      -2.268507     1.156144     0.855628      85.33
 H      -2.803566     0.266142     1.198058      21.51
 O      -1.992235     2.031411     2.038276     245.58
 H      -1.307772     1.539919     2.480691      27.39
 C      -3.291317     1.969503     0.007003      85.56
 H      -2.672165     2.707163    -0.399419      24.58
 O      -3.768310     0.972034    -0.950026     276.32
 H      -3.426313     1.359209    -1.834621      24.39
 C      -4.514250     2.570370     0.818028      91.86
 O      -5.387946     3.208305    -0.084825     267.26
 H      -4.958651     4.119197    -0.416361      28.30
 H      -3.690673     3.429565     1.603072      21.67
 H      -4.890593     1.974608     1.566151      28.79
55
name = lig-etoh-Waterframe_846
 C       5.445860    -0.899182     1.145040      52.88
 H       5.440329     0.203064     1.048781      19.59
 C       4.781976    -3.291205     0.803630      73.63
 H       4.586354    -4.008401     0.093893      22.61
 C       4.831295    -3.617700     2.163189      21.64
 O       4.303384    -4.807284     2.642629     253.21
 C       3.752655    -5.768931     1.750982      85.90
 H       2.911697    -5.346395     1.105958      27.15
 H       3.399680    -6.643099     2.550903      23.55
 H       4.631421    -5.961292     0.993609      25.72
 C       5.516091    -2.603924     2.983369      10.69
 O       5.763834    -2.903701     4.265220      60.77
 H       5.399878    -3.810817     4.440478      18.78
 C       5.767880    -1.345434     2.494742      65.87
 H       6.199151    -0.679796     3.090831      26.55
 C       5.076061    -1.927219     0.268819      25.03
 C       4.952395    -1.671433    -1.341587      73.40
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 H       5.267400    -2.604661    -1.889754      25.34
 O       5.748245    -0.460088    -1.744963     199.89
 H       5.452644     0.413202    -1.480348      25.88
 C       3.399623    -1.468303    -1.906157      89.47
 H       2.983662    -2.500065    -1.665289      24.02
 C       3.027030    -1.513632    -3.460012      89.85
 O       3.226777    -2.976197    -4.028577     232.10
 H       4.065297    -3.078757    -4.649514      24.01
 H       3.515295    -0.641025    -4.054579      25.01
 H       2.104532    -1.020766    -3.701139      26.40
 C      -0.658173    -0.592595    -0.010558      46.17
 H      -1.413904    -1.477588     0.036305      19.59
 C      -0.009368     1.679393    -0.054073      55.60
 H      -0.315030     2.842853     0.021434      18.86
 C       1.296417     1.301509    -0.591728       9.40
 O       2.154961     2.269682    -1.167276     183.56
 C       1.889210     3.745547    -0.947574     105.66
 H       2.425060     4.202337    -1.782951      25.21
 H       0.942379     4.049282    -1.197619      27.15
 H       2.342829     4.403215     0.046636      22.81
 C       1.630651    -0.071988    -0.661984      28.36
 O       2.845138    -0.343467    -1.419702     208.18
 C       0.634397    -0.991384    -0.518474      85.92
 H       0.686413    -2.062660    -0.682751      22.45
 C      -0.895922     0.748552     0.175836      46.39
 C      -2.242315     1.226257     0.880783      74.93
 H      -2.812270     0.336480     1.371967      23.40
 O      -1.968994     2.017422     2.044224     273.47
 H      -1.120879     1.781248     2.367090      30.53
 C      -3.316894     1.952334     0.013604      89.08
 H      -2.942347     2.917174    -0.538719      23.45
 O      -3.786484     1.039937    -0.886998     255.60
 H      -3.661145     1.243369    -1.882982      24.49
 C      -4.390470     2.600294     0.901082      77.61
 O      -5.465469     3.252894    -0.137609     194.21
 H      -4.827972     3.911487    -0.657438      30.07
 H      -3.909202     3.565331     1.470675      23.55
 H      -5.030519     1.882016     1.448118      26.68
55
name = lig-etoh-Waterframe_847
 C       5.535474    -0.888474     1.145911      47.82
 H       5.630012     0.067275     0.738798      19.89
 C       4.840938    -3.250054     0.733784      52.83
 H       4.565720    -4.060658     0.130653      20.18
 C       4.864641    -3.566510     2.163924       9.98
 O       4.303299    -4.809488     2.685062     211.15
 C       3.787112    -5.789255     1.722807     108.94
 H       2.914295    -5.417618     1.325681      28.44
 H       3.350477    -6.597682     2.357677      25.91
 H       4.497705    -6.539029     1.006816      24.52
 C       5.461380    -2.655231     3.001388      10.63
 O       5.814874    -2.957790     4.304962     206.84
 H       5.457829    -3.828471     4.564414      23.40
 C       5.752109    -1.343919     2.482565      65.53
 H       6.101504    -0.837667     3.351948      24.41
 C       5.038183    -1.891690     0.183721      13.78
 C       4.923455    -1.558145    -1.331275      98.12
 H       5.359030    -2.397415    -1.742046      26.54
 O       5.773199    -0.422436    -1.657831     236.54
 H       5.366262     0.405935    -1.332406      26.73
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 C       3.392582    -1.586205    -1.893011      76.05
 H       2.788118    -2.290520    -1.270941      22.97
 C       3.067603    -1.456040    -3.450681      87.50
 O       3.312634    -2.951184    -4.075714     238.67
 H       4.050288    -2.854231    -4.783396      25.42
 H       3.954227    -0.896333    -3.887965      22.53
 H       1.963996    -1.311919    -3.612284      24.18
 C      -0.683323    -0.700443    -0.005048      34.42
 H      -1.484574    -1.550950     0.234377      19.67
 C       0.052723     1.706744    -0.082844      70.54
 H      -0.206828     2.670155     0.274642      20.76
 C       1.222073     1.361499    -0.590955      17.21
 O       2.094852     2.260957    -1.087182     220.85
 C       1.906861     3.680865    -1.032374     104.77
 H       2.448766     4.322350    -1.741100      24.30
 H       0.935561     3.908750    -1.006048      28.20
 H       2.381501     3.924947     0.067187      23.01
 C       1.622723    -0.080707    -0.681498       9.92
 O       2.829670    -0.331562    -1.341339     171.99
 C       0.560404    -1.056496    -0.539865      57.92
 H       0.892071    -2.147249    -0.753706      20.20
 C      -1.087649     0.708197     0.093672      35.30
 C      -2.228311     1.241354     0.927734      77.36
 H      -2.733253     0.197357     1.062801      22.07
 O      -1.917675     2.057134     2.067163     272.79
 H      -1.100082     1.796951     2.455645      30.31
 C      -3.269548     2.016945     0.049045      77.85
 H      -2.806638     2.873266    -0.665599      23.67
 O      -3.868431     1.030865    -0.874368     217.27
 H      -3.574529     1.257429    -1.845725      24.36
 C      -4.383222     2.698036     0.860257      97.27
 O      -5.469324     3.264873    -0.110795     223.33
 H      -4.999794     3.962307    -0.751339      30.97
 H      -4.241390     3.325661     1.501487      30.26
 H      -5.065707     1.921632     1.471880      26.44
55
name = lig-etoh-Waterframe_848
 C       5.579124    -0.994054     1.138177      54.27
 H       6.023865    -0.107594     0.884984      23.69
 C       4.852560    -3.167342     0.664503      66.54
 H       4.466422    -3.940187    -0.050731      21.18
 C       4.849867    -3.574667     2.013173       2.15
 O       4.368057    -4.782907     2.679317     169.15
 C       3.751865    -5.849719     1.758487     118.11
 H       3.055019    -5.414116     1.110136      28.59
 H       3.412604    -6.491235     2.405099      29.14
 H       4.609237    -6.245686     1.019564      27.69
 C       5.415444    -2.688808     3.021234      -5.82
 O       5.847421    -2.987740     4.354518     191.94
 H       5.805083    -3.935417     4.588582      23.19
 C       5.751626    -1.337755     2.503812      44.39
 H       6.156344    -0.465899     3.239761      21.75
 C       5.028587    -1.887711     0.204712      45.73
 C       4.891922    -1.522674    -1.311184     101.93
 H       5.495616    -2.174378    -1.916730      25.27
 O       5.757726    -0.387034    -1.592426     212.35
 H       5.327072     0.359478    -1.109694      26.39
 C       3.366384    -1.632773    -1.821528      64.91
 H       2.937252    -2.545992    -1.371639      24.11
 C       3.210263    -1.594412    -3.402823      99.61
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 O       3.372186    -2.829953    -4.071868     280.14
 H       4.255836    -2.879716    -4.590330      25.04
 H       3.863192    -0.792442    -3.867262      23.94
 H       2.097576    -1.305260    -3.574174      25.26
 C      -0.765326    -0.718940    -0.034111      41.27
 H      -1.494912    -1.478584     0.379276      19.17
 C      -0.095141     1.679644    -0.061686      86.79
 H      -0.098191     2.601577     0.244969      20.14
 C       1.229791     1.316796    -0.614563      10.84
 O       2.146055     2.247909    -1.070366     222.28
 C       1.927229     3.630241    -1.002512      98.95
 H       2.517821     3.895483    -1.947327      23.24
 H       0.680184     3.935803    -0.889812      24.20
 H       2.236423     3.941399    -0.096579      30.30
 C       1.530153    -0.081908    -0.811407      29.98
 O       2.826363    -0.227541    -1.239893     138.82
 C       0.562554    -1.085106    -0.522541      60.57
 H       0.825988    -2.221021    -0.720162      19.56
 C      -1.078700     0.670879     0.098526      47.19
 C      -2.281127     1.187950     0.907106      75.08
 H      -2.934436     0.459989     1.431938      23.20
 O      -1.855082     2.099255     2.090481     211.00
 H      -1.304818     1.504463     2.590055      28.01
 C      -3.225897     2.097052     0.050771      79.76
 H      -2.464928     2.710257    -0.468198      24.78
 O      -3.951530     1.025957    -0.861595     204.97
 H      -3.360267     1.151005    -1.711193      24.37
 C      -4.506076     2.771288     0.745354      91.50
 O      -5.431092     3.268184    -0.053188     248.87
 H      -5.106494     4.227232    -0.382259      26.90
 H      -4.106409     3.551180     1.719163      23.30
 H      -4.897187     1.797906     1.311711      25.96
55
name = lig-etoh-Waterframe_849
 C       5.636944    -1.061901     1.182117      58.22
 H       6.129619    -0.156457     0.938899      23.97
 C       4.744808    -3.211910     0.607575      54.93
 H       4.363482    -3.861301    -0.288702      21.26
 C       4.858862    -3.585063     1.992805      -5.28
 O       4.436722    -4.766854     2.570718     204.41
 C       3.779973    -5.820556     1.806786     130.70
 H       2.988774    -5.410660     1.067350      25.67
 H       3.369916    -6.544820     2.470045      28.54
 H       4.585254    -6.188031     1.290278      30.47
 C       5.441135    -2.636767     3.021857      10.57
 O       5.842555    -3.001230     4.336969     139.09
 H       5.786180    -3.983953     4.468602      21.33
 C       5.736560    -1.409881     2.554435      59.79
 H       6.333314    -0.480340     3.074606      22.97
 C       5.076269    -1.867365     0.201178      31.44
 C       4.922100    -1.561707    -1.277182      79.80
 H       5.280817    -2.497245    -1.968143      24.47
 O       5.677223    -0.317448    -1.540316     231.02
 H       5.532254     0.549755    -1.062961      23.56
 C       3.428819    -1.528815    -1.743792      80.82
 H       2.965346    -2.466090    -1.424862      25.12
 C       3.299891    -1.626401    -3.295602     118.70
 O       3.438177    -2.770974    -4.059198     310.90
 H       4.308013    -2.973248    -4.428211      28.51
 H       3.778841    -0.777021    -3.670927      27.05
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 H       2.312606    -1.189557    -3.549058      27.20
 C      -0.783695    -0.694378    -0.084061      51.21
 H      -1.440532    -1.452329     0.220064      22.73
 C      -0.115390     1.623562    -0.107968      62.11
 H      -0.410966     2.616065     0.210836      21.62
 C       1.121262     1.264025    -0.625639       9.37
 O       2.215513     2.147233    -1.050710     149.41
 C       1.918985     3.618340    -0.933658     106.79
 H       2.429334     4.115714    -1.868964      25.28
 H       0.763787     3.967114    -1.473046      23.01
 H       2.345889     4.293324    -0.243213      26.43
 C       1.414080    -0.070628    -0.940079      18.83
 O       2.852056    -0.228977    -1.189036     132.53
 C       0.525399    -1.075166    -0.495194      65.37
 H       0.694899    -2.194398    -0.571227      21.94
 C      -1.057877     0.629861     0.219735      25.61
 C      -2.389001     1.195300     0.963164      82.93
 H      -2.949484     0.455660     1.483887      25.48
 O      -1.783107     2.085367     2.081491     220.42
 H      -1.707807     1.466434     2.796712      27.91
 C      -3.240305     2.079265     0.029919      92.56
 H      -2.735293     2.766455    -0.554315      27.03
 O      -3.961513     1.097413    -0.853839     207.40
 H      -3.454438     0.757335    -1.687866      25.84
 C      -4.444602     2.717926     0.769443      77.46
 O      -5.457945     3.366606    -0.069804     228.27
 H      -5.326634     4.373258     0.088755      26.84
 H      -3.911795     3.735045     1.557875      21.60
 H      -5.034906     1.912856     1.246830      26.03
55
name = lig-etoh-Waterframe_850
 C       5.694721    -1.062377     1.205875      66.60
 H       5.955860    -0.043671     0.816318      24.95
 C       4.628089    -3.235294     0.621998      60.52
 H       4.225640    -4.111813    -0.039565      23.77
 C       4.877823    -3.537717     1.996010      23.87
 O       4.490113    -4.773191     2.497606     190.29
 C       3.847306    -5.770275     1.804280     129.04
 H       2.836119    -5.387430     1.239263      24.34
 H       3.344748    -6.518574     2.665099      24.96
 H       4.357256    -6.489611     1.198651      28.95
 C       5.459536    -2.707099     2.998445       7.13
 O       5.807535    -3.016335     4.264351     168.47
 H       5.445973    -3.938502     4.556362      23.49
 C       5.792179    -1.391194     2.550279      54.79
 H       6.340689    -0.979042     3.481851      20.11
 C       5.130375    -1.958344     0.220915      26.74
 C       4.948247    -1.510206    -1.204075      96.23
 H       5.541614    -2.356750    -1.836493      23.32
 O       5.628030    -0.290686    -1.561134     237.87
 H       5.150790     0.357481    -0.929919      26.92
 C       3.486378    -1.432670    -1.660619      94.84
 H       2.903349    -2.160512    -1.105090      25.29
 C       3.324390    -1.419433    -3.209146      93.07
 O       3.482498    -2.808624    -4.006036     241.45
 H       4.314756    -2.755539    -4.636764      24.23
 H       4.160784    -0.887926    -3.584903      24.07
 H       2.278205    -1.355265    -3.324834      26.18
 C      -0.805946    -0.704550    -0.077698      53.85
 H      -1.452889    -1.484101     0.028432      25.27
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 C      -0.131642     1.619160    -0.126283      51.54
 H      -0.478281     2.746000     0.053041      21.92
 C       1.092602     1.281399    -0.715464       9.31
 O       2.213117     2.105947    -0.970409     145.17
 C       1.934335     3.626474    -1.036942      88.56
 H       2.684924     3.979706    -1.749655      25.00
 H       0.790809     3.672255    -1.149135      24.20
 H       2.137774     4.138307     0.170819      23.65
 C       1.422211    -0.130097    -0.992634      14.35
 O       2.834187    -0.296503    -1.176935     172.26
 C       0.478122    -1.069479    -0.532460      62.88
 H       0.767577    -2.086914    -0.546749      23.65
 C      -1.133157     0.622862     0.349506      21.30
 C      -2.350398     1.235024     1.038244      94.23
 H      -2.973244     0.376710     1.210057      26.82
 O      -1.759208     2.028124     2.063135     258.16
 H      -1.912159     1.699693     2.928780      29.36
 C      -3.335280     1.999963    -0.020815      96.66
 H      -2.900826     2.823045    -0.598903      26.91
 O      -3.972318     1.154058    -0.861856     231.39
 H      -3.280380     0.909311    -1.597948      25.66
 C      -4.379751     2.701604     0.820052      99.86
 O      -5.471566     3.484145    -0.077754     213.87
 H      -5.438911     4.490444     0.102395      25.71
 H      -3.905466     3.353209     1.612045      26.34
 H      -4.871773     2.117611     1.470786      29.27
55
name = lig-etoh-Waterframe_851
 C       5.711582    -1.055094     1.177021      28.08
 H       5.940182     0.048676     0.866760      19.97
 C       4.590670    -3.206808     0.718094      87.55
 H       4.137064    -4.000216     0.085155      27.03
 C       4.847732    -3.553026     1.977588      41.87
 O       4.583615    -4.794651     2.491400     237.90
 C       3.773604    -5.808727     1.786801     104.35
 H       2.875930    -5.260959     1.283223      26.45
 H       3.477596    -6.366312     2.846284      23.43
 H       4.338112    -6.443530     0.911446      27.48
 C       5.475898    -2.731012     2.896161      23.67
 O       5.746816    -3.060016     4.214833     152.58
 H       5.423026    -3.992261     4.583948      17.44
 C       5.892324    -1.434855     2.595174      43.11
 H       6.269011    -0.753516     3.319172      23.64
 C       5.168685    -2.017780     0.295562      35.57
 C       5.011780    -1.474829    -1.160568      95.46
 H       5.453567    -2.162979    -1.882166      25.60
 O       5.585128    -0.267869    -1.573354     237.97
 H       5.149097     0.612129    -1.182958      22.61
 C       3.481542    -1.478487    -1.592883      78.38
 H       3.086860    -2.488933    -1.274181      25.23
 C       3.348868    -1.355806    -3.177214      83.97
 O       3.493771    -2.783602    -3.862210     237.37
 H       4.177410    -2.760352    -4.676374      23.16
 H       4.050609    -0.549195    -3.689083      23.72
 H       2.386755    -0.840319    -3.489272      25.34
 C      -0.876189    -0.704626    -0.006760      44.55
 H      -1.587788    -1.500458     0.143790      23.78
 C      -0.201462     1.609592    -0.115804      34.97
 H      -0.139586     2.786048     0.018777      21.58
 C       1.130234     1.248896    -0.826969      -2.41
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 O       2.172136     2.142111    -0.894088     193.95
 C       1.948299     3.540714    -1.056369     121.08
 H       2.660921     3.968544    -1.684446      27.43
 H       1.079587     3.817663    -1.402360      28.28
 H       1.952729     3.803122     0.181834      22.77
 C       1.472611    -0.130860    -0.938005      23.66
 O       2.790329    -0.272209    -1.153263     165.67
 C       0.477691    -1.086962    -0.629974      57.81
 H       0.668960    -2.082698    -0.677672      26.11
 C      -1.100307     0.656817     0.310798      38.88
 C      -2.297808     1.191929     1.019176      85.02
 H      -2.992012     0.441104     1.541025      26.61
 O      -1.780475     2.006314     2.082325     241.32
 H      -1.987407     1.652714     2.923633      29.53
 C      -3.387819     2.039563     0.033651      67.40
 H      -2.633354     2.767868    -0.520845      25.55
 O      -3.997157     1.118402    -0.939244     219.00
 H      -3.362956     1.133102    -1.754446      25.75
 C      -4.435860     2.790367     0.868423     112.32
 O      -5.417338     3.530322    -0.001424     280.72
 H      -5.032857     4.473167    -0.066009      27.04
 H      -3.873327     3.364160     1.397346      27.90
 H      -4.994763     2.022976     1.434958      27.07
55
name = lig-etoh-Waterframe_852
 C       5.728353    -1.076673     1.248377      67.19
 H       6.093694    -0.064073     0.810914      20.97
 C       4.583942    -3.168891     0.707624      62.15
 H       4.121009    -3.673618    -0.077124      26.07
 C       4.818385    -3.631139     2.028857       9.64
 O       4.657569    -4.875000     2.506775     262.19
 C       3.670304    -5.803478     1.805523     106.45
 H       2.802651    -5.334249     1.460675      27.96
 H       3.359787    -6.722813     2.371909      25.71
 H       4.452723    -6.227762     1.002333      26.41
 C       5.537692    -2.699673     2.927265       9.77
 O       5.676317    -3.105496     4.195070     138.26
 H       5.668487    -4.163908     4.250689      18.58
 C       5.957397    -1.426044     2.509468      84.03
 H       6.247855    -0.682060     3.110263      26.07
 C       5.191211    -1.896848     0.286671      37.61
 C       4.977839    -1.496296    -1.164369      90.88
 H       5.349491    -2.220292    -1.768600      26.03
 O       5.594907    -0.217658    -1.591344     231.56
 H       5.351355     0.731910    -1.167610      19.86
 C       3.471644    -1.554337    -1.647655      64.57
 H       2.955047    -2.548955    -1.451569      25.11
 C       3.367529    -1.371239    -3.196952      97.76
 O       3.452028    -2.663368    -3.687929     251.29
 H       4.292411    -2.801712    -4.307358      23.05
 H       4.302590    -0.631765    -3.497462      23.41
 H       2.362962    -0.901652    -3.494665      25.07
 C      -0.799015    -0.714423    -0.009058      42.27
 H      -1.613170    -1.407597     0.438407      21.89
 C      -0.053912     1.619861    -0.218961      65.57
 H      -0.374726     2.576386     0.305461      22.08
 C       1.020309     1.233448    -0.795985      33.14
 O       2.153134     2.136328    -0.882272     202.66
 C       1.923474     3.501831    -0.996431     142.54
 H       2.853189     3.907278    -1.423223      27.00
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 H       1.197657     3.837715    -1.809234      26.52
 H       1.934804     4.217562    -0.251838      28.17
 C       1.444076    -0.106256    -0.846612       8.65
 O       2.818502    -0.271169    -1.111985      95.33
 C       0.369013    -1.101454    -0.663951      61.74
 H       0.568059    -2.114698    -0.897625      25.69
 C      -1.081876     0.658763     0.191080      22.37
 C      -2.361528     1.148876     0.999650      72.58
 H      -2.802942     0.188882     1.519756      24.91
 O      -1.814944     2.041125     2.132001     217.51
 H      -1.846897     1.428658     2.848631      28.21
 C      -3.341617     2.036982     0.109345      58.44
 H      -2.695680     2.830618    -0.486183      24.97
 O      -4.002897     1.090215    -1.005552     175.86
 H      -3.668187     1.174402    -1.954674      25.71
 C      -4.508155     2.857517     0.858675      83.49
 O      -5.330492     3.561579     0.106069     275.97
 H      -4.906217     4.345481    -0.263117      28.90
 H      -3.866402     3.726006     1.637497      22.25
 H      -5.239615     2.059854     1.468646      23.90
55
name = lig-etoh-Waterframe_853
 C       5.775200    -0.999303     1.157035      55.40
 H       6.281248    -0.027830     0.942181      24.07
 C       4.634856    -3.094212     0.660852      66.73
 H       4.129095    -3.684048    -0.011610      25.94
 C       4.858437    -3.575788     2.011208     -16.48
 O       4.618149    -5.005849     2.551678     231.56
 C       3.659602    -5.797519     1.805790     131.48
 H       2.827074    -5.265525     1.643206      31.09
 H       3.468804    -6.608508     2.337322      30.81
 H       3.975983    -6.062194     0.753148      30.23
 C       5.536931    -2.738921     2.940673       1.51
 O       5.647786    -3.111384     4.219982       5.80
 H       5.559421    -4.146260     4.528866      16.10
 C       5.983584    -1.423175     2.545221      44.10
 H       6.474288    -0.862225     3.290752      22.77
 C       5.097917    -1.834753     0.263067      42.74
 C       4.898646    -1.475153    -1.201582      82.43
 H       5.563676    -2.249983    -1.712199      25.52
 O       5.640753    -0.225729    -1.630333     191.87
 H       5.297017     0.344033    -0.882161      28.16
 C       3.418975    -1.501465    -1.712525      96.28
 H       2.789559    -2.276242    -1.273380      25.91
 C       3.393944    -1.317119    -3.145229     112.22
 O       3.421939    -2.643895    -3.604261     271.79
 H       4.276745    -2.771988    -4.187416      25.68
 H       4.343131    -0.849766    -3.512796      26.02
 H       2.397623    -0.950533    -3.427797      26.39
 C      -0.781787    -0.672599    -0.016929      59.26
 H      -1.409159    -1.587978     0.417341      21.73
 C      -0.197158     1.653053    -0.193062      56.19
 H      -0.150510     2.719810     0.129860      21.49
 C       1.144499     1.251341    -0.734456       6.30
 O       2.138108     2.081309    -0.870004     160.46
 C       1.958831     3.626943    -1.021581      79.93
 H       3.040938     3.728099    -1.280585      23.29
 H       1.082497     3.577221    -2.048907      22.29
 H       1.465998     4.165213    -0.229110      25.23
 C       1.382590    -0.181068    -0.820765      18.55
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 O       2.827267    -0.323296    -1.053166     147.44
 C       0.385006    -1.109781    -0.687002      60.99
 H       0.549472    -2.199577    -0.957250      23.06
 C      -1.089101     0.671885     0.089351      39.12
 C      -2.336807     1.145430     0.964204      76.11
 H      -2.909929     0.197004     1.139851      25.89
 O      -1.894761     2.032238     2.163528     212.45
 H      -1.405727     1.490108     2.791694      28.40
 C      -3.333292     1.972893     0.113560      79.41
 H      -2.787040     2.772803    -0.381340      25.90
 O      -4.004231     1.102658    -0.978809     209.88
 H      -3.509382     1.389800    -1.792515      26.91
 C      -4.425858     2.818510     0.935257      82.21
 O      -5.342967     3.625777     0.100827     271.36
 H      -4.993185     4.509786    -0.076971      27.95
 H      -4.037571     3.444710     2.044553      22.92
 H      -5.166579     2.118125     1.589361      24.87
55
name = lig-etoh-Waterframe_854
 C       5.847108    -0.922980     1.167002      29.17
 H       6.227038    -0.004172     0.814974      24.34
 C       4.678040    -3.098561     0.692817      62.39
 H       4.209602    -3.816772     0.037615      24.40
 C       4.909331    -3.577377     1.950959      15.63
 O       4.564289    -5.008270     2.534942      77.70
 C       3.629952    -5.766350     1.769911     136.24
 H       2.632112    -5.190893     1.952652      25.40
 H       3.569171    -6.622989     2.413176      28.48
 H       3.784836    -5.961222     0.765227      30.48
 C       5.497527    -2.765533     2.928428       6.34
 O       5.652308    -3.062314     4.307862     159.77
 H       5.433636    -3.974101     4.525838      21.53
 C       5.966747    -1.469541     2.554472      48.39
 H       6.714157    -1.027702     3.308291      21.30
 C       5.000055    -1.747164     0.243692      11.83
 C       4.900731    -1.462295    -1.262052      83.60
 H       5.363649    -2.405268    -1.945365      24.86
 O       5.644676    -0.312681    -1.630407     238.28
 H       5.514359     0.573727    -1.145987      25.09
 C       3.371149    -1.369640    -1.607260     102.16
 H       2.988191    -2.391701    -1.464444      26.34
 C       3.368007    -1.251551    -3.159541     101.43
 O       3.408552    -2.736368    -3.627692     272.04
 H       4.102390    -2.807618    -4.396854      26.03
 H       4.072557    -0.624017    -3.526169      27.28
 H       2.615064    -0.586762    -3.546943      27.64
 C      -0.799758    -0.689890    -0.071984      39.21
 H      -1.578712    -1.489720     0.258640      21.56
 C      -0.169918     1.713291    -0.233880      63.13
 H      -0.445752     2.753288    -0.155366      20.78
 C       1.102126     1.212551    -0.581552       3.39
 O       2.211544     2.115018    -0.851971     153.20
 C       1.960352     3.621443    -1.098292      78.83
 H       2.887405     4.371170    -1.119424      23.55
 H       1.389062     3.938273    -2.230767      22.85
 H       1.307959     3.796265    -0.163581      23.52
 C       1.471382    -0.159679    -0.874725      26.75
 O       2.780710    -0.350454    -0.972801     206.29
 C       0.439024    -1.134656    -0.676852      47.42
 H       0.600508    -2.307002    -0.758525      20.19
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 C      -1.192489     0.701393     0.127993      48.64
 C      -2.302195     1.140417     0.921767      95.32
 H      -2.864640     0.371479     1.369575      27.37
 O      -1.998900     1.954562     2.145496     225.43
 H      -1.185326     1.603133     2.496191      30.29
 C      -3.370645     1.982989     0.098989      92.27
 H      -2.808421     2.668678    -0.421914      27.28
 O      -3.972447     1.166408    -0.871557     268.13
 H      -3.401738     1.228008    -1.684193      27.20
 C      -4.392561     2.713226     1.051056      96.13
 O      -5.351220     3.650731     0.099045     220.67
 H      -5.092760     4.538744     0.192727      28.73
 H      -3.720797     3.290198     1.617338      25.39
 H      -5.027019     1.934909     1.298509      27.43
55
name = lig-etoh-Waterframe_855
 C       5.789969    -0.978476     1.224860      72.71
 H       6.197006    -0.075699     0.948522      24.41
 C       4.685118    -3.098954     0.679420      44.22
 H       4.309239    -3.760857    -0.180914      21.44
 C       4.936155    -3.677136     2.002978      15.99
 O       4.573808    -4.889701     2.441918     252.72
 C       3.526146    -5.719579     1.801586     114.23
 H       2.300705    -5.394060     1.899891      22.21
 H       3.611529    -6.907639     2.142297      25.66
 H       3.836661    -5.810369     0.789823      27.52
 C       5.482106    -2.732534     2.993737      16.21
 O       5.651653    -2.967665     4.335712     103.98
 H       5.601609    -3.956078     4.482752      22.56
 C       5.972854    -1.494394     2.471395      58.35
 H       6.669928    -0.911268     3.259484      22.46
 C       5.043021    -1.708754     0.307170      27.68
 C       4.870677    -1.430893    -1.230941      95.79
 H       5.096768    -2.347417    -1.934105      23.98
 O       5.696290    -0.380049    -1.664559     272.62
 H       5.313244     0.512599    -1.406290      25.59
 C       3.411622    -1.372685    -1.630672      79.34
 H       2.984797    -2.374279    -1.392945      22.95
 C       3.312305    -1.226924    -3.231951      95.84
 O       3.373566    -2.720461    -3.703621     259.54
 H       4.107452    -2.759430    -4.375025      27.56
 H       4.269833    -0.852264    -3.483901      24.41
 H       2.308238    -0.924216    -3.606223      24.52
 C      -0.840084    -0.671531    -0.155795      40.73
 H      -1.618178    -1.367677     0.045471      21.19
 C      -0.180042     1.689647    -0.268908      66.38
 H      -0.516265     2.652820    -0.369357      21.22
 C       1.105980     1.259734    -0.509549      -0.67
 O       2.314471     2.206907    -0.864863     146.87
 C       1.920830     3.569968    -1.128969     117.40
 H       2.776578     4.206961    -0.779090      25.52
 H       1.550660     3.713974    -2.045630      28.81
 H       1.115715     4.076152    -0.331416      24.14
 C       1.417279    -0.103494    -0.844662      24.79
 O       2.777448    -0.304741    -0.858471     167.91
 C       0.458297    -1.104960    -0.609429      47.42
 H       0.763292    -2.234081    -0.674308      19.65
 C      -1.113547     0.678263     0.136720      24.59
 C      -2.420970     1.145256     0.967629      82.52
 H      -2.824745     0.180942     1.316507      24.00
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 O      -2.054975     1.893674     2.090302     278.61
 H      -1.195055     1.618153     2.377499      29.82
 C      -3.345381     2.053779     0.105799      96.11
 H      -2.814894     2.929362    -0.380191      24.98
 O      -3.972359     1.194199    -0.801034     264.25
 H      -3.465974     0.890233    -1.571148      27.34
 C      -4.405417     2.655124     0.969293     114.57
 O      -5.314236     3.571640     0.179292     302.11
 H      -5.011989     4.486796     0.105318      29.14
 H      -3.925883     3.168063     1.660976      28.31
 H      -5.003757     1.997449     1.527601      28.17
55
name = lig-etoh-Waterframe_856
 C       5.688838    -0.989098     1.236022      53.40
 H       6.147043    -0.043385     1.072617      21.52
 C       4.716796    -3.084984     0.698290      66.64
 H       4.309156    -3.749053    -0.176480      22.10
 C       4.930873    -3.577107     2.000940      21.78
 O       4.551418    -4.874831     2.391061     202.41
 C       3.464528    -5.692682     1.764473     101.21
 H       2.354211    -5.259916     2.027745      22.53
 H       3.758943    -6.777936     2.297465      23.29
 H       3.587208    -5.577186     0.654200      24.30
 C       5.479764    -2.707679     2.983227      31.58
 O       5.647543    -2.900268     4.346562     219.07
 H       5.701471    -3.879239     4.666648      24.79
 C       5.995595    -1.518822     2.524153      37.19
 H       6.433903    -0.699788     3.230958      23.09
 C       5.082191    -1.849513     0.311169      39.44
 C       4.847626    -1.449333    -1.144937     100.73
 H       5.345728    -2.263151    -1.495076      25.33
 O       5.761681    -0.398600    -1.729812     243.68
 H       5.288313     0.401264    -1.422159      27.35
 C       3.394642    -1.383160    -1.705880      79.00
 H       2.828100    -2.202923    -1.265574      23.63
 C       3.263424    -1.334491    -3.247982      94.78
 O       3.314605    -2.642214    -3.797337     283.02
 H       4.187849    -2.769635    -4.211616      26.63
 H       4.126143    -0.694213    -3.805713      23.60
 H       2.246017    -0.865488    -3.606317      25.11
 C      -0.866528    -0.674320    -0.216792      61.34
 H      -1.542167    -1.402431    -0.064672      24.21
 C      -0.204769     1.677771    -0.268239      55.47
 H      -0.418942     2.688297    -0.264565      22.60
 C       1.238554     1.377266    -0.590192       5.46
 O       2.303686     2.241791    -0.843558     199.73
 C       1.888775     3.567496    -1.070879     126.46
 H       2.816605     4.075414    -1.014352      25.94
 H       1.658093     3.580161    -2.167817      26.99
 H       0.891123     3.887747    -0.661500      24.79
 C       1.377038    -0.025567    -0.700837      14.14
 O       2.820114    -0.262280    -0.785066     131.84
 C       0.430979    -1.039787    -0.543029      59.99
 H       0.731609    -2.088120    -0.720880      22.53
 C      -1.082547     0.666465     0.135051      27.67
 C      -2.461539     1.108771     0.941548      78.23
 H      -3.170038     0.191538     0.974071      24.31
 O      -2.060611     1.880970     2.079224     247.30
 H      -1.341506     1.465596     2.559834      29.24
 C      -3.302313     2.064949     0.130454      80.48
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 H      -2.671957     2.984618    -0.330358      25.09
 O      -4.026513     1.174232    -0.815027     210.30
 H      -3.315037     0.973083    -1.433329      28.77
 C      -4.461382     2.701920     0.915669      97.66
 O      -5.292608     3.461422     0.264011     291.65
 H      -4.810196     4.251268    -0.057584      28.44
 H      -4.094917     3.320722     1.958126      23.54
 H      -5.098622     1.874942     1.468534      24.62
55
name = lig-etoh-Waterframe_857
 C       5.648739    -0.989448     1.283952      58.19
 H       5.823778     0.044799     0.845250      22.83
 C       4.728647    -3.164458     0.701561      46.56
 H       4.228971    -3.988100     0.084325      20.03
 C       4.860778    -3.492328     2.010821      25.34
 O       4.531290    -4.896868     2.370660     277.59
 C       3.462737    -5.582165     1.736945     135.82
 H       2.630110    -5.260892     2.198079      29.01
 H       3.498657    -6.647528     2.136448      26.09
 H       3.344939    -5.803396     0.608885      26.20
 C       5.514226    -2.711020     2.996546      15.90
 O       5.642870    -2.875201     4.372858      70.39
 H       5.443278    -3.921108     4.510858      19.21
 C       5.969834    -1.417725     2.570598      61.06
 H       6.357491    -0.845490     3.417073      23.14
 C       5.104218    -1.843774     0.286573      36.99
 C       4.927626    -1.534512    -1.162386      86.31
 H       5.339034    -2.388298    -1.672754      26.30
 O       5.760974    -0.410839    -1.750654     204.59
 H       5.754766     0.481762    -1.408594      27.30
 C       3.360956    -1.368319    -1.652366      63.32
 H       2.856922    -2.345577    -1.507505      24.32
 C       3.200285    -1.350350    -3.257062     100.94
 O       3.231523    -2.615859    -3.887584     263.04
 H       4.158327    -2.725496    -4.375769      23.27
 H       3.824301    -0.462311    -3.771595      24.36
 H       2.179197    -0.851699    -3.330691      25.90
 C      -0.907802    -0.689964    -0.210462      13.55
 H      -1.615731    -1.457785    -0.065933      21.55
 C      -0.086981     1.730439    -0.255227      60.78
 H      -0.514390     2.681581     0.126798      22.20
 C       1.164178     1.422693    -0.661782      30.45
 O       2.245605     2.221909    -0.773172     202.79
 C       1.879967     3.622848    -1.130454      99.91
 H       2.540195     4.436245    -0.885795      25.47
 H       1.722094     3.630948    -2.494878      22.88
 H       1.070629     3.891643    -0.514880      26.51
 C       1.552430     0.045731    -0.569701      13.25
 O       2.850846    -0.247959    -0.788086     162.80
 C       0.451140    -0.970660    -0.522791      59.03
 H       0.650123    -1.961701    -0.728141      22.63
 C      -1.188410     0.686353     0.123914      29.57
 C      -2.384763     1.087038     0.839531      88.72
 H      -3.064265     0.273541     1.286399      24.87
 O      -2.047201     1.854003     2.113029     200.62
 H      -1.755427     1.184050     2.768586      27.07
 C      -3.336211     2.051224     0.143858      78.96
 H      -2.671914     2.690454    -0.528356      26.22
 O      -4.042502     1.185567    -0.873703     170.08
 H      -3.478358     1.035797    -1.640681      27.81
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 C      -4.440446     2.648468     1.086735      82.40
 O      -5.376542     3.452742     0.227322     269.56
 H      -4.933244     4.229504    -0.195868      28.54
 H      -3.800203     3.343643     1.973784      21.80
 H      -5.034812     1.643747     1.106655      24.32
55
name = lig-etoh-Waterframe_858
 C       5.626342    -0.954833     1.255055      54.60
 H       5.734000     0.199012     1.003996      21.39
 C       4.729076    -3.185734     0.671971      48.15
 H       4.347029    -3.911304    -0.038041      21.37
 C       4.791304    -3.569012     2.102898       3.34
 O       4.571813    -4.873468     2.356035     278.14
 C       3.405770    -5.534358     1.770542     129.24
 H       2.527313    -5.120172     2.010511      30.18
 H       3.457234    -6.463682     2.052622      26.82
 H       3.524172    -5.518431     0.607984      26.38
 C       5.546953    -2.636611     3.021146       0.85
 O       5.621085    -2.932914     4.371894     109.85
 H       5.298078    -3.914638     4.660077      21.15
 C       5.880323    -1.335256     2.628070      63.12
 H       6.382868    -0.749928     3.305619      24.87
 C       5.111276    -1.867061     0.302349      37.46
 C       4.982560    -1.548728    -1.278519      91.79
 H       5.144102    -2.407950    -2.082878      24.64
 O       5.764613    -0.454067    -1.765196     220.21
 H       5.703341     0.206874    -1.072934      29.16
 C       3.416777    -1.411853    -1.581354      71.59
 H       2.901252    -2.349947    -1.240888      22.36
 C       3.062117    -1.198933    -3.191701      87.70
 O       3.162254    -2.605978    -3.950144     226.70
 H       3.972435    -2.573475    -4.624218      25.35
 H       3.899770    -0.662802    -3.653035      23.84
 H       2.034144    -1.159006    -3.292400      24.88
 C      -0.891391    -0.610288    -0.164450      39.31
 H      -1.636764    -1.461155    -0.082219      20.92
 C      -0.207656     1.723823    -0.136827      50.42
 H      -0.198098     2.868679     0.266117      19.24
 C       1.106958     1.351660    -0.642734       1.30
 O       2.227867     2.317405    -0.728139     170.62
 C       1.877385     3.690038    -1.191943      99.62
 H       2.699397     4.276254    -0.759357      24.05
 H       1.446407     3.810691    -2.425157      23.50
 H       0.992832     3.974042    -0.753319      27.18
 C       1.573574    -0.006805    -0.538151      19.11
 O       2.932166    -0.265343    -0.843055     183.56
 C       0.548717    -0.894004    -0.518097      69.01
 H       0.799344    -1.869011    -0.663082      23.43
 C      -1.139397     0.719179     0.015512      32.50
 C      -2.361532     1.123872     0.881202      83.88
 H      -2.678988     0.095734     1.136112      25.02
 O      -2.003519     1.803002     2.155788     244.76
 H      -2.122065     1.161257     2.886654      26.42
 C      -3.375843     1.991429     0.063696      94.26
 H      -2.946969     2.877139    -0.363246      26.45
 O      -4.068627     1.208938    -0.936132     223.14
 H      -3.630268     1.245546    -1.784585      27.16
 C      -4.391659     2.580676     1.077221      91.15
 O      -5.465358     3.442628     0.210343     240.13
 H      -5.082027     4.353434    -0.020862      27.64
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 H      -4.069281     2.999262     2.099780      24.99
 H      -5.009996     1.879608     1.746108      26.32
55
name = lig-etoh-Waterframe_859
 C       5.599395    -0.919580     1.244773      38.11
 H       5.927272     0.181748     1.043554      22.45
 C       4.746585    -3.155916     0.742385      74.34
 H       4.578000    -3.722072    -0.084519      22.69
 C       4.830045    -3.522277     2.057281      18.59
 O       4.599557    -4.888709     2.418952     270.64
 C       3.378590    -5.484480     1.773496     111.41
 H       2.358761    -4.856509     1.886449      24.72
 H       3.390250    -6.479811     2.154403      24.86
 H       3.654494    -5.363826     0.713375      26.26
 C       5.442391    -2.659025     3.042397      -0.26
 O       5.605588    -2.998312     4.378979      74.22
 H       5.432533    -4.057234     4.503382      20.49
 C       5.771211    -1.280646     2.603546      57.00
 H       6.249871    -0.563903     3.154235      25.46
 C       5.133624    -1.909295     0.236279      25.09
 C       4.939291    -1.582675    -1.374190      96.60
 H       5.447682    -2.594021    -1.832897      23.84
 O       5.774840    -0.487750    -1.755990     213.84
 H       5.594178     0.171143    -1.085126      30.08
 C       3.447699    -1.447125    -1.587513      86.47
 H       3.034073    -2.304132    -1.034724      22.16
 C       2.963984    -1.215536    -3.088406      95.72
 O       3.107419    -2.541429    -3.949581     230.31
 H       4.072835    -2.539073    -4.401470      24.67
 H       3.486751    -0.401818    -3.527021      26.27
 H       2.010223    -0.741781    -3.309995      26.29
 C      -0.694099    -0.555459    -0.187622      41.67
 H      -1.549961    -1.362419    -0.035494      22.58
 C      -0.151032     1.736872    -0.086749      56.07
 H      -0.406267     2.893134     0.243526      21.44
 C       1.155243     1.370209    -0.517323      15.02
 O       2.145703     2.410626    -0.717818     219.33
 C       1.828941     3.730885    -1.197658     132.12
 H       2.825596     4.280355    -1.183242      24.15
 H       1.877269     3.694959    -2.165322      29.47
 H       0.939889     4.241257    -0.789971      26.51
 C       1.582046     0.013990    -0.636873      15.48
 O       2.997889    -0.249049    -0.879612     164.16
 C       0.524451    -0.973261    -0.476424      54.30
 H       0.834970    -2.016848    -0.553755      21.43
 C      -1.160000     0.808560     0.024932      57.87
 C      -2.352175     1.113198     0.917354      88.32
 H      -2.958987     0.228933     1.005315      27.52
 O      -1.959044     1.748001     2.169911     247.78
 H      -2.112870     1.164427     2.945552      26.97
 C      -3.437959     1.957533     0.069983      88.16
 H      -2.987852     2.848478    -0.273946      27.87
 O      -4.104156     1.226178    -1.006656     235.75
 H      -3.587300     1.432198    -1.772010      28.11
 C      -4.501366     2.568061     1.020394     113.01
 O      -5.488687     3.384932     0.277704     267.25
 H      -5.198067     4.350296     0.428962      28.53
 H      -3.917392     3.251368     1.477316      28.06
 H      -5.128391     1.842430     1.499797      28.63
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name = lig-etoh-Waterframe_860
 C       5.563624    -0.938760     1.186393      64.06
 H       5.991072    -0.036481     0.786306      22.61
 C       4.786218    -3.093360     0.691746      71.76
 H       4.558939    -4.005824     0.168140      24.94
 C       4.921450    -3.509773     2.067571     -12.12
 O       4.583914    -4.877862     2.508787     193.68
 C       3.435544    -5.408159     1.746145     102.06
 H       2.450171    -4.681876     2.150383      20.61
 H       3.079382    -6.500100     2.202615      24.35
 H       3.487875    -5.703677     0.726625      26.03
 C       5.305103    -2.624150     3.055832       8.66
 O       5.591773    -3.063982     4.351697     181.91
 H       5.509519    -4.073910     4.515562      21.96
 C       5.648618    -1.315743     2.552684      51.03
 H       5.974413    -0.626158     3.349372      22.32
 C       5.171808    -1.824289     0.204810      37.12
 C       4.963256    -1.656213    -1.303146      86.41
 H       5.359381    -2.562287    -1.890694      22.55
 O       5.778316    -0.506920    -1.747526     220.70
 H       5.563872     0.379958    -1.467504      26.27
 C       3.383430    -1.460986    -1.644642      70.89
 H       2.917629    -2.387073    -1.284010      24.68
 C       2.916592    -1.294954    -3.049651     110.94
 O       3.081296    -2.405627    -3.881767     263.91
 H       4.079291    -2.476161    -4.107526      26.63
 H       3.514689    -0.468518    -3.392407      25.51
 H       1.794281    -0.986040    -2.886274      24.31
 C      -0.690170    -0.491726    -0.176225      34.74
 H      -1.415071    -1.404571     0.032078      19.90
 C      -0.050726     1.802641    -0.073280      54.55
 H      -0.359646     2.849210     0.106438      21.23
 C       1.253269     1.469342    -0.401946      24.05
 O       2.079990     2.455096    -0.675544     212.77
 C       1.829092     3.762557    -1.257260     101.63
 H       2.711670     4.442491    -0.949957      24.65
 H       1.718800     3.550569    -2.355713      24.69
 H       1.044258     4.459371    -0.688035      23.47
 C       1.623342     0.041401    -0.757065      10.15
 O       3.007369    -0.186324    -0.892838     130.67
 C       0.663154    -1.047187    -0.469911      35.11
 H       0.656045    -2.244899    -0.491929      19.66
 C      -1.112784     0.796222     0.109539      32.55
 C      -2.440093     1.069007     0.884535      82.03
 H      -2.988584     0.198342     1.249689      24.40
 O      -1.935501     1.704948     2.156482     228.24
 H      -1.795995     1.002868     2.861580      25.62
 C      -3.502199     1.979749     0.111109      82.57
 H      -2.863816     2.699321    -0.490106      24.52
 O      -4.111637     1.243646    -1.060266     236.45
 H      -3.574583     1.229258    -1.854231      27.51
 C      -4.611377     2.589113     0.945191     120.73
 O      -5.522088     3.340185     0.347518     286.85
 H      -5.461260     4.315937     0.579028      28.72
 H      -3.872720     3.305847     1.505132      24.63
 H      -4.996115     1.759666     1.522579      28.45
55
name = lig-etoh-Waterframe_861
 C       5.569559    -0.918991     1.148981      51.14
 H       5.907494     0.011277     0.897133      22.52
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 C       4.841253    -3.151627     0.692717      56.88
 H       4.439028    -3.926779    -0.099050      21.15
 C       4.947967    -3.556887     2.033493      10.70
 O       4.565259    -4.825467     2.526701     236.14
 C       3.449074    -5.385686     1.809545     101.49
 H       2.607758    -4.489944     1.714361      23.59
 H       3.154396    -6.336233     2.546702      23.23
 H       3.602761    -5.577886     0.769241      25.55
 C       5.239355    -2.604238     3.062578      10.41
 O       5.573004    -3.062876     4.312874     166.49
 H       5.332625    -3.965057     4.516536      31.83
 C       5.531533    -1.343616     2.558951      47.00
 H       5.809806    -0.549818     3.387403      20.40
 C       5.138909    -1.870198     0.190666      40.76
 C       4.966594    -1.607496    -1.237536     107.73
 H       5.216422    -2.394560    -1.807320      25.80
 O       5.789383    -0.531916    -1.779749     223.01
 H       5.243620     0.236591    -1.639747      29.04
 C       3.376104    -1.476257    -1.586459      78.50
 H       2.746453    -2.268144    -1.162824      23.78
 C       2.878796    -1.249274    -3.009251     103.31
 O       3.100959    -2.344988    -3.827132     250.28
 H       4.036436    -2.375257    -4.207267      27.12
 H       3.344617    -0.326116    -3.545037      23.46
 H       1.735788    -1.416938    -2.966912      24.04
 C      -0.673642    -0.567913    -0.134176      40.10
 H      -1.487142    -1.305147     0.062017      19.94
 C      -0.079998     1.824245    -0.026298      59.80
 H      -0.144942     2.792073     0.065399      21.47
 C       1.242820     1.460704    -0.383462      -1.07
 O       2.172987     2.536321    -0.620234     177.95
 C       1.838295     3.807647    -1.284939      81.23
 H       2.832641     4.320759    -1.129941      22.69
 H       1.268724     3.808348    -2.494057      22.30
 H       0.826807     4.168083    -0.807369      22.41
 C       1.645085     0.037265    -0.749844      25.42
 O       3.002353    -0.159491    -0.942962     174.75
 C       0.728969    -0.912476    -0.481816      51.48
 H       0.970012    -2.092311    -0.658282      20.12
 C      -0.996698     0.774822     0.178310      19.37
 C      -2.498989     1.038808     0.886708      63.81
 H      -2.802677    -0.025276     1.084066      23.26
 O      -1.954883     1.680276     2.133775     227.73
 H      -1.410846     0.951008     2.576628      25.98
 C      -3.483501     1.971333     0.007154      84.04
 H      -2.853754     2.955211    -0.337692      22.88
 O      -4.126950     1.240483    -1.069869     272.05
 H      -3.424754     1.018311    -1.704071      27.53
 C      -4.518495     2.583440     1.002019      99.09
 O      -5.677350     3.349680     0.339592     237.52
 H      -5.556352     4.348707     0.504913      27.34
 H      -4.261479     2.986156     2.116240      23.81
 H      -5.055502     1.760062     1.637198      25.61
55
name = lig-etoh-Waterframe_862
 C       5.544751    -0.940785     1.215566      48.00
 H       5.718146     0.065081     1.023496      23.29
 C       4.863741    -3.274185     0.663222      49.62
 H       4.505017    -3.842765    -0.281154      19.96
 C       4.917955    -3.585724     2.001239      31.93
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 O       4.560486    -4.769294     2.511797     268.95
 C       3.422283    -5.346428     1.872136     122.28
 H       2.683786    -4.744688     1.652452      32.46
 H       3.003225    -6.176865     2.510656      25.38
 H       3.923840    -5.798231     0.970737      26.00
 C       5.252957    -2.655872     2.988875       6.23
 O       5.531939    -2.984030     4.292892     185.70
 H       5.335335    -3.917478     4.440215      27.17
 C       5.458453    -1.268983     2.562763      53.69
 H       5.808400    -0.403138     3.294983      23.98
 C       5.137803    -1.926123     0.275877      38.83
 C       4.909334    -1.579402    -1.290559      99.86
 H       5.219794    -2.490403    -1.739487      25.74
 O       5.744939    -0.536732    -1.804599     254.75
 H       5.328775     0.324276    -1.671615      29.64
 C       3.404023    -1.386758    -1.485944      87.47
 H       3.006646    -2.230505    -0.867207      20.29
 C       2.831692    -1.196487    -2.989848      91.38
 O       3.197127    -2.398504    -3.846674     249.60
 H       4.051647    -2.227203    -4.308158      27.49
 H       2.871572    -0.081501    -3.347018      24.97
 H       1.738793    -1.002816    -2.963928      25.53
 C      -0.594313    -0.623647    -0.065959      -3.96
 H      -1.251472    -1.418722    -0.038763      20.51
 C      -0.048540     1.789648     0.014397      49.74
 H      -0.353901     2.760563     0.272885      20.72
 C       1.238646     1.466070    -0.470490      15.42
 O       2.299809     2.567573    -0.587490     177.58
 C       1.767019     3.814219    -1.285878     106.05
 H       2.506659     4.552798    -1.459160      25.14
 H       1.710209     3.493873    -2.487800      22.12
 H       1.123959     4.399517    -0.607500      24.65
 C       1.683067     0.194727    -0.624771      20.33
 O       2.995572    -0.140559    -0.995091     201.15
 C       0.648060    -0.827771    -0.503239      79.98
 H       1.128987    -1.808518    -0.760431      18.75
 C      -1.024045     0.727650     0.222344      67.24
 C      -2.348902     1.025718     0.835436      67.78
 H      -3.070269     0.114790     0.888146      23.07
 O      -2.042112     1.654983     2.101689     210.70
 H      -1.269735     1.127385     2.486528      27.23
 C      -3.426218     1.986364     0.011397      67.14
 H      -2.860388     2.877117    -0.471156      23.29
 O      -4.110448     1.244821    -1.039209     278.89
 H      -3.418412     0.968372    -1.678963      26.75
 C      -4.563261     2.506795     1.114624      68.22
 O      -5.785594     3.345373     0.357249     192.75
 H      -5.417511     4.313367     0.225544      28.23
 H      -3.981389     3.275540     1.818370      22.29
 H      -5.190298     1.604268     1.037615      24.04
55
name = lig-etoh-Waterframe_863
 C       5.445739    -0.970860     1.262068      64.79
 H       5.544314     0.033496     0.807412      23.02
 C       4.879649    -3.282589     0.549839      57.12
 H       4.647005    -4.234006     0.038052      22.19
 C       4.885300    -3.559283     1.972315     -26.12
 O       4.521991    -4.785108     2.550220     294.87
 C       3.409500    -5.409867     1.883446     114.71
 H       2.684440    -4.716435     1.597493      29.28
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 H       2.970683    -5.974284     2.592140      27.07
 H       3.643390    -6.179127     1.026048      25.91
 C       5.339133    -2.576065     2.915052       3.45
 O       5.463628    -2.891433     4.272258      97.17
 H       5.571324    -3.900788     4.504489      17.79
 C       5.450228    -1.252602     2.617398      67.70
 H       5.665567    -0.549635     3.475142      23.39
 C       5.166436    -1.941182     0.280170      40.01
 C       4.887151    -1.573347    -1.267793      90.17
 H       5.145901    -2.532853    -1.977498      23.54
 O       5.681206    -0.512145    -1.833187     238.45
 H       5.555736     0.369818    -1.425589      28.68
 C       3.375276    -1.300700    -1.497374      85.84
 H       2.915608    -2.181442    -0.985235      22.88
 C       2.789875    -1.223002    -2.966123      98.81
 O       3.284165    -2.391762    -3.858533     236.99
 H       4.158234    -2.173119    -4.205775      28.93
 H       3.441778    -0.426059    -3.361467      22.38
 H       1.757241    -1.414062    -2.857190      24.91
 C      -0.610861    -0.625843     0.006099      27.66
 H      -1.133276    -1.484361     0.025824      20.28
 C      -0.050072     1.705995     0.048852      37.99
 H      -0.471904     2.743713     0.443760      19.61
 C       1.319187     1.668551    -0.519713       8.75
 O       2.349179     2.585037    -0.576445     223.74
 C       1.795755     3.788441    -1.293259     112.71
 H       2.594355     4.462935    -1.360864      25.28
 H       1.228244     3.392605    -2.048803      27.83
 H       0.995243     4.248619    -0.804149      27.49
 C       1.691405     0.228923    -0.534378      18.41
 O       2.981556    -0.010007    -0.962330     168.15
 C       0.746840    -0.785257    -0.548721      79.76
 H       0.816394    -1.798130    -0.745560      21.19
 C      -0.991641     0.672535     0.196227      42.25
 C      -2.293349     1.063874     0.766690      77.06
 H      -2.870123     0.118182     0.986048      21.68
 O      -2.155589     1.645102     2.086275     242.40
 H      -1.410584     1.273811     2.661390      27.73
 C      -3.368799     2.028596     0.063843      86.86
 H      -2.927041     2.803505    -0.442720      26.23
 O      -4.062141     1.244364    -0.975681     284.72
 H      -3.540514     1.143920    -1.818598      27.48
 C      -4.652260     2.456115     0.965214      95.63
 O      -5.787202     3.322664     0.415610     242.46
 H      -5.340856     4.140727    -0.067140      29.25
 H      -4.217477     2.966729     1.887165      26.32
 H      -5.060194     1.574206     1.602398      26.46
55
name = lig-etoh-Waterframe_864
 C       5.313951    -0.950515     1.206088      30.25
 H       5.460730     0.169493     0.868614      22.66
 C       4.900553    -3.316437     0.599729      72.69
 H       4.809809    -4.054183    -0.189027      25.56
 C       4.894029    -3.502743     1.937681      -7.50
 O       4.478312    -4.796820     2.555904     154.34
 C       3.343609    -5.539891     1.922988      90.09
 H       2.724453    -4.555725     1.402485      25.15
 H       2.895515    -5.900216     2.758066      26.71
 H       3.605644    -6.214672     1.008863      24.96
 C       5.378809    -2.596464     2.948141       7.45
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 O       5.406833    -2.807269     4.258924      50.77
 H       5.438949    -3.881281     4.490321      14.65
 C       5.493019    -1.216176     2.636441      45.24
 H       5.565505    -0.551645     3.452331      21.66
 C       5.167924    -1.955124     0.135185      24.31
 C       4.869028    -1.531130    -1.228280      95.67
 H       5.078454    -2.484357    -1.995766      22.80
 O       5.640706    -0.453836    -1.851480     163.55
 H       5.549179     0.205042    -1.139494      28.30
 C       3.306220    -1.280402    -1.516873      78.09
 H       2.616185    -1.922584    -0.987701      24.25
 C       2.913043    -1.344336    -2.978132     113.44
 O       3.343340    -2.377176    -3.832032     277.24
 H       4.257577    -2.295980    -4.105594      28.81
 H       3.126577    -0.381453    -3.529628      25.68
 H       1.831940    -1.319441    -3.154311      26.24
 C      -0.534012    -0.654559    -0.023022      32.52
 H      -1.286030    -1.401023     0.223858      19.09
 C       0.027106     1.763067     0.037835      50.01
 H      -0.397928     2.879984     0.387192      21.09
 C       1.306214     1.665143    -0.400226      20.08
 O       2.328883     2.635072    -0.580071     240.48
 C       1.800262     3.755027    -1.273620     111.19
 H       2.716215     4.346303    -1.598446      23.55
 H       1.256975     3.510414    -2.167929      27.64
 H       1.096835     4.189132    -0.558538      24.79
 C       1.712009     0.283666    -0.570811      16.38
 O       3.014008     0.134801    -0.902481     134.30
 C       0.749222    -0.810678    -0.499746      70.49
 H       1.085599    -1.734046    -0.783908      23.49
 C      -0.934878     0.698425     0.159323      53.45
 C      -2.381459     1.082041     0.813140      70.40
 H      -2.744206     0.085515     0.803187      24.01
 O      -2.258700     1.691988     2.113209     251.63
 H      -1.714577     1.047376     2.710108      27.46
 C      -3.402158     2.021240     0.054645      93.41
 H      -2.930717     2.971672    -0.190319      26.80
 O      -4.004357     1.227007    -0.940217     295.19
 H      -3.511796     1.415787    -1.782795      27.61
 C      -4.675166     2.443306     0.904817     112.68
 O      -5.723558     3.241198     0.456554     267.63
 H      -5.285568     4.051423    -0.048577      30.36
 H      -4.353335     3.013766     1.692072      29.07
 H      -5.140544     1.567589     1.440173      28.48
55
name = lig-etoh-Waterframe_865
 C       5.233733    -0.926014     1.145347      49.53
 H       5.256035     0.235318     0.950839      21.76
 C       4.957054    -3.252140     0.567067      54.02
 H       4.752251    -3.983515    -0.197284      25.09
 C       4.908000    -3.584945     2.026390     -13.63
 O       4.457133    -4.774987     2.514398     311.41
 C       3.312404    -5.555368     1.958255      92.97
 H       2.364447    -4.847542     1.367764      24.13
 H       2.753466    -6.134564     2.718257      26.18
 H       3.787181    -6.350000     1.365242      26.18
 C       5.342053    -2.569764     2.954325       2.28
 O       5.368638    -2.788588     4.310180     123.13
 H       5.113188    -3.776022     4.660427      15.94
 C       5.518012    -1.223882     2.477364      57.69
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 H       5.617392    -0.427548     3.095596      24.72
 C       5.143295    -1.919654     0.167493      28.21
 C       4.791339    -1.521435    -1.321968      97.82
 H       5.109958    -2.432693    -1.854386      24.99
 O       5.594398    -0.402523    -1.815503     218.77
 H       5.588465     0.470174    -1.335166      25.75
 C       3.307171    -1.215448    -1.471405      77.73
 H       2.907442    -1.950889    -0.768004      26.81
 C       2.978788    -1.301946    -3.079729     105.61
 O       3.428766    -2.449493    -3.800684     275.17
 H       4.320836    -2.303494    -4.219327      26.05
 H       3.110878    -0.285214    -3.383887      27.10
 H       1.814737    -1.385874    -3.083344      26.72
 C      -0.518879    -0.574076    -0.055223      25.04
 H      -1.235916    -1.490404     0.183596      21.28
 C      -0.008275     1.900834     0.046364      57.88
 H      -0.312166     3.037856     0.213698      19.79
 C       1.341056     1.542742    -0.245345      20.70
 O       2.283596     2.625519    -0.573644     184.01
 C       1.774071     3.781607    -1.256582     103.15
 H       2.710900     4.495033    -1.612007      25.08
 H       1.381648     3.501001    -2.396236      23.67
 H       1.461408     4.663897    -0.578425      23.65
 C       1.684261     0.310012    -0.647423      17.80
 O       3.082935     0.172530    -0.908933     139.99
 C       0.820032    -0.840335    -0.440620      55.08
 H       1.207314    -1.786687    -0.673934      24.27
 C      -0.929592     0.824545     0.186326      39.16
 C      -2.430487     1.075479     0.856294      72.65
 H      -3.064659     0.203825     0.910833      26.09
 O      -2.331772     1.719878     2.167104     218.46
 H      -2.116960     0.950082     2.830060      26.00
 C      -3.486475     1.996687     0.082021      82.40
 H      -2.889651     2.995841    -0.301903      24.52
 O      -3.944780     1.214038    -0.998420     280.82
 H      -3.444944     1.267333    -1.865703      27.27
 C      -4.602577     2.406434     1.033680     103.58
 O      -5.695509     3.168969     0.390765     231.13
 H      -5.416880     4.180235     0.191786      28.57
 H      -4.034311     3.003773     1.781770      25.61
 H      -5.120484     1.513992     0.998819      28.30
55
name = lig-etoh-Waterframe_866
 C       5.224303    -0.863795     1.090613      62.28
 H       5.044619     0.176466     0.684846      21.80
 C       5.001277    -3.213708     0.615845      73.16
 H       4.682043    -4.028883     0.001263      25.93
 C       4.932825    -3.572725     1.986793     -18.98
 O       4.414103    -4.796409     2.509505     271.79
 C       3.328648    -5.584553     1.976258     114.73
 H       2.445541    -5.072790     1.446726      27.57
 H       3.016679    -6.117602     3.011901      23.77
 H       3.722206    -6.277300     1.323595      28.48
 C       5.260470    -2.556958     2.948957      -5.44
 O       5.332548    -2.737922     4.372655     103.77
 H       5.317117    -3.767295     4.605492      16.00
 C       5.513333    -1.275166     2.360154      67.62
 H       5.776279    -0.477074     3.023609      24.30
 C       5.054223    -1.862113     0.165431      20.18
 C       4.812962    -1.477170    -1.335953     113.60
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 H       4.963923    -2.194797    -2.008723      26.29
 O       5.586439    -0.376127    -1.808058     235.52
 H       5.154128     0.497488    -1.456197      23.95
 C       3.399706    -1.158897    -1.480397      87.10
 H       2.880648    -1.977529    -0.957307      26.29
 C       2.922076    -1.199072    -3.072133      83.04
 O       3.528919    -2.520984    -3.770284     212.76
 H       4.315825    -2.248439    -4.371872      24.41
 H       3.534791    -0.476141    -3.595456      24.16
 H       1.838242    -1.516084    -3.123706      24.92
 C      -0.507029    -0.388602    -0.055761      27.03
 H      -1.191770    -1.378797    -0.003266      21.68
 C      -0.068853     1.965973     0.078133      60.70
 H      -0.283300     2.983619     0.150351      21.98
 C       1.315266     1.651088    -0.180933       4.29
 O       2.235317     2.576849    -0.536184     150.47
 C       1.842859     3.895555    -1.283865      69.29
 H       2.929237     4.081489    -1.536892      22.86
 H       0.878731     3.534635    -1.997125      22.74
 H       1.062214     4.591803    -0.759297      22.76
 C       1.744003     0.203741    -0.662018       5.00
 O       3.091639     0.104191    -0.975065     178.63
 C       0.861893    -0.804063    -0.398162      60.18
 H       0.901890    -1.898826    -0.434076      23.57
 C      -1.025786     0.898129     0.269936      26.37
 C      -2.455305     1.115516     0.877275      81.37
 H      -2.905095     0.089778     1.088678      23.48
 O      -2.365832     1.712756     2.230196     200.27
 H      -2.233110     1.082788     3.039119      25.54
 C      -3.426856     1.992923     0.069870      82.20
 H      -2.975863     2.943843    -0.502237      23.86
 O      -3.942175     1.186399    -1.089661     250.12
 H      -3.171415     1.088685    -1.772590      26.10
 C      -4.564337     2.372695     1.073545      93.03
 O      -5.660229     3.126471     0.317141     202.50
 H      -5.540462     4.171960     0.502183      26.45
 H      -4.290129     2.585502     2.262548      23.89
 H      -5.012060     1.403302     1.543041      26.93
55
name = lig-etoh-Waterframe_867
 C       5.226331    -0.834147     1.007511      33.72
 H       5.247272     0.253572     0.810128      21.41
 C       4.973263    -3.223895     0.632000      72.29
 H       4.785556    -3.984543    -0.124006      25.38
 C       4.914987    -3.517913     1.976408      15.14
 O       4.431298    -4.784036     2.518045     293.07
 C       3.377819    -5.649140     1.995152     108.13
 H       2.668466    -5.060382     1.769092      35.54
 H       2.930968    -6.177700     3.008436      24.07
 H       3.597199    -6.301576     1.178378      27.83
 C       5.210868    -2.557690     2.962131       9.67
 O       5.310960    -2.662443     4.341064      91.75
 H       5.484709    -3.532314     4.693929      15.15
 C       5.499832    -1.268182     2.428943      28.81
 H       5.905053    -0.598851     3.282724      21.51
 C       4.983903    -1.877233     0.080533      19.46
 C       4.902951    -1.467750    -1.319425     114.30
 H       5.071562    -2.309906    -1.979402      25.58
 O       5.612855    -0.325645    -1.819864     225.79
 H       5.125320     0.545506    -1.495897      22.62
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 C       3.382161    -1.207575    -1.633604      97.91
 H       2.676129    -1.915824    -1.197358      26.10
 C       2.980460    -1.240843    -3.064338     101.61
 O       3.556512    -2.538616    -3.705964     226.34
 H       4.453922    -2.291904    -4.235617      23.23
 H       3.275762    -0.368257    -3.801907      24.38
 H       1.955532    -0.935193    -3.316388      25.82
 C      -0.515480    -0.255539    -0.024256      35.94
 H      -1.353652    -1.024143     0.037671      22.27
 C      -0.075067     1.983625     0.132386      59.05
 H      -0.352131     2.904280     0.283553      24.00
 C       1.224703     1.652852    -0.267487      14.50
 O       2.214389     2.608258    -0.495525     191.58
 C       1.835247     3.880369    -1.265692     101.44
 H       2.624829     4.323572    -1.812075      25.15
 H       1.303104     3.562760    -2.189432      24.89
 H       1.614598     4.610460    -0.415450      22.09
 C       1.778106     0.275190    -0.525472       5.39
 O       3.049243     0.057458    -1.034087     171.59
 C       0.748359    -0.727625    -0.345086      60.04
 H       0.950275    -1.872617    -0.440038      22.31
 C      -1.062615     0.949913     0.334094      52.05
 C      -2.409662     1.125968     0.941552      68.59
 H      -2.799905     0.021900     0.868437      24.25
 O      -2.375127     1.731097     2.296020     209.45
 H      -1.947035     0.936432     2.836754      24.88
 C      -3.384579     1.963014     0.040938      81.70
 H      -2.915809     2.906803    -0.191435      26.33
 O      -3.945972     1.172564    -1.120444     253.89
 H      -3.111118     0.948364    -1.697690      26.02
 C      -4.630969     2.295464     1.057037      80.61
 O      -5.588296     3.062944     0.312006     195.09
 H      -5.566880     4.056122     0.670548      27.38
 H      -4.299515     3.219250     1.830562      23.30
 H      -5.144897     1.263961     1.383032      25.81
55
name = lig-etoh-Waterframe_868
 C       5.274283    -0.894544     1.125874      72.33
 H       5.591782     0.056250     0.818715      24.93
 C       4.882514    -3.212504     0.518122      53.73
 H       4.887763    -4.107300    -0.160008      23.53
 C       4.810501    -3.551143     2.019391     -26.31
 O       4.536477    -4.778501     2.531923     417.74
 C       3.395584    -5.643664     2.025122     107.20
 H       2.526503    -4.958595     1.838034      28.60
 H       3.176127    -6.494781     2.774627      25.45
 H       3.741092    -6.314097     1.098520      28.67
 C       5.212764    -2.490906     2.943387      10.40
 O       5.302763    -2.582894     4.288739      14.47
 H       5.262489    -3.572213     4.587692      14.04
 C       5.453310    -1.207673     2.450542      52.94
 H       5.822199    -0.382140     3.221361      21.83
 C       5.010762    -1.866125     0.132079      25.70
 C       4.884037    -1.503430    -1.408238      86.59
 H       5.563788    -2.404219    -1.879912      23.09
 O       5.659437    -0.283513    -1.835408     156.06
 H       5.502892     0.631727    -1.334475      23.88
 C       3.312299    -1.300231    -1.748134      70.31
 H       2.905796    -2.160537    -1.204412      24.19
 C       3.079575    -1.255298    -3.241670     107.07
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 O       3.511056    -2.507613    -3.638233     256.16
 H       4.478176    -2.325672    -3.994492      25.57
 H       3.730041    -0.305526    -3.537408      22.73
 H       1.970734    -1.309045    -3.226613      25.28
 C      -0.654737    -0.304944     0.047134      27.05
 H      -1.313004    -1.105274     0.139417      20.35
 C      -0.070287     2.025120     0.199875      40.65
 H      -0.253746     3.065523     0.463823      21.42
 C       1.229251     1.633091    -0.407394      13.67
 O       2.235262     2.694332    -0.491888     215.33
 C       1.870551     3.831550    -1.227559     137.68
 H       2.737999     4.267448    -1.673038      25.64
 H       1.089290     3.752081    -1.863563      30.16
 H       1.625554     4.662431    -0.574775      26.74
 C       1.669767     0.349155    -0.375428      23.77
 O       2.976756     0.081159    -1.068080      99.49
 C       0.686022    -0.586401    -0.303975      60.23
 H       0.925062    -1.704194    -0.595263      20.47
 C      -0.969846     1.053263     0.374357      30.71
 C      -2.384871     1.124246     0.958554      78.27
 H      -2.935291     0.161858     1.114979      23.99
 O      -2.352271     1.703334     2.316874     245.04
 H      -1.621206     1.186051     2.864991      26.13
 C      -3.426026     1.900784     0.097098      94.31
 H      -2.987037     2.777784    -0.195182      27.19
 O      -3.912024     1.200846    -1.063179     281.49
 H      -3.336859     0.951722    -1.904006      23.99
 C      -4.634615     2.287685     0.944895     116.94
 O      -5.584815     3.004570     0.278417     255.50
 H      -5.585820     4.023695     0.574415      28.30
 H      -4.016893     2.778307     1.707046      27.35
 H      -5.127174     1.377939     1.387066      28.68
55
name = lig-etoh-Waterframe_869
 C       5.362851    -0.912709     1.148448      66.47
 H       5.676246    -0.027694     0.779399      27.37
 C       4.771503    -3.236103     0.562680      56.45
 H       4.732158    -4.036180    -0.248552      22.81
 C       4.737056    -3.477249     1.937377      -6.40
 O       4.625746    -4.836898     2.552954     247.38
 C       3.472096    -5.618668     2.040559     112.32
 H       2.298624    -5.109381     1.824713      24.48
 H       3.446637    -6.359566     2.758843      26.86
 H       3.859890    -5.864903     0.924794      28.20
 C       5.176841    -2.457966     2.876481       8.56
 O       5.302392    -2.562795     4.271100      40.88
 H       5.117998    -3.578962     4.496488      16.28
 C       5.411869    -1.139037     2.502832      63.95
 H       5.645505    -0.218472     3.167829      22.80
 C       5.050553    -1.863964     0.155551      18.97
 C       4.888449    -1.453823    -1.403500      82.97
 H       5.356898    -2.286081    -2.204652      21.71
 O       5.707693    -0.273950    -1.847745     144.05
 H       5.400241     0.406426    -1.136466      27.03
 C       3.341482    -1.325524    -1.720627      66.48
 H       2.770241    -2.198347    -1.327379      24.00
 C       3.096122    -1.205454    -3.296058     100.04
 O       3.515032    -2.535823    -3.665643     242.44
 H       4.452016    -2.567949    -4.068156      28.24
 H       3.777745    -0.495623    -3.820220      23.99
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 H       2.050363    -1.164391    -3.754212      24.98
 C      -0.726271    -0.364234     0.124636      24.22
 H      -1.359233    -1.138397     0.242858      21.46
 C       0.058019     2.107010     0.201284      36.41
 H      -0.109119     3.266233     0.590863      21.39
 C       1.253332     1.815422    -0.396702      19.41
 O       2.249423     2.692226    -0.492260     246.79
 C       1.894575     3.913310    -1.195719     105.59
 H       2.898867     3.983384    -1.795632      22.25
 H       0.938245     3.678508    -1.710190      27.22
 H       1.542574     4.682785    -0.559398      26.81
 C       1.661933     0.364647    -0.424313      14.66
 O       2.863669     0.074377    -1.076944     107.08
 C       0.574316    -0.575762    -0.263661      54.95
 H       0.886208    -1.602142    -0.630756      22.25
 C      -1.014529     0.992770     0.427422      21.28
 C      -2.396652     1.133289     1.012983      79.76
 H      -2.616451     0.100612     1.128686      25.88
 O      -2.305717     1.700771     2.322317     271.24
 H      -1.568629     1.335098     2.948484      27.69
 C      -3.423656     1.876866     0.096282      98.75
 H      -2.980265     2.848652    -0.325758      24.84
 O      -3.912445     1.186937    -1.003830     276.02
 H      -3.211003     1.307392    -1.758968      24.84
 C      -4.553676     2.231333     0.936638     116.93
 O      -5.662433     3.006249     0.202338     224.39
 H      -5.485027     4.062139     0.301758      28.19
 H      -4.293254     2.586765     1.846026      29.96
 H      -5.034953     1.425448     1.373774      30.72
55
name = lig-etoh-Waterframe_870
 C       5.452482    -0.864767     1.024305      32.69
 H       5.555064     0.122978     0.749069      24.59
 C       4.680990    -3.180569     0.582958      75.31
 H       4.321102    -3.975900    -0.133026      25.02
 C       4.740495    -3.453029     1.955612      16.27
 O       4.662855    -4.794902     2.533465     283.83
 C       3.597130    -5.595328     2.003348     123.54
 H       2.583642    -4.945647     2.349072      25.19
 H       3.514477    -6.458537     2.517003      27.54
 H       3.650118    -5.973573     0.936862      27.48
 C       5.106646    -2.422563     2.899426       3.48
 O       5.284578    -2.609150     4.218261      73.29
 H       5.423552    -3.576119     4.696247      18.39
 C       5.376892    -1.087795     2.506338      25.34
 H       5.540354    -0.428531     3.371440      20.36
 C       5.079625    -1.907152     0.110861      19.35
 C       4.904039    -1.398272    -1.354386      88.81
 H       4.961729    -2.282885    -2.008264      25.86
 O       5.689411    -0.301172    -1.798464     191.48
 H       5.429729     0.637357    -1.427354      23.48
 C       3.338474    -1.191075    -1.711364      78.64
 H       2.672753    -2.006870    -1.348050      27.27
 C       3.115566    -1.180350    -3.309483      99.01
 O       3.531502    -2.623415    -3.765694     241.93
 H       4.380588    -2.353435    -4.271583      26.19
 H       3.751797    -0.528080    -3.809715      27.00
 H       2.194474    -0.668013    -3.638207      27.40
 C      -0.720333    -0.326338     0.203318      32.17
 H      -1.476110    -1.073424     0.356710      21.11
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 C       0.007715     2.071704     0.232946      93.11
 H      -0.263657     3.241656     0.604569      19.08
 C       1.301266     1.801864    -0.257440      15.41
 O       2.325093     2.718500    -0.501508     196.14
 C       1.897704     3.995218    -1.181619      81.46
 H       2.626664     4.466709    -2.073716      24.13
 H       1.117781     3.636992    -2.025676      22.80
 H       2.001335     4.819352    -0.431061      21.99
 C       1.545286     0.379135    -0.587303      17.70
 O       2.793042     0.034039    -1.083570     159.44
 C       0.616171    -0.645242    -0.292520      58.74
 H       0.763638    -1.674804    -0.467022      23.28
 C      -0.997774     0.996692     0.444192      41.08
 C      -2.351749     1.113985     1.065156      70.37
 H      -2.850684     0.144901     1.075747      26.20
 O      -2.282943     1.765674     2.361579     239.81
 H      -1.687218     1.043496     2.805416      25.77
 C      -3.360842     1.934362     0.116196      72.05
 H      -2.755462     2.954623    -0.177456      25.15
 O      -3.910082     1.129759    -0.980555     247.98
 H      -3.235879     1.173753    -1.780009      24.66
 C      -4.639785     2.218931     1.010476      87.07
 O      -5.701958     3.005672     0.169154     174.90
 H      -5.275785     3.977996     0.023123      29.18
 H      -4.535080     3.024629     1.853829      24.97
 H      -5.101109     1.250507     0.984853      27.85
55
name = lig-etoh-Waterframe_871
 C       5.479380    -0.835274     1.042311      61.23
 H       5.491775     0.135184     0.553010      22.71
 C       4.607700    -3.110076     0.582679      53.42
 H       4.098575    -3.862090    -0.012382      22.79
 C       4.782953    -3.446070     2.021802      25.80
 O       4.715514    -4.708905     2.477205     266.37
 C       3.654978    -5.585404     2.005170     125.93
 H       2.728383    -5.114629     2.290031      27.36
 H       3.760090    -6.597314     2.496457      25.34
 H       3.577774    -5.635696     0.988799      27.81
 C       5.062010    -2.409517     2.900887       9.95
 O       5.284128    -2.659721     4.231824     136.83
 H       5.366918    -3.667695     4.345622      22.40
 C       5.342562    -1.095218     2.357928      58.53
 H       5.559423    -0.413150     3.089789      24.88
 C       5.102291    -1.847887     0.084110       3.92
 C       4.790795    -1.392601    -1.307792      90.78
 H       5.174456    -2.117930    -1.888549      25.73
 O       5.675931    -0.330405    -1.743117     207.29
 H       5.338725     0.610831    -1.627978      25.50
 C       3.271470    -1.054336    -1.727514      94.58
 H       2.885742    -1.997469    -1.299448      27.77
 C       3.199416    -1.158214    -3.285790      98.52
 O       3.503571    -2.590951    -3.889457     232.92
 H       4.330020    -2.356646    -4.393282      27.06
 H       4.002486    -0.567413    -3.562419      24.49
 H       2.112495    -1.105697    -3.379189      26.56
 C      -0.574041    -0.310730     0.218893      33.39
 H      -1.374153    -1.095857     0.503846      21.57
 C      -0.079434     2.010509     0.293967      59.25
 H      -0.443400     3.084617     0.514636      20.50
 C       1.298750     1.674787    -0.149829     -16.14
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 O       2.407864     2.771293    -0.539316     103.56
 C       1.946856     4.049281    -1.232936      81.50
 H       2.912277     4.292016    -1.775881      23.22
 H       0.768587     4.146361    -1.508187      22.86
 H       1.693875     4.856366    -0.385065      22.59
 C       1.438057     0.348343    -0.736294       7.75
 O       2.795494     0.065379    -1.108044     169.18
 C       0.597474    -0.717529    -0.323245      61.71
 H       0.903326    -1.682303    -0.423660      23.88
 C      -0.961640     1.024504     0.473003      27.84
 C      -2.379996     1.182145     1.055366      80.88
 H      -2.947187     0.241818     1.270287      23.35
 O      -2.251550     1.803396     2.404542     210.64
 H      -1.986818     1.147018     3.164006      24.82
 C      -3.334550     2.000049     0.219217      70.50
 H      -2.870538     2.937421    -0.299695      24.87
 O      -3.864903     1.100929    -0.937455     234.58
 H      -3.392051     0.817186    -1.796677      25.62
 C      -4.784477     2.292916     0.937115      85.71
 O      -5.698973     2.992466     0.174726     220.98
 H      -5.229447     3.886274    -0.171323      28.13
 H      -4.448358     2.720481     2.170439      24.09
 H      -5.223588     1.228601     1.251058      26.03
55
name = lig-etoh-Waterframe_872
 C       5.423625    -0.844622     0.973965      62.84
 H       5.629355     0.139368     0.621719      23.52
 C       4.586581    -3.024258     0.631942      91.05
 H       4.196744    -3.662887    -0.098763      23.82
 C       4.793438    -3.362362     1.914965      12.32
 O       4.784140    -4.689753     2.456817     250.15
 C       3.655848    -5.554339     2.000058     115.76
 H       2.740006    -5.440086     2.339592      29.03
 H       4.113049    -6.607690     2.490446      24.54
 H       3.759917    -5.499450     0.948529      29.51
 C       5.089168    -2.377362     2.881171       7.20
 O       5.289452    -2.662285     4.222031     136.31
 H       5.105059    -3.589037     4.573119      21.58
 C       5.340791    -1.109769     2.354804      52.81
 H       5.572031    -0.241584     2.846201      23.44
 C       5.012507    -1.804552     0.133550      20.97
 C       4.708422    -1.369883    -1.323555      94.92
 H       4.988939    -2.207007    -2.027412      24.51
 O       5.677167    -0.331242    -1.704323     201.31
 H       5.280789     0.531682    -1.422779      26.45
 C       3.288383    -1.159288    -1.706596      87.19
 H       2.606896    -1.945694    -1.338910      25.45
 C       3.239019    -1.196352    -3.243751     107.34
 O       3.478578    -2.464168    -3.981588     278.56
 H       4.377425    -2.492499    -4.329056      28.85
 H       3.725847    -0.316239    -3.798086      24.68
 H       2.251161    -1.011469    -3.785626      26.03
 C      -0.547358    -0.354670     0.271162      30.88
 H      -1.170112    -1.288836     0.703564      20.90
 C      -0.004922     2.031710     0.317881      53.38
 H      -0.241115     2.991869     0.490048      22.27
 C       1.251359     1.664716    -0.189435      -7.90
 O       2.354770     2.737133    -0.563428     120.06
 C       1.961959     4.096262    -1.132212      96.57
 H       2.678429     4.272422    -1.842924      27.16
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 H       1.072062     3.922753    -1.840933      25.19
 H       2.072834     4.832439    -0.260421      23.68
 C       1.491770     0.333109    -0.773150      13.69
 O       2.803045     0.188719    -1.152189     120.15
 C       0.632757    -0.754269    -0.410413      57.84
 H       0.928734    -1.760181    -0.500624      22.95
 C      -1.014725     0.939401     0.520602      34.88
 C      -2.397996     1.267044     1.140323      73.58
 H      -2.700399     0.166805     1.174443      23.77
 O      -2.230152     1.869208     2.451992     231.81
 H      -2.130516     1.149859     3.165649      25.05
 C      -3.452345     2.017263     0.211352      95.66
 H      -3.073669     2.928358    -0.150781      27.73
 O      -3.824078     1.078941    -0.846626     283.48
 H      -3.025901     1.087509    -1.455811      27.80
 C      -4.764750     2.289712     0.928384      97.50
 O      -5.717651     3.013984     0.181802     239.66
 H      -5.340607     3.937588    -0.192472      29.02
 H      -4.622660     2.862164     1.937041      26.23
 H      -5.413458     1.311033     1.207082      25.54
55
name = lig-etoh-Waterframe_873
 C       5.341803    -0.829845     0.998507      51.50
 H       5.549312     0.204916     0.611595      21.86
 C       4.555674    -3.012728     0.550076      63.16
 H       4.350649    -3.807871    -0.128148      24.93
 C       4.797666    -3.351359     1.925910      13.48
 O       4.798579    -4.652605     2.441874     266.24
 C       3.758338    -5.549107     1.990114     113.85
 H       2.795885    -5.391319     2.550321      26.28
 H       4.091449    -6.724229     2.167149      24.01
 H       3.622942    -5.734962     0.811775      26.03
 C       5.161857    -2.361757     2.885367       8.55
 O       5.292990    -2.607798     4.202101     179.77
 H       5.084562    -3.477675     4.581872      22.86
 C       5.395661    -1.033246     2.406316      43.81
 H       5.578126    -0.271746     3.210657      21.22
 C       4.834381    -1.749213     0.064121      39.40
 C       4.760719    -1.408575    -1.333693     102.12
 H       4.879227    -2.438803    -1.978706      23.40
 O       5.638565    -0.323211    -1.678622     218.38
 H       5.461441     0.531678    -1.267803      25.69
 C       3.257375    -1.224821    -1.715497      64.46
 H       2.535253    -1.908332    -1.257795      22.37
 C       3.151661    -1.160862    -3.353306      86.10
 O       3.496794    -2.348406    -4.024742     285.82
 H       4.424559    -2.178948    -4.208278      29.27
 H       3.954831    -0.262929    -3.674683      21.98
 H       2.067665    -0.759403    -3.415884      24.87
 C      -0.592803    -0.450005     0.330730      35.82
 H      -1.196555    -1.350431     0.738984      18.00
 C       0.038241     1.982223     0.322415      54.19
 H      -0.053163     2.938875     0.586208      23.73
 C       1.239814     1.752608    -0.372112      17.99
 O       2.218578     2.634643    -0.563130     221.35
 C       1.998022     4.037230    -1.038827     118.07
 H       2.731831     4.334585    -1.761160      25.26
 H       1.148273     4.014471    -1.613390      28.41
 H       2.067751     4.841687    -0.343616      25.92
 C       1.597021     0.346035    -0.682887      14.92
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 O       2.855066     0.259970    -1.265578     115.94
 C       0.686232    -0.694097    -0.484552      65.00
 H       0.772704    -1.791877    -0.671092      20.39
 C      -0.975134     0.953378     0.558827      38.11
 C      -2.366366     1.268135     1.235706      64.32
 H      -3.016250     0.344953     1.407708      22.09
 O      -2.236196     1.952878     2.495246     252.00
 H      -1.904825     1.196321     3.052133      26.27
 C      -3.556280     1.984108     0.226297      92.89
 H      -3.181683     2.908660    -0.096139      26.08
 O      -3.749352     1.076468    -0.766869     299.35
 H      -2.949029     1.124828    -1.356957      25.65
 C      -4.768246     2.294859     1.008511     107.88
 O      -5.780857     3.063007     0.152137     261.14
 H      -5.429037     4.067968     0.022669      29.07
 H      -4.503858     2.834856     1.716885      30.55
 H      -5.218935     1.302898     1.076236      27.79
55
name = lig-etoh-Waterframe_874
 C       5.223505    -0.736270     1.095503      54.06
 H       5.439788     0.313853     0.705709      20.53
 C       4.537686    -3.100010     0.509019      58.17
 H       4.403902    -3.993577    -0.135242      20.05
 C       4.794109    -3.336304     1.930416      11.05
 O       4.804001    -4.635472     2.413072     286.50
 C       3.844661    -5.624887     1.948646     103.30
 H       2.875489    -5.218397     2.609459      22.62
 H       4.198888    -6.588739     2.379342      21.44
 H       3.419018    -5.315964     0.880541      20.15
 C       5.221088    -2.333396     2.837082      10.23
 O       5.313906    -2.541156     4.232653     137.62
 H       5.242195    -3.489723     4.310397      20.64
 C       5.447750    -1.011760     2.436587      55.93
 H       5.717465    -0.267182     3.324880      21.13
 C       4.726740    -1.705033     0.116635      27.04
 C       4.744674    -1.451186    -1.391790     125.63
 H       5.501129    -2.187770    -1.876435      26.33
 O       5.616548    -0.336505    -1.705609     227.76
 H       5.291971     0.421492    -1.227393      28.47
 C       3.244552    -1.138602    -1.822131      89.86
 H       2.766446    -1.920948    -1.240334      20.77
 C       3.028736    -1.022060    -3.346685      94.86
 O       3.531135    -2.250408    -4.056692     283.84
 H       4.395218    -2.051914    -4.478298      29.98
 H       3.882096    -0.243184    -3.498934      20.68
 H       1.943356    -0.867364    -3.614376      24.62
 C      -0.551477    -0.422039     0.295645      22.68
 H      -1.243794    -1.206242     0.445205      18.24
 C       0.018500     1.924891     0.300101      43.55
 H      -0.212918     2.959228     0.781954      19.21
 C       1.165088     1.691183    -0.507618      32.42
 O       2.169015     2.624699    -0.576235     234.35
 C       2.001057     3.954893    -0.988646     110.95
 H       3.079194     4.095624    -1.514541      20.75
 H       1.021143     4.215732    -1.300346      26.24
 H       1.899926     4.516067    -0.081185      25.54
 C       1.674361     0.399033    -0.624198       9.66
 O       2.915774     0.224674    -1.400991     160.59
 C       0.603672    -0.619334    -0.415664      51.58
 H       0.906130    -1.611821    -0.956590      17.39
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 C      -0.919961     0.904091     0.623404      26.78
 C      -2.386967     1.271079     1.284335      74.19
 H      -2.815213     0.322137     1.630372      21.17
 O      -2.230690     2.028705     2.549342     288.13
 H      -1.646055     1.655445     3.206917      28.69
 C      -3.445937     2.003171     0.320870      73.24
 H      -3.065075     2.988419    -0.210331      22.03
 O      -3.698961     1.035014    -0.752800     298.00
 H      -3.133654     0.879127    -1.556911      23.94
 C      -4.866045     2.312106     1.021085      99.85
 O      -5.815494     3.089583     0.157319     273.53
 H      -5.600113     4.124574     0.317500      27.33
 H      -4.490627     2.771440     2.073362      25.42
 H      -5.344938     1.505783     1.477149      28.70
55
name = lig-etoh-Waterframe_875
 C       5.061069    -0.674611     1.117746      63.16
 H       5.158865     0.442505     0.788231      21.34
 C       4.574360    -3.079532     0.580825      45.74
 H       4.373356    -3.810998    -0.262647      19.53
 C       4.789379    -3.338481     1.864736      18.61
 O       4.857746    -4.641386     2.404486     295.51
 C       3.827491    -5.588660     1.981690     146.52
 H       2.803131    -5.695626     2.615135      25.06
 H       4.222487    -6.491084     2.086882      27.10
 H       3.743063    -5.631891     0.835954      28.55
 C       5.250019    -2.310851     2.852824      17.47
 O       5.349335    -2.525049     4.225612     137.18
 H       5.417536    -3.433988     4.521465      16.21
 C       5.468769    -1.020634     2.438232      48.21
 H       5.943425    -0.138893     3.069169      19.13
 C       4.696555    -1.728075     0.241398      24.09
 C       4.767804    -1.405093    -1.432752      84.99
 H       5.052433    -2.362936    -1.917348      24.09
 O       5.607913    -0.311586    -1.744834     305.11
 H       5.215881     0.506919    -1.455346      25.94
 C       3.272929    -1.099338    -1.932845     102.35
 H       2.553700    -1.828458    -1.511562      23.27
 C       3.000637    -0.942420    -3.373294     118.34
 O       3.527426    -2.152854    -4.079766     298.69
 H       4.401712    -1.962988    -4.536373      28.54
 H       3.223639    -0.013224    -3.757135      25.85
 H       2.066880    -0.812021    -3.827669      25.45
 C      -0.571195    -0.364054     0.234331       4.72
 H      -1.219409    -1.126187     0.121433      16.97
 C      -0.063917     1.882561     0.279588      64.50
 H      -0.306594     3.078219     0.629955      19.02
 C       1.124621     1.642384    -0.481954      48.23
 O       2.175718     2.587408    -0.618657     220.23
 C       1.982855     3.961195    -0.851268     104.61
 H       2.889745     4.450427    -1.630414      20.42
 H       1.128890     4.167615    -1.732862      22.45
 H       2.165938     4.459429     0.130763      22.77
 C       1.642849     0.341256    -0.683510      32.03
 O       2.900514     0.183557    -1.446509     191.15
 C       0.701441    -0.571875    -0.393951      77.21
 H       0.712188    -1.671305    -0.851146      17.31
 C      -0.937463     0.906176     0.708069      43.84
 C      -2.330802     1.255852     1.378725      77.82
 H      -2.685287     0.261208     1.522795      23.66
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 O      -2.226144     2.146439     2.578526     301.82
 H      -1.597650     1.675279     3.122345      27.34
 C      -3.324938     1.963126     0.374327      58.55
 H      -2.827294     3.039844     0.037270      22.40
 O      -3.702059     0.972845    -0.731546     248.99
 H      -3.091605     1.074744    -1.492029      25.17
 C      -4.902430     2.352108     1.043011      75.86
 O      -5.799864     3.089793     0.222991     234.34
 H      -5.785437     4.132342     0.387900      27.24
 H      -4.730771     3.190083     2.103210      22.62
 H      -5.521881     1.467848     1.315657      26.23
55
name = lig-etoh-Waterframe_876
 C       4.924041    -0.674237     1.136630      57.94
 H       4.941025     0.393367     0.693143      22.50
 C       4.610913    -2.978397     0.585695      46.52
 H       4.355057    -3.791822    -0.188016      21.41
 C       4.849718    -3.356595     1.993049      20.66
 O       4.875261    -4.671133     2.414223     237.67
 C       3.847549    -5.627077     1.975567     129.30
 H       2.884962    -5.529692     2.531633      25.58
 H       4.358511    -6.562557     2.074357      24.29
 H       3.653751    -5.546171     0.951045      28.21
 C       5.242866    -2.366355     2.879138      13.23
 O       5.409336    -2.538468     4.221441     189.63
 H       5.445246    -3.424078     4.579906      23.43
 C       5.452598    -0.975511     2.367139      48.26
 H       5.972734    -0.284474     3.107710      20.58
 C       4.699527    -1.651272     0.164893      34.55
 C       4.678844    -1.356966    -1.374585      97.25
 H       4.864535    -2.226568    -1.905662      23.45
 O       5.628604    -0.295347    -1.798232     307.85
 H       5.278697     0.575659    -1.678249      27.83
 C       3.267579    -1.086523    -1.971660      70.47
 H       2.585532    -1.935990    -1.737109      21.45
 C       2.990043    -0.898046    -3.566639     103.63
 O       3.512314    -2.051229    -4.124205     282.16
 H       4.540573    -1.882211    -4.235624      26.22
 H       3.349762     0.015009    -3.985202      23.89
 H       1.889714    -1.112306    -3.352740      22.59
 C      -0.598931    -0.339258     0.172664      50.94
 H      -1.271470    -1.159630     0.138637      18.91
 C      -0.079512     1.943285     0.251001      76.16
 H      -0.274143     3.151683     0.318067      16.97
 C       1.176309     1.670110    -0.358102      20.06
 O       2.198082     2.518650    -0.684816     187.82
 C       1.991975     4.048409    -0.785630      80.26
 H       2.894324     4.344260    -1.360323      22.83
 H       0.852642     4.171190    -1.363164      22.10
 H       1.809118     4.826587     0.066559      22.98
 C       1.625089     0.323083    -0.824252      12.05
 O       2.801819     0.217480    -1.386530     175.26
 C       0.717763    -0.698290    -0.395572      50.64
 H       0.825163    -1.807614    -0.608226      19.21
 C      -0.993126     0.932796     0.751440      27.58
 C      -2.275114     1.241868     1.449604      92.02
 H      -2.839963     0.389821     1.864236      21.10
 O      -2.202355     2.219357     2.561843     280.63
 H      -1.833269     1.683486     3.267319      26.61
 C      -3.339055     1.884460     0.434204      68.17
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 H      -2.788885     2.777366    -0.016205      23.98
 O      -3.687470     0.976849    -0.663783     266.47
 H      -3.036123     1.120854    -1.366648      26.20
 C      -4.850672     2.409670     1.074699      83.29
 O      -5.791955     3.091366     0.256378     273.44
 H      -5.614405     4.140171     0.260216      26.31
 H      -4.455230     2.959362     2.138987      23.42
 H      -5.181348     1.329505     1.150283      26.18
55
name = lig-etoh-Waterframe_877
 C       4.867728    -0.634047     1.102340      39.84
 H       4.934560     0.453353     0.774432      22.38
 C       4.659641    -2.930356     0.634973      54.77
 H       4.487089    -3.820798    -0.012287      23.16
 C       4.886308    -3.349921     1.995858      14.57
 O       4.879596    -4.723903     2.446706     190.06
 C       3.882902    -5.652081     1.930783     113.77
 H       3.124347    -5.424415     2.554625      28.48
 H       4.213601    -6.754233     2.374476      22.18
 H       3.542575    -5.395762     1.003769      28.44
 C       5.263243    -2.324654     2.894139      11.22
 O       5.497979    -2.558134     4.257115     202.21
 H       5.374592    -3.502406     4.357982      23.05
 C       5.379896    -1.038902     2.380601      54.20
 H       5.664057    -0.280618     3.068951      22.34
 C       4.671044    -1.610969     0.060369      27.34
 C       4.565725    -1.270276    -1.363942     105.69
 H       5.152633    -2.087628    -1.776085      22.71
 O       5.652790    -0.321819    -1.854928     238.73
 H       5.383847     0.562743    -1.591215      26.80
 C       3.237772    -0.981070    -1.995021      85.50
 H       2.733060    -1.913424    -1.651278      23.41
 C       2.963140    -0.881415    -3.604203      82.89
 O       3.531233    -2.010822    -4.228501     260.70
 H       4.588562    -1.971014    -4.322463      25.15
 H       3.356751     0.080900    -4.084494      23.30
 H       1.681484    -0.950464    -3.649691      22.35
 C      -0.607498    -0.359842     0.165742      39.15
 H      -1.330680    -1.176493     0.560506      20.61
 C      -0.032144     2.042610     0.240663      56.68
 H      -0.340625     3.050142     0.428045      20.18
 C       1.236425     1.631534    -0.276898       9.16
 O       2.231849     2.584708    -0.725748     164.16
 C       1.934637     4.087647    -0.752779     101.44
 H       2.730213     4.387344    -1.184930      27.71
 H       1.026584     4.249870    -1.344369      27.38
 H       1.838353     4.367702     0.361323      24.85
 C       1.430779     0.325312    -0.809641       9.93
 O       2.756542     0.235743    -1.347544     152.26
 C       0.624292    -0.787591    -0.410872      54.48
 H       0.990040    -1.751000    -0.465648      21.17
 C      -0.938255     0.927560     0.651965      17.95
 C      -2.356982     1.259478     1.508621      73.43
 H      -2.621259     0.293035     2.079890      22.44
 O      -2.137693     2.261543     2.542352     265.79
 H      -2.084962     1.887002     3.394390      29.21
 C      -3.395402     1.888887     0.452184     102.11
 H      -2.911331     2.653525     0.005626      27.69
 O      -3.674591     0.990421    -0.582756     262.11
 H      -3.008679     0.844000    -1.267769      27.06
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 C      -4.658171     2.357053     1.098368     106.29
 O      -5.756701     3.103277     0.292948     287.96
 H      -5.370935     4.032560     0.009774      28.05
 H      -4.570340     2.717085     1.953912      30.02
 H      -5.317092     1.473796     1.515754      25.51
55
name = lig-etoh-Waterframe_878
 C       4.903087    -0.641965     1.062539      53.10
 H       4.993606     0.470094     0.937918      21.95
 C       4.700468    -2.970908     0.630675      61.09
 H       4.607605    -3.724719    -0.106814      23.98
 C       4.909506    -3.340343     1.936137      -5.89
 O       4.929761    -4.713570     2.462995     207.21
 C       3.850871    -5.619917     1.980741     103.66
 H       2.948241    -5.501653     2.521184      27.91
 H       4.194631    -6.884708     1.979118      22.88
 H       3.739154    -5.671919     0.828347      25.61
 C       5.287977    -2.321845     2.942628       5.94
 O       5.590956    -2.595474     4.261594     197.23
 H       5.394897    -3.518149     4.476858      24.62
 C       5.240799    -1.009309     2.404484      58.72
 H       5.339030    -0.238868     3.054203      25.43
 C       4.615074    -1.589069     0.160754      24.37
 C       4.634194    -1.203730    -1.491793      78.89
 H       4.762569    -2.333037    -1.979261      22.93
 O       5.650508    -0.327577    -1.882902     289.95
 H       5.629479     0.527033    -1.415437      26.21
 C       3.137875    -0.893875    -2.017499      96.64
 H       2.488195    -1.692103    -1.650820      25.30
 C       2.946240    -0.863199    -3.541130      97.73
 O       3.539915    -2.028114    -4.349924     239.85
 H       4.503399    -1.723601    -4.597777      25.78
 H       3.329227     0.225522    -3.877384      24.02
 H       2.054210    -0.761066    -4.164882      24.45
 C      -0.661281    -0.424796     0.269876      61.48
 H      -1.266786    -1.289189     0.838590      19.76
 C      -0.002409     2.034379     0.292875      63.17
 H      -0.197835     2.917291     0.621272      22.07
 C       1.242423     1.713597    -0.305718       5.28
 O       2.233206     2.649889    -0.752306     197.40
 C       1.866736     4.027030    -0.688091     122.49
 H       2.684156     4.715884    -1.071032      26.07
 H       1.163010     4.332445    -1.272393      30.90
 H       1.906134     4.303370     0.380924      25.98
 C       1.339359     0.304887    -0.717831      14.69
 O       2.688250     0.239885    -1.322671     147.67
 C       0.510052    -0.760791    -0.441603      52.38
 H       0.829371    -1.704515    -0.504478      22.72
 C      -0.889871     0.987254     0.517397      30.72
 C      -2.347928     1.297661     1.519835      49.02
 H      -2.635776     0.221501     1.795450      24.26
 O      -2.069413     2.312894     2.515895     266.39
 H      -1.991997     1.808575     3.307155      28.07
 C      -3.357828     1.911794     0.467428      87.22
 H      -2.905373     2.879486     0.197750      25.40
 O      -3.712980     0.936575    -0.552189     232.27
 H      -2.875915     0.714786    -0.978694      28.21
 C      -4.650116     2.299673     1.154482      92.45
 O      -5.639745     3.081900     0.351341     288.30
 H      -5.296555     3.942004    -0.084791      29.02
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 H      -4.342191     3.062152     1.990232      24.26
 H      -5.305007     1.436508     1.436735      24.84
55
name = lig-etoh-Waterframe_879
 C       4.976053    -0.621422     1.145548      45.24
 H       4.914078     0.389408     0.768585      18.12
 C       4.705312    -2.997692     0.525212      44.87
 H       4.604697    -3.740539    -0.205482      20.62
 C       4.962444    -3.355244     1.986501      13.77
 O       4.951977    -4.670055     2.444138     187.97
 C       3.847492    -5.618718     1.978253      88.32
 H       2.770882    -5.508818     2.379070      25.02
 H       4.428250    -6.546368     2.349646      21.55
 H       3.811731    -5.378997     0.770835      23.20
 C       5.259160    -2.363347     2.906177      10.63
 O       5.672654    -2.632501     4.239839     212.71
 H       5.484895    -3.524190     4.596503      24.78
 C       5.100750    -0.941646     2.496339      52.13
 H       5.199112    -0.181164     3.216802      25.60
 C       4.603667    -1.638250     0.126335      10.97
 C       4.618446    -1.261830    -1.541437      71.02
 H       4.811524    -2.178382    -2.328034      22.33
 O       5.667522    -0.327601    -1.910420     250.89
 H       5.541933     0.446269    -1.304092      26.23
 C       3.022517    -0.923782    -1.986819      77.66
 H       2.500620    -1.820439    -1.652905      22.79
 C       2.981334    -0.788906    -3.600972      94.23
 O       3.526808    -1.990032    -4.413940     248.71
 H       4.526149    -1.893865    -4.660994      27.95
 H       3.773891    -0.050554    -3.738530      21.65
 H       1.947701    -0.763396    -3.715872      24.88
 C      -0.703021    -0.396754     0.393677      28.03
 H      -1.399082    -1.252992     0.773350      19.23
 C       0.042845     2.017709     0.348412      58.24
 H      -0.139702     2.968720     0.804259      20.75
 C       1.186684     1.775358    -0.403765      15.66
 O       2.202403     2.643878    -0.776784     208.26
 C       1.846230     4.035522    -0.590792      88.50
 H       2.910956     4.663722    -1.022425      20.95
 H       0.806305     4.241087    -1.112345      23.65
 H       1.483023     4.456191     0.316431      25.29
 C       1.453909     0.392048    -0.679793      11.05
 O       2.575849     0.275307    -1.306767     157.24
 C       0.407284    -0.712267    -0.432766      49.32
 H       0.564571    -1.731551    -0.749202      19.84
 C      -1.001402     0.965637     0.549457      54.57
 C      -2.203792     1.360779     1.367448      92.96
 H      -2.725609     0.528456     1.884825      23.02
 O      -2.009335     2.306688     2.499007     258.54
 H      -1.598239     1.846113     3.231044      28.07
 C      -3.330400     1.899841     0.513809      59.75
 H      -2.902924     2.919091    -0.077450      22.68
 O      -3.722759     0.896752    -0.529982     196.39
 H      -2.922786     0.556509    -0.942973      26.49
 C      -4.728581     2.339651     1.228869      91.83
 O      -5.527345     3.027576     0.388148     301.13
 H      -5.133502     3.938865     0.181869      27.42
 H      -4.097237     3.046070     2.203474      21.55
 H      -5.060203     1.431828     1.623137      27.00
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name = lig-etoh-Waterframe_880
 C       4.954888    -0.642806     1.160065      27.83
 H       4.876772     0.366023     0.922758      15.44
 C       4.705236    -3.015983     0.513960      49.85
 H       4.547507    -3.855329    -0.145531      21.18
 C       4.964752    -3.353013     1.899116      17.22
 O       4.939554    -4.633493     2.433552     223.66
 C       3.940902    -5.567772     1.959860     125.04
 H       2.953214    -5.255957     2.572751      25.48
 H       4.119501    -6.454930     2.322207      24.99
 H       3.750761    -5.605543     0.786109      25.04
 C       5.215367    -2.327792     2.905827       4.30
 O       5.731558    -2.648303     4.185424     204.61
 H       5.519879    -3.593423     4.384371      24.57
 C       5.025082    -0.962715     2.597257      48.24
 H       5.177631    -0.189301     3.421159      24.36
 C       4.720237    -1.688814     0.035767      17.29
 C       4.516844    -1.340354    -1.502137      99.54
 H       4.980084    -2.161917    -1.984336      25.87
 O       5.650336    -0.333179    -1.911643     210.87
 H       5.444652     0.571778    -1.480480      24.27
 C       3.069385    -1.033037    -1.953200      82.87
 H       2.440123    -1.888584    -1.639661      21.76
 C       3.067714    -0.783923    -3.617584      99.43
 O       3.464327    -1.922142    -4.413156     295.30
 H       4.452846    -1.895308    -4.420470      29.23
 H       3.580864     0.120011    -3.909534      24.27
 H       2.053958    -0.410706    -3.833100      25.17
 C      -0.721434    -0.336452     0.417847      23.78
 H      -1.506920    -1.054399     0.538852      18.40
 C      -0.010193     1.984396     0.393987      55.73
 H      -0.266344     3.099735     0.821067      17.85
 C       1.111411     1.756885    -0.442054      12.54
 O       2.144433     2.641400    -0.758294     194.10
 C       1.775747     4.105926    -0.525225      70.11
 H       2.805012     4.706964    -1.032751      20.80
 H       0.923661     4.182149    -1.450368      20.86
 H       1.655515     4.223949     0.520134      24.47
 C       1.360147     0.387118    -0.642175      24.55
 O       2.588448     0.263289    -1.388375     178.31
 C       0.429364    -0.570162    -0.395661      69.48
 H       0.434200    -1.588736    -0.962509      17.07
 C      -0.987262     0.988302     0.687029      45.95
 C      -2.175901     1.416445     1.333677      94.67
 H      -2.488618     0.482895     1.777868      23.08
 O      -1.923435     2.306726     2.473110     270.21
 H      -1.283513     1.843562     3.020705      28.94
 C      -3.371204     1.925528     0.476188      75.42
 H      -3.054692     2.773836    -0.290894      21.97
 O      -3.727216     0.864193    -0.481054     230.10
 H      -3.013273     0.616550    -1.071746      25.45
 C      -4.556640     2.334926     1.351309     107.84
 O      -5.485477     3.008395     0.393723     277.90
 H      -5.245941     3.974238     0.433112      29.05
 H      -4.707763     2.963204     2.363093      23.61
 H      -5.194452     1.546552     1.741228      26.44
55
name = lig-etoh-Waterframe_881
 C       4.854010    -0.725851     1.140223      58.16
 H       4.875607     0.277859     1.000249      26.48
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 C       4.717729    -3.049174     0.531490      52.97
 H       4.467702    -3.896202    -0.161284      22.88
 C       4.944044    -3.276765     1.836031      14.35
 O       4.976759    -4.623199     2.409693     248.41
 C       3.964254    -5.511568     1.975107     129.36
 H       2.964689    -5.091256     2.376747      24.56
 H       4.105145    -6.536163     2.295566      25.41
 H       3.898985    -5.695033     0.952699      28.36
 C       5.187499    -2.321469     2.912531       9.16
 O       5.749065    -2.672222     4.097643     222.71
 H       5.626916    -3.651110     4.272444      27.19
 C       5.006658    -1.020071     2.542616      59.17
 H       5.117669    -0.179020     3.372833      22.64
 C       4.855987    -1.636225     0.094118      40.05
 C       4.559251    -1.379382    -1.376777      98.30
 H       4.714995    -2.293803    -1.811845      22.19
 O       5.563953    -0.365130    -1.892892     268.56
 H       5.275703     0.607774    -1.691116      22.72
 C       3.152010    -1.081369    -2.005231      84.28
 H       2.391123    -1.842996    -1.775446      22.73
 C       3.092150    -0.761240    -3.546730     103.79
 O       3.420888    -1.849573    -4.375335     301.83
 H       4.388897    -1.910433    -4.511328      29.40
 H       3.711408     0.096268    -3.629789      23.49
 H       2.076646    -0.570839    -4.064025      23.34
 C      -0.727941    -0.282973     0.346580      39.24
 H      -1.435590    -0.999369     0.358100      19.06
 C      -0.049152     2.039320     0.386575      66.86
 H      -0.375714     3.226786     0.638314      15.42
 C       1.057013     1.751422    -0.357046      38.15
 O       2.057270     2.665525    -0.720612     254.23
 C       1.748637     4.089600    -0.584444     121.01
 H       2.561822     4.727606    -0.724704      25.18
 H       0.826090     4.717290    -1.085686      25.12
 H       1.586701     4.441286     0.461586      26.29
 C       1.360710     0.408361    -0.733738      36.10
 O       2.620900     0.195617    -1.480309     197.69
 C       0.407101    -0.551706    -0.351335      66.47
 H       0.593175    -1.609906    -0.911414      17.90
 C      -0.856589     1.038100     0.798783      53.30
 C      -2.276463     1.416441     1.451595      83.54
 H      -2.721860     0.469866     1.727748      24.13
 O      -1.840340     2.342432     2.444872     295.17
 H      -1.212845     1.840088     2.980155      26.86
 C      -3.334481     1.951010     0.443007      83.91
 H      -3.148357     2.882986     0.003756      26.10
 O      -3.766398     0.817734    -0.416316     245.23
 H      -3.104852     0.950253    -1.091849      27.20
 C      -4.520691     2.323289     1.418574      91.15
 O      -5.464904     3.019652     0.421559     283.37
 H      -5.506610     3.990459     0.385175      30.25
 H      -4.150855     2.925290     2.145970      27.20
 H      -5.052883     1.305319     1.515561      25.64
55
name = lig-etoh-Waterframe_882
 C       4.772315    -0.705198     1.163386      76.48
 H       4.756400     0.257036     0.778214      29.65
 C       4.750380    -2.991989     0.500929      76.11
 H       4.533028    -3.814585    -0.267990      23.06
 C       4.931727    -3.319528     1.918005      19.71
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 O       5.063897    -4.605457     2.372415     278.01
 C       3.914142    -5.485080     1.968503     108.39
 H       2.893716    -5.220529     2.123452      25.74
 H       4.304368    -6.453053     2.718592      22.37
 H       4.051982    -5.549860     0.962827      28.43
 C       5.186077    -2.368374     2.851303      24.14
 O       5.746756    -2.708173     4.039318     208.10
 H       5.727000    -3.686598     4.271509      24.37
 C       5.005540    -1.035361     2.446076      67.52
 H       5.055450    -0.107533     3.148867      18.68
 C       4.858024    -1.693881     0.171420      39.22
 C       4.670409    -1.373170    -1.311668      81.41
 H       4.874391    -2.338770    -1.916348      19.98
 O       5.466789    -0.432950    -1.890480     308.23
 H       5.066916     0.446317    -1.493435      24.10
 C       3.121423    -1.074305    -2.010504      70.27
 H       2.568248    -2.015765    -1.820219      21.84
 C       3.109844    -0.719851    -3.474388      99.51
 O       3.450592    -1.842136    -4.359896     284.69
 H       4.374250    -1.826342    -4.657950      28.58
 H       3.863842     0.031777    -3.581027      23.14
 H       1.963063    -0.450683    -3.412094      23.28
 C      -0.733171    -0.231923     0.282131      39.89
 H      -1.457617    -0.958999     0.471739      20.75
 C      -0.059830     2.164658     0.378311      49.71
 H      -0.325886     3.316761     0.552309      17.99
 C       1.130571     1.754647    -0.308661      15.84
 O       1.958820     2.751138    -0.710942     213.34
 C       1.720184     4.152380    -0.574009     116.19
 H       2.572945     4.500575    -0.866249      27.85
 H       0.899855     4.339587    -1.205044      28.58
 H       1.391185     4.320916     0.509249      25.01
 C       1.440928     0.422906    -0.852867      13.27
 O       2.597400     0.177089    -1.510998     172.72
 C       0.481701    -0.631133    -0.427386      47.28
 H       0.575573    -1.805361    -0.555621      19.57
 C      -0.960212     1.019977     0.892197      26.32
 C      -2.233742     1.348926     1.499923      99.08
 H      -2.858235     0.651282     2.149538      22.14
 O      -1.809645     2.411697     2.462656     246.07
 H      -1.387119     1.945230     3.223998      27.14
 C      -3.319996     1.963023     0.536153      82.74
 H      -2.939299     2.755059    -0.021325      27.67
 O      -3.764301     0.836138    -0.363636     210.36
 H      -3.424009     0.810879    -1.259880      27.61
 C      -4.532235     2.344691     1.290075     110.68
 O      -5.476151     3.021844     0.492118     330.58
 H      -5.294221     3.960030     0.514554      31.40
 H      -3.975589     2.794340     2.071752      27.25
 H      -4.918136     1.397896     1.931265      27.14
55
name = lig-etoh-Waterframe_883
 C       4.737221    -0.633692     1.096435      42.03
 H       4.484856     0.422580     0.886181      20.45
 C       4.800467    -3.050557     0.581941      55.77
 H       4.819148    -3.773777    -0.292055      22.54
 C       4.910151    -3.394951     1.866010      34.33
 O       5.102735    -4.653380     2.351524     272.36
 C       3.952815    -5.484731     1.968485     103.97
 H       3.059679    -5.004068     2.214713      28.43
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 H       3.896190    -6.606693     2.687562      23.37
 H       4.095087    -5.935811     0.891447      25.38
 C       5.219248    -2.373735     2.809129       4.23
 O       5.746388    -2.716701     4.044463     163.78
 H       5.660816    -3.720363     4.181335      23.95
 C       5.014265    -0.981865     2.462374      49.97
 H       5.117428    -0.264431     3.291319      25.93
 C       4.735952    -1.695438     0.123217      38.07
 C       4.639724    -1.454809    -1.362501      85.94
 H       5.226288    -2.419115    -1.851307      23.84
 O       5.439044    -0.404954    -1.888592     226.03
 H       5.443650     0.503886    -1.363010      25.09
 C       3.152189    -1.127090    -1.893001      80.97
 H       2.405572    -1.941362    -1.678732      24.21
 C       3.147391    -0.746552    -3.414163      99.44
 O       3.464247    -1.842217    -4.342161     290.46
 H       4.405365    -1.692001    -4.506529      27.93
 H       3.640373     0.230601    -3.708372      23.55
 H       2.181798    -0.255555    -3.789498      24.64
 C      -0.681677    -0.223368     0.250414      54.05
 H      -1.349682    -1.066806     0.610961      20.81
 C      -0.092771     2.085154     0.411309      58.95
 H      -0.211900     3.088451     0.663345      19.82
 C       1.128696     1.793498    -0.297569       3.91
 O       1.967240     2.799138    -0.744263     199.01
 C       1.634930     4.194797    -0.567939     105.63
 H       2.612794     4.737565    -1.022616      24.29
 H       0.996385     4.361796    -1.333723      28.14
 H       1.507327     4.577974     0.526620      23.47
 C       1.385299     0.337804    -0.829736      20.57
 O       2.601150     0.215935    -1.496412     159.33
 C       0.544023    -0.620040    -0.498918      62.12
 H       0.732659    -1.665519    -0.580369      23.05
 C      -0.970047     1.038204     0.772258      22.77
 C      -2.210538     1.369720     1.621173      80.52
 H      -2.459935     0.405735     2.272608      22.32
 O      -1.813835     2.504906     2.519517     251.29
 H      -1.774018     2.086987     3.430075      26.64
 C      -3.266395     1.866991     0.555822      84.23
 H      -2.692775     2.598918    -0.091455      25.45
 O      -3.763056     0.856765    -0.324816     249.25
 H      -3.343044     0.890059    -1.189922      28.38
 C      -4.497311     2.384858     1.269692      98.91
 O      -5.523281     3.050214     0.571489     305.14
 H      -5.161052     3.902276     0.447434      31.96
 H      -4.419569     3.297745     2.203891      22.07
 H      -5.129447     1.605293     1.779893      25.65
55
name = lig-etoh-Waterframe_884
 C       4.708647    -0.620008     1.070092      45.03
 H       4.318241     0.457889     0.936295      18.68
 C       4.833052    -3.078110     0.502391      37.40
 H       5.007964    -3.991253    -0.100725      21.63
 C       4.968155    -3.392953     1.893705      -7.94
 O       5.118719    -4.793110     2.338740     202.62
 C       3.983405    -5.561982     1.991303     107.37
 H       3.190614    -4.825099     2.027965      28.16
 H       3.843714    -6.333784     2.739278      25.91
 H       3.912711    -6.036759     0.818842      24.42
 C       5.249613    -2.327783     2.801515       9.36
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 O       5.728029    -2.701249     4.051456     181.47
 H       5.605403    -3.696966     4.249515      22.36
 C       5.036181    -0.983133     2.479477      55.62
 H       5.157163    -0.341718     3.269703      26.00
 C       4.595784    -1.648382     0.112398      30.52
 C       4.561385    -1.487848    -1.413512      81.60
 H       4.789757    -2.488987    -1.986139      24.42
 O       5.496807    -0.333943    -1.898036     139.64
 H       5.454523     0.407489    -1.148726      23.47
 C       3.160360    -1.144016    -1.869026      77.32
 H       2.372222    -1.822850    -1.525327      23.77
 C       3.123366    -0.785723    -3.440609      97.07
 O       3.501876    -1.822635    -4.300810     293.15
 H       4.480322    -2.039877    -4.445716      27.59
 H       3.954763     0.040819    -3.355320      20.82
 H       2.119536    -0.728978    -3.762752      25.28
 C      -0.618617    -0.298848     0.256078      59.24
 H      -1.234449    -1.261538     0.582116      21.33
 C      -0.015530     2.006179     0.411635      75.87
 H      -0.230778     2.817622     0.884579      25.59
 C       1.063175     1.762329    -0.356041      26.83
 O       2.029350     2.802534    -0.765084     174.41
 C       1.601195     4.245148    -0.639928      90.71
 H       2.596092     5.051248    -0.876131      22.06
 H       0.604904     4.742190    -1.126181      23.86
 H       1.325608     4.654550     0.367468      24.76
 C       1.419499     0.462227    -0.754230       8.83
 O       2.644584     0.255909    -1.421946     114.09
 C       0.451647    -0.625256    -0.479612      43.01
 H       0.730783    -1.511380    -0.793997      23.13
 C      -0.946206     1.010552     0.628128      55.19
 C      -2.121328     1.408513     1.707826      77.30
 H      -2.373730     0.408875     2.172324      24.98
 O      -1.853110     2.560880     2.580721     251.67
 H      -2.008209     2.247182     3.525082      27.25
 C      -3.219189     1.791746     0.615831      69.00
 H      -2.718955     2.745843     0.076701      23.13
 O      -3.757451     0.833751    -0.312745     269.90
 H      -3.123712     0.956324    -1.012800      28.10
 C      -4.548131     2.472138     1.395527      82.25
 O      -5.594141     3.128031     0.564059     310.19
 H      -5.416356     3.912713     0.119830      32.51
 H      -3.933385     3.203699     2.283538      22.84
 H      -4.878582     1.532544     1.658662      27.64
55
name = lig-etoh-Waterframe_885
 C       4.651149    -0.674884     1.160954      44.07
 H       4.454288     0.384888     0.743540      18.10
 C       4.849790    -3.038312     0.479448      45.08
 H       4.905600    -3.784965    -0.289927      21.48
 C       5.076318    -3.399934     1.872042       0.74
 O       5.168936    -4.839698     2.310898     230.60
 C       3.926015    -5.621462     2.002654     112.86
 H       2.915684    -5.048984     1.908006      26.89
 H       3.823369    -6.209405     2.729934      28.78
 H       4.193413    -6.104090     0.972760      26.40
 C       5.272345    -2.378459     2.836806      10.75
 O       5.701673    -2.647767     4.073700     195.98
 H       5.582886    -3.630653     4.365131      22.35
 C       5.051129    -0.988309     2.409372      52.45
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 H       5.143949    -0.200398     3.069369      23.98
 C       4.555633    -1.743264     0.096827      45.36
 C       4.481728    -1.375714    -1.423231      87.63
 H       4.713566    -2.227708    -1.961522      26.04
 O       5.545135    -0.353096    -1.883146     229.58
 H       5.274228     0.406619    -1.223641      26.11
 C       3.061652    -1.060929    -1.922706      82.33
 H       2.563466    -1.943814    -1.545534      22.66
 C       3.100985    -0.855311    -3.401261     108.15
 O       3.550603    -1.895098    -4.290783     271.42
 H       4.643547    -1.865690    -4.335315      23.46
 H       3.736030     0.112964    -3.583028      22.03
 H       2.105264    -0.499530    -3.521824      25.31
 C      -0.683690    -0.422151     0.311036      27.15
 H      -1.477643    -1.254097     0.564822      18.53
 C       0.005343     2.001113     0.421115      44.02
 H      -0.122586     2.946122     0.996481      19.79
 C       1.157804     1.835082    -0.492244      13.13
 O       2.044488     2.840806    -0.773405     172.15
 C       1.560055     4.326087    -0.638260      68.25
 H       2.552288     4.790295    -1.170458      21.40
 H       0.567198     4.338389    -1.428177      22.02
 H       1.430903     4.248737     0.361424      24.70
 C       1.470383     0.470632    -0.730356      22.87
 O       2.703529     0.285673    -1.314727     138.38
 C       0.518320    -0.560085    -0.512093      58.53
 H       0.543107    -1.523382    -0.913246      21.11
 C      -0.943861     0.954835     0.684619      37.18
 C      -2.034751     1.382009     1.634760      93.31
 H      -2.376058     0.706418     2.352378      22.46
 O      -1.893278     2.566463     2.605551     230.56
 H      -1.850233     2.146128     3.544341      25.95
 C      -3.297556     1.900074     0.756545      67.11
 H      -2.828608     2.681941     0.036602      22.17
 O      -3.695849     0.808804    -0.291425     240.71
 H      -3.186834     0.642686    -1.081418      27.23
 C      -4.518360     2.509555     1.438357     103.56
 O      -5.641137     3.172486     0.573816     279.78
 H      -5.198731     3.993940     0.227009      29.77
 H      -4.158713     3.072932     2.281499      27.31
 H      -5.122323     1.779973     2.016681      26.80
55
name = lig-etoh-Waterframe_886
 C       4.576015    -0.803741     1.087339      55.29
 H       4.555631     0.331633     0.956608      21.06
 C       4.855456    -3.060843     0.500272      42.45
 H       4.778914    -3.717031    -0.314861      23.31
 C       5.173473    -3.454323     1.808832      15.37
 O       5.170632    -4.770635     2.263540     185.73
 C       3.923843    -5.665084     1.976721      96.50
 H       2.934107    -5.020900     1.905287      23.00
 H       3.804660    -6.473498     2.893299      23.72
 H       4.151764    -6.341716     1.252077      26.41
 C       5.279990    -2.429622     2.806742       6.06
 O       5.677431    -2.580675     4.150523     219.84
 H       5.629030    -3.573297     4.473698      21.98
 C       5.076147    -1.038573     2.414318      41.03
 H       5.217727    -0.186124     3.121914      17.42
 C       4.579121    -1.728367     0.109171      39.87
 C       4.480690    -1.274484    -1.398463     102.74
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 H       4.829577    -2.098172    -1.901664      22.60
 O       5.529204    -0.410626    -1.812866     297.27
 H       5.477145     0.587256    -1.701968      25.85
 C       3.063125    -0.960416    -1.892353     102.29
 H       2.327879    -1.729111    -1.647716      21.82
 C       3.029093    -0.817711    -3.432391     102.06
 O       3.559339    -1.990049    -4.240638     261.34
 H       4.539825    -1.703161    -4.493250      24.68
 H       3.556785     0.047394    -3.759558      23.69
 H       2.029577    -0.562378    -3.948017      23.64
 C      -0.706675    -0.387373     0.317387      15.92
 H      -1.424788    -1.236010     0.338428      17.02
 C       0.040934     1.982930     0.370195      48.62
 H      -0.131534     3.123465     0.818345      16.37
 C       1.155259     1.907907    -0.474746      23.74
 O       2.073190     2.892894    -0.812499     228.46
 C       1.566200     4.232723    -0.677029     113.52
 H       2.214696     4.961580    -1.047690      25.36
 H       0.587484     4.344777    -1.368634      24.65
 H       1.413554     4.721830     0.292000      25.45
 C       1.491894     0.448681    -0.768477      20.71
 O       2.768630     0.258889    -1.244209     192.80
 C       0.516877    -0.540334    -0.492823      48.14
 H       0.724381    -1.542709    -1.027176      18.09
 C      -0.856075     0.918963     0.835844      48.52
 C      -2.129633     1.402603     1.606552      85.09
 H      -2.406010     0.498119     2.126888      23.44
 O      -1.884781     2.536908     2.595225     282.20
 H      -1.374105     1.952865     3.314573      24.91
 C      -3.329095     1.962634     0.731380      78.49
 H      -2.992816     2.839357     0.205134      24.69
 O      -3.663496     0.782826    -0.201888     222.14
 H      -3.020963     0.892234    -0.916658      26.05
 C      -4.601752     2.509192     1.489577     109.25
 O      -5.585339     3.196070     0.620278     289.13
 H      -5.133189     4.090805     0.429841      29.36
 H      -4.314340     3.317587     2.018714      27.39
 H      -5.298649     1.861958     2.130362      26.00
55
name = lig-etoh-Waterframe_887
 C       4.591208    -0.783208     1.146055      37.42
 H       4.304142     0.236183     0.810551      21.73
 C       4.850255    -3.117870     0.445548      50.86
 H       4.766454    -4.030156    -0.137823      24.27
 C       5.198741    -3.461775     1.780298       7.52
 O       5.128115    -4.766775     2.218907     183.38
 C       3.999567    -5.694010     1.988105      92.07
 H       3.109154    -5.004019     1.730537      23.79
 H       3.861915    -6.229057     3.218281      21.34
 H       4.054188    -6.287562     1.145014      26.51
 C       5.321809    -2.415180     2.814067      11.44
 O       5.636080    -2.536411     4.194729     201.06
 H       5.676851    -3.504997     4.579082      20.54
 C       5.064678    -1.170284     2.402245      50.55
 H       5.243959    -0.384423     3.258812      20.27
 C       4.604461    -1.719189     0.064507      35.36
 C       4.519642    -1.322242    -1.357636     102.03
 H       4.697218    -2.317722    -1.953530      20.85
 O       5.553915    -0.423495    -1.765594     284.68
 H       5.218867     0.528545    -1.641609      26.23
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 C       3.114460    -0.910462    -1.894811      85.31
 H       2.368820    -1.652744    -1.558340      22.50
 C       2.962430    -0.751426    -3.586114      90.67
 O       3.514542    -2.044143    -4.131467     274.18
 H       4.477893    -2.100608    -4.463588      26.86
 H       3.573051     0.038068    -3.769716      25.10
 H       1.857286    -0.976546    -3.859759      23.08
 C      -0.617989    -0.276651     0.255651      85.98
 H      -1.300654    -1.049431     0.326858      19.75
 C       0.042628     2.013764     0.366302      74.03
 H      -0.473574     3.097385     0.639327      16.46
 C       1.162520     1.785791    -0.402638      19.54
 O       2.098035     2.928033    -0.837147     199.35
 C       1.553336     4.233300    -0.742441     123.42
 H       2.218418     4.819076    -1.187838      26.49
 H       0.627952     4.293062    -1.155581      29.42
 H       1.274751     4.680461     0.322591      24.50
 C       1.451283     0.543723    -0.783413      20.68
 O       2.787242     0.276683    -1.193901     178.82
 C       0.492237    -0.540167    -0.470302      55.07
 H       0.761820    -1.652690    -0.848583      17.90
 C      -0.784157     0.976908     0.922835      24.15
 C      -2.252594     1.452928     1.631969      83.93
 H      -2.736460     0.472622     1.945512      20.81
 O      -1.844001     2.435050     2.558807     294.56
 H      -1.159402     2.097088     3.274858      27.27
 C      -3.356068     1.945551     0.689993      77.25
 H      -3.098355     2.778368     0.134194      26.52
 O      -3.638782     0.815033    -0.106442     245.11
 H      -2.977964     0.926676    -0.804893      26.47
 C      -4.702241     2.555639     1.544540      84.75
 O      -5.522635     3.189606     0.644302     301.04
 H      -5.273485     4.126761     0.264829      27.30
 H      -4.021189     3.383356     2.231258      23.54
 H      -5.021404     1.601889     2.109447      26.49
55
name = lig-etoh-Waterframe_888
 C       4.641348    -0.753233     1.145964      41.73
 H       4.221775     0.219440     1.036088      20.13
 C       4.856521    -3.135999     0.423078      42.43
 H       4.757500    -3.982243    -0.331393      21.18
 C       5.139885    -3.422568     1.798729      21.45
 O       5.140379    -4.828473     2.202018     216.34
 C       4.044980    -5.616586     2.010113     116.18
 H       3.127937    -5.148628     1.814048      29.86
 H       3.794718    -6.272278     3.022342      24.40
 H       4.303437    -6.430310     1.166041      25.42
 C       5.386458    -2.525918     2.833234       6.35
 O       5.593517    -2.521609     4.192109     190.37
 H       5.559793    -3.498380     4.552134      21.72
 C       5.029158    -1.157277     2.414067      48.28
 H       5.020019    -0.375130     3.301462      24.08
 C       4.637101    -1.809683     0.099305      26.23
 C       4.526472    -1.436340    -1.418376      67.44
 H       4.759980    -2.462807    -2.066307      22.07
 O       5.593610    -0.406061    -1.740139     207.87
 H       5.211985     0.340837    -1.209647      26.63
 C       3.143310    -0.898462    -1.948092      71.12
 H       2.596510    -1.828644    -1.645523      25.04
 C       2.975088    -0.822578    -3.603160     106.61
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 O       3.446727    -2.103014    -4.026903     299.84
 H       4.413561    -1.929643    -4.159820      25.69
 H       3.296581     0.095239    -4.089330      26.54
 H       1.850158    -0.570377    -3.719173      25.61
 C      -0.586442    -0.182706     0.273908      60.40
 H      -1.255802    -0.903688     0.518407      22.19
 C      -0.045460     2.094285     0.452722      53.33
 H      -0.272017     3.195812     0.500740      17.67
 C       1.220303     1.868538    -0.343636       3.56
 O       2.072786     2.843423    -0.826700     162.41
 C       1.488945     4.294631    -0.781641      85.10
 H       2.328074     4.800798    -1.418806      24.24
 H       0.622760     4.285721    -1.293195      28.34
 H       1.640966     4.304681     0.327382      22.26
 C       1.464690     0.460218    -0.792290      36.35
 O       2.762976     0.356485    -1.167913     155.70
 C       0.587785    -0.498789    -0.512215      67.02
 H       0.552836    -1.663226    -0.663429      20.73
 C      -0.852511     1.065907     0.880763      14.06
 C      -2.226135     1.431050     1.628741      82.77
 H      -2.747531     0.653586     2.314155      18.85
 O      -1.825798     2.396972     2.538879     250.31
 H      -1.403357     1.775463     3.319362      23.04
 C      -3.390072     2.011350     0.735108      82.85
 H      -3.027384     2.760102    -0.051689      23.90
 O      -3.653664     0.836504    -0.082869     195.98
 H      -3.074012     0.474164    -0.754574      26.11
 C      -4.550801     2.568057     1.543745      95.67
 O      -5.558110     3.174629     0.641623     262.07
 H      -4.933072     3.972906     0.303946      24.96
 H      -4.331374     3.024111     2.743868      24.37
 H      -5.299475     1.787009     1.919961      24.25
55
name = lig-etoh-Waterframe_889
 C       4.687608    -0.815382     1.106793      52.95
 H       4.386925     0.165900     0.991067      21.60
 C       4.871640    -3.134629     0.480751      48.71
 H       4.855603    -3.854839    -0.421140      22.17
 C       5.073972    -3.529061     1.850927      18.99
 O       5.229588    -4.808805     2.213415     258.93
 C       3.997750    -5.644703     2.010675     109.48
 H       3.165071    -5.115020     1.738829      31.14
 H       3.863057    -6.143422     2.783947      28.56
 H       4.372534    -6.538329     1.240731      24.57
 C       5.365079    -2.463728     2.796143       1.08
 O       5.562147    -2.587398     4.174870     189.14
 H       5.492836    -3.481291     4.641966      23.78
 C       5.016901    -1.132177     2.454436      42.98
 H       4.817615    -0.368098     3.238060      22.89
 C       4.646892    -1.807174     0.096708      27.39
 C       4.568450    -1.452374    -1.478994      78.67
 H       4.987042    -2.333065    -2.113729      23.01
 O       5.601176    -0.421086    -1.703040     183.78
 H       5.675933     0.302213    -1.075703      27.14
 C       3.189171    -0.910113    -1.987831      95.60
 H       2.297410    -1.554845    -1.755292      23.94
 C       2.953004    -0.844784    -3.457451     104.69
 O       3.387064    -2.149586    -3.954571     258.96
 H       4.301587    -2.050138    -4.284919      26.33
 H       3.655652    -0.162152    -4.152748      24.43
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 H       1.892791    -0.820595    -3.738438      26.35
 C      -0.587913    -0.136421     0.339504      27.88
 H      -1.162171    -1.027677     0.599808      20.35
 C       0.034552     2.258462     0.441130      75.42
 H      -0.206861     3.186649     0.776097      24.37
 C       1.120403     1.910798    -0.256502      16.48
 O       2.021199     2.773336    -0.835963     166.47
 C       1.537127     4.220014    -0.803175      91.46
 H       2.311058     5.092220    -1.396603      22.36
 H       0.462190     4.395705    -1.181255      24.69
 H       1.493093     4.866068     0.149508      24.67
 C       1.530967     0.518897    -0.722893      -2.13
 O       2.803420     0.352412    -1.247310     113.03
 C       0.536949    -0.514864    -0.474215      48.87
 H       0.822978    -1.529073    -0.860284      21.19
 C      -1.010569     1.112301     0.749684      64.47
 C      -2.157167     1.418453     1.604742      94.00
 H      -2.466507     0.398986     2.026888      24.55
 O      -1.787943     2.432469     2.608373     238.05
 H      -1.845968     1.879896     3.506629      24.40
 C      -3.279689     2.027808     0.756050      67.91
 H      -2.850623     3.030252     0.196048      22.58
 O      -3.777888     0.814735    -0.093535     151.62
 H      -2.873324     0.561780    -0.386364      26.59
 C      -4.535169     2.448482     1.548029      93.68
 O      -5.534300     3.200854     0.660499     273.91
 H      -5.266944     4.072545     0.069704      26.34
 H      -4.268166     3.248877     2.264265      26.16
 H      -5.052677     1.519542     1.737675      26.76
55
name = lig-etoh-Waterframe_890
 C       4.717042    -0.840062     1.087168      53.12
 H       4.595720     0.131106     0.692315      21.64
 C       4.877407    -3.147495     0.530731      45.66
 H       4.956769    -4.076638    -0.115423      22.70
 C       5.073079    -3.489270     1.859108      14.80
 O       5.255747    -4.822754     2.247648     245.94
 C       4.010325    -5.718606     1.999280      83.48
 H       3.279947    -5.000159     1.591425      29.18
 H       3.771592    -6.097221     3.044784      24.43
 H       4.149907    -6.389405     1.069353      26.13
 C       5.243279    -2.425952     2.820295       4.60
 O       5.544628    -2.660004     4.144055     203.67
 H       5.554352    -3.622241     4.384854      20.88
 C       4.994932    -1.111244     2.421595      63.49
 H       4.945695    -0.413005     3.187469      25.55
 C       4.656867    -1.790927     0.040363      33.25
 C       4.642598    -1.368701    -1.415380     104.65
 H       4.836152    -2.199075    -1.998694      26.31
 O       5.643978    -0.451003    -1.710491     227.01
 H       5.603282     0.211089    -1.018032      30.29
 C       3.152294    -0.928161    -1.913727      91.76
 H       2.455973    -1.703267    -1.469581      24.35
 C       2.983011    -0.870927    -3.417853      99.27
 O       3.349927    -2.244324    -3.911023     276.56
 H       4.089832    -2.298416    -4.501400      28.96
 H       3.716525     0.058602    -3.769830      24.21
 H       1.965615    -0.713834    -3.673689      27.00
 C      -0.620957    -0.186563     0.362275      52.33
 H      -1.299893    -1.081284     0.710059      18.21
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 C      -0.054364     2.292555     0.473230      53.60
 H      -0.107119     3.166284     0.961110      21.16
 C       1.137925     1.859236    -0.285005       1.81
 O       1.977511     2.846379    -0.831209     161.92
 C       1.597114     4.200879    -0.794163      74.56
 H       2.475187     4.529444    -1.660473      20.40
 H       0.458588     4.134065    -1.327052      22.55
 H       1.522882     4.633629     0.210440      24.95
 C       1.485223     0.554314    -0.591290      11.85
 O       2.856568     0.360606    -1.360007     117.98
 C       0.566103    -0.420784    -0.419513      56.33
 H       0.660078    -1.420510    -0.738930      22.46
 C      -0.931712     1.248147     0.587629      42.89
 C      -2.106043     1.437386     1.601560      84.66
 H      -2.422677     0.468872     1.917151      25.60
 O      -1.775178     2.475160     2.676417     248.55
 H      -1.787547     1.997491     3.586911      24.82
 C      -3.254644     1.985661     0.779658      69.68
 H      -2.828217     2.847832     0.119710      22.69
 O      -3.837427     0.857107    -0.103450     127.01
 H      -3.015853     0.339966    -0.348383      27.84
 C      -4.553881     2.422639     1.450020     114.30
 O      -5.531118     3.165632     0.680660     316.36
 H      -4.921305     4.018350     0.357060      25.82
 H      -4.205007     2.960543     2.197087      29.30
 H      -4.862087     1.575058     1.991819      29.53
55
name = lig-etoh-Waterframe_891
 C       4.733399    -0.795791     1.006826      38.44
 H       4.719655     0.312991     0.811342      19.03
 C       4.867427    -3.164385     0.495400      57.91
 H       4.900976    -4.033599    -0.139808      23.39
 C       5.105316    -3.386227     1.870627       4.90
 O       5.200802    -4.852017     2.278286     183.39
 C       4.066260    -5.683734     1.972206      90.23
 H       3.138160    -4.975847     1.725745      21.52
 H       3.528000    -6.364239     3.051332      21.03
 H       4.293602    -6.484193     1.338022      23.77
 C       5.093297    -2.460841     2.875883      13.99
 O       5.532908    -2.698583     4.089719     203.41
 H       5.640962    -3.651552     4.331462      27.23
 C       4.965943    -1.078691     2.399517      53.31
 H       5.187331    -0.303113     3.035344      22.73
 C       4.709841    -1.861196     0.075189      38.22
 C       4.625410    -1.362796    -1.361084     100.29
 H       4.742476    -2.201027    -1.924578      24.30
 O       5.731701    -0.434950    -1.729040     257.42
 H       5.505169     0.405246    -1.306198      27.31
 C       3.143063    -0.971244    -1.752132      81.52
 H       2.713762    -1.816035    -1.252497      23.49
 C       3.045493    -0.936369    -3.387846      98.20
 O       3.318164    -2.317251    -3.897590     286.94
 H       4.081611    -2.171895    -4.436639      28.03
 H       3.685711    -0.063878    -3.746885      24.96
 H       2.101520    -0.528218    -3.673952      27.01
 C      -0.628699    -0.102803     0.305135      31.93
 H      -1.440018    -0.897253     0.649425      17.86
 C      -0.018782     2.261552     0.403873      63.24
 H      -0.153382     3.204756     0.901794      18.63
 C       1.190256     1.954902    -0.321182      20.69
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 O       1.992272     2.837904    -0.791234     235.40
 C       1.623345     4.175540    -0.847848     128.16
 H       2.322305     4.726923    -1.396286      25.61
 H       0.611894     4.477061    -1.395760      25.58
 H       1.818594     4.561158     0.096209      27.00
 C       1.566451     0.579139    -0.585363      18.01
 O       2.782706     0.416973    -1.402467     169.99
 C       0.531606    -0.437635    -0.303736      45.22
 H       0.704570    -1.401931    -0.578867      21.77
 C      -0.913595     1.191288     0.645410      45.23
 C      -2.071356     1.514080     1.608177      83.47
 H      -2.324046     0.701539     2.208836      23.64
 O      -1.787378     2.507675     2.675550     280.74
 H      -1.478150     1.776893     3.256914      25.76
 C      -3.340027     1.926178     0.701374      91.63
 H      -3.031171     2.604147     0.001070      24.54
 O      -3.811362     0.887668    -0.107300     227.09
 H      -3.406995     0.150258    -0.569098      26.65
 C      -4.528706     2.443172     1.471584     104.31
 O      -5.495832     3.097164     0.703432     283.43
 H      -5.068102     3.996620     0.342519      27.52
 H      -4.169961     3.035021     2.429101      25.77
 H      -5.223939     1.645058     1.902129      25.29
55
name = lig-etoh-Waterframe_892
 C       4.779254    -0.775372     1.056107      35.33
 H       4.729968     0.330539     0.667218      18.53
 C       4.873814    -3.198848     0.471132      40.79
 H       4.814547    -3.861618    -0.329899      22.81
 C       5.067118    -3.494438     1.838220       6.82
 O       5.136785    -4.802809     2.310403     237.83
 C       4.052771    -5.648244     1.992101     109.52
 H       3.073483    -5.210799     1.475877      23.96
 H       3.881981    -6.289027     3.029749      21.96
 H       4.433574    -6.338652     1.318972      23.72
 C       4.996374    -2.393032     2.837629       8.39
 O       5.533667    -2.691446     4.097914     159.23
 H       5.515359    -3.650413     4.493773      26.96
 C       4.938686    -1.066976     2.373601      61.81
 H       5.261474    -0.235885     3.005069      21.86
 C       4.767554    -1.810281     0.092633      28.56
 C       4.623311    -1.401517    -1.347364      89.32
 H       4.897611    -2.239718    -2.089052      21.17
 O       5.780313    -0.408505    -1.729694     224.95
 H       5.517214     0.500441    -1.775388      27.36
 C       3.209796    -0.974787    -1.698239      83.67
 H       2.416322    -1.514918    -1.284999      21.78
 C       3.081823    -1.022505    -3.267022     106.72
 O       3.316897    -2.309085    -3.912621     276.47
 H       4.232199    -2.339798    -4.195066      27.71
 H       3.894294    -0.625866    -3.668448      25.37
 H       2.037229    -0.788658    -3.629973      25.06
 C      -0.692884    -0.045661     0.260245     104.85
 H      -1.399853    -0.949863     0.383376      20.90
 C       0.064269     2.218515     0.328548      75.79
 H      -0.312803     3.261406     0.526430      18.45
 C       1.182936     1.922007    -0.321340      21.10
 O       2.127801     2.855294    -0.824306     204.20
 C       1.684093     4.299396    -0.876214     125.02
 H       2.378165     4.780129    -1.354371      26.77
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 H       0.658198     4.423594    -1.104520      28.01
 H       1.635711     4.790088     0.116505      25.87
 C       1.572028     0.575573    -0.617747      11.24
 O       2.647010     0.438124    -1.378654     137.15
 C       0.644724    -0.466132    -0.253267      61.69
 H       0.813281    -1.488615    -0.433808      20.73
 C      -0.925569     1.198919     0.843240      38.15
 C      -2.131113     1.588298     1.576183      90.98
 H      -2.474212     0.576317     2.004938      21.12
 O      -1.783361     2.524848     2.620670     302.44
 H      -1.310153     2.079719     3.324635      29.32
 C      -3.331786     1.910491     0.646851      79.37
 H      -3.102379     2.794115     0.082185      25.47
 O      -3.854715     0.807636    -0.138887     188.93
 H      -2.965649     0.436572    -0.479410      26.54
 C      -4.540172     2.424463     1.604715      75.59
 O      -5.487522     3.090789     0.676480     272.85
 H      -5.228716     3.908979     0.241873      30.16
 H      -4.104355     3.325183     2.390056      22.59
 H      -5.070775     1.402414     1.867697      24.37
55
name = lig-etoh-Waterframe_893
 C       4.820157    -0.765425     1.044859      49.02
 H       4.793281     0.335027     0.635174      20.08
 C       4.883273    -3.164224     0.444148      42.87
 H       4.853461    -3.931139    -0.296757      21.05
 C       4.949651    -3.519696     1.803464      21.95
 O       5.095525    -4.720907     2.365214     381.90
 C       4.039979    -5.721073     1.997826     101.51
 H       3.161901    -5.143169     1.637861      30.40
 H       3.821521    -6.140541     2.814057      30.03
 H       4.445021    -6.346780     1.119492      28.00
 C       5.033237    -2.443679     2.768455       9.94
 O       5.509159    -2.622488     4.109815     216.92
 H       5.374188    -3.627642     4.295946      25.02
 C       4.942780    -1.053998     2.435975      46.75
 H       5.021118    -0.275778     3.315415      22.76
 C       4.820823    -1.767387     0.104909      40.34
 C       4.710811    -1.371000    -1.325535      75.65
 H       4.900728    -2.374943    -2.029628      21.39
 O       5.776886    -0.409503    -1.734270     239.98
 H       5.319064     0.410671    -1.822774      28.56
 C       3.185412    -0.937968    -1.732483      86.63
 H       2.512687    -1.700066    -1.253669      23.36
 C       3.133905    -1.096884    -3.192679     104.92
 O       3.333813    -2.348477    -3.914434     292.39
 H       4.278178    -2.469368    -4.048979      27.34
 H       3.794411    -0.275884    -3.533943      25.66
 H       2.079065    -0.645419    -3.514746      25.50
 C      -0.652537    -0.109176     0.269990      64.56
 H      -1.363610    -0.904008     0.319775      23.20
 C      -0.018977     2.205014     0.371835      39.20
 H      -0.153724     3.323645     0.235185      19.42
 C       1.278796     1.891241    -0.377308     -10.83
 O       2.236262     2.927448    -0.863622     117.34
 C       1.734873     4.391385    -0.819331      82.94
 H       2.524779     4.798215    -1.642315      23.24
 H       0.880570     4.273960    -1.356312      27.70
 H       1.727850     4.745417     0.296094      22.39
 C       1.482513     0.529004    -0.625148      27.80
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 O       2.657318     0.413627    -1.391672     141.25
 C       0.662928    -0.442171    -0.209562      65.71
 H       0.808639    -1.511981    -0.353588      22.15
 C      -0.823691     1.249085     0.874339      34.80
 C      -2.206004     1.538530     1.566247      78.87
 H      -2.680440     0.552294     2.024882      22.22
 O      -1.804849     2.591224     2.538589     253.12
 H      -1.542019     2.077133     3.312513      27.62
 C      -3.378820     2.038975     0.722882      60.69
 H      -3.104912     2.920159    -0.074005      23.65
 O      -3.816720     0.709514    -0.154193      75.02
 H      -2.916557     0.576887    -0.595740      28.34
 C      -4.528391     2.424815     1.564979     101.65
 O      -5.523149     3.070516     0.658212     292.56
 H      -4.964931     3.751313     0.476028      32.46
 H      -4.192136     3.053656     2.544290      25.17
 H      -4.882078     1.653361     2.313751      26.45
55
name = lig-etoh-Waterframe_894
 C       4.867461    -0.713051     1.105795      46.50
 H       4.835806     0.375405     0.823572      21.86
 C       4.873710    -3.112491     0.427107      57.31
 H       4.954361    -3.963477    -0.284832      20.63
 C       4.854791    -3.390708     1.809162      30.29
 O       5.043883    -4.741741     2.421203     272.00
 C       4.046494    -5.737850     1.978570     101.02
 H       3.185569    -5.199689     1.792436      31.95
 H       3.714653    -6.417192     2.801908      26.28
 H       4.414012    -6.584333     1.148206      26.54
 C       5.141774    -2.424231     2.771613      13.66
 O       5.437800    -2.587060     4.066727     153.80
 H       5.601620    -3.567706     4.383069      20.50
 C       4.942816    -1.090153     2.447281      45.60
 H       4.770369    -0.345869     3.356251      21.44
 C       4.878029    -1.774959     0.097318      34.80
 C       4.775025    -1.314487    -1.323814      87.05
 H       4.883271    -2.328061    -1.889638      22.10
 O       5.728113    -0.415954    -1.747640     272.59
 H       5.429432     0.479174    -1.564866      28.24
 C       3.197039    -0.994826    -1.700454      75.70
 H       2.811636    -1.899457    -1.129174      24.10
 C       3.129257    -1.038831    -3.271917      94.33
 O       3.370310    -2.363653    -3.876280     264.46
 H       4.292833    -2.292039    -4.262298      24.84
 H       3.716017    -0.086039    -3.706568      24.45
 H       2.007571    -0.858004    -3.550476      25.98
 C      -0.581092    -0.121555     0.413993      52.89
 H      -1.299815    -0.803204     0.593446      26.66
 C       0.107211     2.283847     0.309751      39.22
 H      -0.332845     3.281341     0.680054      21.61
 C       1.265962     1.994223    -0.372789      18.89
 O       2.254610     2.944876    -0.853822     172.22
 C       1.808448     4.328346    -0.803850      93.83
 H       2.797186     5.140753    -1.332406      22.34
 H       0.880648     4.558074    -1.364975      26.23
 H       1.825347     4.909304     0.238806      23.39
 C       1.561884     0.594806    -0.686027     -11.94
 O       2.747216     0.325689    -1.420171     121.14
 C       0.558275    -0.520688    -0.187786      44.95
 H       0.893659    -1.538083    -0.495296      22.93
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 C      -0.869358     1.141802     0.761251      23.03
 C      -2.186565     1.514657     1.546117      99.79
 H      -2.490793     0.702057     2.245516      24.65
 O      -1.863415     2.640357     2.482182     251.38
 H      -1.837432     2.071925     3.243497      28.51
 C      -3.394215     2.055524     0.745923      55.59
 H      -3.091316     2.816135    -0.145515      24.10
 O      -3.719119     0.699610    -0.125694      68.62
 H      -3.151993     0.407211    -0.900674      28.32
 C      -4.582380     2.453252     1.566268     117.80
 O      -5.536447     3.045086     0.694255     289.53
 H      -5.235612     3.929318     0.344630      29.22
 H      -4.193349     3.227801     2.069494      27.84
 H      -5.102491     1.573648     1.943424      27.16
55
name = lig-etoh-Waterframe_895
 C       4.909730    -0.699947     1.134375      66.29
 H       4.776982     0.319378     0.936331      24.12
 C       4.857294    -3.084081     0.471943      43.47
 H       4.916107    -3.861077    -0.378046      20.41
 C       4.864578    -3.416216     1.881059      15.40
 O       4.971766    -4.755843     2.424685     246.76
 C       4.029798    -5.743961     1.989453      92.40
 H       3.094770    -5.437471     1.597524      29.52
 H       3.932187    -6.608870     3.018384      22.61
 H       4.525666    -6.223408     1.002211      24.89
 C       5.195988    -2.372772     2.788358       9.66
 O       5.387596    -2.608282     4.103420     138.47
 H       5.642614    -3.598336     4.290137      21.76
 C       4.932128    -1.063343     2.431350      58.93
 H       4.866118    -0.260178     3.236984      22.40
 C       4.930575    -1.662023     0.119810      38.68
 C       4.737828    -1.339999    -1.334360     104.84
 H       5.029990    -2.069504    -1.994405      25.17
 O       5.707617    -0.349453    -1.790385     217.21
 H       5.716845     0.442244    -1.253108      28.53
 C       3.329456    -1.101982    -1.733480      88.26
 H       2.505485    -1.727439    -1.275156      23.87
 C       3.013100    -0.995772    -3.352741      94.39
 O       3.450925    -2.300580    -3.846681     261.42
 H       4.193321    -2.211210    -4.546025      25.55
 H       3.817396    -0.376475    -3.904555      23.00
 H       1.974349    -0.884649    -3.564660      26.31
 C      -0.593206    -0.202493     0.589882      14.78
 H      -1.211916    -0.947115     1.014800      19.88
 C       0.083399     2.261793     0.329902      62.79
 H      -0.034398     3.248771     0.920794      23.04
 C       1.299182     2.050145    -0.408256      12.68
 O       2.204296     2.941369    -0.819451     188.53
 C       1.930321     4.338612    -0.773863      91.14
 H       2.984350     4.826880    -1.142422      22.09
 H       0.907316     4.672299    -1.217258      24.43
 H       1.709645     4.472008     0.301109      25.23
 C       1.569709     0.552446    -0.692562       4.05
 O       2.805647     0.270269    -1.386152     109.81
 C       0.720689    -0.465273    -0.318586      48.81
 H       0.704987    -1.602599    -0.529992      22.13
 C      -0.889486     1.246889     0.623517      19.83
 C      -2.106581     1.581394     1.509692      98.54
 H      -2.440706     0.635721     1.895675      27.22
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 O      -1.917697     2.656686     2.457474     282.47
 H      -1.857068     2.403249     3.354803      31.83
 C      -3.303167     1.869771     0.630075      90.22
 H      -3.103239     2.831381     0.119112      26.92
 O      -3.672301     0.719869    -0.075728     236.33
 H      -3.117604     0.833564    -0.912348      26.98
 C      -4.629039     2.508161     1.505789     102.01
 O      -5.618782     3.047595     0.685849     283.46
 H      -5.503280     3.924556     0.247421      30.45
 H      -4.265122     3.160921     2.292240      27.93
 H      -5.096421     1.644115     1.955925      28.76
55
name = lig-etoh-Waterframe_896
 C       4.915543    -0.623695     1.074326      53.22
 H       4.747627     0.344561     0.795815      23.59
 C       4.859868    -3.006116     0.569633      55.80
 H       4.677565    -3.783346    -0.255817      22.12
 C       4.958715    -3.482999     1.884618      23.76
 O       4.892550    -4.703033     2.427811     309.45
 C       4.043946    -5.779528     1.935874     107.95
 H       2.962450    -5.451898     1.807922      27.67
 H       4.065987    -6.614494     2.935290      23.98
 H       4.523498    -6.227532     1.135987      28.64
 C       5.152095    -2.385082     2.836508      -2.35
 O       5.373962    -2.661899     4.203436     122.23
 H       5.361830    -3.686930     4.258032      21.68
 C       4.970308    -0.990790     2.490407      50.17
 H       5.086767    -0.235115     3.222270      24.14
 C       4.934078    -1.675590     0.134282      41.75
 C       4.771118    -1.369357    -1.377855      79.17
 H       5.083457    -2.245471    -1.861737      24.92
 O       5.702370    -0.249153    -1.838178     150.67
 H       5.679514     0.390784    -1.131886      27.87
 C       3.268929    -1.062843    -1.878187      79.78
 H       2.693523    -1.974659    -1.503638      25.25
 C       3.012024    -1.035897    -3.365167     120.58
 O       3.469530    -2.259365    -3.861554     285.11
 H       4.385912    -2.166378    -4.454842      21.45
 H       3.412101    -0.035993    -3.718957      25.71
 H       2.040223    -0.735772    -3.503336      28.11
 C      -0.430581    -0.140663     0.560813      43.80
 H      -0.906395    -0.985304     1.165933      21.02
 C       0.096140     2.241407     0.326939      64.38
 H       0.021101     3.283737     0.676435      23.86
 C       1.256381     1.906151    -0.418123      16.12
 O       2.182984     2.894851    -0.827529     193.87
 C       2.018477     4.357845    -0.640731     120.54
 H       2.763140     4.773404    -1.018299      28.17
 H       1.297226     4.611399    -1.486305      24.18
 H       1.915292     4.646605     0.357110      27.46
 C       1.630836     0.544547    -0.730000      18.63
 O       2.852023     0.285126    -1.305282     126.72
 C       0.665827    -0.413578    -0.294936      49.75
 H       1.055299    -1.471167    -0.651368      22.97
 C      -0.857586     1.247294     0.635500      34.12
 C      -2.046584     1.597781     1.484792      97.56
 H      -2.196391     0.692354     2.023729      25.86
 O      -1.952924     2.697332     2.437740     267.10
 H      -1.794807     2.208193     3.236114      30.35
 C      -3.311316     1.892945     0.620352      93.66
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 H      -3.044314     2.536341    -0.170911      26.46
 O      -3.643995     0.723801    -0.095305     246.08
 H      -3.247138     0.801119    -1.019935      26.76
 C      -4.577614     2.463556     1.437332      89.13
 O      -5.763198     3.062610     0.624275     253.46
 H      -5.130330     3.848550     0.389827      27.64
 H      -4.316532     3.104077     2.424054      25.28
 H      -5.062503     1.653038     2.029726      27.37
55
name = lig-etoh-Waterframe_897
 C       4.909691    -0.580716     1.101702      44.96
 H       4.853623     0.419093     0.731559      20.66
 C       4.856510    -3.013120     0.592593      46.35
 H       4.558605    -3.808258    -0.104546      22.10
 C       5.048851    -3.368784     1.913179      15.88
 O       4.836175    -4.686580     2.460245     275.40
 C       4.072250    -5.819448     1.903435     117.23
 H       2.958102    -5.440022     1.887120      25.17
 H       4.097988    -6.549820     2.624750      25.48
 H       4.322596    -6.293123     1.044107      26.43
 C       5.078642    -2.368074     2.941703       5.06
 O       5.354312    -2.731356     4.262468     214.67
 H       5.188868    -3.686910     4.529490      29.24
 C       5.066569    -0.963783     2.483760      52.45
 H       5.188675    -0.310020     3.244629      23.58
 C       4.877424    -1.650944     0.118716      20.21
 C       4.829769    -1.336478    -1.436329      77.64
 H       5.117221    -2.345229    -1.931255      21.43
 O       5.672229    -0.216591    -1.860919     187.89
 H       5.481682     0.574109    -1.324711      25.40
 C       3.208332    -1.005949    -1.904337      78.18
 H       2.776962    -1.863471    -1.449166      24.79
 C       3.027882    -0.950285    -3.362445     104.96
 O       3.440316    -2.233114    -3.931396     288.69
 H       4.425984    -2.232795    -4.265282      23.20
 H       3.492272    -0.091426    -3.803950      25.62
 H       1.870567    -1.123681    -3.553747      23.80
 C      -0.304191    -0.014576     0.484563      47.12
 H      -0.888860    -0.935066     0.973769      20.37
 C       0.129097     2.221358     0.263080      68.22
 H      -0.191274     3.218362     0.238675      25.91
 C       1.262251     1.832827    -0.430246      23.20
 O       2.203764     2.826522    -0.831012     163.45
 C       2.072401     4.321167    -0.544589     108.08
 H       2.959571     4.794366    -0.936066      24.13
 H       1.160436     4.765757    -1.104184      23.65
 H       1.905988     4.834621     0.363636      26.50
 C       1.618060     0.551849    -0.747332      23.98
 O       2.908526     0.282456    -1.240976     145.36
 C       0.715414    -0.424583    -0.297719      57.73
 H       0.963254    -1.536935    -0.285131      22.41
 C      -0.750963     1.218980     0.762127      47.43
 C      -2.074901     1.572491     1.479787      97.70
 H      -2.360323     0.763786     2.133174      24.71
 O      -1.940620     2.723898     2.445052     247.25
 H      -1.655232     2.213923     3.190745      29.75
 C      -3.342269     2.022992     0.606031      76.53
 H      -3.026375     2.704176    -0.172193      24.70
 O      -3.656147     0.651093    -0.154847     197.34
 H      -3.446911     0.577785    -1.137368      25.60
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 C      -4.578685     2.353493     1.412437      82.80
 O      -5.778374     3.070970     0.590852     169.84
 H      -5.468983     3.996489     0.037091      26.70
 H      -4.212216     3.379275     1.836138      22.12
 H      -5.021909     1.358278     1.746700      25.65
55
name = lig-etoh-Waterframe_898
 C       4.930217    -0.644326     1.141013      49.51
 H       5.039698     0.483594     0.996428      20.73
 C       4.840089    -3.003049     0.542092      35.12
 H       4.737804    -3.836939    -0.094292      22.55
 C       5.016787    -3.300952     1.986768      -4.08
 O       4.836449    -4.681880     2.486198     251.03
 C       4.067052    -5.792595     1.889067     110.44
 H       2.937997    -5.562495     1.753993      26.86
 H       4.190359    -6.526725     2.524407      25.09
 H       4.397643    -6.005331     0.735718      24.01
 C       5.075267    -2.321672     3.010517      18.44
 O       5.313820    -2.747793     4.315593     226.15
 H       5.220058    -3.743900     4.321150      23.33
 C       5.160810    -0.999972     2.510510      56.53
 H       5.202640    -0.185665     3.205179      22.02
 C       4.815331    -1.592713     0.105920      23.39
 C       4.776161    -1.260665    -1.438571      95.39
 H       5.247334    -2.046655    -2.216743      18.98
 O       5.641761    -0.212560    -1.869321     230.83
 H       5.205922     0.680366    -1.767552      25.27
 C       3.295512    -0.973898    -1.774289      88.50
 H       2.530641    -1.583507    -1.397489      23.64
 C       2.988552    -0.905906    -3.420047      86.93
 O       3.380846    -2.213227    -3.990772     277.40
 H       4.231743    -2.208867    -4.512842      25.60
 H       3.484103    -0.188985    -3.994521      25.83
 H       1.750430    -0.817571    -3.677691      23.22
 C      -0.345057    -0.061562     0.503626      54.48
 H      -1.148725    -0.892587     0.754069      19.91
 C       0.091596     2.243027     0.183203      66.69
 H      -0.239607     3.209542     0.026961      20.37
 C       1.334854     1.939801    -0.457236      17.87
 O       2.248514     2.820586    -0.817345     177.76
 C       2.051109     4.261201    -0.490779      77.72
 H       3.130065     4.790453    -1.133462      20.45
 H       1.128668     4.666377    -0.941465      23.64
 H       2.086962     4.175854     0.619511      23.63
 C       1.661183     0.491822    -0.773154      11.55
 O       2.951023     0.278659    -1.203714     168.37
 C       0.858897    -0.512791    -0.308076      62.77
 H       0.903503    -1.519409    -0.207066      22.08
 C      -0.680893     1.309919     0.889060      29.13
 C      -2.148367     1.595828     1.504090      71.09
 H      -2.653293     0.623697     1.793879      22.08
 O      -1.892967     2.710473     2.461656     266.76
 H      -1.547399     2.484111     3.299128      29.81
 C      -3.320237     1.980018     0.462199      68.58
 H      -3.157776     3.036584     0.023521      22.43
 O      -3.685507     0.602326    -0.187014     210.51
 H      -3.432301     0.826024    -1.134754      25.38
 C      -4.617504     2.399505     1.251841      94.60
 O      -5.750781     3.008889     0.553814     225.50
 H      -5.314824     3.984496     0.126978      25.00
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 H      -4.341919     2.913618     2.277210      25.22
 H      -5.045825     1.570564     1.916072      26.58
55
name = lig-etoh-Waterframe_899
 C       4.994071    -0.708220     1.203471      38.21
 H       5.072904     0.445721     0.929713      21.66
 C       4.836135    -2.950461     0.580323      46.57
 H       4.958884    -3.685011    -0.162628      19.16
 C       4.856539    -3.340828     1.940638      24.66
 O       4.868587    -4.638805     2.510668     303.39
 C       4.060759    -5.684713     1.813676     127.30
 H       2.979547    -5.511653     1.889445      27.21
 H       4.328480    -6.736861     2.409062      25.41
 H       4.740456    -5.820938     0.755785      26.25
 C       5.141066    -2.329295     3.025639       4.54
 O       5.257006    -2.737572     4.349873     151.15
 H       5.325120    -3.705766     4.265348      20.40
 C       5.206627    -1.010077     2.569292      54.95
 H       5.327502    -0.081128     3.238622      22.42
 C       4.806190    -1.628009     0.109580      35.74
 C       4.704172    -1.208522    -1.405796      94.56
 H       4.888265    -2.276772    -1.869643      22.34
 O       5.609332    -0.147231    -1.874219     221.94
 H       5.138781     0.737163    -1.933184      24.89
 C       3.320072    -0.932418    -1.785525      82.21
 H       2.748261    -1.822370    -1.408283      23.19
 C       2.971599    -0.918491    -3.451869     103.14
 O       3.271265    -2.198344    -4.041822     288.42
 H       4.092583    -2.081877    -4.534342      26.34
 H       3.537779    -0.069664    -3.844048      26.32
 H       1.960815    -0.443068    -3.462974      25.74
 C      -0.377093    -0.121436     0.516025      37.65
 H      -1.124619    -0.883119     0.742671      21.74
 C       0.099366     2.331918     0.104700      39.06
 H      -0.209567     3.363886     0.209044      18.36
 C       1.331723     1.898830    -0.476843       8.50
 O       2.330726     2.859431    -0.871362     177.62
 C       2.048559     4.138571    -0.472215      98.37
 H       2.953111     5.014913    -1.037890      22.46
 H       1.112060     4.544347    -0.733286      26.90
 H       2.341671     4.295038     0.664974      24.44
 C       1.743385     0.540788    -0.721568       2.72
 O       3.016723     0.340801    -1.189469     139.47
 C       0.782259    -0.559705    -0.170676      41.84
 H       1.085317    -1.478200    -0.474456      21.62
 C      -0.707907     1.248427     0.876963       7.04
 C      -2.142027     1.638907     1.482834      77.14
 H      -2.398160     0.681195     2.123941      21.92
 O      -1.888131     2.693073     2.461695     261.93
 H      -1.593101     2.126921     3.173455      28.34
 C      -3.355546     1.916296     0.427222      64.77
 H      -2.992013     2.518827    -0.591359      22.83
 O      -3.678516     0.674852    -0.238463     225.34
 H      -3.461062     0.666463    -1.222100      25.69
 C      -4.654480     2.406425     1.235147      99.83
 O      -5.670995     2.957113     0.489554     288.91
 H      -5.395980     3.982658     0.292183      26.05
 H      -4.350011     2.996150     2.052563      26.13
 H      -5.141767     1.412844     1.432870      26.28
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name = lig-etoh-Waterframe_900
 C       5.064338    -0.697758     1.216557      55.09
 H       5.020742     0.395263     0.835913      23.88
 C       4.828325    -2.983099     0.592441      53.96
 H       4.907242    -3.760173    -0.184857      22.21
 C       4.745679    -3.321255     1.982427      20.15
 O       4.881021    -4.605153     2.505018     206.23
 C       4.164758    -5.575609     1.758263     112.07
 H       3.159005    -5.332033     1.750722      28.53
 H       4.282810    -6.757245     2.357581      23.64
 H       4.276391    -5.707787     0.594629      25.62
 C       5.161269    -2.403301     2.963052      -0.48
 O       5.211245    -2.729295     4.339260     163.73
 H       5.289738    -3.640377     4.620935      24.20
 C       5.228901    -1.002060     2.604174      45.60
 H       5.552911    -0.247779     3.474612      21.21
 C       4.845797    -1.594777     0.215921      32.71
 C       4.716293    -1.225283    -1.333615      85.81
 H       5.022347    -2.090688    -1.865362      25.35
 O       5.576775    -0.118928    -1.879014     178.83
 H       5.185386     0.803545    -1.567804      22.57
 C       3.261632    -0.927032    -1.897232      85.34
 H       2.760829    -1.793970    -1.327094      25.35
 C       3.007673    -0.858780    -3.350977     112.18
 O       3.140754    -2.154104    -4.091400     280.53
 H       4.065512    -2.246977    -4.361372      26.47
 H       3.808175    -0.172502    -3.794723      24.96
 H       2.016500    -0.746537    -3.537626      28.91
 C      -0.423033    -0.155824     0.549511      43.37
 H      -0.981767    -0.906030     0.926963      23.62
 C       0.078896     2.251087     0.147960      41.12
 H      -0.047242     3.333951     0.454935      19.89
 C       1.338863     1.889702    -0.501700       1.96
 O       2.369594     2.817373    -0.955294     167.80
 C       2.093664     4.179471    -0.448892     109.96
 H       2.608557     4.751764    -1.088919      26.55
 H       1.089301     4.383683    -0.580115      27.69
 H       2.329108     4.588940     0.668663      24.56
 C       1.665405     0.533276    -0.540452      14.14
 O       3.030275     0.400660    -1.189696     103.33
 C       0.804141    -0.434288    -0.108092      64.94
 H       0.922799    -1.516045    -0.505020      23.74
 C      -0.740288     1.239980     0.657379      32.47
 C      -2.057011     1.621577     1.410066      83.72
 H      -2.472938     0.759059     2.030277      23.89
 O      -1.900268     2.664405     2.469088     258.34
 H      -1.731064     2.073100     3.206596      28.99
 C      -3.335239     1.879524     0.400340      77.30
 H      -2.890511     2.631095    -0.359935      25.19
 O      -3.698622     0.694019    -0.282872     242.19
 H      -3.324828     0.620201    -1.221464      26.47
 C      -4.609093     2.308446     1.225577     102.80
 O      -5.634593     2.980007     0.367960     323.42
 H      -5.496723     3.916562     0.130646      30.20
 H      -4.358361     2.998231     1.931408      27.79
 H      -4.948927     1.317294     1.493268      28.28
55
name = lig-etoh-Waterframe_901
 C       5.121792    -0.577647     1.283318      49.56
 H       5.145879     0.496784     1.081376      25.12
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 C       4.790611    -3.005512     0.607023      62.88
 H       4.607132    -3.857895    -0.130707      24.07
 C       4.767708    -3.309906     1.993512      22.66
 O       4.895864    -4.612104     2.462235     226.81
 C       4.167504    -5.526709     1.679061     135.42
 H       3.143697    -5.267497     1.815921      26.83
 H       4.361943    -6.581434     2.235363      26.21
 H       4.503132    -5.560075     0.738713      28.62
 C       5.112079    -2.378851     2.979161      22.12
 O       5.188479    -2.699869     4.312700     138.35
 H       5.159874    -3.646109     4.464672      22.65
 C       5.269864    -1.066626     2.608533      52.74
 H       5.591487    -0.330003     3.456717      23.13
 C       4.883256    -1.622326     0.247693       7.53
 C       4.769463    -1.234297    -1.320082      86.23
 H       5.238303    -1.945786    -1.862756      26.20
 O       5.530648    -0.112968    -1.843028     113.23
 H       5.449021     0.726874    -1.240393      25.29
 C       3.261393    -0.953797    -1.782001      86.64
 H       2.304573    -1.491373    -1.525089      24.95
 C       3.042186    -0.825640    -3.328539      96.48
 O       3.074878    -2.118039    -4.101372     287.80
 H       3.981482    -2.393720    -4.299050      27.01
 H       3.692375    -0.021439    -3.888466      25.05
 H       2.063286    -0.449569    -3.572776      27.79
 C      -0.436382    -0.110157     0.552085      36.30
 H      -0.944039    -0.856687     1.041925      23.75
 C       0.162944     2.167096     0.184558      58.20
 H      -0.203538     3.220156     0.542034      24.36
 C       1.338494     1.951610    -0.461985      30.15
 O       2.300690     2.765348    -0.959781     191.07
 C       2.107975     4.267682    -0.489738     102.15
 H       2.606093     4.726947    -1.124734      29.45
 H       1.034707     4.419039    -0.612284      25.42
 H       2.546216     4.172199     0.555543      25.56
 C       1.730135     0.577788    -0.483119      15.61
 O       2.912578     0.385105    -1.188702     118.07
 C       0.794831    -0.413246    -0.078788      56.47
 H       0.968310    -1.637864    -0.081577      23.99
 C      -0.853659     1.209997     0.504925      38.31
 C      -2.046305     1.553661     1.338191      91.25
 H      -2.305322     0.577694     1.623960      27.05
 O      -1.899378     2.612965     2.446871     244.06
 H      -1.848061     2.261538     3.328209      29.71
 C      -3.239641     1.938957     0.414767      92.87
 H      -3.170368     2.853049     0.009602      27.50
 O      -3.722824     0.658613    -0.341099     195.52
 H      -3.091415     0.656328    -1.130917      27.40
 C      -4.542987     2.273643     1.136306      97.14
 O      -5.606152     2.955946     0.260563     309.90
 H      -5.201998     3.753184     0.057178      32.62
 H      -4.283724     2.833367     2.129069      26.20
 H      -5.076390     1.553408     1.756519      27.06
55
name = lig-etoh-Waterframe_902
 C       5.160069    -0.579067     1.303250      46.99
 H       5.317590     0.430298     1.202258      21.00
 C       4.720058    -2.937667     0.643374      59.14
 H       4.400015    -3.649190    -0.199535      22.97
 C       4.885458    -3.325322     1.969900      23.36
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 O       4.920810    -4.627996     2.434503     204.33
 C       4.138883    -5.557855     1.625175     129.74
 H       2.972494    -5.405990     1.632751      25.81
 H       4.293562    -6.457212     1.952587      30.91
 H       4.622763    -5.576562     0.699522      28.27
 C       5.032089    -2.338573     3.014577      17.28
 O       5.181243    -2.693892     4.308925     209.68
 H       5.071941    -3.641114     4.258566      23.21
 C       5.326563    -1.025527     2.606340      52.80
 H       5.502682    -0.306982     3.400438      24.24
 C       4.931599    -1.572780     0.236299      28.46
 C       4.761204    -1.250618    -1.271138      91.06
 H       4.967505    -2.248537    -1.823432      24.62
 O       5.501040    -0.114469    -1.769192     150.84
 H       5.456871     0.776588    -1.230693      21.71
 C       3.224619    -0.949958    -1.654392      68.89
 H       2.590885    -1.837428    -1.391403      26.27
 C       3.057094    -0.781434    -3.394108      86.83
 O       3.064451    -2.073057    -4.049329     264.71
 H       3.979127    -2.126802    -4.440795      25.55
 H       3.905867    -0.097881    -3.736405      24.95
 H       2.063736    -0.208641    -3.297325      26.24
 C      -0.412174    -0.096161     0.500680      42.72
 H      -1.070000    -0.860413     1.002662      21.57
 C       0.123509     2.210872     0.229500      56.44
 H      -0.190627     3.325431     0.305816      22.47
 C       1.376021     1.909992    -0.378571      31.69
 O       2.198148     2.835881    -0.945744     211.14
 C       2.119878     4.214452    -0.572802     103.85
 H       2.946205     4.951766    -1.199175      22.65
 H       1.076046     4.793101    -0.465802      23.10
 H       2.534756     4.329927     0.430604      26.12
 C       1.745326     0.568240    -0.508388      23.74
 O       2.833022     0.335961    -1.207841     142.65
 C       0.805515    -0.476989    -0.015950      59.80
 H       1.428738    -1.451809     0.214783      23.86
 C      -0.867863     1.216441     0.492311      43.78
 C      -2.114183     1.490822     1.307419      99.94
 H      -2.361721     0.629253     1.870458      25.54
 O      -1.891046     2.529039     2.363394     245.98
 H      -1.911600     1.847196     3.076411      25.65
 C      -3.282189     1.941047     0.457682      69.54
 H      -3.026293     2.765141    -0.382857      21.87
 O      -3.672128     0.705982    -0.409113     192.22
 H      -3.069399     0.378583    -1.152439      25.45
 C      -4.566847     2.298008     1.150230      89.45
 O      -5.504431     2.893155     0.215004     275.17
 H      -5.235317     3.852933    -0.102581      27.42
 H      -4.230037     3.270441     1.831969      22.76
 H      -5.153625     1.319255     1.383058      24.59
55
name = lig-etoh-Waterframe_903
 C       5.224626    -0.625052     1.248065      57.27
 H       5.413544     0.329984     0.928753      23.50
 C       4.668613    -2.808600     0.644299      56.60
 H       4.426309    -3.562090    -0.145228      22.49
 C       4.985870    -3.296365     1.971736      -0.92
 O       4.910464    -4.675907     2.411092     195.12
 C       4.151312    -5.630740     1.568678     100.42
 H       2.993142    -5.249876     1.498292      25.23
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 H       4.244110    -6.561622     1.994375      26.03
 H       4.422106    -5.603229     0.354814      23.56
 C       5.023103    -2.311720     2.975887      10.61
 O       5.170742    -2.732736     4.328084     212.93
 H       5.074709    -3.655213     4.563691      24.50
 C       5.329397    -0.949492     2.654378      60.43
 H       5.478286    -0.235707     3.355806      24.29
 C       4.948455    -1.495707     0.259738      51.31
 C       4.647907    -1.210581    -1.181608      88.50
 H       4.978287    -2.165110    -1.916678      21.19
 O       5.519493    -0.158380    -1.703630     186.45
 H       5.061678     0.718674    -1.344237      22.58
 C       3.240962    -0.996950    -1.682671      97.82
 H       2.812711    -1.836454    -1.168373      24.41
 C       3.086295    -0.750785    -3.281802      90.65
 O       3.110513    -2.008997    -3.988751     267.76
 H       3.823049    -1.967953    -4.684697      26.81
 H       3.972530    -0.230106    -3.574296      26.02
 H       2.023847    -0.318915    -3.663763      23.60
 C      -0.396793    -0.157336     0.454320      38.45
 H      -1.164518    -0.999233     0.841947      20.02
 C       0.042572     2.298961     0.225574      50.05
 H      -0.145288     3.367369     0.156415      20.09
 C       1.316031     1.885956    -0.262228      -5.41
 O       2.121335     2.924661    -0.971623     176.41
 C       2.167450     4.239229    -0.560843      91.00
 H       3.024893     4.774078    -1.550425      21.98
 H       1.102465     4.812601    -0.791470      23.08
 H       2.481530     4.483575     0.379861      27.74
 C       1.606760     0.497209    -0.499993      20.22
 O       2.846099     0.283086    -1.236651     151.05
 C       0.949630    -0.497875     0.055785      66.53
 H       1.286271    -1.496287     0.293423      22.13
 C      -0.803423     1.245392     0.590766      17.56
 C      -2.198005     1.472927     1.294712      78.40
 H      -2.629890     0.557870     1.815405      22.48
 O      -1.883081     2.410873     2.285791     249.33
 H      -1.652827     1.893727     3.156312      24.98
 C      -3.338172     1.853062     0.349704      70.58
 H      -2.682923     2.632363    -0.401337      21.83
 O      -3.643271     0.752416    -0.447520     240.81
 H      -2.878709     0.616420    -1.095973      25.29
 C      -4.598895     2.398921     1.107441     101.34
 O      -5.433603     2.847193     0.158870     278.89
 H      -5.450056     3.933820     0.020085      24.08
 H      -4.491977     2.983093     2.148960      25.20
 H      -4.898225     1.388027     1.652726      26.79
55
name = lig-etoh-Waterframe_904
 C       5.333271    -0.541005     1.271561      47.34
 H       5.499540     0.459481     0.890953      23.75
 C       4.674895    -2.822079     0.679035      40.79
 H       4.464658    -3.544634    -0.080610      21.30
 C       4.969425    -3.293963     1.927323       0.82
 O       4.900054    -4.689895     2.344807     230.08
 C       4.145385    -5.636001     1.495875      90.58
 H       3.088016    -5.322013     1.792421      25.48
 H       4.228911    -6.695255     2.100669      23.35
 H       4.635041    -5.784215     0.318418      22.08
 C       5.133244    -2.331560     3.031742       5.03
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 O       5.158997    -2.735416     4.348816     210.64
 H       5.044274    -3.703191     4.394678      25.83
 C       5.276776    -0.920805     2.644100      57.33
 H       5.480208    -0.217774     3.372960      23.41
 C       4.862484    -1.511087     0.267222      41.15
 C       4.646185    -1.163702    -1.214496     102.14
 H       5.140302    -2.127074    -1.642453      21.54
 O       5.526064    -0.178515    -1.622037     188.09
 H       5.160142     0.790498    -1.743755      22.43
 C       3.212482    -1.037369    -1.731416      95.70
 H       2.411262    -1.679459    -1.451006      24.47
 C       3.124553    -0.794018    -3.151633     114.54
 O       3.186411    -2.002085    -3.956947     288.08
 H       3.853848    -1.958923    -4.703588      26.12
 H       3.826436    -0.067660    -3.363781      27.17
 H       2.233263    -0.100213    -3.420156      25.16
 C      -0.369412    -0.152905     0.460255      49.15
 H      -1.094244    -1.079751     0.700303      21.52
 C       0.011617     2.329819     0.213662      56.10
 H      -0.352070     3.281371     0.310104      21.68
 C       1.243599     1.970331    -0.259099      11.89
 O       2.055180     2.854041    -0.977859     175.45
 C       2.177536     4.360630    -0.597733     100.22
 H       3.149595     4.536600    -1.227950      23.96
 H       1.268808     4.819659    -0.952524      25.32
 H       2.505161     4.503945     0.408629      27.02
 C       1.674600     0.535530    -0.547493     -12.84
 O       2.814751     0.311768    -1.191591     106.38
 C       0.920792    -0.580937     0.184637      52.64
 H       1.149138    -1.558572     0.027709      23.07
 C      -0.819230     1.130500     0.708601      25.18
 C      -2.216547     1.383807     1.281404      79.81
 H      -2.517366     0.307962     1.526717      23.03
 O      -1.901547     2.368045     2.275501     251.15
 H      -1.462607     1.951841     3.111859      25.84
 C      -3.261355     1.892230     0.288480      85.46
 H      -3.192879     2.861044    -0.246694      23.14
 O      -3.654430     0.747133    -0.507699     230.26
 H      -2.918731     0.717873    -1.201854      25.65
 C      -4.521718     2.371145     1.122865      99.85
 O      -5.500450     2.864293     0.102473     290.85
 H      -5.259673     3.941372     0.026448      24.76
 H      -4.310661     3.093152     1.850958      26.38
 H      -5.137079     1.583525     1.538015      26.35
55
name = lig-etoh-Waterframe_905
 C       5.341808    -0.513888     1.261616      50.32
 H       5.574079     0.618174     1.180222      24.10
 C       4.693511    -2.899999     0.651818      43.05
 H       4.406951    -3.592549    -0.079331      19.93
 C       4.904576    -3.322755     2.009705       9.58
 O       4.918985    -4.650201     2.259629     241.47
 C       4.138278    -5.626709     1.515878     101.53
 H       3.132644    -5.533106     1.332029      31.57
 H       4.461795    -6.746425     2.040406      23.71
 H       4.496190    -5.700664     0.449103      26.74
 C       5.250366    -2.335361     3.007097      11.26
 O       5.157318    -2.740591     4.365043     193.58
 H       5.000275    -3.697863     4.244694      24.99
 C       5.266824    -0.966209     2.634197      42.94
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 H       5.465292    -0.248435     3.486794      20.77
 C       4.789910    -1.442670     0.345745      28.17
 C       4.699093    -1.255478    -1.201602      88.17
 H       4.967482    -2.074883    -1.744518      25.82
 O       5.571348    -0.136239    -1.587227     174.36
 H       5.208656     0.832978    -1.630669      21.15
 C       3.134654    -1.011786    -1.661780      71.42
 H       2.427790    -1.873919    -1.517723      25.30
 C       3.161594    -0.752176    -3.184908     111.05
 O       3.261552    -2.023274    -3.932884     275.65
 H       4.156824    -1.889545    -4.404554      24.12
 H       4.013406    -0.119584    -3.462710      25.30
 H       2.184303    -0.415192    -3.201883      27.39
 C      -0.389686    -0.215175     0.569609      50.79
 H      -1.147148    -0.993071     0.771938      23.83
 C      -0.093738     2.192267     0.295586      56.33
 H      -0.466506     3.131979     0.481371      22.69
 C       1.219477     1.972699    -0.372986       5.86
 O       2.050076     2.832743    -0.970904     164.23
 C       2.201222     4.373888    -0.674030     106.54
 H       2.940617     4.746632    -1.085952      29.35
 H       1.486284     4.996435    -0.951386      27.23
 H       2.209363     4.488954     0.499650      25.25
 C       1.651187     0.531931    -0.413165      -2.19
 O       2.824855     0.379842    -1.155828     117.50
 C       0.945776    -0.508201     0.134636      78.16
 H       1.085818    -1.498920    -0.140691      24.74
 C      -0.806325     1.102517     0.701253      44.86
 C      -2.118302     1.305683     1.226929      91.57
 H      -2.643233     0.493009     1.851006      23.15
 O      -1.963329     2.377841     2.305836     221.45
 H      -1.714685     1.701350     3.047688      24.32
 C      -3.271884     1.964067     0.332533      74.36
 H      -2.996305     2.711352    -0.306424      25.93
 O      -3.665490     0.758833    -0.591810     195.45
 H      -3.248123     0.437888    -1.455194      24.27
 C      -4.500889     2.320325     1.065124     105.79
 O      -5.559617     2.919840     0.131234     316.90
 H      -5.428838     3.855813    -0.402071      27.01
 H      -4.111825     3.132090     1.510455      26.32
 H      -5.015964     1.534762     1.546347      27.06
55
name = lig-etoh-Waterframe_906
 C       5.238146    -0.556686     1.329964      56.71
 H       5.482892     0.566445     1.000868      24.80
 C       4.697731    -2.845359     0.688947      67.99
 H       4.423770    -3.528418    -0.074211      23.26
 C       4.847956    -3.288646     1.964511      18.79
 O       4.920710    -4.649147     2.251106     218.18
 C       4.185546    -5.631420     1.481952     118.48
 H       3.148203    -5.471630     1.529079      29.01
 H       4.407626    -6.642279     2.093182      24.27
 H       4.582347    -5.649918     0.609837      30.07
 C       5.263434    -2.368437     2.976393      20.26
 O       5.179206    -2.752291     4.343405     158.73
 H       4.989944    -3.691869     4.559945      27.03
 C       5.346885    -1.021113     2.644616      48.94
 H       5.447562    -0.241965     3.543909      19.76
 C       4.801275    -1.489302     0.347700      37.50
 C       4.673403    -1.264047    -1.138059      88.61
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 H       4.995479    -2.047686    -1.734187      24.63
 O       5.625246    -0.117545    -1.583992     163.03
 H       5.135816     0.623113    -1.167857      27.28
 C       3.228514    -0.912283    -1.607562      80.01
 H       2.642501    -1.772630    -1.119450      24.16
 C       3.133725    -0.746290    -3.226252      90.49
 O       3.358164    -2.034322    -3.904802     286.03
 H       4.317145    -2.259168    -4.250169      24.47
 H       3.938338     0.012289    -3.633476      24.40
 H       2.232888    -0.430404    -3.728278      26.67
 C      -0.372411    -0.315478     0.688982      56.01
 H      -0.973147    -1.081159     0.969432      25.02
 C      -0.019891     2.115845     0.296078      74.63
 H      -0.440544     3.093640     0.496765      25.27
 C       1.095168     1.884858    -0.387556      17.92
 O       2.108071     2.921215    -1.001039     121.75
 C       2.148698     4.296531    -0.699847     112.09
 H       3.128734     4.708952    -1.079361      25.21
 H       1.266245     4.765354    -1.149725      24.83
 H       2.148329     4.456641     0.545639      23.51
 C       1.667289     0.642099    -0.316836      19.25
 O       2.831825     0.392925    -1.108407     121.49
 C       0.858056    -0.468231     0.045834      48.69
 H       1.336051    -1.487972    -0.042237      24.86
 C      -0.830379     0.990492     0.671190      21.25
 C      -2.191623     1.395504     1.288227      93.33
 H      -2.564742     0.417734     1.728392      26.78
 O      -2.025277     2.370438     2.339408     238.08
 H      -2.035797     2.046339     3.298484      26.32
 C      -3.222725     1.841948     0.230855      85.00
 H      -2.582144     2.581284    -0.291295      26.61
 O      -3.728789     0.772987    -0.645365     220.62
 H      -3.093110     0.730206    -1.436846      27.70
 C      -4.546294     2.410388     0.932028      98.71
 O      -5.621025     2.914596     0.181386     300.70
 H      -5.234575     3.894766     0.026454      24.88
 H      -4.239724     3.112368     1.924533      23.72
 H      -4.774375     1.610336     1.655122      26.56
55
name = lig-etoh-Waterframe_907
 C       5.103042    -0.624917     1.365508      42.89
 H       5.258089     0.471333     1.018851      20.68
 C       4.645606    -2.804306     0.667025      70.11
 H       4.484483    -3.542932    -0.132951      24.39
 C       4.862143    -3.300602     1.950548      33.10
 O       4.917066    -4.649589     2.307527     178.21
 C       4.230717    -5.633600     1.481258     122.58
 H       3.153813    -5.343663     1.677982      26.60
 H       4.326143    -6.547490     1.930308      28.63
 H       4.619372    -5.789050     0.382170      27.03
 C       5.172423    -2.454298     3.011241      17.60
 O       5.229184    -2.741412     4.325233     200.89
 H       5.077673    -3.723142     4.421212      23.35
 C       5.443148    -1.039997     2.685593      36.42
 H       5.651746    -0.265436     3.570408      25.27
 C       4.868223    -1.518901     0.322254      46.31
 C       4.707978    -1.130044    -1.139019     100.06
 H       5.049528    -2.167442    -1.600706      23.26
 O       5.626858    -0.156925    -1.551642     222.03
 H       5.535518     0.740269    -1.158679      25.54
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 C       3.320839    -0.799254    -1.617598      89.26
 H       2.592032    -1.564084    -1.232071      25.98
 C       3.134358    -0.797308    -3.271873      87.61
 O       3.432766    -2.084182    -3.853716     266.80
 H       4.417414    -1.987365    -4.322047      21.81
 H       3.890695     0.102518    -3.424438      24.46
 H       2.117306    -0.348364    -3.666282      26.15
 C      -0.362392    -0.391499     0.751560      46.73
 H      -0.728697    -1.235805     1.201010      25.55
 C      -0.046270     2.084854     0.297304      47.23
 H      -0.410161     3.198120     0.390066      23.79
 C       1.210328     1.966346    -0.432920      14.12
 O       2.125013     2.877278    -1.012754     159.12
 C       2.019631     4.242642    -0.675295      97.11
 H       3.144373     4.702736    -1.234779      21.84
 H       1.080135     4.726091    -1.256413      23.18
 H       2.074269     4.604317     0.457501      23.74
 C       1.710984     0.599124    -0.385176      15.48
 O       2.852980     0.432855    -1.029141     131.29
 C       0.831835    -0.499780     0.009937      55.03
 H       1.465808    -1.480299     0.167106      25.37
 C      -0.924695     0.952840     0.739735      13.87
 C      -2.282609     1.370286     1.401517      95.98
 H      -2.652397     0.451339     1.748494      29.76
 O      -2.107764     2.429708     2.344943     236.25
 H      -1.992685     1.853533     3.203217      25.75
 C      -3.212020     1.788067     0.142150      70.16
 H      -2.737448     2.639610    -0.588389      25.77
 O      -3.765577     0.805853    -0.689453     221.20
 H      -3.054153     0.654174    -1.403450      27.56
 C      -4.511986     2.457030     0.921445      67.93
 O      -5.651013     2.928389     0.228836     224.76
 H      -5.755132     3.947479     0.111487      26.52
 H      -4.242615     3.377470     1.786521      22.14
 H      -5.027980     1.429496     1.253946      24.45
55
name = lig-etoh-Waterframe_908
 C       5.058773    -0.619524     1.420750      56.36
 H       5.070325     0.442595     1.346430      22.82
 C       4.612142    -2.911375     0.613537      51.48
 H       4.461105    -3.659571    -0.234970      22.40
 C       4.887824    -3.351830     1.972239       9.36
 O       4.919999    -4.676584     2.356877     158.30
 C       4.224893    -5.629458     1.524073     115.80
 H       3.089818    -5.425425     1.257604      25.17
 H       4.370392    -6.519240     1.910579      27.92
 H       4.568541    -5.612812     0.242788      24.30
 C       5.111137    -2.361720     3.028602      23.15
 O       5.286951    -2.786596     4.347816     203.59
 H       5.232221    -3.789273     4.420694      24.02
 C       5.444290    -1.109736     2.693728      60.49
 H       5.880491    -0.434636     3.455659      24.16
 C       4.870214    -1.468771     0.311881      24.58
 C       4.755715    -1.048314    -1.133584      96.29
 H       4.968156    -2.010841    -1.897305      21.55
 O       5.713761    -0.161963    -1.554893     257.44
 H       5.564255     0.792002    -1.386001      26.32
 C       3.283884    -0.770884    -1.670146      77.27
 H       2.672868    -1.645842    -1.444889      26.69
 C       3.183684    -0.767564    -3.221101      96.33
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 O       3.488219    -2.104936    -3.791433     251.48
 H       4.270901    -1.998781    -4.445488      24.83
 H       3.901536    -0.145638    -3.814896      24.58
 H       2.027225    -0.663945    -3.215789      25.46
 C      -0.365297    -0.344172     0.744794      39.55
 H      -0.724560    -1.210284     1.381733      24.53
 C      -0.099866     2.056526     0.258593      12.10
 H      -0.621304     3.141789     0.353814      20.72
 C       1.282141     1.922584    -0.374756       8.07
 O       2.114162     2.793588    -0.991351     139.62
 C       1.909957     4.265618    -0.697235      93.42
 H       2.748745     4.943125    -1.353752      23.02
 H       0.887544     4.774317    -1.082951      23.96
 H       1.903130     4.401545     0.320629      26.92
 C       1.611045     0.525483    -0.512710       7.25
 O       2.966671     0.487030    -0.994363     141.10
 C       0.933145    -0.530340     0.055218      55.18
 H       1.279795    -1.628384     0.129160      23.59
 C      -0.914638     0.979562     0.854483      25.78
 C      -2.317930     1.289439     1.363368      87.04
 H      -2.890023     0.668049     1.969647      27.72
 O      -2.209392     2.465237     2.358171     203.94
 H      -1.643855     2.088677     3.126205      26.64
 C      -3.306315     1.913858     0.170115      71.03
 H      -2.720257     2.637019    -0.569401      24.87
 O      -3.784114     0.803770    -0.745952     170.55
 H      -3.228443     0.268571    -1.366807      26.64
 C      -4.489951     2.432412     0.904824      92.66
 O      -5.724398     2.967616     0.224157     258.04
 H      -5.640083     3.926433    -0.085309      26.37
 H      -3.959078     3.098902     1.660438      24.28
 H      -4.892488     1.521460     1.518248      25.08
55
name = lig-etoh-Waterframe_909
 C       5.085893    -0.568373     1.429566      49.99
 H       5.098324     0.439355     1.322691      23.04
 C       4.675052    -2.941637     0.629299      50.22
 H       4.459272    -3.664468    -0.229235      19.92
 C       4.860833    -3.335743     1.936768       5.09
 O       4.883074    -4.715214     2.397121     137.66
 C       4.191024    -5.626788     1.473720     125.85
 H       3.042074    -5.383802     1.600465      24.05
 H       4.330102    -6.651044     1.924358      25.78
 H       4.985036    -5.557048     0.618602      26.98
 C       5.105900    -2.447827     3.056887       9.75
 O       5.346263    -2.845648     4.374532     195.87
 H       5.305915    -3.858190     4.493488      23.52
 C       5.394946    -1.077815     2.695207      48.65
 H       5.843868    -0.501638     3.413753      24.97
 C       4.774860    -1.528666     0.351653      16.08
 C       4.728158    -1.092593    -1.180969      82.10
 H       5.120102    -2.028748    -1.701682      22.62
 O       5.871649    -0.083716    -1.597833     206.44
 H       5.361518     0.704570    -1.560171      28.25
 C       3.377002    -0.769715    -1.673516      96.36
 H       2.756845    -1.536801    -1.275249      24.12
 C       3.210840    -0.753714    -3.187394     107.24
 O       3.482567    -2.124216    -3.712982     294.79
 H       4.317848    -2.147380    -4.192091      27.66
 H       3.503930     0.042619    -3.789437      27.02
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 H       2.172125    -0.584917    -3.544882      26.55
 C      -0.291294    -0.256427     0.726673      49.88
 H      -0.960107    -1.118916     1.256108      22.66
 C      -0.107928     2.052776     0.215969      61.38
 H      -0.580210     3.096126     0.271970      21.54
 C       1.107431     1.769405    -0.240498       5.07
 O       2.088632     2.807157    -0.961953     105.77
 C       1.770990     4.269747    -0.731937     118.43
 H       2.601845     4.774046    -1.153141      26.13
 H       0.743111     4.318749    -1.002769      27.24
 H       1.935456     4.391463     0.226249      29.88
 C       1.621265     0.517540    -0.613846      -7.82
 O       3.002344     0.470794    -1.004500     125.45
 C       0.920082    -0.580619     0.165379      47.32
 H       1.309090    -1.569091    -0.083857      21.80
 C      -0.823443     0.999607     0.889955      33.64
 C      -2.341514     1.358393     1.308093      67.08
 H      -2.830742     0.394741     1.753748      24.90
 O      -2.285144     2.478671     2.339985     224.69
 H      -1.633894     2.321922     3.079490      27.90
 C      -3.343141     1.915329     0.146584      85.73
 H      -2.785923     2.765135    -0.210234      26.18
 O      -3.834887     0.806403    -0.765612     212.25
 H      -2.970816     0.563131    -1.160418      28.34
 C      -4.561306     2.437130     0.923321     114.63
 O      -5.738121     2.997627     0.220432     340.78
 H      -5.344109     3.731461    -0.103286      32.21
 H      -4.207996     3.126236     1.498686      28.81
 H      -4.845229     1.761572     1.676181      27.30
55
name = lig-etoh-Waterframe_910
 C       5.106227    -0.595370     1.360674      37.03
 H       5.302020     0.381011     0.994137      22.83
 C       4.750821    -2.879345     0.650229      67.00
 H       4.564690    -3.645390    -0.142153      16.89
 C       4.830337    -3.394991     2.021675      29.35
 O       4.815137    -4.713461     2.427663     232.99
 C       4.217306    -5.636497     1.478605     124.19
 H       3.172460    -5.313214     1.262171      27.28
 H       4.212218    -6.784184     1.956403      24.43
 H       4.495901    -5.733278     0.518257      30.63
 C       5.169574    -2.527236     3.050029       4.00
 O       5.401165    -2.905399     4.373329     190.61
 H       5.193927    -3.911884     4.493514      22.99
 C       5.314184    -1.070624     2.748738      47.11
 H       5.592161    -0.422318     3.492763      25.26
 C       4.706158    -1.521731     0.383800      47.03
 C       4.874780    -1.180680    -1.182830      81.77
 H       5.119266    -2.063320    -1.624041      28.26
 O       5.933582    -0.040450    -1.610050     170.28
 H       5.618734     0.855525    -1.670932      27.34
 C       3.451405    -0.767402    -1.654246      84.49
 H       2.832450    -1.577386    -1.263005      24.92
 C       3.152249    -0.752723    -3.241797     100.90
 O       3.467844    -2.114739    -3.642191     306.76
 H       4.333643    -2.054811    -4.013399      29.13
 H       3.861390     0.057988    -3.497759      25.42
 H       2.106265    -0.615348    -3.370017      27.53
 C      -0.278621    -0.261444     0.791790      56.44
 H      -0.995314    -1.206145     0.980350      20.11
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 C      -0.169342     2.100518     0.265349      54.73
 H      -0.352568     3.124884     0.196898      21.32
 C       1.142739     1.774433    -0.342070      -3.11
 O       1.991462     2.799774    -0.875484     195.63
 C       1.646115     4.156867    -0.722922     121.78
 H       2.198836     4.688000    -1.342246      27.99
 H       0.723175     4.474770    -1.122139      28.12
 H       1.744312     4.677259     0.374890      24.94
 C       1.666363     0.424041    -0.513271      18.48
 O       2.939305     0.443054    -1.039823     178.83
 C       0.975907    -0.563417     0.116266      75.07
 H       1.144855    -1.607239     0.128189      22.79
 C      -0.847057     1.099526     0.837858      42.29
 C      -2.296154     1.443459     1.288291      71.02
 H      -2.633053     0.310083     1.578530      23.84
 O      -2.358717     2.473316     2.270127     252.39
 H      -1.879616     1.985084     3.003350      25.35
 C      -3.384785     1.854916     0.188916      86.17
 H      -3.068735     2.632533    -0.449787      26.10
 O      -3.816146     0.885511    -0.735832     269.20
 H      -3.113127     0.614830    -1.391165      26.53
 C      -4.666637     2.491072     1.004650      99.33
 O      -5.701008     2.989527     0.205379     303.39
 H      -5.638347     3.851826    -0.155381      30.77
 H      -4.335989     3.463166     1.504692      23.86
 H      -5.138953     1.717753     1.542864      26.80
55
name = lig-etoh-Waterframe_911
 C       5.125408    -0.655110     1.392415      46.58
 H       5.516523     0.380219     1.074819      23.97
 C       4.762380    -2.915293     0.751001      60.13
 H       4.731711    -3.564393    -0.100317      21.71
 C       4.834716    -3.404342     2.043066      12.67
 O       4.751027    -4.748972     2.416680     179.68
 C       4.164159    -5.670762     1.455930     109.89
 H       3.162978    -5.374915     1.395317      26.83
 H       4.164789    -6.700127     2.162080      22.95
 H       4.645701    -5.776981     0.490685      26.66
 C       5.246557    -2.444497     3.076685      11.17
 O       5.452517    -2.968004     4.349461     208.85
 H       5.014478    -3.884521     4.577600      23.34
 C       5.211556    -1.112182     2.728945      71.67
 H       5.309884    -0.393595     3.566984      23.49
 C       4.795456    -1.486802     0.328773      26.82
 C       5.004796    -1.126080    -1.152442      93.43
 H       5.323117    -1.908930    -1.731057      25.65
 O       5.954152    -0.094392    -1.595899     214.78
 H       5.557287     0.785426    -1.387109      27.28
 C       3.438065    -0.829759    -1.661177      72.21
 H       2.909419    -1.777911    -1.356385      24.07
 C       3.148362    -0.749547    -3.160978      97.24
 O       3.457952    -2.085315    -3.625184     273.58
 H       4.205417    -2.096478    -4.282415      26.88
 H       3.976114    -0.178412    -3.809813      23.05
 H       2.122222    -0.392748    -3.323905      25.97
 C      -0.319140    -0.216738     0.803113      40.43
 H      -0.888137    -1.111229     1.109959      22.50
 C      -0.012879     2.195797     0.227317      57.50
 H      -0.449835     3.102136     0.318962      23.44
 C       1.144820     1.808147    -0.449922      28.46
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 O       1.911117     2.773175    -0.784968     180.35
 C       1.506088     4.125941    -0.736217     100.12
 H       2.231097     4.572895    -1.474350      24.50
 H       0.454587     4.310891    -1.086183      25.29
 H       1.544005     4.653735     0.491277      22.41
 C       1.726057     0.484838    -0.361934      12.42
 O       2.901736     0.407717    -1.092121     151.19
 C       0.904617    -0.606155     0.124175      60.17
 H       1.295918    -1.589658     0.231519      23.95
 C      -0.929810     1.079788     0.771047      24.89
 C      -2.291371     1.420106     1.210246     102.08
 H      -2.783065     0.658157     1.874537      23.70
 O      -2.385282     2.435058     2.244604     217.68
 H      -2.294401     2.068335     3.158257      27.72
 C      -3.424762     1.911317     0.251063      77.60
 H      -3.064901     2.783256    -0.419614      24.22
 O      -3.815799     0.902281    -0.688614     276.11
 H      -3.366819     0.741787    -1.542163      28.13
 C      -4.705668     2.549823     1.057482      82.26
 O      -5.728342     2.975776     0.114432     252.30
 H      -5.704541     3.995009     0.074620      26.58
 H      -4.135115     3.238109     2.022123      21.64
 H      -5.212798     1.727187     1.688256      26.67
55
name = lig-etoh-Waterframe_912
 C       5.158699    -0.656830     1.416455      42.87
 H       5.375966     0.512721     1.503902      23.30
 C       4.733169    -2.921385     0.720338      69.51
 H       4.682008    -3.707327     0.027846      25.40
 C       4.892000    -3.357914     2.060238      -1.22
 O       4.720775    -4.760827     2.403048     178.23
 C       4.061610    -5.716738     1.470223     116.27
 H       3.044477    -5.517697     1.297009      26.46
 H       4.143334    -6.707596     1.977823      26.05
 H       4.965173    -5.797491     0.703317      26.67
 C       5.219851    -2.494484     3.099582      20.33
 O       5.512174    -2.979161     4.343456     236.73
 H       4.934399    -3.832575     4.448268      24.08
 C       5.144900    -1.112854     2.752960      27.34
 H       5.235533    -0.285981     3.606718      21.28
 C       5.026159    -1.556294     0.338431      22.55
 C       4.996042    -1.067070    -1.173676      92.17
 H       5.378099    -2.049520    -1.716866      23.00
 O       5.945628    -0.132506    -1.538041     229.25
 H       5.620757     0.746884    -1.158413      26.15
 C       3.458657    -0.897629    -1.645669      79.69
 H       2.867800    -1.769185    -1.233598      25.81
 C       3.255840    -0.757228    -3.115815     101.06
 O       3.410836    -2.109032    -3.666318     283.22
 H       4.025356    -1.994535    -4.463697      26.51
 H       3.706714     0.166289    -3.706738      24.51
 H       2.201116    -0.409732    -3.373395      25.99
 C      -0.404267    -0.208496     0.761639      55.54
 H      -0.929044    -0.805087     1.367039      25.47
 C      -0.064616     2.118282     0.265712      76.33
 H      -0.349280     3.127964     0.354499      25.04
 C       1.091861     1.778012    -0.395604       6.83
 O       1.987220     2.826221    -0.790051     144.96
 C       1.361823     4.166506    -0.773924      98.58
 H       2.290173     4.826567    -1.251285      22.91
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 H       0.302560     4.021502    -1.158831      23.83
 H       1.494643     4.450360     0.343689      24.69
 C       1.711389     0.496316    -0.289724       7.41
 O       2.894083     0.367435    -1.118272     133.29
 C       0.854129    -0.548927     0.198036      58.20
 H       1.340088    -1.502885     0.224635      26.06
 C      -0.862092     1.097411     0.641037      26.59
 C      -2.415999     1.361747     1.240058      71.77
 H      -2.741564     0.384534     1.518068      26.94
 O      -2.348270     2.468827     2.278347     216.63
 H      -2.342597     2.054696     3.174780      27.49
 C      -3.450701     2.027740     0.250622      78.69
 H      -2.892769     3.024917    -0.036204      23.94
 O      -3.867428     0.875952    -0.620228     261.25
 H      -3.335517     1.159463    -1.369054      29.34
 C      -4.695977     2.474929     1.078136      73.94
 O      -5.746257     3.010469     0.091702     222.26
 H      -5.482264     4.054084    -0.077377      24.20
 H      -4.503572     3.521690     1.776320      22.44
 H      -5.146687     1.591168     1.711354      25.21
55
name = lig-etoh-Waterframe_913
 C       5.201773    -0.642827     1.488719      27.86
 H       5.028820     0.458604     1.110205      21.02
 C       4.760403    -2.911461     0.653376      54.92
 H       4.441627    -3.633267    -0.074557      23.94
 C       4.905936    -3.408908     2.005380      -1.20
 O       4.689935    -4.739345     2.414588     190.78
 C       4.066771    -5.748285     1.522691     125.71
 H       3.129830    -5.486812     1.040527      26.90
 H       4.025986    -6.588482     2.018381      29.13
 H       4.512829    -5.914270     0.347478      26.40
 C       5.151449    -2.519295     3.110990      11.37
 O       5.550795    -2.964699     4.354876     186.86
 H       5.206519    -3.901760     4.672775      20.88
 C       5.135075    -1.124745     2.822050      47.01
 H       5.265595    -0.336634     3.718113      21.84
 C       5.220701    -1.603297     0.365179      16.97
 C       4.928177    -1.172705    -1.141740      78.23
 H       5.147713    -2.191479    -1.855968      22.40
 O       5.936926    -0.109544    -1.471458     202.15
 H       5.802649     0.878359    -1.286299      23.37
 C       3.503323    -0.899156    -1.554689      78.93
 H       2.926051    -1.785535    -1.218326      26.19
 C       3.273110    -0.766531    -3.146207      99.98
 O       3.361654    -2.106466    -3.772657     259.65
 H       4.213148    -2.111099    -4.408270      24.81
 H       4.086095    -0.069396    -3.304663      24.76
 H       2.182926    -0.666093    -3.056897      26.37
 C      -0.470240    -0.241753     0.710679      54.76
 H      -0.981639    -0.878065     1.361540      24.17
 C      -0.154758     2.121023     0.267631      37.17
 H      -0.393576     3.184183     0.403125      20.84
 C       1.231627     1.829910    -0.292757      -4.45
 O       2.056068     2.867222    -0.835586     164.37
 C       1.327816     4.167498    -0.760538     116.27
 H       1.709543     5.137941    -1.328780      25.11
 H       0.400746     4.286069    -1.407190      26.87
 H       1.000602     4.506319     0.072398      30.15
 C       1.662857     0.457188    -0.365929      16.91
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 O       2.870428     0.345859    -1.075314     154.08
 C       0.880980    -0.484554     0.297047      70.39
 H       1.077759    -1.560808     0.382861      23.62
 C      -1.039206     1.058793     0.652075      21.92
 C      -2.433611     1.405341     1.265420      91.00
 H      -2.740681     0.431449     1.516108      26.97
 O      -2.286812     2.456682     2.327997     230.45
 H      -1.988260     1.976043     3.133982      27.57
 C      -3.466039     2.042392     0.358710      90.34
 H      -3.102236     2.786069    -0.429177      25.03
 O      -3.881264     0.950763    -0.560441     238.26
 H      -3.572104     0.928868    -1.484032      27.77
 C      -4.740775     2.483393     1.002685     108.50
 O      -5.731446     3.034475     0.151196     292.80
 H      -5.498256     3.930742    -0.416492      25.29
 H      -4.528666     3.227561     1.680896      27.62
 H      -5.212680     1.596018     1.481813      26.50
55
name = lig-etoh-Waterframe_914
 C       5.231899    -0.694500     1.482264      42.87
 H       5.062313     0.342196     1.174097      22.29
 C       4.861130    -2.961049     0.661201      63.80
 H       4.411619    -3.383029    -0.253837      23.00
 C       4.867114    -3.459300     1.939638      12.30
 O       4.663251    -4.757716     2.392441     243.90
 C       4.062883    -5.726469     1.506327     128.57
 H       2.978442    -5.289355     1.552858      24.20
 H       3.950740    -6.547163     2.156158      27.65
 H       4.764356    -5.993345     0.643573      27.10
 C       5.114886    -2.539916     3.090341       2.62
 O       5.570809    -2.931456     4.377641     226.26
 H       5.328497    -3.850219     4.716448      21.84
 C       5.172564    -1.126442     2.862047      49.26
 H       5.199309    -0.515684     3.807744      22.75
 C       5.239614    -1.604733     0.399579      33.95
 C       4.956530    -1.216727    -1.031775      85.81
 H       5.250976    -1.956778    -1.814746      23.05
 O       5.941328    -0.123241    -1.446771     194.97
 H       5.298360     0.686826    -1.369516      24.39
 C       3.461339    -0.918691    -1.475265      83.54
 H       2.889969    -1.773711    -1.143672      24.97
 C       3.280640    -0.861794    -3.059670      97.67
 O       3.338383    -2.070499    -3.911682     253.31
 H       4.376313    -2.171386    -4.166811      23.56
 H       3.961402    -0.248763    -3.604688      25.14
 H       2.385633    -0.207392    -3.364679      25.86
 C      -0.532959    -0.229778     0.704900      36.23
 H      -0.980506    -1.289631     0.979830      21.86
 C      -0.093023     2.135256     0.192030      37.30
 H      -0.668483     3.075034     0.389985      20.48
 C       1.248046     1.921862    -0.162087       6.72
 O       2.056976     2.934536    -0.849018     143.62
 C       1.263895     4.212471    -0.822313      90.36
 H       2.182880     4.879790    -1.014134      23.97
 H       0.499192     3.829732    -1.525599      25.78
 H       0.814315     4.429939     0.182125      25.30
 C       1.637507     0.496372    -0.455399      -7.30
 O       2.877351     0.323215    -0.998493     143.43
 C       0.843100    -0.500533     0.376720      38.35
 H       1.262420    -1.559519     0.459539      22.09
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 C      -1.174567     1.015848     0.687967      20.84
 C      -2.398550     1.502930     1.318688     104.75
 H      -2.988293     0.803619     1.919339      25.03
 O      -2.205941     2.396113     2.398437     242.87
 H      -1.640562     2.014865     3.082794      29.47
 C      -3.475879     1.993329     0.297756      95.69
 H      -3.066132     2.836096    -0.283157      26.68
 O      -3.922914     0.974670    -0.510959     244.87
 H      -3.545939     0.898577    -1.406871      27.17
 C      -4.780442     2.530333     0.995370     107.65
 O      -5.761888     3.036643     0.156086     280.53
 H      -5.410570     4.040161    -0.112409      23.88
 H      -4.429250     3.000244     1.945373      25.87
 H      -5.276224     1.676828     1.372745      27.73
55
name = lig-etoh-Waterframe_915
 C       5.252660    -0.712467     1.507287      52.28
 H       5.424610     0.280611     1.465337      24.23
 C       4.966723    -3.003020     0.644958      69.57
 H       4.711849    -3.760751    -0.197520      19.96
 C       4.842705    -3.468278     2.010126      21.09
 O       4.688277    -4.785556     2.385502     268.13
 C       4.015444    -5.694754     1.564756     130.29
 H       2.897956    -5.447819     1.097019      24.95
 H       4.005611    -6.759394     2.177629      24.16
 H       4.547147    -5.870980     0.724198      29.33
 C       5.151881    -2.566676     3.069512      13.45
 O       5.555167    -2.885084     4.359293     230.73
 H       5.194650    -3.750875     4.597471      24.45
 C       5.211647    -1.189343     2.827686      50.98
 H       5.241355    -0.507166     3.598857      25.25
 C       5.131806    -1.629086     0.454277      42.03
 C       5.054296    -1.171279    -0.991028      96.73
 H       5.297412    -2.062075    -1.403303      27.58
 O       5.874910    -0.145691    -1.418984     239.87
 H       5.423126     0.817224    -1.492304      23.41
 C       3.385078    -0.987778    -1.450221      69.95
 H       2.791996    -1.762202    -1.000149      24.91
 C       3.311308    -0.884194    -3.053074      90.62
 O       3.302254    -2.051545    -3.984651     259.26
 H       4.319276    -2.057739    -4.367623      22.90
 H       4.180795    -0.227222    -3.365262      24.40
 H       2.364787    -0.329837    -3.336472      26.12
 C      -0.560048    -0.288766     0.724292      38.43
 H      -1.386844    -1.205952     0.777047      20.89
 C      -0.183045     2.048136     0.219383      53.84
 H      -0.440723     3.163641     0.145075      19.60
 C       1.217380     1.941151    -0.189183       4.42
 O       2.004342     2.946586    -0.763126     174.20
 C       1.282302     4.209332    -0.904963     101.83
 H       2.008386     4.982837    -1.086098      26.43
 H       0.539868     4.292295    -1.742836      26.15
 H       0.904907     4.392078     0.279632      22.05
 C       1.557217     0.531983    -0.334132       4.56
 O       2.921268     0.319758    -0.916146     140.61
 C       0.845424    -0.434795     0.298826      58.08
 H       1.327799    -1.454366     0.458475      22.13
 C      -1.001200     1.049035     0.651035      22.19
 C      -2.476098     1.509735     1.411053      58.88
 H      -2.978335     0.474635     1.771313      24.88
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 O      -2.094310     2.437740     2.475104     232.10
 H      -1.571659     1.872323     3.064192      28.28
 C      -3.492530     2.087200     0.270378      88.63
 H      -2.995938     2.882613    -0.182891      26.58
 O      -3.982650     0.910495    -0.530049     212.59
 H      -3.239642     0.896289    -1.158593      28.37
 C      -4.772559     2.464402     1.067461      70.93
 O      -5.778216     3.103926     0.145271     210.45
 H      -5.796860     4.162461     0.008054      23.62
 H      -4.516719     3.333534     2.153094      22.12
 H      -5.184512     1.542228     1.418260      26.15
55
name = lig-etoh-Waterframe_916
 C       5.269970    -0.700515     1.543161      54.55
 H       5.640233     0.244356     1.324454      22.90
 C       5.006377    -3.071388     0.727759      52.82
 H       5.249414    -3.888464    -0.050795      17.52
 C       4.868376    -3.455144     2.049009      27.52
 O       4.720620    -4.813346     2.432482     199.28
 C       3.963605    -5.730749     1.540846     103.04
 H       2.938984    -5.318341     1.216249      25.63
 H       3.906049    -6.816210     2.184008      22.66
 H       4.489356    -5.902234     0.610687      26.51
 C       5.207142    -2.578718     3.085534      18.55
 O       5.503520    -2.863969     4.341292     209.74
 H       5.264742    -3.751451     4.734813      21.54
 C       5.262034    -1.230491     2.789424      68.13
 H       5.474295    -0.604995     3.555950      26.90
 C       5.023871    -1.610819     0.457824      32.70
 C       4.992373    -1.199166    -0.977138      87.61
 H       5.387688    -2.053642    -1.595904      24.40
 O       5.840573    -0.126233    -1.426182     229.93
 H       5.540818     0.880741    -1.166427      22.12
 C       3.387629    -1.050227    -1.433996      47.65
 H       2.827260    -1.892239    -1.018978      22.33
 C       3.320884    -0.851859    -3.078123      93.26
 O       3.285983    -2.031380    -3.995123     283.16
 H       4.107140    -2.024235    -4.634746      25.85
 H       4.243735    -0.238673    -3.029724      21.20
 H       2.342395    -0.449780    -3.090774      26.73
 C      -0.511761    -0.293935     0.672449      35.47
 H      -1.300354    -1.063777     1.076127      20.39
 C      -0.154804     2.107263     0.220916      62.27
 H      -0.729237     3.113560     0.157926      20.65
 C       1.088946     1.862960    -0.294756      26.88
 O       1.925113     2.921919    -0.673437     213.06
 C       1.356505     4.250939    -0.925691     122.72
 H       2.007574     4.963413    -1.195834      27.08
 H       0.513136     4.308776    -1.629026      26.76
 H       0.683951     4.780782    -0.027079      24.41
 C       1.660333     0.611346    -0.208547      13.58
 O       2.927173     0.319050    -0.819201     143.86
 C       0.753486    -0.475650     0.230636      61.04
 H       1.273503    -1.461453     0.228888      21.62
 C      -0.977286     1.044605     0.716620      28.51
 C      -2.441056     1.473171     1.371176      61.78
 H      -2.778708     0.398046     1.772303      23.32
 O      -2.012028     2.468392     2.501788     193.25
 H      -1.830900     1.944215     3.322961      25.39
 C      -3.522672     2.131507     0.421443      74.90
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 H      -3.208069     2.798267    -0.386519      24.16
 O      -3.968323     0.903260    -0.576424     124.31
 H      -3.253974     0.442506    -1.047841      26.25
 C      -4.798611     2.495990     1.073968      87.82
 O      -5.792013     3.122677     0.180166     267.02
 H      -5.494009     4.112317     0.091189      25.34
 H      -4.488584     3.333341     2.027405      22.85
 H      -5.242016     1.579845     1.524322      25.42
55
name = lig-etoh-Waterframe_917
 C       5.266093    -0.714769     1.436731      49.78
 H       5.468248     0.378059     1.166497      18.73
 C       5.017002    -3.024265     0.788278      56.21
 H       5.317835    -3.689644    -0.034259      18.07
 C       4.924554    -3.548627     2.089484      21.18
 O       4.743432    -4.861040     2.477272     295.25
 C       3.943904    -5.727867     1.517543     105.42
 H       3.100598    -5.251322     1.568291      31.45
 H       3.731601    -6.657115     2.177327      24.45
 H       4.616961    -6.038695     0.566678      24.97
 C       5.207755    -2.575024     3.093158       1.35
 O       5.464840    -2.861445     4.418526     114.01
 H       5.267730    -3.906667     4.651441      18.73
 C       5.365485    -1.182896     2.843050      48.45
 H       5.782042    -0.677713     3.721818      27.07
 C       4.998948    -1.663906     0.464493      45.14
 C       4.843704    -1.263733    -1.012194      98.31
 H       5.260677    -1.977465    -1.857157      22.68
 O       5.823109    -0.080457    -1.429175     148.08
 H       5.368385     0.673252    -0.875629      22.81
 C       3.459477    -1.069517    -1.431233      55.83
 H       2.822811    -1.932802    -1.091576      20.48
 C       3.293488    -0.825198    -3.008563     100.25
 O       3.261398    -1.987710    -3.955173     265.51
 H       4.182583    -1.843228    -4.380836      24.05
 H       3.970570    -0.129182    -3.596833      21.37
 H       2.472265    -0.177301    -3.268186      25.22
 C      -0.542662    -0.221127     0.670402      37.41
 H      -0.800977    -1.100428     1.167795      21.35
 C      -0.239310     2.155011     0.240011      46.88
 H      -0.668611     3.195450     0.251039      20.29
 C       1.026569     1.882192    -0.376929       2.20
 O       1.872138     2.933826    -0.616338     180.01
 C       1.347148     4.309855    -0.928524     105.32
 H       2.360049     4.649512    -1.229056      24.21
 H       0.783355     3.897641    -1.696176      25.95
 H       1.071606     4.786578     0.004061      25.90
 C       1.735746     0.498274    -0.156791       4.97
 O       2.935744     0.301028    -0.729045     133.62
 C       0.811015    -0.539562     0.134662      52.01
 H       1.000310    -1.609130     0.027947      20.22
 C      -1.055266     1.080058     0.778754      46.87
 C      -2.269877     1.465564     1.351393     103.16
 H      -2.865712     0.781159     1.935030      24.09
 O      -1.988135     2.450685     2.473241     214.77
 H      -2.253965     2.094795     3.327090      26.94
 C      -3.502018     1.995873     0.465883      59.74
 H      -3.170856     2.964384    -0.188377      23.66
 O      -3.949919     0.933038    -0.575177     164.47
 H      -3.115919     0.505174    -0.836915      28.20
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 C      -4.854928     2.571376     1.105069     112.53
 O      -5.762991     3.122037     0.243523     327.98
 H      -5.412927     3.954032    -0.152407      28.25
 H      -4.498785     3.050633     1.790410      30.43
 H      -5.427309     1.727900     1.633264      25.23
55
name = lig-etoh-Waterframe_918
 C       5.263696    -0.729307     1.464087      43.20
 H       5.100318     0.431906     1.182779      18.72
 C       5.009038    -3.060781     0.788921      50.85
 H       4.855100    -3.705008    -0.036657      19.74
 C       5.002505    -3.571310     2.137006       5.78
 O       4.784301    -4.933205     2.495639     319.77
 C       3.962767    -5.699623     1.606174     119.72
 H       3.033668    -5.209010     1.247007      27.19
 H       3.785360    -6.574051     2.064266      26.74
 H       4.387432    -5.897176     0.435502      24.68
 C       5.211505    -2.537384     3.159875       6.34
 O       5.432643    -2.850890     4.491359     174.88
 H       5.109568    -3.849227     4.797569      21.66
 C       5.486749    -1.145182     2.773462      45.66
 H       5.876809    -0.403324     3.621529      20.70
 C       5.031053    -1.692714     0.422889      29.88
 C       4.872089    -1.276488    -1.079178      82.47
 H       5.077269    -2.336822    -1.544026      23.64
 O       5.740139    -0.117835    -1.386013     238.63
 H       5.427345     0.857819    -1.164497      22.12
 C       3.426058    -0.968537    -1.499830      70.75
 H       2.752302    -1.830770    -1.187522      21.96
 C       3.224094    -0.717919    -3.002952      90.10
 O       3.249477    -1.933751    -3.859954     291.58
 H       4.192218    -2.039058    -4.117358      27.77
 H       4.147496    -0.099035    -3.313618      21.79
 H       2.152690    -0.297094    -3.077507      25.10
 C      -0.483003    -0.212087     0.684309      41.85
 H      -1.024946    -0.936675     1.170662      21.50
 C      -0.299756     2.140663     0.207453      53.24
 H      -0.461491     3.166048     0.324740      20.05
 C       1.016921     1.873851    -0.294261      -1.15
 O       1.887313     2.924391    -0.565380     218.35
 C       1.412989     4.250115    -0.932689     111.02
 H       2.397208     4.849379    -1.492763      22.33
 H       0.605557     4.437294    -1.698943      26.35
 H       1.115783     4.828830    -0.163663      27.65
 C       1.658452     0.421970    -0.243550      10.40
 O       3.013348     0.256877    -0.672121     175.81
 C       0.793065    -0.568529     0.083358      60.71
 H       0.978516    -1.593574    -0.022230      21.19
 C      -1.009856     1.094253     0.734914      31.99
 C      -2.341973     1.477384     1.506845      83.12
 H      -2.593900     0.524106     1.917483      25.21
 O      -1.996489     2.467392     2.404806     281.12
 H      -2.375305     2.069437     3.185879      26.83
 C      -3.507624     1.900652     0.402487      81.35
 H      -2.939840     2.844264     0.048481      23.95
 O      -3.891409     0.985729    -0.521140     244.52
 H      -3.049362     0.683846    -0.930145      26.29
 C      -4.809574     2.511977     1.191776      80.57
 O      -5.750230     3.150558     0.246580     305.40
 H      -5.514867     3.961348    -0.175654      29.06
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 H      -4.413425     3.381434     2.075794      22.71
 H      -5.458517     1.685870     1.654264      24.07
55
name = lig-etoh-Waterframe_919
 C       5.233970    -0.759276     1.454127      43.70
 H       5.133248     0.416314     1.290257      20.65
 C       4.959793    -3.148274     0.773824      44.30
 H       4.496586    -3.865632     0.161816      21.74
 C       5.075972    -3.480081     2.160986       2.65
 O       4.836463    -4.943947     2.504737     129.33
 C       3.954763    -5.676568     1.628416     119.00
 H       2.864648    -5.084648     1.326213      23.50
 H       3.770603    -6.580569     2.027297      27.15
 H       4.665929    -5.883206     0.772686      26.18
 C       5.288113    -2.521092     3.213791      21.05
 O       5.387692    -2.792989     4.547840     281.85
 H       5.210939    -3.731199     4.777985      26.98
 C       5.572459    -1.192254     2.730171      51.79
 H       5.670508    -0.247915     3.472995      20.40
 C       5.070239    -1.682992     0.417101      21.85
 C       4.901361    -1.273249    -1.050852      99.15
 H       5.359043    -2.017855    -1.733620      22.63
 O       5.698493    -0.207802    -1.379186     246.37
 H       5.141812     0.603233    -1.449404      25.69
 C       3.334302    -0.874459    -1.503763      76.86
 H       2.708862    -1.752050    -1.246179      24.07
 C       3.165059    -0.598065    -3.010099      96.63
 O       3.243483    -1.885284    -3.727522     295.13
 H       4.139373    -2.026969    -4.034576      28.18
 H       3.842191     0.262212    -3.179575      25.29
 H       2.067418    -0.248246    -3.130742      25.70
 C      -0.470912    -0.237463     0.712419      41.04
 H      -1.258986    -0.913434     0.990705      21.75
 C      -0.218599     2.143834     0.123390      71.29
 H      -0.553746     3.077688     0.339125      21.77
 C       1.091584     1.800257    -0.165726      10.31
 O       1.934420     2.900089    -0.551564     192.10
 C       1.491113     4.225335    -0.945889      82.04
 H       2.380664     4.895700    -1.523614      22.27
 H       0.401254     4.202051    -1.383813      24.59
 H       1.327565     4.822409     0.002747      24.29
 C       1.587047     0.522945    -0.430023      -1.39
 O       3.051826     0.220191    -0.637232     179.42
 C       0.693556    -0.628382     0.082849      36.66
 H       1.122011    -1.570720     0.073417      20.80
 C      -1.012069     1.068632     0.705681      10.89
 C      -2.432030     1.346417     1.530856      77.72
 H      -2.546075     0.423098     2.104993      24.92
 O      -2.052646     2.512857     2.383103     237.68
 H      -2.046979     2.379826     3.343024      27.94
 C      -3.480092     1.975461     0.529492      94.77
 H      -3.063367     2.695954    -0.114492      25.33
 O      -3.821864     0.979554    -0.506045     236.04
 H      -3.199331     0.787655    -1.227108      26.80
 C      -4.719974     2.460308     1.189939      82.12
 O      -5.737196     3.147416     0.252184     270.47
 H      -5.423403     4.005362     0.192425      29.63
 H      -4.456559     3.415035     2.177406      22.50
 H      -5.233052     1.626859     1.701483      26.33
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name = lig-etoh-Waterframe_920
 C       5.247461    -0.806859     1.407049      51.48
 H       5.394777     0.256882     1.140473      22.21
 C       4.899290    -3.091945     0.818104      58.08
 H       4.588849    -3.865885     0.098830      23.86
 C       5.101283    -3.486903     2.154508      10.68
 O       4.881224    -4.843248     2.548534     152.18
 C       3.998881    -5.665915     1.611100     109.48
 H       2.973939    -5.003986     1.593426      23.81
 H       3.665493    -6.581027     2.261877      25.86
 H       4.412846    -5.941676     0.725073      29.15
 C       5.426065    -2.519073     3.200687      18.48
 O       5.343285    -2.723075     4.592981     197.19
 H       5.265560    -3.661852     4.745080      23.33
 C       5.566608    -1.219904     2.765379      50.74
 H       5.644296    -0.511622     3.657420      21.52
 C       5.048555    -1.796411     0.403943      34.67
 C       4.829668    -1.325586    -1.057014      99.38
 H       5.052476    -2.116512    -1.712715      24.32
 O       5.727470    -0.206134    -1.412763     221.19
 H       5.220932     0.632388    -1.351981      25.26
 C       3.318349    -0.889544    -1.439080      76.98
 H       2.649647    -1.711180    -1.275299      24.79
 C       3.082373    -0.486051    -2.978158     103.38
 O       3.256137    -1.809621    -3.609705     292.86
 H       4.106837    -1.714645    -3.981900      28.92
 H       3.595298     0.202220    -3.609158      25.92
 H       2.080676    -0.125110    -3.292459      25.62
 C      -0.580332    -0.287744     0.710088      26.61
 H      -1.079453    -1.298037     0.975973      20.74
 C      -0.224953     2.062135     0.167850      62.07
 H      -0.523783     3.084119     0.184039      21.47
 C       1.234178     1.870723    -0.187961      -4.35
 O       2.055637     2.838696    -0.557430     169.11
 C       1.502647     4.218753    -0.851713      84.81
 H       2.212979     4.402299    -1.631472      25.20
 H       0.621427     3.908847    -1.497437      24.19
 H       1.632335     4.807205     0.160037      22.77
 C       1.528307     0.449229    -0.500736      11.64
 O       2.972195     0.247432    -0.609334     175.48
 C       0.735734    -0.548440     0.045514      37.41
 H       1.055137    -1.588462     0.167241      21.36
 C      -1.051644     1.066369     0.699784      28.34
 C      -2.349103     1.307838     1.472214      89.94
 H      -2.973824     0.634003     2.136546      23.86
 O      -2.134439     2.560448     2.389356     207.84
 H      -1.687448     2.193186     3.190657      26.60
 C      -3.390940     1.998326     0.587950      79.32
 H      -2.933812     2.896862     0.183186      25.23
 O      -3.808830     0.927010    -0.492301     215.91
 H      -3.145133     1.164479    -1.153770      28.63
 C      -4.742762     2.471559     1.175158     112.49
 O      -5.659930     3.091193     0.302311     327.44
 H      -5.542518     4.024783     0.219048      29.33
 H      -4.258679     3.053112     2.020274      25.83
 H      -5.169001     1.621658     1.612698      29.08
55
name = lig-etoh-Waterframe_921
 C       5.353758    -0.862773     1.411614      51.27
 H       5.513549     0.061326     1.038019      24.41
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 C       4.844708    -3.107457     0.863786      57.22
 H       4.870217    -3.856816    -0.003849      23.18
 C       5.115282    -3.513224     2.183121      26.55
 O       4.909478    -4.769842     2.563975     161.78
 C       4.024372    -5.610054     1.690618     106.22
 H       3.136081    -5.064798     1.405298      27.57
 H       3.804485    -6.598813     2.433971      24.54
 H       4.248418    -5.907764     0.705282      27.54
 C       5.503353    -2.580407     3.170576      12.98
 O       5.317699    -2.686811     4.584964     149.62
 H       5.194843    -3.593766     4.953808      20.05
 C       5.509397    -1.178723     2.768451      62.51
 H       5.757052    -0.508029     3.515921      26.26
 C       4.986547    -1.778875     0.386074      32.14
 C       4.721422    -1.361114    -1.095976      88.20
 H       4.769455    -2.280123    -1.647309      24.79
 O       5.760477    -0.203760    -1.456335     152.62
 H       5.567660     0.657213    -1.117570      26.82
 C       3.328983    -0.849038    -1.403449      73.45
 H       2.678245    -1.684274    -1.264256      25.56
 C       3.003056    -0.450854    -2.953488     100.06
 O       3.280229    -1.737049    -3.550229     286.20
 H       4.096834    -1.719103    -3.997567      30.61
 H       3.822507     0.201325    -3.337464      23.90
 H       1.967997    -0.222963    -2.884372      26.39
 C      -0.574724    -0.345814     0.586763      45.39
 H      -1.094517    -1.182600     1.272842      22.58
 C      -0.130248     2.024091     0.232270      52.66
 H      -0.571224     3.080231     0.206938      21.71
 C       1.142959     1.827086    -0.271508       7.20
 O       2.214852     2.795020    -0.555429     189.63
 C       1.584009     4.110981    -0.809663     123.17
 H       2.114983     4.549464    -1.506663      28.41
 H       0.535782     4.251442    -1.126283      26.79
 H       1.406412     4.981440    -0.029710      25.00
 C       1.580527     0.460458    -0.415027      19.17
 O       2.853735     0.272249    -0.599895     177.17
 C       0.662615    -0.490826     0.078281      57.85
 H       1.102830    -1.564269     0.032474      22.45
 C      -1.076719     0.933012     0.751075      28.15
 C      -2.316591     1.480806     1.445141      85.31
 H      -2.672461     0.420848     1.903274      24.30
 O      -2.182773     2.543380     2.406674     252.69
 H      -1.614557     2.069842     3.045974      28.07
 C      -3.382342     1.955749     0.497217      86.72
 H      -2.853805     2.900313     0.131234      24.67
 O      -3.759092     0.944117    -0.457546     239.92
 H      -3.238730     1.047074    -1.277744      27.72
 C      -4.697357     2.447752     1.243489     107.37
 O      -5.597064     3.033454     0.335586     324.60
 H      -5.423120     3.949582    -0.033732      27.88
 H      -4.577037     3.048861     1.997652      28.77
 H      -5.319540     1.595223     1.545014      26.56
55
name = lig-etoh-Waterframe_922
 C       5.458538    -0.846731     1.375016      49.73
 H       5.583694     0.154333     1.222225      25.22
 C       4.846588    -3.128385     0.811154      48.26
 H       4.764873    -4.075895     0.160341      20.09
 C       5.127769    -3.463052     2.176318      11.46
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 O       4.917229    -4.822071     2.577628     169.04
 C       4.018599    -5.547035     1.792254     109.40
 H       3.151391    -5.099681     1.654008      29.30
 H       3.793163    -6.591987     2.406060      24.64
 H       4.814050    -5.907120     0.926467      23.26
 C       5.455266    -2.536453     3.205340      18.35
 O       5.321229    -2.685233     4.548944     192.75
 H       5.182703    -3.636295     4.878966      22.03
 C       5.511599    -1.202348     2.753480      59.31
 H       5.778167    -0.399318     3.293807      26.05
 C       4.916968    -1.745214     0.419825      32.57
 C       4.691616    -1.275063    -1.057017      92.01
 H       5.020358    -2.020184    -1.865626      22.81
 O       5.775933    -0.291475    -1.510902     189.06
 H       5.544977     0.446052    -1.000856      30.55
 C       3.251089    -0.792690    -1.407200      95.63
 H       2.664689    -1.705380    -1.133077      24.45
 C       3.045397    -0.493469    -2.817250     101.17
 O       3.278938    -1.706305    -3.573924     292.02
 H       4.151695    -1.622274    -3.963303      28.35
 H       3.515073     0.581250    -2.933709      24.09
 H       1.999274    -0.184173    -2.977117      27.56
 C      -0.643033    -0.368295     0.559699      35.97
 H      -1.168657    -1.259517     1.119952      22.53
 C      -0.131192     1.990680     0.316136      54.66
 H      -0.523446     3.083058     0.557158      21.51
 C       1.087615     1.766674    -0.355415       9.07
 O       2.240689     2.779604    -0.544765     152.38
 C       1.661995     4.101970    -0.796363     105.92
 H       2.197434     4.791404    -1.504359      25.92
 H       0.644700     3.828077    -1.034410      25.73
 H       1.865328     4.453288     0.266169      24.27
 C       1.527843     0.508612    -0.232531      25.03
 O       2.866391     0.283764    -0.602974     200.24
 C       0.691931    -0.577059     0.056472      48.17
 H       1.130691    -1.667741     0.004592      22.04
 C      -0.961059     1.008309     0.733606      30.29
 C      -2.313568     1.516536     1.429444      88.20
 H      -2.642513     0.619294     1.999827      25.11
 O      -2.181416     2.489600     2.427516     284.38
 H      -1.807714     2.306092     3.303399      29.70
 C      -3.403189     1.987694     0.420396      84.43
 H      -3.190906     2.788342    -0.379693      24.31
 O      -3.717194     0.957211    -0.445850     240.46
 H      -3.264083     0.796777    -1.278596      27.36
 C      -4.640677     2.381083     1.283938      82.79
 O      -5.597090     3.000785     0.294356     282.73
 H      -5.026175     3.796714     0.011071      27.26
 H      -4.520508     3.102317     2.205016      23.90
 H      -5.105291     1.370337     1.686411      25.25
55
name = lig-etoh-Waterframe_923
 C       5.480633    -0.823195     1.355169      45.01
 H       5.602067     0.272592     1.177306      23.47
 C       4.888935    -3.108547     0.795367      65.66
 H       4.401559    -3.799276     0.054324      20.79
 C       5.102452    -3.460651     2.151884      -1.82
 O       4.956391    -4.807999     2.676327     177.51
 C       4.053284    -5.605527     1.868647     105.34
 H       3.132206    -5.067228     1.595363      29.53
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 H       3.742880    -6.454586     2.420321      27.35
 H       4.511958    -5.963393     0.705620      24.80
 C       5.314906    -2.449065     3.197965       9.86
 O       5.339554    -2.723328     4.551497     165.82
 H       5.276356    -3.736186     4.669279      21.77
 C       5.604485    -1.181575     2.699900      58.48
 H       5.761376    -0.439521     3.514288      23.55
 C       4.911847    -1.739682     0.402865      17.97
 C       4.758512    -1.190640    -1.037740      98.62
 H       4.831151    -2.236230    -1.679232      23.19
 O       5.742977    -0.366448    -1.513916     197.74
 H       5.702128     0.535065    -1.244286      28.44
 C       3.197215    -0.854586    -1.298677      81.76
 H       2.566373    -1.769504    -1.027122      23.97
 C       3.018095    -0.474756    -2.739689      97.58
 O       3.307102    -1.657390    -3.651484     268.05
 H       4.250183    -1.535675    -3.972592      26.35
 H       3.699175     0.339236    -3.217297      23.28
 H       1.975481    -0.348532    -3.084368      25.78
 C      -0.630759    -0.363277     0.563435      39.53
 H      -1.387336    -1.131968     0.618189      23.04
 C      -0.101107     2.125916     0.349623      50.56
 H      -0.306568     3.159462     0.826166      20.70
 C       1.137869     1.861741    -0.332212       0.86
 O       2.168991     2.684428    -0.580974     185.31
 C       1.741570     4.100151    -0.681691      98.76
 H       2.392424     4.561862    -1.653255      23.56
 H       0.711990     4.128857    -1.109935      25.29
 H       1.829829     4.610730     0.285306      25.53
 C       1.556733     0.387793    -0.154911      -2.79
 O       2.903741     0.341486    -0.556343     170.54
 C       0.672117    -0.705877     0.069196      62.02
 H       1.071141    -1.766751     0.059821      23.02
 C      -0.977460     1.043906     0.760220      34.53
 C      -2.260329     1.434267     1.424497      92.38
 H      -2.890533     0.722395     1.767970      26.97
 O      -2.149668     2.523329     2.462382     242.14
 H      -2.195349     1.938264     3.296726      25.31
 C      -3.385576     2.056156     0.385794      64.07
 H      -3.101179     3.057865    -0.087496      23.79
 O      -3.746983     0.856808    -0.471738     212.10
 H      -2.951591     0.877453    -1.031674      27.51
 C      -4.651515     2.323043     1.211438      81.78
 O      -5.578595     2.927718     0.297756     285.48
 H      -5.340116     3.969154     0.012358      25.14
 H      -3.915732     2.983829     2.081909      20.01
 H      -4.982005     1.314689     1.706223      26.59
55
name = lig-etoh-Waterframe_924
 C       5.440045    -0.780913     1.354046      49.58
 H       5.637463     0.271583     0.832272      21.06
 C       4.874123    -3.054597     0.793693      60.62
 H       4.436460    -3.684123     0.045281      23.55
 C       5.046910    -3.470920     2.186366      12.39
 O       4.988029    -4.747179     2.747231     142.12
 C       4.052730    -5.698553     1.899377      96.57
 H       3.128097    -4.927162     1.655515      24.87
 H       3.823435    -6.432118     2.483631      28.28
 H       4.436613    -6.050400     0.913503      26.15
 C       5.204908    -2.448360     3.108877       2.58
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 O       5.354436    -2.768516     4.530007     167.43
 H       5.321803    -3.784469     4.773227      21.52
 C       5.686260    -1.118067     2.708751      47.98
 H       5.936482    -0.374325     3.613868      21.22
 C       5.037669    -1.681217     0.419585      39.37
 C       4.698025    -1.300869    -0.992454      93.82
 H       4.786544    -2.262436    -1.621683      22.46
 O       5.739550    -0.369067    -1.522289     163.01
 H       5.567815     0.561955    -1.490686      27.10
 C       3.290591    -0.888768    -1.192327      68.82
 H       2.615484    -1.740766    -0.880876      23.12
 C       2.985071    -0.528016    -2.846445      91.54
 O       3.331510    -1.610253    -3.718657     274.61
 H       4.369924    -1.589348    -4.024560      23.43
 H       3.728374     0.281231    -2.950178      23.08
 H       1.972455    -0.128785    -2.799607      25.33
 C      -0.624818    -0.291287     0.530998      24.30
 H      -1.424216    -0.895809     0.443550      22.40
 C      -0.019221     2.266173     0.383897     101.70
 H      -0.238978     3.275849     0.691383      21.63
 C       1.137906     1.752755    -0.119783       7.52
 O       2.091540     2.640266    -0.647692     145.28
 C       1.796189     4.107867    -0.622071     112.60
 H       2.795035     4.461946    -1.286247      23.33
 H       0.870004     4.530247    -0.994770      25.76
 H       1.856684     4.774248     0.169896      26.67
 C       1.580377     0.382180    -0.191611      13.09
 O       2.909551     0.350650    -0.470471     161.56
 C       0.655547    -0.740313     0.121445      63.77
 H       0.816630    -1.791292     0.095470      22.23
 C      -0.986308     1.008174     0.794063      62.27
 C      -2.311338     1.452099     1.374069      90.48
 H      -2.683640     0.477807     1.769797      25.99
 O      -2.093908     2.492866     2.499345     220.35
 H      -2.381231     1.990498     3.341466      26.14
 C      -3.344702     1.990909     0.413162      96.47
 H      -2.886104     2.858567    -0.029787      26.40
 O      -3.729834     0.819962    -0.526093     188.26
 H      -2.928541     0.482540    -1.000240      26.39
 C      -4.556951     2.330596     1.111209     113.11
 O      -5.608904     2.851202     0.322414     263.12
 H      -5.660513     3.920636     0.250123      26.92
 H      -4.649515     3.137878     2.008284      23.92
 H      -5.155247     1.524720     1.476012      27.08
55
name = lig-etoh-Waterframe_925
 C       5.453253    -0.665911     1.402486      27.69
 H       5.794104     0.426641     1.022236      19.73
 C       4.834481    -3.033226     0.836537      73.37
 H       4.775707    -3.794606     0.126943      24.00
 C       4.959078    -3.436974     2.155550       4.35
 O       4.967706    -4.746506     2.722282     199.44
 C       4.083577    -5.703669     1.970468     113.73
 H       2.951461    -5.206001     1.815443      23.08
 H       3.861036    -6.535908     2.659023      26.68
 H       4.648975    -6.019994     1.263243      29.37
 C       5.250314    -2.419201     3.157380      10.33
 O       5.358598    -2.772776     4.451365     165.28
 H       5.253288    -3.790229     4.712050      20.16
 C       5.651804    -1.116017     2.733199      46.79
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 H       6.231118    -0.301319     3.394735      22.07
 C       5.141541    -1.729601     0.455059      38.62
 C       4.713464    -1.416489    -0.960647      93.45
 H       4.866097    -2.153191    -1.629130      23.88
 O       5.720856    -0.361758    -1.541812     167.29
 H       5.191417     0.403246    -1.475310      28.33
 C       3.315300    -0.870803    -1.216316      88.25
 H       2.730514    -1.686403    -0.784355      24.65
 C       3.071930    -0.575872    -2.806960      98.35
 O       3.295879    -1.588521    -3.781877     281.99
 H       4.340324    -1.438791    -4.057678      21.54
 H       3.531922     0.351308    -2.946907      25.88
 H       2.024825    -0.200432    -3.019762      25.25
 C      -0.668592    -0.220142     0.490638      55.90
 H      -1.371030    -1.012927     0.694567      21.97
 C      -0.078506     2.160134     0.515022      68.39
 H      -0.242582     3.154869     0.421494      20.88
 C       1.168681     1.703939     0.074916      -0.94
 O       2.025608     2.665597    -0.698419     138.78
 C       1.906482     4.142768    -0.598290     109.71
 H       2.765764     4.593636    -1.115881      26.41
 H       1.037237     4.314322    -1.232714      25.14
 H       2.073831     4.228813     0.542837      26.11
 C       1.528721     0.344636    -0.185590      23.96
 O       2.949437     0.275600    -0.412581     179.36
 C       0.683951    -0.639724     0.147665      62.42
 H       0.818844    -1.629225    -0.008815      23.57
 C      -0.907302     1.208363     0.779021      18.38
 C      -2.314522     1.429008     1.433704      83.18
 H      -2.606113     0.490029     2.057782      20.74
 O      -2.065109     2.410257     2.468716     267.74
 H      -2.144631     2.123102     3.442406      26.60
 C      -3.256695     1.863171     0.364469      86.22
 H      -2.860247     2.531150    -0.361019      25.20
 O      -3.695636     0.834746    -0.568074     207.72
 H      -2.962376     0.384362    -1.040853      26.48
 C      -4.653646     2.384975     1.121980      99.67
 O      -5.719145     2.793570     0.274202     315.92
 H      -5.408069     3.823639     0.083755      25.53
 H      -4.369545     2.955356     1.957790      26.85
 H      -4.793598     1.386033     1.504069      28.23
55
name = lig-etoh-Waterframe_926
 C       5.497777    -0.684498     1.432076      50.44
 H       5.766305     0.421616     1.261370      22.49
 C       4.841747    -3.081699     0.865955      62.82
 H       4.928466    -3.813410     0.093249      22.42
 C       4.896493    -3.366782     2.230922      14.26
 O       4.900445    -4.734992     2.661457     240.63
 C       4.123992    -5.706454     2.099409     115.46
 H       3.152211    -5.474813     1.567990      25.86
 H       4.050030    -6.686698     2.881948      24.33
 H       4.618308    -6.097506     1.124132      25.06
 C       5.341788    -2.404978     3.153345       9.67
 O       5.373770    -2.762203     4.447061      85.51
 H       5.171687    -3.806755     4.428794      18.07
 C       5.600952    -1.082535     2.746537      49.58
 H       6.145587    -0.546570     3.582278      21.99
 C       5.153017    -1.695999     0.475123      20.54
 C       4.859907    -1.413633    -0.997921      91.41
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 H       4.894246    -2.343160    -1.520370      24.04
 O       5.644008    -0.362631    -1.532007     186.70
 H       5.317642     0.525868    -1.459394      27.28
 C       3.282947    -0.938049    -1.267865      76.98
 H       2.637696    -1.774651    -1.134280      26.32
 C       3.100702    -0.536553    -2.715256      93.33
 O       3.261699    -1.580850    -3.824342     269.17
 H       4.184408    -1.676620    -4.195613      25.90
 H       3.684851     0.259638    -3.132823      24.98
 H       1.994473    -0.540065    -2.846188      26.21
 C      -0.658702    -0.127453     0.497804      61.90
 H      -1.308719    -0.924857     1.047110      24.08
 C       0.013969     2.159634     0.591395      70.64
 H      -0.397306     3.133417     0.505580      23.85
 C       1.278983     1.815597     0.088239       6.20
 O       1.994849     2.636250    -0.736158     189.82
 C       2.009489     4.084296    -0.551084     124.00
 H       2.792663     4.535509    -0.919591      28.51
 H       1.067148     4.640829    -0.935745      25.39
 H       1.738269     4.377294     0.652588      24.17
 C       1.626482     0.433304    -0.108858      -3.21
 O       2.976952     0.169356    -0.391641     157.63
 C       0.586399    -0.578993     0.145826      59.98
 H       0.927379    -1.553991    -0.043331      24.72
 C      -1.049412     1.106857     0.830224      40.96
 C      -2.194551     1.363418     1.554312      74.37
 H      -2.777551     0.416900     1.865099      25.13
 O      -2.060475     2.401969     2.436776     272.43
 H      -1.900845     1.823609     3.266609      25.88
 C      -3.311339     1.847358     0.273329      57.35
 H      -2.725119     2.700908    -0.234593      25.07
 O      -3.680814     0.790267    -0.604916     194.17
 H      -2.825263     0.677625    -1.089160      28.37
 C      -4.665756     2.323697     1.110005      87.46
 O      -5.798465     2.776654     0.230882     299.78
 H      -5.542023     3.491455    -0.461444      28.54
 H      -4.224551     3.013107     1.706888      26.99
 H      -5.015670     1.379462     1.683798      25.03
55
name = lig-etoh-Waterframe_927
 C       5.534014    -0.754511     1.430492      61.57
 H       5.618446     0.225422     1.027645      27.60
 C       4.914823    -3.020387     0.869443      61.52
 H       4.702375    -3.860061     0.137434      21.55
 C       4.868844    -3.381526     2.229247      18.10
 O       4.856630    -4.646476     2.678035     203.02
 C       4.144985    -5.807526     2.087393      88.43
 H       3.208462    -5.463153     1.944042      29.63
 H       4.064709    -6.582465     3.087513      23.85
 H       4.722404    -6.376296     1.103564      23.39
 C       5.367207    -2.404876     3.135034      12.10
 O       5.407737    -2.769461     4.503766     131.40
 H       5.241519    -3.806485     4.687174      21.13
 C       5.601134    -1.073328     2.841028      69.08
 H       5.790491    -0.401134     3.615119      21.50
 C       5.097651    -1.678909     0.474122      32.46
 C       4.870348    -1.349489    -0.999522      94.48
 H       5.234349    -2.342026    -1.614004      23.22
 O       5.627104    -0.338872    -1.557243     221.40
 H       5.416649     0.529155    -1.191623      28.29
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 C       3.344962    -1.101112    -1.306014      70.80
 H       2.655735    -1.928563    -1.223243      24.36
 C       3.068188    -0.538897    -2.763624      90.12
 O       3.194646    -1.609436    -3.811963     283.35
 H       4.142608    -1.458052    -4.030700      25.48
 H       3.676490     0.460902    -2.924404      23.16
 H       2.064545    -0.067739    -2.593765      26.52
 C      -0.668961    -0.243790     0.578741      34.18
 H      -1.445857    -1.125043     0.860966      22.07
 C       0.053293     2.175001     0.629117      62.55
 H      -0.260419     3.238544     0.862534      22.93
 C       1.302410     1.879961     0.027998       2.07
 O       2.043817     2.674997    -0.786523     205.70
 C       1.997561     4.056382    -0.443063     117.91
 H       2.960829     4.387314    -0.755156      26.38
 H       1.227395     4.630883    -1.088721      25.02
 H       2.076936     4.432916     0.685982      24.99
 C       1.687548     0.472419     0.018104      19.66
 O       2.981944     0.064236    -0.385315     140.25
 C       0.661461    -0.462785     0.069579      50.01
 H       0.762398    -1.621360     0.112324      23.25
 C      -0.958944     1.072815     0.871885      17.94
 C      -2.316137     1.334223     1.509961      71.40
 H      -2.675055     0.404028     2.016618      24.94
 O      -2.071454     2.415822     2.477598     255.35
 H      -1.863388     2.142763     3.442839      27.36
 C      -3.435751     1.874569     0.333928      75.86
 H      -2.971163     2.855807    -0.086128      23.66
 O      -3.622592     0.737901    -0.655734     165.40
 H      -2.934644     0.648562    -1.368131      26.85
 C      -4.624489     2.258660     0.992675     105.48
 O      -5.848356     2.713105     0.202471     270.83
 H      -5.455717     3.396486    -0.439927      30.14
 H      -4.506913     3.301694     1.568411      23.77
 H      -5.312895     1.727342     1.693577      24.64
55
name = lig-etoh-Waterframe_928
 C       5.530053    -0.769454     1.441744      53.67
 H       5.627494     0.177085     1.137323      25.94
 C       4.928212    -2.997428     0.847098      64.27
 H       4.453801    -3.728936     0.083288      18.15
 C       4.937434    -3.367916     2.150557      20.54
 O       4.830806    -4.637906     2.743932     225.62
 C       4.138617    -5.865740     2.103810     113.43
 H       3.134502    -5.706940     1.885951      31.55
 H       4.181717    -6.563002     2.961487      26.67
 H       4.830608    -6.323335     1.243411      27.15
 C       5.324368    -2.453473     3.260939       6.08
 O       5.452834    -2.765308     4.566862     175.92
 H       5.384585    -3.796975     4.752502      20.69
 C       5.608833    -1.061578     2.851055      56.61
 H       5.596170    -0.256185     3.468288      25.13
 C       5.072079    -1.688879     0.468888      51.09
 C       4.813920    -1.368236    -0.993209     104.42
 H       5.304416    -2.217643    -1.698381      24.26
 O       5.669354    -0.226689    -1.588839     181.83
 H       5.461879     0.504825    -0.996370      28.29
 C       3.373231    -1.195365    -1.368911      70.92
 H       2.887532    -2.130126    -0.951382      21.45
 C       3.011159    -0.546560    -2.769074      92.12
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 O       3.123635    -1.578725    -3.748173     292.92
 H       3.987994    -1.472646    -4.238956      26.90
 H       3.927334     0.228743    -2.939398      20.05
 H       2.052533    -0.034439    -2.925224      25.46
 C      -0.586962    -0.351557     0.620261      43.37
 H      -1.320047    -1.198548     0.390482      21.47
 C       0.023499     2.139433     0.658776      65.63
 H      -0.116795     3.216969     1.047108      20.49
 C       1.265649     1.810343    -0.027873      -4.97
 O       2.119408     2.732551    -0.789628     170.27
 C       2.052432     4.136411    -0.381092      99.24
 H       3.083395     4.604433    -0.857471      23.25
 H       1.249220     4.529181    -0.999153      24.93
 H       1.993647     4.050083     0.632921      27.34
 C       1.730801     0.448863     0.035948      19.90
 O       2.997721    -0.014258    -0.371446     127.19
 C       0.681536    -0.483185     0.090222      35.43
 H       1.212463    -1.598413    -0.124534      20.73
 C      -0.840472     1.123603     0.925432      12.24
 C      -2.428470     1.404089     1.459397      86.88
 H      -2.751888     0.557949     2.000638      25.08
 O      -2.122739     2.464941     2.496704     251.41
 H      -2.260203     1.953101     3.412499      24.53
 C      -3.413663     1.804289     0.392582      84.82
 H      -3.111301     2.623130    -0.281960      24.50
 O      -3.582341     0.722787    -0.675378     163.85
 H      -2.813216     0.756528    -1.313370      25.98
 C      -4.829222     2.315015     0.964901      92.92
 O      -5.848325     2.628789     0.106636     291.92
 H      -5.674661     3.588694    -0.133414      28.63
 H      -4.225110     3.270728     1.682576      23.08
 H      -4.866849     1.459299     1.733681      26.76
55
name = lig-etoh-Waterframe_929
 C       5.484505    -0.736958     1.465456      64.01
 H       5.705199     0.278429     1.361345      20.76
 C       4.848801    -3.047754     0.794327      47.59
 H       4.519801    -3.802770    -0.014526      21.23
 C       5.066045    -3.386635     2.262407     -11.71
 O       4.775911    -4.700642     2.779718     243.77
 C       4.181151    -5.864086     2.159614     135.53
 H       3.190322    -5.836108     1.557348      28.26
 H       4.212989    -6.567001     2.802041      27.74
 H       4.766542    -6.071458     1.338032      28.09
 C       5.293268    -2.402044     3.273872      23.00
 O       5.489573    -2.783679     4.644464     210.24
 H       5.400981    -3.779117     4.582003      23.33
 C       5.567100    -1.131370     2.807444      54.64
 H       5.751793    -0.331027     3.538154      26.60
 C       5.109052    -1.652284     0.441094      20.54
 C       4.886699    -1.338319    -1.088576      77.30
 H       5.060570    -2.306703    -1.575701      25.18
 O       5.679805    -0.129737    -1.558013     200.02
 H       5.537686     0.733228    -1.117608      25.70
 C       3.295777    -1.142243    -1.350383      67.38
 H       2.788099    -2.178391    -1.168362      23.35
 C       3.037659    -0.586611    -2.737981     109.52
 O       3.049335    -1.590056    -3.740793     292.27
 H       3.841203    -1.586850    -4.328185      28.27
 H       3.888835     0.116635    -2.943022      24.50
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 H       2.062283    -0.151768    -2.794078      27.61
 C      -0.495499    -0.263974     0.602455      43.39
 H      -1.286994    -0.950275     0.453568      24.18
 C       0.084374     2.093580     0.647740      54.37
 H      -0.333946     3.151337     0.865868      21.25
 C       1.316802     1.771220    -0.090950       5.97
 O       2.171192     2.721414    -0.739123     187.11
 C       2.091962     4.185572    -0.378049     114.24
 H       3.036289     4.967710    -0.635571      23.34
 H       1.207044     4.736935    -0.513529      26.20
 H       1.964154     4.330848     0.621837      27.84
 C       1.746074     0.409827    -0.077031      13.75
 O       3.025814    -0.048044    -0.349277     140.37
 C       0.780251    -0.648004     0.177186      45.18
 H       1.047532    -1.629705    -0.410832      21.38
 C      -0.943477     0.993895     0.981293      26.86
 C      -2.328432     1.489623     1.459039      91.28
 H      -2.828854     0.605143     1.832419      24.91
 O      -2.248306     2.505360     2.489732     284.53
 H      -2.469018     1.900186     3.288684      24.65
 C      -3.401420     1.797746     0.296247      76.30
 H      -2.889320     2.612550    -0.195151      25.38
 O      -3.563376     0.709717    -0.636161     206.10
 H      -2.657509     0.742723    -1.052109      27.88
 C      -4.850061     2.281651     1.049062      84.61
 O      -5.850364     2.581972    -0.014517     267.20
 H      -5.972580     3.532636     0.009843      30.73
 H      -4.716850     3.282308     1.690721      24.82
 H      -5.398957     1.416602     1.599113      25.80
55
name = lig-etoh-Waterframe_930
 C       5.425922    -0.711181     1.458867      31.94
 H       5.709859     0.371151     1.153492      19.75
 C       4.825820    -3.031056     0.898734      52.67
 H       4.741518    -3.868840     0.218688      22.42
 C       5.067948    -3.485074     2.259153      -5.35
 O       4.731247    -4.715394     2.849301     253.69
 C       4.262130    -5.842681     2.094987     108.67
 H       3.083081    -5.442250     1.872511      23.39
 H       4.122457    -6.678081     2.818685      24.38
 H       4.924770    -6.125508     1.357400      26.24
 C       5.310408    -2.446141     3.268095       5.31
 O       5.498041    -2.794643     4.639089     148.98
 H       5.395939    -3.745296     4.721947      27.34
 C       5.521775    -1.133315     2.810026      53.47
 H       6.077323    -0.512636     3.652146      24.65
 C       5.139126    -1.684647     0.394091      16.66
 C       4.925716    -1.244839    -1.111804      92.72
 H       5.343402    -1.898811    -1.797508      26.76
 O       5.686255    -0.109539    -1.531496     209.38
 H       5.219131     0.702598    -1.180523      26.40
 C       3.318086    -1.038502    -1.280393      88.56
 H       2.601352    -1.897398    -1.217036      27.09
 C       3.076455    -0.580184    -2.719848     111.93
 O       2.964228    -1.676416    -3.782504     273.23
 H       3.891546    -1.514467    -4.098372      26.24
 H       3.625562     0.229517    -2.971965      30.20
 H       2.151628    -0.022625    -2.566840      28.66
 C      -0.518429    -0.266273     0.581115      35.09
 H      -1.186692    -1.016218     0.799495      25.84
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 C       0.105932     1.971013     0.596957      67.44
 H      -0.175764     3.033158     0.506325      23.81
 C       1.343921     1.784794    -0.073779      -6.21
 O       2.219304     2.747461    -0.669532     149.51
 C       2.050570     4.233183    -0.273479      92.06
 H       2.936788     4.593047    -0.991792      24.02
 H       1.118334     4.599868    -0.785795      24.15
 H       2.389535     4.375426     0.831829      24.74
 C       1.716240     0.286971    -0.205171       2.11
 O       3.059925    -0.044733    -0.359544     174.26
 C       0.883530    -0.716430     0.210653      62.40
 H       0.699585    -1.672298    -0.010804      25.43
 C      -0.887386     1.047504     0.967706      35.44
 C      -2.261802     1.450339     1.455679      80.26
 H      -2.722831     0.521282     1.962571      24.23
 O      -2.405263     2.528080     2.455002     275.60
 H      -2.221143     2.235942     3.380543      29.25
 C      -3.398083     1.909555     0.290484      74.09
 H      -3.204075     2.859460    -0.238047      25.72
 O      -3.532954     0.704596    -0.557435     141.09
 H      -2.750847     0.363681    -1.082663      27.36
 C      -4.839817     2.201841     1.005427      95.83
 O      -5.851852     2.534856    -0.113298     280.71
 H      -5.889772     3.495963    -0.212442      30.92
 H      -4.743116     2.918759     1.617116      30.73
 H      -5.413912     1.475733     1.556474      28.09
55
name = lig-etoh-Waterframe_931
 C       5.381459    -0.759228     1.404238       1.22
 H       5.658922     0.371430     1.022806      23.10
 C       4.887173    -3.032883     0.982353      82.09
 H       4.718160    -3.756087     0.261337      25.23
 C       4.972187    -3.497726     2.280533      23.66
 O       4.748385    -4.703296     2.922786     265.71
 C       4.272888    -5.790963     2.042337      90.65
 H       3.196642    -5.526636     1.516689      26.75
 H       4.105617    -6.739724     2.877957      23.88
 H       4.877648    -6.163089     1.111550      25.42
 C       5.353262    -2.553638     3.235344      -6.64
 O       5.488290    -2.781279     4.570402     104.17
 H       5.436542    -3.722298     4.672808      26.65
 C       5.525759    -1.125744     2.835875       1.23
 H       6.035039    -0.316435     3.571379      16.55
 C       5.152284    -1.723345     0.456176      46.14
 C       4.928990    -1.248145    -1.066831      91.27
 H       5.182619    -2.017474    -1.799198      26.13
 O       5.674234    -0.056326    -1.481216     224.05
 H       5.196941     0.820383    -1.274297      24.95
 C       3.469498    -1.016325    -1.310575      85.15
 H       2.997781    -1.883115    -0.912361      27.17
 C       3.017445    -0.520058    -2.742967      89.52
 O       2.931896    -1.696007    -3.765367     250.26
 H       3.800794    -1.884523    -4.235302      27.41
 H       3.741055     0.108793    -3.210243      27.28
 H       1.933449    -0.213411    -2.810260      27.13
 C      -0.522213    -0.337887     0.636381      50.07
 H      -1.063777    -1.168478     1.085536      25.04
 C       0.167621     2.027605     0.466510      70.13
 H      -0.110802     3.034395     0.573761      23.45
 C       1.389694     1.646532    -0.049395      12.21
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 O       2.224640     2.750591    -0.545379     150.33
 C       2.057311     4.190435    -0.269488     104.97
 H       2.626819     4.577162    -0.990239      28.15
 H       0.938847     4.542309    -0.525722      24.37
 H       2.381113     4.473690     0.910406      24.57
 C       1.734187     0.289350    -0.259624       4.23
 O       3.085049     0.042780    -0.377847     162.07
 C       0.715897    -0.713970     0.229712      32.94
 H       1.103038    -1.719704     0.392971      24.89
 C      -0.773197     1.078055     0.893089      20.10
 C      -2.325451     1.449524     1.462676      68.79
 H      -2.641592     0.405941     1.898688      24.88
 O      -2.518138     2.560583     2.404865     275.68
 H      -2.040213     2.191842     3.157469      29.98
 C      -3.391962     1.931404     0.377399      83.68
 H      -3.241299     2.784892    -0.326484      26.41
 O      -3.533257     0.701398    -0.481313     121.75
 H      -2.684102     0.556780    -1.016991      28.03
 C      -4.840984     2.117776     0.841034     102.26
 O      -5.819651     2.492847    -0.167888     327.82
 H      -5.457474     3.329534    -0.440118      31.17
 H      -4.603169     2.925953     1.591920      25.78
 H      -4.934629     1.180250     1.302256      27.28
55
name = lig-etoh-Waterframe_932
 C       5.405915    -0.795036     1.484660      65.31
 H       5.497012     0.348103     1.159462      23.63
 C       4.937977    -3.118061     0.907214      66.77
 H       4.556399    -3.774405     0.165586      19.02
 C       4.894916    -3.438584     2.359953       6.65
 O       4.763007    -4.737863     2.901253     207.49
 C       4.220962    -5.758794     1.994183      89.65
 H       3.374874    -5.565181     1.500455      33.41
 H       4.090583    -6.817661     2.688534      23.65
 H       5.165175    -5.870474     1.219186      25.96
 C       5.413486    -2.421686     3.202362      13.75
 O       5.480602    -2.791598     4.519623     134.58
 H       5.499615    -3.748076     4.664393      23.94
 C       5.548677    -1.167656     2.763902      82.05
 H       5.632726    -0.358973     3.546972      20.08
 C       5.129055    -1.758585     0.507630      18.49
 C       4.964830    -1.275350    -1.011286      80.42
 H       5.166126    -2.272506    -1.557463      23.76
 O       5.693004    -0.025827    -1.423007     211.19
 H       5.308467     0.903241    -1.146439      23.21
 C       3.528024    -1.007552    -1.347200      65.56
 H       3.117874    -1.984006    -1.110454      23.45
 C       2.996025    -0.594418    -2.847197      86.37
 O       2.907272    -1.707430    -3.710449     264.41
 H       3.793743    -1.775561    -4.204488      26.49
 H       3.760219     0.255359    -3.218446      23.32
 H       1.929177    -0.090343    -2.770793      24.92
 C      -0.552010    -0.344222     0.789572      35.43
 H      -1.335728    -1.054895     1.282451      21.68
 C       0.149749     2.100192     0.386321      52.75
 H      -0.004863     3.094232     0.665103      22.55
 C       1.438939     1.654919    -0.086940      19.72
 O       2.257307     2.680807    -0.418562     198.80
 C       2.002733     4.107863    -0.278003     119.17
 H       2.510055     4.767287    -0.885972      27.32
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 H       0.967887     4.459165    -0.099916      25.66
 H       2.419259     4.565339     0.743226      25.20
 C       1.701860     0.285057    -0.199122      11.13
 O       3.103307     0.145111    -0.414437     135.43
 C       0.718121    -0.696931     0.173127      49.78
 H       1.422499    -1.529863     0.586457      21.64
 C      -0.823603     1.067595     0.813301       6.49
 C      -2.380140     1.520090     1.415586      76.58
 H      -2.769986     0.579772     1.864820      25.63
 O      -2.544562     2.552070     2.374261     274.24
 H      -2.231336     2.271117     3.239874      29.32
 C      -3.365581     1.832107     0.341136     103.59
 H      -2.700831     2.617799    -0.132416      25.34
 O      -3.517088     0.690602    -0.451311     184.25
 H      -2.667234     0.759654    -0.990048      28.47
 C      -4.793353     2.048563     0.758462      73.32
 O      -5.738844     2.463413    -0.207351     298.47
 H      -5.417944     3.250894    -0.611293      30.18
 H      -5.065165     2.918930     1.794137      21.69
 H      -5.207005     1.014198     1.053919      23.78
55
name = lig-etoh-Waterframe_933
 C       5.426602    -0.781566     1.451505      52.88
 H       5.389074     0.310100     1.289311      22.84
 C       4.926597    -3.186326     0.875167      59.39
 H       4.586209    -3.980237     0.157641      14.15
 C       4.898401    -3.414814     2.267518      14.11
 O       4.735396    -4.730632     2.859163     259.05
 C       4.252502    -5.729456     1.942662     104.57
 H       3.357143    -5.396445     1.558827      35.26
 H       4.035863    -6.674678     2.474143      25.47
 H       5.053308    -5.964364     1.136503      28.69
 C       5.389371    -2.457648     3.224219      -5.40
 O       5.496988    -2.771291     4.530152     156.33
 H       5.478736    -3.775594     4.615053      20.02
 C       5.590966    -1.088763     2.825143      59.04
 H       5.555272    -0.400092     3.603020      22.84
 C       5.104544    -1.773618     0.497280      26.94
 C       4.997592    -1.267793    -0.943907      91.38
 H       5.640043    -1.866428    -1.667613      23.35
 O       5.770338    -0.070479    -1.363987     170.78
 H       5.248286     0.672636    -0.860148      25.69
 C       3.451390    -0.993110    -1.375212      68.06
 H       2.657825    -1.786334    -1.224372      23.91
 C       3.050369    -0.628184    -2.841046      91.39
 O       2.910410    -1.747756    -3.693747     270.89
 H       3.769175    -1.609374    -4.217472      25.41
 H       3.657047     0.288589    -3.373864      23.56
 H       2.070953    -0.149261    -2.567469      25.89
 C      -0.534263    -0.232592     0.884831      18.32
 H      -1.327519    -1.054063     1.250846      20.43
 C       0.048855     2.029729     0.387153      79.04
 H      -0.145884     3.072831     0.588883      23.86
 C       1.287974     1.796425    -0.091917      10.38
 O       2.386565     2.640715    -0.350244     198.27
 C       1.945414     4.064330    -0.177438     100.46
 H       2.385002     4.588512    -1.270062      23.65
 H       0.898107     4.144511    -0.305178      25.03
 H       2.532161     4.236601     0.601845      26.51
 C       1.718116     0.327035    -0.133249       1.63
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 O       3.086483     0.156558    -0.491818     168.22
 C       0.828589    -0.677414     0.220236      48.12
 H       0.912267    -1.882526     0.309772      20.26
 C      -0.960899     1.116197     0.783256      34.18
 C      -2.364157     1.480046     1.437351      93.27
 H      -2.680286     0.617737     1.929506      26.62
 O      -2.510076     2.574298     2.374069     276.96
 H      -2.541082     2.109694     3.225133      27.97
 C      -3.306149     1.798964     0.285204      86.75
 H      -3.072111     2.749807    -0.349704      24.85
 O      -3.448487     0.632811    -0.528752     161.06
 H      -2.754699     0.309138    -1.203712      24.38
 C      -4.832935     2.017828     0.788478      74.29
 O      -5.662952     2.460563    -0.306373     268.87
 H      -5.549691     3.394148    -0.471225      28.99
 H      -4.836017     2.593339     1.948497      23.74
 H      -5.363175     1.001282     1.032859      24.65
55
name = lig-etoh-Waterframe_934
 C       5.419129    -0.762920     1.442269      43.32
 H       5.451614     0.155322     1.029716      24.74
 C       4.878656    -3.127931     0.853877      69.31
 H       4.831716    -3.991770     0.077280      23.30
 C       4.986918    -3.475087     2.200394       5.55
 O       4.712088    -4.674573     2.802317     235.29
 C       4.276231    -5.720717     1.873374     120.54
 H       3.180954    -5.277256     1.372171      23.03
 H       4.062359    -6.450186     2.450945      25.72
 H       4.794516    -5.984048     1.031186      27.04
 C       5.326146    -2.476895     3.206368      -0.83
 O       5.517800    -2.763124     4.572372     199.74
 H       5.443081    -3.762183     4.859158      19.54
 C       5.588946    -1.077012     2.912350      63.01
 H       5.828908    -0.334752     3.575985      28.56
 C       5.109676    -1.779663     0.470065      24.43
 C       5.001164    -1.270835    -0.979050      79.14
 H       5.182015    -2.220097    -1.673293      21.80
 O       5.822091    -0.121126    -1.247731     193.82
 H       5.541998     0.832427    -0.895030      22.58
 C       3.388324    -0.993363    -1.378583      76.10
 H       2.770058    -1.881094    -0.962077      23.04
 C       3.075590    -0.559975    -2.764988     100.22
 O       2.955731    -1.794491    -3.713855     265.54
 H       3.670531    -1.918448    -4.406304      28.46
 H       3.813780     0.057438    -3.304244      24.94
 H       2.082993    -0.293551    -2.827340      28.07
 C      -0.424392    -0.148945     0.843430      49.85
 H      -1.009556    -1.059443     1.177033      24.40
 C      -0.125225     2.086389     0.424093      42.89
 H      -0.602142     3.110379     0.438578      22.34
 C       1.262907     1.720422    -0.081838       3.98
 O       2.414633     2.615614    -0.292444     182.88
 C       1.966173     4.001412    -0.162942      96.70
 H       2.343433     4.573004    -1.303295      23.05
 H       0.903776     4.091540    -0.094142      25.82
 H       2.258035     4.609547     0.670781      26.45
 C       1.757901     0.421184    -0.096479      -0.81
 O       3.030923     0.158751    -0.578693     166.18
 C       0.764717    -0.626267     0.395741      54.21
 H       0.809259    -1.610777    -0.193723      22.30
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 C      -1.030924     1.094538     0.863777      44.00
 C      -2.323531     1.434150     1.424793      95.26
 H      -2.649840     0.519135     1.878143      26.73
 O      -2.435116     2.587143     2.402999     256.46
 H      -2.621247     2.100046     3.210210      27.83
 C      -3.363907     1.786776     0.246211      68.78
 H      -3.294443     2.676876    -0.400003      24.43
 O      -3.392144     0.517550    -0.658896     141.11
 H      -2.528599     0.422568    -1.229249      25.45
 C      -4.838276     1.949037     0.809800     103.82
 O      -5.608857     2.508605    -0.367924     276.60
 H      -5.452966     3.441155    -0.262039      29.94
 H      -4.759861     2.603252     1.468794      30.35
 H      -5.100424     0.900420     1.072483      26.64
55
name = lig-etoh-Waterframe_935
 C       5.402070    -0.794413     1.508521      69.41
 H       5.708672     0.115436     1.175155      22.86
 C       4.872141    -3.057289     0.821901      64.35
 H       4.848270    -3.801557    -0.065373      22.03
 C       5.083517    -3.444349     2.223512      -6.59
 O       4.713178    -4.672936     2.703843     207.39
 C       4.213395    -5.691258     1.813512     104.18
 H       3.036252    -5.409201     1.286274      24.00
 H       4.052664    -6.548466     2.459174      24.28
 H       5.001008    -5.881563     1.127653      25.00
 C       5.306833    -2.431816     3.239859       7.69
 O       5.519620    -2.758236     4.594163     137.52
 H       5.521363    -3.766369     4.929824      23.17
 C       5.535219    -1.132843     2.812589      60.98
 H       6.077907    -0.511929     3.531634      24.76
 C       5.119741    -1.721581     0.474514      26.08
 C       4.880578    -1.288564    -1.023457      89.60
 H       5.126170    -2.121073    -1.726421      24.55
 O       5.900470    -0.198414    -1.165736     214.41
 H       5.410943     0.751763    -1.113089      23.61
 C       3.402355    -1.005951    -1.280376      79.32
 H       3.027020    -2.049181    -1.068677      22.68
 C       3.088083    -0.611224    -2.838879     102.33
 O       2.997050    -1.839272    -3.712670     280.33
 H       3.893806    -1.712537    -4.209410      25.27
 H       3.850225     0.072465    -2.922615      27.67
 H       2.228376     0.019218    -3.007842      28.15
 C      -0.461717    -0.229972     0.860078      58.69
 H      -1.107677    -0.986816     1.152370      27.39
 C      -0.195703     2.168310     0.420186      33.86
 H      -0.569847     3.229614     0.199723      20.20
 C       1.276779     1.726882     0.011603      -9.55
 O       2.318727     2.618288    -0.207214     170.61
 C       1.978340     3.998993    -0.204906     120.47
 H       2.321302     4.636634    -1.039137      26.71
 H       0.904505     4.067287    -0.144525      24.91
 H       2.374076     4.682554     0.716481      25.03
 C       1.696525     0.370963    -0.057372      36.35
 O       2.960091     0.215618    -0.620534     184.93
 C       0.855729    -0.482024     0.401388      74.94
 H       0.952903    -1.546936     0.150054      24.32
 C      -0.913540     1.126246     0.954041      30.76
 C      -2.411336     1.440501     1.388471      82.68
 H      -2.876389     0.540751     1.922661      26.31
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 O      -2.340592     2.543476     2.412380     248.51
 H      -2.390091     2.210325     3.305494      28.57
 C      -3.433751     1.672166     0.216624      92.32
 H      -2.945721     2.471289    -0.262757      26.89
 O      -3.340806     0.471726    -0.728086     135.38
 H      -2.466731     0.704240    -1.185289      29.51
 C      -4.788227     1.890820     0.691771     110.32
 O      -5.576433     2.535392    -0.338601     301.67
 H      -5.266213     3.475046    -0.511352      27.48
 H      -4.803790     2.694740     1.523290      24.80
 H      -5.362294     1.080232     1.138839      26.32
55
name = lig-etoh-Waterframe_936
 C       5.411362    -0.752988     1.456692      51.20
 H       5.881382     0.247473     1.433136      21.55
 C       4.938061    -3.005773     0.858156      62.41
 H       4.585086    -3.767575     0.142074      20.73
 C       5.074964    -3.368291     2.197793      11.81
 O       4.719726    -4.701386     2.647408     203.42
 C       4.166910    -5.681072     1.759376     105.26
 H       3.198692    -5.394535     1.263583      29.20
 H       4.009675    -6.757358     2.385054      23.62
 H       4.972487    -5.925780     0.949930      26.89
 C       5.320250    -2.502490     3.277059      24.90
 O       5.506353    -2.726143     4.600530     128.23
 H       5.663627    -3.764050     4.651647      21.66
 C       5.526403    -1.201527     2.799684      19.37
 H       6.021940    -0.434844     3.557565      22.95
 C       5.062027    -1.680990     0.451926      33.24
 C       4.856128    -1.270986    -0.961684     114.20
 H       5.200774    -1.916576    -1.661612      27.60
 O       5.940111    -0.269546    -1.151688     205.77
 H       5.397469     0.620169    -1.325953      25.31
 C       3.364382    -0.996320    -1.287996      76.28
 H       2.694732    -1.772695    -0.942388      25.04
 C       3.118647    -0.702638    -2.859804      96.57
 O       3.094871    -1.811072    -3.700488     275.82
 H       4.022859    -1.808692    -4.165930      25.18
 H       4.029745    -0.158506    -3.204491      24.78
 H       2.218879     0.016929    -2.872778      26.65
 C      -0.541994    -0.245803     0.933149      43.30
 H      -1.188768    -0.999101     1.152251      25.18
 C      -0.027616     2.172998     0.383088      78.31
 H      -0.451934     3.221287     0.296907      21.82
 C       1.195470     1.855831     0.145122      38.27
 O       2.223445     2.650049    -0.149204     205.23
 C       1.956566     4.099734    -0.211941     129.44
 H       2.398181     4.364537    -1.038722      30.31
 H       0.876894     4.377214    -0.361665      24.95
 H       2.610064     4.168755     0.747854      23.97
 C       1.704884     0.488354    -0.072049      -6.32
 O       2.917691     0.256635    -0.620584     151.23
 C       0.817735    -0.628120     0.410425      46.86
 H       1.327272    -1.487863     0.719251      23.83
 C      -0.919017     1.117440     1.010959      21.63
 C      -2.456605     1.388325     1.447807      79.42
 H      -2.797546     0.455274     2.084119      24.57
 O      -2.270619     2.499260     2.377429     253.83
 H      -2.115666     1.953502     3.156608      27.79
 C      -3.344673     1.535389     0.192415      93.28
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 H      -3.054506     2.486609    -0.350603      26.17
 O      -3.307860     0.519337    -0.708467     200.03
 H      -2.510519     0.371198    -1.341570      24.18
 C      -4.819900     1.946518     0.597393      88.12
 O      -5.593217     2.553581    -0.334268     268.85
 H      -5.098587     3.379107    -0.676730      26.09
 H      -4.520062     2.504373     1.869643      22.13
 H      -5.467637     1.102020     0.849243      24.75
55
name = lig-etoh-Waterframe_937
 C       5.454707    -0.711827     1.469718      38.05
 H       5.640381     0.422328     1.030221      22.02
 C       4.961139    -2.991600     0.891823      73.66
 H       4.509149    -3.722623     0.303883      18.17
 C       4.976695    -3.445617     2.222885      18.48
 O       4.744915    -4.716554     2.625126     238.46
 C       4.184851    -5.700897     1.674551      79.42
 H       3.302437    -5.361427     1.521740      34.79
 H       3.880145    -6.657231     2.449240      22.99
 H       4.676771    -5.993153     0.646201      25.84
 C       5.362703    -2.501884     3.223655      22.28
 O       5.479914    -2.738851     4.598535     171.96
 H       5.813328    -3.686972     4.938624      22.04
 C       5.566257    -1.192897     2.820917      56.28
 H       5.694767    -0.348102     3.650428      22.26
 C       5.014512    -1.641463     0.487934      23.73
 C       4.898475    -1.266427    -0.919573      98.07
 H       4.991360    -2.223250    -1.470340      26.44
 O       5.916414    -0.284696    -1.200121     204.78
 H       5.759454     0.737041    -1.293858      23.80
 C       3.278840    -0.925978    -1.336623      79.11
 H       2.629135    -1.674867    -0.956002      25.36
 C       3.215369    -0.696191    -2.797095      90.26
 O       3.174880    -1.844366    -3.713725     280.50
 H       4.021933    -1.889451    -4.279541      26.28
 H       3.960605     0.055568    -3.315226      23.67
 H       2.114935    -0.352214    -3.016904      24.99
 C      -0.492288    -0.250996     0.973327      43.30
 H      -1.179378    -1.005491     1.377949      23.99
 C      -0.121572     2.118361     0.516952      43.88
 H      -0.321844     3.209357     0.620605      21.07
 C       1.291778     1.815223     0.172950      21.96
 O       2.168328     2.756532    -0.158779     214.65
 C       2.001873     4.175231    -0.197842     115.34
 H       2.715635     4.415331    -1.112965      24.16
 H       0.990377     4.733547    -0.216271      24.04
 H       2.296083     4.928057     0.643425      24.39
 C       1.575922     0.456584    -0.012644      -4.82
 O       2.929925     0.332891    -0.615738     131.63
 C       0.753441    -0.676027     0.464928      63.00
 H       1.308915    -1.468983     0.887550      22.75
 C      -0.984692     1.061337     0.958258      36.48
 C      -2.320636     1.292802     1.484766      91.13
 H      -2.714454     0.389082     2.033296      25.51
 O      -2.254142     2.451338     2.350010     260.10
 H      -1.999722     2.109921     3.234638      28.50
 C      -3.274820     1.607769     0.218259      72.35
 H      -2.955790     2.588423    -0.313318      24.77
 O      -3.317465     0.483430    -0.713755     171.47
 H      -2.423360     0.221301    -1.123628      25.73
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 C      -4.797130     1.882244     0.634271      84.59
 O      -5.629195     2.612431    -0.398656     249.62
 H      -5.319617     3.645599    -0.514339      24.46
 H      -4.802965     2.718016     1.495678      22.75
 H      -5.222599     0.898568     0.749128      24.92
55
name = lig-etoh-Waterframe_938
 C       5.461346    -0.705147     1.512194      59.89
 H       5.370434     0.469585     1.162620      21.55
 C       4.874860    -3.028801     0.906996      62.46
 H       4.711617    -3.607430     0.048959      18.42
 C       4.928778    -3.475352     2.260842      14.26
 O       4.800794    -4.796727     2.609188     226.74
 C       4.120428    -5.707287     1.649164     108.59
 H       3.096942    -5.338326     1.520664      27.54
 H       4.192070    -6.697539     2.213588      23.13
 H       4.800107    -5.848362     0.755099      25.98
 C       5.416240    -2.502049     3.191684      -4.53
 O       5.436724    -2.755122     4.601275     172.13
 H       5.956325    -3.604687     4.951889      22.76
 C       5.605796    -1.066953     2.816494      43.47
 H       5.662941    -0.471413     3.759077      22.51
 C       5.038316    -1.633434     0.618121      21.87
 C       4.822705    -1.248484    -0.921270      78.33
 H       5.118330    -2.248868    -1.545815      23.06
 O       5.911308    -0.298434    -1.315432     187.53
 H       5.444800     0.596531    -1.050270      25.50
 C       3.337759    -0.840177    -1.285821      84.53
 H       2.802248    -1.781267    -1.145100      23.00
 C       3.208317    -0.634376    -2.866836      87.14
 O       3.238242    -1.924094    -3.709117     293.06
 H       4.102434    -1.757053    -4.170663      24.44
 H       3.808512     0.336830    -2.865182      24.15
 H       2.180178    -0.200822    -3.010113      26.73
 C      -0.465262    -0.321704     1.007698      53.60
 H      -1.022859    -1.068448     1.708316      22.00
 C      -0.146628     2.065100     0.698345      53.63
 H      -0.533841     3.036327     0.919411      20.89
 C       1.194858     1.761296     0.202292     -20.30
 O       2.185473     2.878543    -0.174362     143.37
 C       2.031563     4.341574    -0.192727      61.09
 H       2.716724     4.932026    -1.159134      21.84
 H       0.992709     4.383198    -0.647269      22.75
 H       2.409349     4.654489     0.833707      22.72
 C       1.584153     0.357313     0.004135      13.65
 O       2.892208     0.383441    -0.599320     176.95
 C       0.777049    -0.599608     0.542865      63.28
 H       0.986556    -1.712705     0.551348      21.30
 C      -0.948571     0.973025     0.869479      40.72
 C      -2.267380     1.256587     1.474371      92.62
 H      -2.664141     0.392336     1.914206      27.09
 O      -2.265438     2.418541     2.341654     271.18
 H      -2.214002     2.233492     3.307379      28.82
 C      -3.273308     1.726453     0.280927      69.42
 H      -2.636169     2.506651    -0.196891      24.64
 O      -3.350414     0.447634    -0.689652     129.35
 H      -2.383835     0.355407    -0.907475      29.26
 C      -4.753893     1.903739     0.613160     101.57
 O      -5.640377     2.623535    -0.465396     250.76
 H      -5.495394     3.610041    -0.180313      25.79
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 H      -4.906224     2.311472     1.438463      29.23
 H      -5.267841     0.969858     0.917606      25.46
55
name = lig-etoh-Waterframe_939
 C       5.412411    -0.632281     1.574772      27.57
 H       5.492673     0.515361     1.446777      21.37
 C       4.770856    -3.019564     0.912337      70.60
 H       4.831026    -3.718234     0.063852      25.40
 C       4.961938    -3.462197     2.245276      -8.88
 O       4.848480    -4.881665     2.621809     209.63
 C       4.116622    -5.719302     1.674489     132.14
 H       2.910346    -5.514863     1.284648      23.18
 H       4.162189    -6.650272     1.947002      23.51
 H       4.630742    -5.593381     0.742568      27.46
 C       5.442187    -2.455535     3.218833       7.93
 O       5.397969    -2.756006     4.584373     140.72
 H       5.984828    -3.609690     4.638507      22.55
 C       5.624202    -1.098017     2.927271      45.95
 H       5.918712    -0.352847     3.610265      23.67
 C       5.043041    -1.691785     0.588338      20.71
 C       4.805768    -1.245329    -0.863779      94.06
 H       4.974191    -2.115421    -1.668684      21.18
 O       5.839955    -0.301533    -1.428426     167.06
 H       5.620729     0.650562    -1.059389      24.43
 C       3.431562    -0.835819    -1.288245      67.81
 H       2.731005    -1.663244    -0.895708      20.60
 C       3.122605    -0.546841    -2.875630      88.31
 O       3.300617    -1.888688    -3.640133     266.50
 H       4.173700    -1.958237    -4.198132      26.27
 H       3.959357    -0.070514    -3.446622      21.39
 H       2.148047    -0.156882    -3.020922      26.24
 C      -0.485704    -0.394218     1.062513      41.59
 H      -1.028198    -1.299808     1.621974      21.37
 C      -0.042998     2.046010     0.794826      72.44
 H      -0.511465     2.922469     1.021326      23.54
 C       1.124509     1.859756     0.196265       5.18
 O       2.221594     2.859964    -0.191248     137.15
 C       1.971600     4.434305    -0.210105      86.89
 H       2.888116     4.823654    -0.865362      22.93
 H       0.948035     4.747478    -0.482318      25.11
 H       2.058218     4.669136     0.779001      26.45
 C       1.685605     0.470228    -0.004597      -3.34
 O       2.848334     0.350809    -0.589663     149.01
 C       0.884825    -0.670079     0.583730      52.16
 H       1.076909    -1.721403     0.095768      20.74
 C      -0.958802     0.877774     0.925800      36.36
 C      -2.377078     1.277199     1.451890      96.93
 H      -2.734110     0.432976     1.970287      26.39
 O      -2.284996     2.409519     2.358171     279.48
 H      -2.465538     1.894358     3.189627      26.04
 C      -3.271227     1.686297     0.302389      89.85
 H      -2.938888     2.551468    -0.269982      25.36
 O      -3.365351     0.496954    -0.602825     172.43
 H      -2.523884     0.289220    -1.096604      27.74
 C      -4.780321     1.992421     0.570461      84.92
 O      -5.598930     2.557572    -0.449532     274.84
 H      -5.454898     3.598353    -0.511084      26.17
 H      -4.832016     2.444448     1.725796      24.13
 H      -5.182093     0.925020     0.513245      24.36
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name = lig-etoh-Waterframe_940
 C       5.338778    -0.687124     1.639371      57.30
 H       5.626035     0.238804     1.323977      23.89
 C       4.754078    -3.010970     0.934380      56.41
 H       4.487856    -3.866776     0.216249      21.92
 C       5.029899    -3.457635     2.246316      -4.03
 O       4.869135    -4.871550     2.646919     137.68
 C       4.146475    -5.732662     1.617369     112.49
 H       2.961880    -5.340831     1.954382      23.04
 H       4.190086    -6.727664     1.942606      26.68
 H       4.471780    -5.658712     0.621388      28.14
 C       5.376587    -2.476411     3.262252      14.26
 O       5.402696    -2.787704     4.568592     138.98
 H       5.733799    -3.734661     4.845846      22.38
 C       5.632790    -1.112543     2.937389      60.68
 H       6.093333    -0.522773     3.652055      25.40
 C       5.034123    -1.583005     0.559723      19.33
 C       4.871740    -1.222778    -0.900653      98.01
 H       4.880090    -2.186946    -1.339993      22.93
 O       5.752937    -0.297313    -1.510433     257.77
 H       5.858768     0.660824    -1.246376      25.68
 C       3.355143    -0.818510    -1.320700      67.97
 H       2.712974    -1.771711    -1.063480      22.06
 C       3.163202    -0.583743    -2.889566      98.00
 O       3.278228    -1.837105    -3.527175     288.45
 H       4.195946    -1.735016    -4.023485      24.66
 H       3.781685     0.182116    -3.465598      23.59
 H       2.182138    -0.225221    -3.015864      27.34
 C      -0.388157    -0.507908     1.067386      31.84
 H      -1.181882    -1.320541     1.123402      21.64
 C      -0.079216     2.002785     0.848608      36.42
 H      -0.318410     3.024294     1.024728      23.04
 C       1.316330     1.935521     0.137360       7.95
 O       2.185851     2.846963    -0.211933     163.81
 C       1.887612     4.394385    -0.166556     115.23
 H       2.710377     4.733341    -0.618270      27.53
 H       1.067031     4.884750    -0.625077      27.02
 H       1.896675     4.845353     0.760836      27.18
 C       1.616075     0.525321     0.083250      11.95
 O       2.915170     0.354280    -0.612275     164.13
 C       0.976474    -0.633840     0.515522      54.30
 H       1.451331    -1.682047     0.287086      20.94
 C      -0.983074     0.885911     1.120066       8.56
 C      -2.450525     1.302883     1.436952      92.54
 H      -3.033607     0.463987     1.950753      25.09
 O      -2.329629     2.382406     2.411077     249.21
 H      -2.417548     2.053807     3.374149      26.54
 C      -3.318885     1.654572     0.217612      98.98
 H      -2.926120     2.529273    -0.284242      26.92
 O      -3.382025     0.528322    -0.545326     222.60
 H      -2.644184     0.481192    -1.199733      27.90
 C      -4.810105     1.975684     0.581914      75.45
 O      -5.545368     2.539515    -0.448141     296.92
 H      -5.191814     3.413719    -0.770158      28.11
 H      -4.923257     2.839120     1.648963      21.88
 H      -5.270756     0.927972     0.733310      24.18
55
name = lig-etoh-Waterframe_941
 C       5.329724    -0.730863     1.610676      62.47
 H       5.660688     0.160760     1.327180      24.26
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 C       4.810182    -2.933295     0.965688      57.00
 H       4.255415    -3.500256     0.144762      20.79
 C       5.059030    -3.473202     2.248217      20.41
 O       4.917905    -4.807379     2.628161     176.78
 C       4.143549    -5.703353     1.667210     110.07
 H       3.028944    -5.483109     1.803501      26.78
 H       4.446058    -6.805736     2.103202      24.01
 H       4.341181    -5.637388     0.610484      26.79
 C       5.303643    -2.543285     3.271534      10.25
 O       5.432252    -2.845280     4.634692     165.80
 H       5.399236    -3.830834     4.884126      23.49
 C       5.616592    -1.182229     2.933831      50.49
 H       6.033140    -0.622334     3.739323      24.06
 C       4.965750    -1.566612     0.603943      27.59
 C       4.818422    -1.192569    -0.961136      92.40
 H       5.211735    -2.039848    -1.409337      25.31
 O       5.743701    -0.305079    -1.618031     235.73
 H       5.460640     0.531510    -1.161951      27.76
 C       3.280556    -0.808022    -1.350976      82.75
 H       2.679565    -1.710836    -1.268952      24.22
 C       3.176154    -0.558176    -2.838255     106.60
 O       3.267451    -1.824560    -3.467024     288.91
 H       4.168405    -1.974414    -4.013564      25.20
 H       3.713039     0.329606    -2.904373      26.10
 H       2.086457    -0.290186    -2.940812      27.04
 C      -0.324846    -0.476705     0.991907      45.01
 H      -0.833852    -1.393251     0.873431      23.44
 C      -0.017175     1.989092     0.820726      44.40
 H      -0.497138     3.025526     1.017839      20.50
 C       1.248864     1.839812     0.257775      20.00
 O       2.142114     2.939770    -0.248842     167.79
 C       1.825666     4.299239    -0.128666     110.26
 H       2.641975     4.757640    -0.538431      26.75
 H       1.042852     4.309605    -0.908727      25.34
 H       1.784286     4.558232     1.048007      23.16
 C       1.728103     0.544200     0.061621       7.58
 O       2.975365     0.395569    -0.608815     167.39
 C       0.935698    -0.560462     0.482328      62.82
 H       1.588265    -1.421531     0.656635      22.67
 C      -0.877980     0.857563     1.279859      16.69
 C      -2.455105     1.298413     1.534030      69.54
 H      -3.099671     0.350868     1.843129      23.73
 O      -2.412799     2.389237     2.465904     260.52
 H      -2.256456     1.997921     3.422849      25.25
 C      -3.373337     1.743935     0.212952      77.55
 H      -2.813812     2.500075    -0.358161      25.44
 O      -3.400969     0.466541    -0.601189     187.44
 H      -2.632208     0.594450    -1.193800      28.93
 C      -4.815197     1.953723     0.657547     101.18
 O      -5.521752     2.538090    -0.530733     317.76
 H      -5.065116     3.395370    -0.523041      29.52
 H      -4.776531     2.734615     1.528984      25.03
 H      -5.359776     1.265363     1.234544      26.69
55
name = lig-etoh-Waterframe_942
 C       5.419611    -0.679550     1.624345      37.32
 H       5.623758     0.424555     1.530960      22.24
 C       4.826577    -2.892746     0.953819      59.01
 H       4.521213    -3.599156     0.110046      20.05
 C       5.029635    -3.457464     2.227862      30.38
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 O       4.955857    -4.778716     2.561488     249.47
 C       4.138337    -5.663525     1.770206     136.94
 H       3.191269    -5.688671     1.763593      31.87
 H       4.452506    -6.875455     2.116954      24.35
 H       4.546598    -5.478048     0.730886      27.09
 C       5.300085    -2.585059     3.339688      13.64
 O       5.452053    -2.899367     4.691368     179.97
 H       5.356101    -3.895792     4.765087      23.54
 C       5.559140    -1.287444     2.930834      51.83
 H       5.824360    -0.494700     3.671073      22.52
 C       4.889925    -1.572315     0.571331      29.59
 C       4.720881    -1.260826    -0.993277      77.43
 H       4.909726    -2.211816    -1.592145      24.15
 O       5.724838    -0.251345    -1.655436     173.96
 H       5.528347     0.708812    -1.507358      26.05
 C       3.302798    -0.874665    -1.321055      83.44
 H       2.587909    -1.468552    -0.871119      24.29
 C       3.094405    -0.460917    -2.736511      91.89
 O       3.293936    -1.836888    -3.481254     245.09
 H       4.210948    -1.836585    -4.026345      25.61
 H       3.923212     0.103402    -3.204374      22.88
 H       2.029569    -0.106764    -3.063138      24.87
 C      -0.367752    -0.372176     0.926286      52.08
 H      -0.773186    -1.269943     1.240715      25.01
 C      -0.042587     1.963810     0.874040      56.69
 H      -0.573214     3.032837     0.887335      19.71
 C       1.236184     1.831215     0.337285       7.93
 O       2.114348     2.868797    -0.255678     182.06
 C       1.740390     4.205780    -0.126712      96.52
 H       2.611286     4.998900    -0.388160      22.62
 H       0.681207     4.543434    -0.647418      24.13
 H       1.168415     4.572615     0.988158      22.22
 C       1.860595     0.537494     0.011705      16.53
 O       3.017372     0.442174    -0.585403     164.05
 C       1.037733    -0.494021     0.458775      60.25
 H       1.307595    -1.502262     0.571677      23.26
 C      -0.794390     0.863468     1.297761      37.76
 C      -2.391646     1.273519     1.592579      72.26
 H      -2.805555     0.343594     2.118842      23.14
 O      -2.516040     2.397163     2.527319     261.89
 H      -2.295891     1.926975     3.435558      24.84
 C      -3.341413     1.676935     0.312925      61.47
 H      -3.119228     2.606602    -0.314315      23.95
 O      -3.409432     0.438712    -0.675958     156.26
 H      -2.614262     0.307762    -1.238617      26.75
 C      -4.804299     2.066851     0.711388     103.87
 O      -5.488683     2.525869    -0.565840     262.45
 H      -5.504219     3.491156    -0.599921      28.99
 H      -4.645876     2.799600     1.300020      29.50
 H      -5.309504     1.175836     1.042355      27.03
55
name = lig-etoh-Waterframe_943
 C       5.454066    -0.715409     1.623060      54.29
 H       5.520289     0.512229     1.593303      22.88
 C       4.800830    -2.959780     0.898424      39.41
 H       4.936147    -3.806043     0.207250      20.41
 C       4.976892    -3.389669     2.254147      10.59
 O       4.975440    -4.797037     2.544771     166.48
 C       4.197813    -5.673192     1.794721     115.03
 H       3.033503    -5.473355     2.000910      24.37
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 H       4.446932    -6.760364     2.190522      22.53
 H       4.489612    -5.710448     0.654459      24.69
 C       5.329523    -2.612303     3.368260       8.07
 O       5.451603    -2.958440     4.690153     204.94
 H       5.569261    -3.892278     5.003637      22.91
 C       5.509463    -1.236375     2.918643      44.91
 H       5.696013    -0.551233     3.837806      23.45
 C       4.937977    -1.465598     0.532099      12.70
 C       4.703141    -1.287123    -0.993252      74.38
 H       4.678940    -2.336241    -1.555583      21.38
 O       5.680081    -0.244746    -1.647637     163.53
 H       5.449815     0.692008    -1.561876      26.24
 C       3.294897    -0.822162    -1.221799      85.73
 H       2.642257    -1.616848    -0.865557      24.60
 C       3.049975    -0.507059    -2.777272      86.11
 O       3.294449    -1.815645    -3.511863     257.72
 H       4.117709    -1.493433    -4.020493      23.89
 H       3.894707     0.189531    -3.243180      22.87
 H       2.091635     0.132927    -2.948692      25.05
 C      -0.303520    -0.335162     0.915725      56.15
 H      -0.883160    -1.056039     1.504177      25.50
 C      -0.028212     2.028381     0.927970      46.34
 H      -0.445343     3.107219     0.891144      21.69
 C       1.343611     1.848615     0.302287      15.20
 O       2.068897     2.758806    -0.233444     151.81
 C       1.508940     4.226758    -0.086626      76.36
 H       2.592672     4.889458    -0.251381      22.83
 H       0.818709     4.595117    -0.968253      23.33
 H       1.366471     4.299712     1.050354      23.17
 C       1.818730     0.571838     0.068079      16.22
 O       3.128794     0.492091    -0.583041     152.92
 C       1.053123    -0.545136     0.468728      61.98
 H       1.255629    -1.519007     0.150623      23.04
 C      -0.897511     0.974676     1.234529      26.18
 C      -2.303293     1.235240     1.632999      93.01
 H      -2.688046     0.380110     2.116088      26.28
 O      -2.600860     2.377595     2.572963     251.36
 H      -2.477011     2.170891     3.576210      26.75
 C      -3.272685     1.511792     0.373768      70.42
 H      -2.749094     2.428734    -0.100642      25.38
 O      -3.435017     0.461798    -0.682839     187.60
 H      -2.572428     0.305944    -1.100680      30.05
 C      -4.772896     2.153107     0.645741      87.26
 O      -5.455209     2.508851    -0.558402     268.89
 H      -5.717368     3.407185    -0.628285      29.76
 H      -4.757712     3.097515     1.528841      23.60
 H      -5.428065     1.258636     1.009236      25.06
55
name = lig-etoh-Waterframe_944
 C       5.389732    -0.734208     1.602680      31.43
 H       5.608457     0.460123     1.365023      23.92
 C       4.832939    -2.922200     0.888143      63.84
 H       4.940740    -3.621101     0.097669      23.14
 C       4.925962    -3.432330     2.243591      -6.18
 O       5.040287    -4.775710     2.570378     211.65
 C       4.205701    -5.755297     1.770584     104.92
 H       3.016309    -5.249926     2.008933      22.46
 H       4.280844    -6.591158     2.288531      23.54
 H       4.232442    -5.855182     0.653553      27.73
 C       5.351798    -2.549160     3.314331      -3.81
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 O       5.453431    -2.981782     4.677454     121.28
 H       5.570620    -3.904270     4.903060      25.82
 C       5.482317    -1.201496     3.016042      37.80
 H       5.739608    -0.407735     3.821460      19.94
 C       5.048845    -1.589337     0.526254      29.35
 C       4.752298    -1.193230    -0.952567      90.88
 H       5.119602    -2.135359    -1.494003      22.55
 O       5.632481    -0.311000    -1.625161     229.79
 H       5.239053     0.459244    -1.270481      30.20
 C       3.283762    -0.702393    -1.235842      91.87
 H       2.660459    -1.606084    -0.990533      25.73
 C       3.064179    -0.583901    -2.797955     110.06
 O       3.259999    -1.731009    -3.555521     291.41
 H       4.007951    -1.803903    -4.230493      26.44
 H       3.723303     0.342589    -2.880983      26.05
 H       2.007104    -0.350313    -2.919658      28.27
 C      -0.284826    -0.271062     1.027232      44.37
 H      -0.848802    -1.325316     1.186929      22.55
 C       0.075713     2.148653     0.903187      79.41
 H      -0.258837     3.149686     1.066830      25.66
 C       1.255032     1.814625     0.337801      13.86
 O       2.046101     2.853534    -0.251679     165.54
 C       1.433828     4.194400    -0.063144     111.64
 H       2.418181     4.823829    -0.234630      24.03
 H       0.719147     4.234754    -0.819808      28.16
 H       1.032109     4.368475     0.846909      28.82
 C       1.826851     0.526699     0.131413       3.50
 O       3.144020     0.514007    -0.534829     169.62
 C       0.960473    -0.598516     0.458192      48.73
 H       1.326379    -1.544469     0.101992      23.81
 C      -0.861446     1.060607     1.114969       9.15
 C      -2.352791     1.163246     1.724587      80.79
 H      -2.602127     0.233820     2.132081      27.01
 O      -2.657885     2.358049     2.570311     267.49
 H      -2.487455     1.930475     3.485419      25.59
 C      -3.220456     1.489064     0.382642      81.98
 H      -2.455504     2.083482    -0.087176      26.51
 O      -3.450367     0.493509    -0.613139     215.00
 H      -2.593900     0.381603    -1.035440      30.90
 C      -4.717623     2.132135     0.598251      83.92
 O      -5.430021     2.497296    -0.577884     290.64
 H      -5.364118     3.441702    -0.512171      27.87
 H      -4.699486     3.161734     1.532265      22.15
 H      -5.345997     1.444556     1.287489      25.26
55
name = lig-etoh-Waterframe_945
 C       5.320650    -0.741363     1.651758      34.91
 H       5.629705     0.284111     1.307495      21.83
 C       4.893035    -2.986636     0.909532      63.70
 H       4.555348    -3.576394     0.096742      23.42
 C       4.962878    -3.445824     2.206237      -9.17
 O       5.092858    -4.786656     2.547394     233.74
 C       4.142579    -5.773022     1.811595     120.12
 H       2.947902    -5.470310     1.790905      25.33
 H       4.166691    -6.637193     2.300090      24.23
 H       4.604379    -5.840395     0.848253      27.33
 C       5.314600    -2.532187     3.301833     -13.68
 O       5.462364    -2.948288     4.610953     195.66
 H       5.245484    -3.871159     4.592569      26.19
 C       5.473713    -1.113841     2.994980      37.48
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 H       5.793808    -0.390199     3.783812      24.06
 C       5.144030    -1.648207     0.577197      30.66
 C       4.829512    -1.214038    -0.911536     103.73
 H       4.821438    -2.141824    -1.473635      25.85
 O       5.620930    -0.282831    -1.573322     234.57
 H       5.730231     0.604881    -1.331688      28.60
 C       3.364436    -0.771192    -1.290973      76.13
 H       2.573520    -1.341065    -0.737630      26.26
 C       3.047685    -0.534520    -2.753031     114.27
 O       3.233242    -1.713769    -3.641709     265.18
 H       4.141799    -1.698698    -4.090026      26.62
 H       3.461287     0.270571    -3.371905      27.16
 H       2.023281    -0.492201    -2.847876      29.40
 C      -0.323900    -0.242451     1.096464      48.87
 H      -1.172093    -1.094882     1.020926      23.91
 C       0.021201     2.178071     0.906327      76.13
 H      -0.210966     3.130148     1.149128      27.21
 C       1.297545     1.851609     0.300740      -5.22
 O       2.024150     2.953323    -0.221504     177.41
 C       1.423973     4.169587    -0.105020     143.45
 H       1.950930     5.002902    -0.314996      29.08
 H       0.572971     4.255107    -0.696471      29.93
 H       0.908526     4.525611     0.759918      28.29
 C       1.820859     0.472639     0.175553      23.65
 O       3.030477     0.515525    -0.450505     134.77
 C       0.948988    -0.547399     0.421199      62.46
 H       1.070961    -1.673652     0.542037      25.40
 C      -0.773397     1.054764     1.136711       5.33
 C      -2.421799     1.149974     1.702769      73.43
 H      -2.574506     0.202692     2.278694      25.26
 O      -2.672560     2.264893     2.564339     269.96
 H      -2.540016     2.072368     3.547705      27.22
 C      -3.213617     1.569387     0.392409      85.03
 H      -2.746856     2.425051    -0.095253      27.15
 O      -3.441033     0.462738    -0.530183     198.00
 H      -2.732297     0.254324    -1.136674      29.36
 C      -4.605083     2.097952     0.662224     102.00
 O      -5.387700     2.518939    -0.592608     311.65
 H      -5.114079     3.402191    -0.788718      31.55
 H      -4.343622     3.064904     1.017673      25.20
 H      -5.161870     1.278651     1.132067      26.03
55
name = lig-etoh-Waterframe_946
 C       5.326170    -0.693448     1.645508      49.68
 H       5.439483     0.285645     1.493749      22.36
 C       4.930626    -3.065598     0.877196      23.53
 H       4.449342    -3.811415     0.255423      20.49
 C       5.082599    -3.437500     2.247952     -15.89
 O       5.064054    -4.841784     2.529978     265.43
 C       4.136956    -5.754146     1.850793     118.69
 H       3.202429    -5.384647     1.655214      30.67
 H       4.201769    -6.791203     2.454368      22.17
 H       4.666834    -5.988139     0.962932      24.80
 C       5.253518    -2.466326     3.256143      15.23
 O       5.462688    -2.912337     4.508176     236.98
 H       5.045769    -3.744359     4.747731      21.95
 C       5.458076    -1.118548     2.964083      77.80
 H       5.707958    -0.451343     3.741950      29.83
 C       5.148638    -1.634652     0.602785      26.89
 C       4.816155    -1.280267    -0.859416      89.97
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 H       4.933395    -2.135949    -1.481794      26.23
 O       5.725662    -0.213222    -1.569667     147.19
 H       5.851982     0.586377    -1.086198      28.06
 C       3.423609    -0.820566    -1.183141      59.44
 H       2.763567    -1.776692    -1.040800      26.03
 C       2.973026    -0.493496    -2.795226      89.36
 O       3.236314    -1.730573    -3.720917     242.67
 H       4.184342    -1.539573    -3.851385      25.74
 H       3.380967     0.382630    -3.295435      27.34
 H       1.916568    -0.204755    -2.587089      27.43
 C      -0.361184    -0.248021     1.020206      51.73
 H      -1.137496    -0.969994     1.325900      26.93
 C       0.009476     2.123823     0.891389      50.27
 H      -0.435043     3.037282     1.054662      26.55
 C       1.297195     1.938927     0.292697      20.02
 O       2.069283     2.966037    -0.165936     164.48
 C       1.310725     4.297444    -0.179510      80.15
 H       1.995052     4.962703    -0.597369      26.58
 H       0.377123     4.231994    -0.912843      24.85
 H       1.303305     4.438615     1.121771      21.59
 C       1.763373     0.581824     0.165551       9.57
 O       2.977844     0.471057    -0.424938      97.36
 C       0.861567    -0.544020     0.519797      53.89
 H       1.315925    -1.652173     0.529966      24.16
 C      -0.866347     1.038954     1.320552      34.22
 C      -2.350232     1.222715     1.601618      79.01
 H      -2.854545     0.164316     1.926208      25.43
 O      -2.675170     2.198007     2.583870     273.04
 H      -2.479472     1.925818     3.530315      27.93
 C      -3.203712     1.610279     0.356286      89.09
 H      -2.701554     2.502121    -0.117782      27.49
 O      -3.411912     0.396272    -0.463493     162.25
 H      -2.655130     0.293869    -1.038989      30.35
 C      -4.550649     2.135613     0.665012     112.72
 O      -5.306666     2.504042    -0.583879     324.69
 H      -5.113976     3.409147    -0.795735      31.95
 H      -4.472754     2.881846     1.331983      28.74
 H      -5.242401     1.495450     1.173011      27.72
55
name = lig-etoh-Waterframe_947
 C       5.363005    -0.642597     1.585668      35.54
 H       5.276070     0.344309     1.428000      24.83
 C       4.975588    -3.033002     0.917203      67.75
 H       4.926932    -3.801888     0.078164      22.06
 C       5.159977    -3.497277     2.182478      25.44
 O       5.026794    -4.844759     2.585034     180.14
 C       4.205263    -5.756597     1.835814     108.10
 H       3.334739    -5.281590     1.701151      31.12
 H       3.847904    -6.605465     2.795119      23.24
 H       4.431692    -6.223168     0.841506      25.82
 C       5.232793    -2.497785     3.210901      -6.08
 O       5.460637    -2.860903     4.492550     215.07
 H       5.122402    -3.717105     4.818351      20.13
 C       5.430640    -1.119378     2.946678      51.82
 H       5.527686    -0.497789     3.760879      25.44
 C       5.065133    -1.675506     0.564385      25.28
 C       4.870540    -1.232913    -0.877488      79.42
 H       5.242485    -2.088026    -1.442355      23.79
 O       5.846388    -0.190692    -1.536644     156.39
 H       5.645238     0.432585    -0.886645      29.41
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 C       3.361611    -0.834996    -1.148324      80.05
 H       2.820176    -1.790108    -0.941676      26.57
 C       2.941483    -0.510165    -2.787091      82.19
 O       3.222970    -1.662422    -3.723298     255.21
 H       4.130597    -1.755962    -4.053547      26.78
 H       3.576677     0.347197    -2.885436      27.09
 H       1.741676    -0.391906    -2.779131      27.18
 C      -0.510679    -0.296261     1.028160      44.55
 H      -0.780422    -1.198636     1.392270      26.69
 C      -0.057562     2.068263     0.920724      52.34
 H      -0.519808     3.082907     0.812906      22.71
 C       1.219181     1.976121     0.337151      16.74
 O       2.101179     3.005500    -0.138113     126.50
 C       1.304569     4.386378    -0.246900      61.48
 H       2.065813     4.879327    -0.891022      23.84
 H       0.145850     4.177438    -0.614056      23.56
 H       1.130099     4.968223     0.982601      21.75
 C       1.623079     0.629467     0.148144       1.27
 O       3.005218     0.359132    -0.441017     122.75
 C       0.905402    -0.465687     0.606655      42.32
 H       1.381624    -1.474867     0.277737      24.25
 C      -0.877179     1.042515     1.405746      39.50
 C      -2.324685     1.270246     1.539341      87.93
 H      -2.777232     0.216361     1.613168      25.99
 O      -2.668664     2.174627     2.637944     264.62
 H      -2.378893     1.641552     3.389143      28.55
 C      -3.147496     1.635306     0.292153      78.62
 H      -2.524737     2.138463    -0.501814      27.34
 O      -3.353835     0.356871    -0.422503     117.62
 H      -2.530007     0.224913    -0.881674      31.37
 C      -4.621042     2.214787     0.664917      92.04
 O      -5.206600     2.497692    -0.559387     294.24
 H      -5.275307     3.469812    -0.519876      27.50
 H      -4.690565     3.008771     1.657206      23.05
 H      -5.158951     1.308253     1.080929      26.10
55
name = lig-etoh-Waterframe_948
 C       5.337964    -0.697006     1.542182      76.89
 H       5.308704     0.385352     1.205923      26.94
 C       5.045058    -3.005702     0.837205      47.49
 H       5.320012    -3.620994    -0.074168      20.84
 C       5.168427    -3.546752     2.166074      19.20
 O       5.048457    -4.831640     2.643076     181.27
 C       4.146726    -5.749950     1.852790      95.45
 H       3.181349    -5.138263     1.554312      26.28
 H       3.792617    -6.619203     2.657876      25.06
 H       4.796056    -6.298845     1.031766      26.51
 C       5.287269    -2.571745     3.184788     -18.86
 O       5.450466    -2.808498     4.556659     204.22
 H       5.344287    -3.807756     4.686187      21.24
 C       5.382552    -1.112313     2.866139      43.77
 H       5.399248    -0.487560     3.721749      23.83
 C       5.032775    -1.586308     0.559604      -4.47
 C       4.953295    -1.183044    -0.985310      71.48
 H       4.983463    -2.143163    -1.636586      23.41
 O       5.902537    -0.199261    -1.408491     201.26
 H       5.816205     0.735693    -1.220664      26.22
 C       3.261058    -0.890992    -1.233240      90.31
 H       2.739825    -1.566502    -0.642754      27.51
 C       3.000200    -0.604761    -2.685636     105.34
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 O       3.193668    -1.581231    -3.702433     284.08
 H       4.057814    -1.580223    -4.102566      29.00
 H       3.505293     0.341888    -3.015934      27.26
 H       1.891999    -0.364632    -3.043798      26.34
 C      -0.466877    -0.368216     1.121007      55.58
 H      -1.041853    -1.243217     1.399928      25.98
 C      -0.108252     2.130731     0.943840      29.09
 H      -0.630933     3.208128     0.933132      21.10
 C       1.200131     1.983714     0.360722       0.99
 O       2.008285     3.073955    -0.084640     169.84
 C       1.368020     4.402719    -0.273814     110.97
 H       1.708155     5.114940    -1.162528      25.67
 H       0.302908     4.228173    -0.686303      27.06
 H       1.384451     5.125155     0.433662      28.00
 C       1.655249     0.617288     0.088531       9.34
 O       2.981328     0.294136    -0.418893     141.56
 C       0.856980    -0.387336     0.630678      59.43
 H       1.143537    -1.405082     0.443185      26.62
 C      -0.867562     0.966571     1.333830      17.08
 C      -2.388652     1.281806     1.558670      96.92
 H      -2.722144     0.383473     1.935855      28.05
 O      -2.650634     2.143419     2.678678     284.08
 H      -2.476577     1.842210     3.580714      29.00
 C      -3.095346     1.677669     0.236654      72.57
 H      -2.717187     2.429018    -0.519885      26.85
 O      -3.309082     0.329050    -0.402663     127.74
 H      -2.497529     0.018779    -0.795178      31.92
 C      -4.613081     2.160637     0.696336      80.06
 O      -5.165466     2.575914    -0.563620     251.46
 H      -5.519574     3.483217    -0.614152      28.69
 H      -4.560678     3.317402     1.275419      21.43
 H      -4.982482     1.155993     1.040753      24.99
55
name = lig-etoh-Waterframe_949
 C       5.251227    -0.684102     1.523325      41.45
 H       5.523182     0.504197     1.334305      23.80
 C       5.146624    -2.990025     0.729853      66.07
 H       5.163815    -3.761332    -0.082709      26.45
 C       5.150632    -3.490213     2.158997     -41.66
 O       5.055649    -4.859875     2.664028     171.75
 C       4.105065    -5.743837     1.909876     113.56
 H       3.282471    -5.226517     1.147434      25.30
 H       3.749077    -6.470567     2.468014      28.11
 H       4.863559    -6.138602     1.143265      27.04
 C       5.382695    -2.510432     3.203974       8.95
 O       5.420220    -2.787870     4.583366     122.74
 H       5.563162    -3.781578     4.905715      20.04
 C       5.332833    -1.206844     2.827967      61.25
 H       5.434419    -0.395752     3.605670      22.86
 C       5.071699    -1.606521     0.430089      13.73
 C       4.881929    -1.156338    -1.012304      87.03
 H       5.175223    -1.998784    -1.783479      24.75
 O       5.953239    -0.206413    -1.289989     199.11
 H       5.575282     0.652585    -1.560736      28.66
 C       3.272421    -0.928379    -1.231007      63.14
 H       2.795038    -1.896614    -0.962778      26.53
 C       2.977737    -0.596560    -2.681719     116.11
 O       3.200109    -1.584124    -3.706215     285.80
 H       4.057752    -1.378627    -4.010273      29.54
 H       3.599740     0.336033    -2.939303      27.01
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 H       1.990745    -0.191941    -2.480068      28.42
 C      -0.383664    -0.322990     1.251782      48.31
 H      -1.211231    -1.094117     1.324493      23.94
 C      -0.093559     2.141600     0.940605      61.96
 H      -0.610347     3.150884     1.290782      24.28
 C       1.189517     2.010156     0.344901      15.64
 O       1.907678     3.145808    -0.027938     205.78
 C       1.380035     4.407244    -0.370456     109.76
 H       2.026001     4.627001    -1.360729      23.89
 H       0.364570     4.305226    -0.499984      28.32
 H       1.605881     4.978761     0.479961      26.64
 C       1.717079     0.636210     0.074917       9.12
 O       2.932786     0.325914    -0.396665     128.21
 C       0.831563    -0.481111     0.583467      44.62
 H       1.229977    -1.408239     0.608425      27.37
 C      -0.950683     0.982196     1.223617       9.54
 C      -2.377702     1.216633     1.671224      90.36
 H      -2.968523     0.330880     1.846168      28.43
 O      -2.639167     2.206287     2.695344     265.30
 H      -2.552171     1.794017     3.565354      27.96
 C      -3.153799     1.676824     0.291164      80.67
 H      -2.667138     2.537210    -0.196793      27.37
 O      -3.277761     0.349069    -0.407643     125.99
 H      -2.402464     0.106360    -0.710025      31.71
 C      -4.489837     2.138320     0.594029     110.78
 O      -5.196871     2.626649    -0.613844     284.53
 H      -5.390089     3.619145    -0.460310      25.34
 H      -4.323832     2.799136     1.542592      24.73
 H      -5.229776     1.618474     1.241614      26.29
55
name = lig-etoh-Waterframe_950
 C       5.174209    -0.721603     1.478557      38.07
 H       5.329064     0.497490     1.424399      22.13
 C       5.206582    -3.053377     0.743281      76.03
 H       4.873557    -3.800347     0.037974      23.03
 C       5.170511    -3.414704     2.133441     -14.99
 O       5.013681    -4.825413     2.638776     164.72
 C       4.175590    -5.742485     1.882728     109.97
 H       3.238188    -5.021560     1.484095      25.73
 H       3.638449    -6.337498     2.545111      27.20
 H       4.605722    -6.402594     1.147558      27.13
 C       5.415141    -2.558654     3.232805       0.32
 O       5.402542    -2.758420     4.585901     122.46
 H       5.441613    -3.816538     4.826199      19.21
 C       5.323106    -1.159526     2.798120      25.65
 H       5.539263    -0.415720     3.697693      21.26
 C       5.153129    -1.672602     0.354598      13.66
 C       4.811798    -1.200104    -0.989005      99.49
 H       5.032528    -2.041802    -1.675050      26.04
 O       5.956373    -0.162433    -1.217616     146.07
 H       5.469617     0.577875    -1.612517      27.41
 C       3.405804    -0.921102    -1.193875      75.01
 H       2.864547    -1.923942    -1.072940      25.66
 C       2.926507    -0.468298    -2.683545      98.24
 O       3.198948    -1.598009    -3.691600     268.62
 H       4.029356    -1.566974    -4.131703      28.78
 H       3.620392     0.363094    -2.887703      26.80
 H       1.882808    -0.311424    -2.737941      28.11
 C      -0.393792    -0.210146     1.273742      34.75
 H      -0.836444    -1.250723     1.562141      22.30
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 C      -0.110960     2.081649     0.949500      66.01
 H      -0.293673     3.117733     1.251852      24.34
 C       1.150706     2.003965     0.309258      20.11
 O       1.891116     3.097491     0.033723     198.65
 C       1.371116     4.403266    -0.471523      89.05
 H       2.005041     4.629508    -1.371256      24.47
 H       0.376768     4.591344    -0.541703      27.07
 H       1.803895     5.270591     0.483558      21.45
 C       1.601831     0.592906     0.167626       5.94
 O       2.942200     0.357451    -0.425549      89.14
 C       0.933881    -0.535939     0.529501      48.84
 H       1.439280    -1.467314     0.532243      24.45
 C      -0.973397     1.051261     1.215709      41.76
 C      -2.420120     1.190079     1.709409      81.34
 H      -2.825924     0.107480     1.977832      25.20
 O      -2.610065     2.279619     2.712963     279.80
 H      -2.551124     1.826223     3.565738      27.66
 C      -3.167695     1.563947     0.423539      95.77
 H      -2.477595     2.166941    -0.137911      26.17
 O      -3.227266     0.423367    -0.444312     172.74
 H      -2.330229     0.282598    -0.738077      30.04
 C      -4.516523     2.199953     0.565628     111.71
 O      -5.224566     2.684216    -0.625446     325.61
 H      -5.085603     3.729868    -0.581775      26.64
 H      -4.226342     2.961631     1.122494      26.31
 H      -5.221602     1.396330     0.946456      24.96
55
name = lig-etoh-Waterframe_951
 C       5.154752    -0.793270     1.449840      46.64
 H       4.843464     0.205212     1.016986      21.78
 C       5.184130    -3.107808     0.803389      64.73
 H       4.934371    -3.870823     0.106772      22.44
 C       5.227775    -3.488609     2.158605      10.81
 O       5.002319    -4.746373     2.573529     321.53
 C       4.168595    -5.701908     1.860839      91.96
 H       3.339528    -5.140389     1.399057      29.08
 H       3.659637    -6.324038     2.896841      22.56
 H       4.582124    -6.363443     1.162805      25.55
 C       5.372389    -2.488465     3.181842       0.98
 O       5.396508    -2.763810     4.569975     139.12
 H       5.278003    -3.808038     4.725704      19.88
 C       5.365767    -1.139069     2.809968      53.25
 H       5.412085    -0.297630     3.628297      22.55
 C       5.205487    -1.747093     0.473339      28.72
 C       4.926008    -1.263986    -0.986329      87.44
 H       4.916236    -2.022821    -1.692607      25.99
 O       5.875722    -0.136780    -1.193473     206.90
 H       5.688175     0.800206    -1.443262      24.61
 C       3.366548    -0.788908    -1.239732      81.60
 H       2.814246    -1.596651    -0.666004      23.94
 C       2.983220    -0.422761    -2.701842     107.25
 O       3.175370    -1.596444    -3.651186     279.61
 H       4.018005    -1.593776    -4.086055      28.62
 H       3.286898     0.529741    -3.106332      27.22
 H       1.940207    -0.305934    -2.945264      27.21
 C      -0.303749    -0.269222     1.155453      55.76
 H      -0.820610    -0.952339     1.927989      22.39
 C      -0.109151     2.153669     0.929031      62.02
 H      -0.438442     3.114149     1.055924      24.93
 C       1.069949     1.879926     0.302273      10.46
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 O       1.923563     3.039953     0.065331     173.07
 C       1.427336     4.405289    -0.501822      89.93
 H       1.746667     4.604617    -1.461061      26.67
 H       0.322649     4.458485    -0.757512      25.36
 H       1.825125     5.500852     0.135438      21.79
 C       1.650525     0.571889     0.141904      12.88
 O       2.951955     0.398847    -0.450135     153.30
 C       0.881467    -0.499769     0.628252      63.91
 H       1.298712    -1.555279     0.479330      22.67
 C      -0.961075     1.012286     1.338733       5.90
 C      -2.447087     1.198454     1.767640      98.21
 H      -2.561273     0.308401     2.493437      23.24
 O      -2.574895     2.308196     2.711984     288.86
 H      -2.512643     2.043568     3.648445      28.52
 C      -3.126164     1.493158     0.448760      86.79
 H      -2.511842     2.332908     0.049793      25.37
 O      -3.178532     0.446058    -0.501403     200.70
 H      -2.315567     0.265259    -0.882966      29.52
 C      -4.622903     2.280882     0.564077      95.00
 O      -5.212836     2.732272    -0.645656     299.56
 H      -5.179845     3.768942    -0.774612      27.14
 H      -4.636213     3.240300     1.170149      23.05
 H      -5.189734     1.433221     1.006810      24.79
55
name = lig-etoh-Waterframe_952
 C       5.159555    -0.804541     1.460579      46.99
 H       4.786863     0.083692     1.180165      23.61
 C       5.143701    -3.190690     0.853578      62.44
 H       5.260342    -3.911311     0.064849      19.55
 C       5.276437    -3.493034     2.172809      18.99
 O       5.028494    -4.756838     2.557190     222.17
 C       4.092990    -5.636497     1.873031      95.09
 H       3.360183    -5.346477     1.308892      32.56
 H       3.771711    -6.580139     2.765064      21.03
 H       4.833798    -6.152338     1.246721      18.88
 C       5.326648    -2.431106     3.180218      -1.79
 O       5.383240    -2.774941     4.507484     208.80
 H       5.433525    -3.784364     4.678881      22.81
 C       5.388436    -1.081202     2.801655      65.83
 H       5.221873    -0.308843     3.568180      23.21
 C       5.180227    -1.833759     0.487406      32.90
 C       4.983859    -1.216339    -0.960785      83.71
 H       5.297802    -1.947769    -1.744798      23.43
 O       5.836199    -0.151373    -1.212090     213.69
 H       5.299903     0.711752    -1.008054      24.48
 C       3.302458    -0.645315    -1.227467      65.26
 H       2.631806    -1.526580    -1.012067      25.00
 C       2.993425    -0.453421    -2.781933     104.99
 O       3.174074    -1.585892    -3.604185     286.18
 H       4.070637    -1.489152    -3.956016      27.52
 H       3.514539     0.447521    -3.154648      26.32
 H       1.883167    -0.264272    -2.479949      25.37
 C      -0.424299    -0.291468     1.201754      50.77
 H      -0.857261    -1.236189     1.667212      24.18
 C      -0.234109     2.140701     0.934594      50.86
 H      -0.643984     3.087822     0.882881      21.49
 C       1.123893     1.874548     0.277529     -17.83
 O       1.975160     3.016449     0.053654     168.10
 C       1.461804     4.341599    -0.574174      81.89
 H       1.896249     4.242577    -1.514419      25.61
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 H       0.297108     4.134274    -0.397678      23.71
 H       1.773723     5.036487     0.181799      24.69
 C       1.737522     0.561725     0.058610      18.57
 O       2.970537     0.505803    -0.462879     205.98
 C       0.942264    -0.491750     0.665894      35.48
 H       1.119529    -1.688072     0.649965      21.21
 C      -0.844398     1.010277     1.433650      29.27
 C      -2.336611     1.180444     1.938518      69.06
 H      -2.949523     0.285657     2.277091      23.57
 O      -2.550030     2.378704     2.683521     278.64
 H      -2.482120     1.978028     3.603637      25.76
 C      -3.178061     1.619209     0.441219      38.81
 H      -2.541975     2.493506     0.118964      23.84
 O      -3.142223     0.430592    -0.545958     159.15
 H      -2.270921     0.340991    -0.955392      29.74
 C      -4.683800     2.299915     0.599108      90.46
 O      -5.197446     2.739772    -0.717687     302.02
 H      -5.323094     3.734353    -0.449707      24.05
 H      -4.650410     2.964952     1.682596      22.93
 H      -5.536898     1.715936     0.984602      25.79
55
name = lig-etoh-Waterframe_953
 C       5.164634    -0.792134     1.456774      44.17
 H       5.085893     0.213855     1.340052      22.24
 C       5.165357    -3.203171     0.782128      50.88
 H       5.350365    -4.069045     0.109030      18.94
 C       5.255179    -3.427669     2.204969      -9.27
 O       5.048591    -4.824089     2.646241     234.67
 C       4.127055    -5.666005     1.860003      86.53
 H       3.232984    -5.126875     1.448490      28.28
 H       3.615649    -6.393854     2.551300      23.79
 H       4.697233    -6.236204     0.994903      19.48
 C       5.328983    -2.463361     3.188047      10.84
 O       5.372965    -2.780146     4.473144     244.73
 H       5.488290    -3.734881     4.553502      23.90
 C       5.348640    -1.042722     2.825627      54.00
 H       5.269259    -0.334475     3.558155      22.14
 C       5.093442    -1.812700     0.416051      21.86
 C       4.904095    -1.211669    -0.923402      93.35
 H       5.175607    -2.058030    -1.705920      22.37
 O       5.818831    -0.098722    -1.239624     162.77
 H       5.467447     0.695731    -0.648533      24.26
 C       3.374025    -0.682945    -1.261806      72.85
 H       2.667420    -1.466622    -1.016014      24.46
 C       2.975692    -0.409156    -2.757313      89.00
 O       3.184012    -1.596124    -3.567202     267.96
 H       4.096254    -1.612393    -3.982620      27.18
 H       3.648855     0.353986    -3.219572      24.61
 H       1.800951    -0.084922    -2.980019      24.11
 C      -0.401216    -0.338316     1.275801      41.43
 H      -1.026690    -1.197243     1.268334      23.94
 C      -0.159367     2.061385     0.857970      37.15
 H      -0.720061     3.032666     0.922245      19.83
 C       1.149094     1.982310     0.298084      12.95
 O       2.029773     2.959675     0.019388     230.84
 C       1.480355     4.124712    -0.556799     121.72
 H       1.879119     4.379403    -1.641986      25.39
 H       0.269461     4.403381    -0.663130      23.71
 H       1.854091     4.882698    -0.077877      28.28
 C       1.643857     0.593901     0.104662      -7.17
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 O       3.033496     0.614391    -0.500245     131.20
 C       0.946836    -0.504989     0.659971      47.31
 H       1.528608    -1.545557     0.632503      21.23
 C      -0.903901     0.982462     1.541452      28.31
 C      -2.297733     1.225275     1.908793      74.32
 H      -2.835343     0.336290     2.169906      24.79
 O      -2.517460     2.430788     2.707850     259.24
 H      -2.524308     2.289388     3.717080      25.87
 C      -3.252335     1.710380     0.476979      42.40
 H      -2.700890     2.431882    -0.162302      23.90
 O      -3.121419     0.465800    -0.504331     166.36
 H      -2.302183     0.647412    -0.983311      29.04
 C      -4.716174     2.181803     0.670084      93.08
 O      -5.162535     2.780402    -0.708256     256.11
 H      -5.399398     3.772716    -0.778498      27.15
 H      -4.403319     3.224964     1.152257      21.23
 H      -5.429094     1.368095     0.851973      24.96
55
name = lig-etoh-Waterframe_954
 C       5.166226    -0.770744     1.466367      46.64
 H       5.384632     0.273269     1.030653      20.92
 C       5.215275    -3.115627     0.755112      49.32
 H       5.089068    -3.975900     0.020896      20.39
 C       5.176657    -3.506417     2.143535     -19.12
 O       5.081702    -4.844708     2.722818     180.11
 C       4.145987    -5.691983     1.836647      93.59
 H       3.395384    -4.751765     1.611769      23.83
 H       3.757448    -6.289709     2.433396      29.55
 H       4.426621    -6.234859     0.828916      27.63
 C       5.344355    -2.435011     3.167746      -3.55
 O       5.373274    -2.796572     4.514180     167.26
 H       5.301668    -3.756794     4.715267      19.12
 C       5.281144    -1.112128     2.833717      75.37
 H       5.462652    -0.384605     3.522678      24.34
 C       5.004676    -1.730080     0.429710      30.15
 C       4.782047    -1.182351    -0.994441      88.87
 H       4.845399    -2.038078    -1.789909      24.82
 O       5.800904    -0.079882    -1.259175     195.20
 H       5.870419     0.849786    -0.797547      23.19
 C       3.404775    -0.730709    -1.284569      79.54
 H       2.857274    -1.421136    -0.723188      24.72
 C       3.039236    -0.347647    -2.766821      91.85
 O       3.179072    -1.646046    -3.547519     254.97
 H       4.161198    -1.616886    -3.934037      26.18
 H       3.678475     0.525843    -3.085307      24.44
 H       2.001191     0.016958    -3.025650      25.35
 C      -0.298391    -0.372460     1.306171      45.62
 H      -0.990186    -1.128622     1.398346      21.78
 C      -0.098636     2.020572     0.860953      43.80
 H      -0.511940     3.120774     1.007407      20.43
 C       1.150910     1.919976     0.350315      26.83
 O       2.064852     2.900461    -0.038748     222.07
 C       1.514718     4.068848    -0.592708      97.66
 H       1.830272     4.045174    -1.803484      23.08
 H       0.359432     3.991241    -0.606968      24.45
 H       1.977624     5.092652    -0.117025      23.19
 C       1.629230     0.674990     0.186086       4.00
 O       3.019107     0.640700    -0.519674      68.66
 C       0.925802    -0.476325     0.646990      65.16
 H       1.475221    -1.403318     0.546108      22.39
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 C      -0.880110     0.921031     1.480972      21.28
 C      -2.414705     1.361666     1.783392      85.81
 H      -2.677261     0.524382     2.387306      23.69
 O      -2.483075     2.488601     2.745897     256.80
 H      -2.437138     2.054104     3.708362      24.79
 C      -3.233137     1.660473     0.465914      94.27
 H      -2.854714     2.600699     0.008549      24.51
 O      -3.121277     0.537772    -0.379464     219.93
 H      -2.533317     0.789340    -1.107214      26.82
 C      -4.668353     2.165016     0.597088     107.98
 O      -5.135974     2.748864    -0.677987     298.53
 H      -5.140786     3.749016    -0.458163      25.55
 H      -4.923889     2.876218     1.406200      25.72
 H      -5.254266     1.388597     1.150503      26.62
55
name = lig-etoh-Waterframe_955
 C       5.175331    -0.744360     1.451680      49.27
 H       5.299719     0.473163     1.151141      21.72
 C       5.162627    -3.055528     0.781610      64.52
 H       4.963266    -3.621385    -0.164033      19.54
 C       5.161378    -3.535745     2.132928       6.14
 O       5.115315    -4.840714     2.664519     201.23
 C       4.135471    -5.628439     1.857846     108.19
 H       3.139876    -5.002020     1.384550      23.64
 H       3.748050    -6.489440     2.506527      25.49
 H       4.788071    -5.969999     1.017062      27.44
 C       5.298299    -2.571332     3.171778     -15.09
 O       5.378296    -2.772718     4.547908     170.96
 H       5.265846    -3.808899     4.755068      19.64
 C       5.256252    -1.131414     2.790867      44.02
 H       5.582091    -0.433369     3.590285      22.61
 C       4.963082    -1.667592     0.461798       9.91
 C       4.765325    -1.081202    -1.033205      98.10
 H       5.067322    -1.815729    -1.746192      25.11
 O       5.824009    -0.150770    -1.338876     185.00
 H       5.330241     0.782540    -1.082682      24.59
 C       3.282076    -0.634121    -1.238129      82.52
 H       2.642597    -1.526984    -1.040675      24.76
 C       3.116042    -0.374136    -2.764796     107.08
 O       3.180248    -1.647109    -3.534569     258.70
 H       4.183120    -1.698704    -3.965469      23.78
 H       3.915181     0.319582    -3.064481      25.14
 H       2.180086    -0.051464    -2.651572      28.87
 C      -0.297812    -0.356869     1.318670      47.72
 H      -0.597119    -1.296835     1.803295      21.27
 C      -0.136356     2.049400     0.985608      63.59
 H      -0.490717     3.150071     1.079563      21.56
 C       1.217033     1.886501     0.388414       4.47
 O       2.096052     2.847754    -0.067568     194.41
 C       1.521168     4.064535    -0.718447      91.11
 H       1.848702     3.951228    -1.797631      23.75
 H       0.576065     4.015106    -0.501280      28.14
 H       1.877430     5.086951     0.003305      22.00
 C       1.801447     0.579960     0.192943      25.30
 O       2.932598     0.591174    -0.509286     210.89
 C       0.979724    -0.461839     0.625707      61.47
 H       1.162758    -1.426291     0.479159      24.60
 C      -0.844576     0.963588     1.288200      28.34
 C      -2.468091     1.438104     1.755671      78.01
 H      -3.083981     0.566245     2.235637      23.69
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 O      -2.446474     2.538006     2.757744     255.32
 H      -2.354950     1.877852     3.556105      24.12
 C      -3.169603     1.729783     0.508264      95.55
 H      -2.502795     2.517616     0.105142      25.62
 O      -3.125397     0.565532    -0.295900     179.90
 H      -2.726652     0.676914    -1.163694      29.01
 C      -4.680548     2.142198     0.620229      98.41
 O      -5.117268     2.692687    -0.600471     320.73
 H      -5.106113     3.716511    -0.545376      26.74
 H      -4.771918     2.683229     1.470102      27.65
 H      -5.370741     1.189661     0.588646      24.53
55
name = lig-etoh-Waterframe_956
 C       5.173423    -0.668577     1.507365      40.59
 H       4.999889     0.542639     1.474758      21.02
 C       5.006575    -2.995786     0.763924      47.99
 H       5.045370    -3.818310     0.022655      20.20
 C       5.191537    -3.496678     2.164279      -1.23
 O       5.091100    -4.826442     2.538579     210.08
 C       4.168061    -5.606670     1.844835     108.00
 H       3.180251    -5.159674     1.532366      26.66
 H       3.816623    -6.693865     2.546180      22.88
 H       4.699124    -6.027423     1.049624      24.99
 C       5.225888    -2.562131     3.184039       8.23
 O       5.372506    -2.755274     4.538267     164.85
 H       5.518800    -3.780381     4.860465      18.11
 C       5.305155    -1.223728     2.779356      40.88
 H       5.390753    -0.444907     3.688980      22.52
 C       4.982206    -1.620421     0.424776      23.11
 C       4.798170    -1.104845    -0.955643      97.30
 H       4.781580    -1.966471    -1.563198      24.72
 O       5.801708    -0.167696    -1.415768     165.22
 H       5.497006     0.873108    -1.570155      22.38
 C       3.245155    -0.602129    -1.246202      85.54
 H       2.450959    -1.431345    -1.133160      24.88
 C       3.160326    -0.422357    -2.742589     101.48
 O       3.158737    -1.622446    -3.510506     280.30
 H       4.123602    -1.652236    -3.934031      24.07
 H       3.877613     0.234197    -3.250071      24.64
 H       2.204403     0.113741    -3.058732      26.71
 C      -0.256796    -0.274210     1.263639      34.54
 H      -0.602559    -1.123438     2.000100      22.56
 C       0.018223     2.158217     1.001172      42.15
 H      -0.590660     3.036089     1.169839      24.12
 C       1.254764     1.867290     0.452205      17.25
 O       2.122833     2.852502    -0.090903     194.65
 C       1.520125     4.025938    -0.775244     113.77
 H       1.747778     4.212355    -1.722531      28.53
 H       0.457875     4.196653    -0.798123      27.43
 H       2.085445     5.010828    -0.368193      24.77
 C       1.799173     0.525057     0.251948      16.50
 O       2.922154     0.491656    -0.543419     205.23
 C       1.010148    -0.555324     0.651708      67.90
 H       1.258364    -1.551990     0.436110      25.20
 C      -1.003225     0.959682     1.249552       2.82
 C      -2.395749     1.399597     1.834957      87.55
 H      -3.063630     0.483189     2.084070      25.62
 O      -2.407655     2.528334     2.731481     256.21
 H      -2.385833     2.375333     3.747239      26.18
 C      -3.130512     1.904042     0.513958      70.87
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 H      -2.638269     2.598554    -0.174592      26.66
 O      -3.131590     0.516687    -0.276817     109.13
 H      -2.554046     0.670017    -1.045048      29.76
 C      -4.667889     2.063135     0.667345      90.48
 O      -5.125466     2.710676    -0.557023     322.61
 H      -5.213987     3.679959    -0.724286      27.08
 H      -4.840109     2.755134     1.535942      25.54
 H      -5.023912     0.993743     0.571252      24.32
55
name = lig-etoh-Waterframe_957
 C       5.128766    -0.668990     1.576943      47.31
 H       4.971901     0.398280     1.409839      22.50
 C       4.890410    -2.985246     0.806260      41.09
 H       4.952079    -3.784911     0.081473      21.04
 C       5.152051    -3.416287     2.090843      13.84
 O       5.085378    -4.790143     2.452538     120.50
 C       4.172392    -5.720322     1.752162     105.49
 H       3.395204    -5.137003     1.673000      29.77
 H       4.046677    -6.493723     2.729436      23.18
 H       4.316089    -6.164350     0.812983      26.59
 C       5.221450    -2.511755     3.213905       3.08
 O       5.371294    -2.749493     4.540443     192.66
 H       5.386731    -3.797249     4.756021      19.49
 C       5.349470    -1.196988     2.829542      59.58
 H       5.183870    -0.484208     3.790164      22.81
 C       5.038025    -1.540006     0.484392      36.88
 C       4.719827    -1.182677    -0.936962      89.24
 H       4.752155    -2.116118    -1.563153      23.37
 O       5.787326    -0.199363    -1.508406     127.57
 H       5.553385     0.867882    -1.402327      21.39
 C       3.311081    -0.731964    -1.313259      77.10
 H       2.712362    -1.558915    -0.846888      24.65
 C       3.134268    -0.353575    -2.827998      82.04
 O       3.120480    -1.649115    -3.492814     322.31
 H       4.025551    -1.667801    -3.857071      27.58
 H       4.050567     0.268555    -3.005876      21.50
 H       2.154519     0.256784    -3.244562      24.70
 C      -0.297598    -0.209179     1.249257      41.52
 H      -1.062816    -1.052067     1.597938      22.38
 C       0.010017     2.122654     1.000586      24.81
 H      -0.079357     3.188845     1.033722      23.70
 C       1.321186     1.889726     0.479023       7.08
 O       2.118023     2.895456    -0.130136     184.73
 C       1.573943     4.032519    -0.816437     106.15
 H       1.917401     3.821071    -1.836279      25.20
 H       0.287735     4.121138    -0.749847      24.27
 H       1.953381     4.831663    -0.349408      28.09
 C       1.691353     0.520257     0.299118       1.32
 O       2.926190     0.486930    -0.536465     127.67
 C       1.002957    -0.620504     0.703827      64.97
 H       1.499676    -1.675535     0.667526      23.01
 C      -0.906368     1.046235     1.313107      34.57
 C      -2.300893     1.375776     1.829895      88.77
 H      -2.699341     0.513879     2.399329      24.73
 O      -2.363258     2.536276     2.698874     247.76
 H      -2.382566     2.141602     3.669098      25.72
 C      -3.126974     1.904612     0.503647      72.11
 H      -2.833593     2.795646    -0.075294      24.68
 O      -3.123189     0.517167    -0.288878     138.61
 H      -2.295287     0.481650    -0.813916      29.60
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 C      -4.594296     2.089934     0.677875     101.66
 O      -5.174012     2.721072    -0.560250     275.62
 H      -5.220099     3.605598    -0.186421      27.63
 H      -5.240693     2.467086     1.653748      23.54
 H      -4.955417     1.143119     0.997315      26.21
55
name = lig-etoh-Waterframe_958
 C       5.098137    -0.648762     1.596630      48.57
 H       5.121298     0.300859     1.367973      23.31
 C       4.867693    -2.907135     0.801940      60.64
 H       4.652204    -3.482559    -0.059707      23.65
 C       5.046797    -3.409433     2.103536      15.36
 O       5.135944    -4.766397     2.359479     241.69
 C       4.123949    -5.783929     1.723134     108.36
 H       3.167803    -5.358800     1.653804      28.94
 H       4.033563    -6.632219     2.338446      25.56
 H       4.521472    -6.194511     0.684633      24.68
 C       5.289053    -2.487694     3.187598       1.15
 O       5.362856    -2.784935     4.556299     161.48
 H       5.312143    -3.777689     4.772178      19.71
 C       5.317405    -1.058371     2.964189      31.55
 H       5.382647    -0.299045     3.806901      24.19
 C       5.008748    -1.580345     0.550531      40.94
 C       4.723251    -1.193476    -1.012793      87.13
 H       5.163107    -2.089787    -1.547674      22.67
 O       5.741149    -0.266063    -1.574170     143.20
 H       5.510088     0.483192    -0.994507      27.77
 C       3.288526    -0.800674    -1.300331      62.17
 H       2.696173    -1.711132    -1.175791      24.16
 C       3.104696    -0.320260    -2.870738      87.58
 O       3.077710    -1.680658    -3.513854     290.05
 H       3.946645    -1.695185    -3.907083      28.96
 H       4.041522     0.220435    -3.083044      22.23
 H       2.099899     0.263715    -2.733490      25.77
 C      -0.396398    -0.276301     1.236184      39.86
 H      -1.168880    -1.075210     1.168967      23.33
 C       0.078936     2.170971     0.959761      45.87
 H      -0.234548     3.204333     1.091216      21.31
 C       1.316553     1.892140     0.458432      18.43
 O       2.120240     2.879060    -0.104231     178.26
 C       1.609318     4.031035    -0.870091      99.06
 H       1.944952     3.798236    -2.012795      23.76
 H       0.322352     3.923692    -0.722402      24.99
 H       1.884194     4.949105    -0.508340      27.97
 C       1.760205     0.524211     0.216661       4.81
 O       2.899400     0.486993    -0.477066     122.55
 C       0.911545    -0.551231     0.806485      42.13
 H       1.321153    -1.699873     0.972369      22.36
 C      -0.696327     1.150380     1.421476      34.09
 C      -2.218879     1.450646     1.753713      88.81
 H      -2.591714     0.568382     2.213609      26.09
 O      -2.304836     2.542362     2.701077     282.49
 H      -2.289963     2.007494     3.562974      25.52
 C      -3.118004     1.726401     0.548412      89.52
 H      -2.472439     2.560403     0.157445      26.02
 O      -3.103002     0.592763    -0.325077     187.06
 H      -2.189811     0.375415    -0.588005      31.23
 C      -4.649688     2.074160     0.716370      93.27
 O      -5.217772     2.712701    -0.482663     264.93
 H      -5.458085     3.652694    -0.345225      27.89
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 H      -4.619823     2.946341     1.586530      22.66
 H      -5.147426     1.099755     0.633692      24.49
55
name = lig-etoh-Waterframe_959
 C       5.123404    -0.577295     1.652505      47.80
 H       5.227166     0.428245     1.413385      25.11
 C       4.856823    -2.907568     0.788603      38.56
 H       4.488130    -3.591530     0.033916      18.95
 C       4.956654    -3.407201     2.151474      -4.81
 O       5.143826    -4.815038     2.281904     206.54
 C       4.114751    -5.792717     1.698867     112.70
 H       2.956018    -5.547163     1.467290      25.00
 H       4.185774    -6.635428     2.192453      25.98
 H       4.800040    -5.952118     0.679113      23.87
 C       5.331588    -2.425893     3.214222     -13.64
 O       5.358028    -2.839801     4.551763     161.09
 H       5.558370    -3.770349     4.700295      24.11
 C       5.253421    -0.986386     2.991812      55.33
 H       5.552049    -0.368603     3.765332      21.75
 C       4.906050    -1.516210     0.501833      25.93
 C       4.849290    -1.238094    -1.005265      94.38
 H       4.809267    -2.248027    -1.560128      24.21
 O       5.654436    -0.286399    -1.566754     222.93
 H       5.875277     0.516463    -1.145000      28.97
 C       3.245192    -0.781660    -1.337045      76.31
 H       2.404315    -1.456241    -1.221248      25.27
 C       3.079297    -0.396241    -2.746806     102.69
 O       3.011344    -1.659140    -3.564085     283.13
 H       3.915175    -1.614735    -3.964168      27.35
 H       3.625007     0.298862    -3.376056      24.90
 H       2.120962     0.069971    -2.966740      27.56
 C      -0.452681    -0.234601     1.207768      52.03
 H      -1.128565    -1.015474     1.357979      24.40
 C       0.166189     2.294643     0.982595      31.03
 H      -0.454638     3.125971     1.135748      23.25
 C       1.350253     1.877387     0.334685      22.82
 O       2.190077     2.885508    -0.072816     188.20
 C       1.586096     3.946705    -0.911130     105.89
 H       1.872570     4.072828    -2.067287      24.80
 H       0.522122     4.039832    -1.018766      27.06
 H       2.002844     5.045266    -0.584987      25.40
 C       1.730716     0.522048     0.231085      14.74
 O       2.941866     0.384719    -0.454556     154.25
 C       0.900261    -0.444639     0.856363      54.36
 H       1.179068    -1.594028     0.731851      22.77
 C      -0.709318     1.101282     1.494929       8.88
 C      -2.130354     1.457647     1.764711      93.76
 H      -2.544452     0.524548     2.154429      25.98
 O      -2.251474     2.548033     2.720501     287.38
 H      -2.276630     2.279649     3.660796      27.50
 C      -3.075758     1.628744     0.552105      85.22
 H      -2.705247     2.522943    -0.100882      26.37
 O      -3.078192     0.624891    -0.398702     181.73
 H      -2.129502     0.412523    -0.529656      31.18
 C      -4.642951     2.109066     0.730983      97.80
 O      -5.264057     2.706771    -0.406939     312.70
 H      -5.372287     3.643773    -0.598972      28.83
 H      -4.525009     2.695767     1.637105      26.12
 H      -5.379592     1.250431     1.049555      24.99
55
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name = lig-etoh-Waterframe_960
 C       5.145895    -0.530598     1.594917      46.78
 H       5.213124     0.646510     1.486135      23.22
 C       4.796614    -2.914243     0.865493      40.70
 H       4.706967    -3.743771     0.111474      18.93
 C       4.946928    -3.351483     2.144545       4.71
 O       5.085545    -4.831862     2.279287     189.68
 C       4.216537    -5.783556     1.612320      86.80
 H       3.055183    -5.246259     1.620370      23.03
 H       4.315584    -6.680010     2.341084      22.90
 H       4.380296    -6.084207     0.464238      23.98
 C       5.258561    -2.442075     3.245519      -1.82
 O       5.386886    -2.872385     4.538447     160.52
 H       5.654118    -3.771436     4.517306      26.07
 C       5.235630    -1.044744     2.948121      56.47
 H       5.468364    -0.436903     3.696785      23.13
 C       4.858903    -1.439307     0.536813      22.39
 C       4.748340    -1.261707    -0.934515      85.88
 H       5.001442    -2.176283    -1.566089      24.27
 O       5.653011    -0.274911    -1.591008     160.80
 H       5.633427     0.543281    -1.107819      29.88
 C       3.235482    -0.755362    -1.289112      90.17
 H       2.602610    -1.602368    -0.945594      25.52
 C       2.945794    -0.445948    -2.781472      98.49
 O       2.966424    -1.623071    -3.615749     284.41
 H       3.924020    -1.689946    -3.985002      26.60
 H       3.747187     0.323390    -3.049395      23.88
 H       1.947674    -0.176015    -2.829361      29.08
 C      -0.405562    -0.147666     1.227614      57.30
 H      -0.959710    -0.876592     1.695388      25.03
 C       0.119559     2.190605     1.086791      55.11
 H      -0.005067     3.286114     1.017537      24.90
 C       1.327896     1.954259     0.272919     -17.30
 O       2.282103     2.933952    -0.121282     196.12
 C       1.600383     3.937808    -0.980191     102.38
 H       2.134896     3.573274    -1.868103      24.28
 H       0.642829     3.887552    -0.902592      28.20
 H       1.968245     4.904639    -0.255584      21.25
 C       1.710098     0.538282     0.252894      -1.05
 O       2.998280     0.281070    -0.424710     175.37
 C       0.924463    -0.461663     0.787118      62.75
 H       1.279660    -1.431740     0.514374      24.20
 C      -0.748511     1.196534     1.421808      42.70
 C      -2.145819     1.387897     1.897997      80.28
 H      -2.566320     0.527450     2.515940      24.24
 O      -2.211237     2.586801     2.724952     276.45
 H      -2.309600     2.134823     3.576091      27.22
 C      -3.112043     1.759348     0.465601      62.24
 H      -2.839943     2.724076    -0.014856      27.11
 O      -3.039419     0.568763    -0.495126     135.05
 H      -2.135476     0.303750    -0.779805      30.35
 C      -4.590441     2.133897     0.836454      99.74
 O      -5.309916     2.686701    -0.372474     318.22
 H      -4.950538     3.547817    -0.241825      29.83
 H      -4.677809     2.845857     1.568442      27.47
 H      -5.185619     1.318860     1.366767      25.52
55
name = lig-etoh-Waterframe_961
 C       5.132216    -0.552624     1.560333      41.55
 H       5.158518     0.678412     1.371699      20.45
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 C       4.734822    -2.801688     0.906729      67.42
 H       4.915120    -3.474779     0.009118      20.89
 C       4.981407    -3.401508     2.155656       8.51
 O       5.059577    -4.770034     2.329063     221.63
 C       4.255288    -5.728671     1.539078     104.74
 H       3.181731    -5.372073     1.763014      26.63
 H       4.144872    -6.830899     2.196037      22.92
 H       4.445833    -6.013715     0.577337      26.36
 C       5.122610    -2.489449     3.219426      13.18
 O       5.443500    -2.892140     4.524197     216.24
 H       5.405301    -3.852834     4.649786      23.18
 C       5.259954    -1.118219     2.872084      44.65
 H       5.270179    -0.436906     3.703189      24.27
 C       4.859559    -1.506099     0.607507      32.29
 C       4.621691    -1.184302    -0.957278      76.78
 H       4.961761    -2.131310    -1.295694      22.66
 O       5.664986    -0.251679    -1.577255     184.75
 H       5.339232     0.568457    -1.301678      29.79
 C       3.225157    -0.903456    -1.200213      68.33
 H       2.785344    -1.893975    -0.940317      23.75
 C       2.797604    -0.469840    -2.801008      96.22
 O       2.947726    -1.604685    -3.679288     255.04
 H       3.989437    -1.593436    -3.959122      23.42
 H       3.571961     0.323932    -2.969373      24.06
 H       1.821157    -0.021583    -2.673325      27.35
 C      -0.265577    -0.118422     1.289130      33.75
 H      -0.892589    -0.874079     1.780099      23.93
 C       0.191926     2.204595     1.046511      55.91
 H      -0.022038     3.323912     1.404327      23.10
 C       1.341647     1.923712     0.344976      20.60
 O       2.295065     2.911368    -0.136439     212.75
 C       1.713098     3.931019    -0.985495      99.16
 H       1.953467     3.934626    -2.047273      26.02
 H       0.560363     3.670428    -1.011831      26.14
 H       1.827441     5.122869    -0.896862      23.86
 C       1.794557     0.624224     0.166603      13.82
 O       2.993741     0.299743    -0.327587     141.57
 C       0.915633    -0.509794     0.649402      50.69
 H       1.183552    -1.467813     0.686618      24.87
 C      -0.832057     1.224427     1.352256      18.05
 C      -2.240628     1.447786     1.935350      79.56
 H      -2.632417     0.485919     2.445929      24.57
 O      -2.192282     2.609039     2.757530     276.32
 H      -2.311985     2.373868     3.686980      27.89
 C      -3.133629     1.835677     0.448791      52.35
 H      -2.437232     2.556876     0.133487      26.89
 O      -3.044003     0.597105    -0.549590     134.40
 H      -2.101742     0.520558    -0.841715      31.59
 C      -4.551543     2.126265     0.933218     101.24
 O      -5.320531     2.653641    -0.286817     297.21
 H      -5.073425     3.572259    -0.493115      28.86
 H      -4.397780     3.092831     1.516427      23.25
 H      -5.010323     1.173367     1.147484      24.72
55
name = lig-etoh-Waterframe_962
 C       5.104324    -0.607055     1.619177      49.23
 H       5.180690     0.550684     1.310263      20.72
 C       4.735039    -2.847612     0.887231      51.63
 H       4.639580    -3.504264    -0.025082      21.14
 C       4.963293    -3.439501     2.132988      12.93
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 O       5.070549    -4.759547     2.398499     240.36
 C       4.195165    -5.664129     1.547914     124.21
 H       3.231450    -5.482065     1.374472      30.36
 H       4.526816    -6.736095     2.015689      24.00
 H       4.707288    -5.592620     0.711911      27.48
 C       5.064121    -2.550920     3.213610      -5.62
 O       5.487849    -2.899509     4.501148     231.54
 H       5.122896    -3.780375     4.772372      23.91
 C       5.257087    -1.131126     2.853028      49.21
 H       5.260209    -0.448890     3.823836      23.10
 C       4.851084    -1.451950     0.527193      33.08
 C       4.701838    -1.157403    -0.951147      99.45
 H       4.712056    -2.077972    -1.527983      22.60
 O       5.608292    -0.235562    -1.514924     254.49
 H       5.509060     0.686130    -1.596600      25.99
 C       3.143945    -0.999851    -1.214228      57.45
 H       2.428271    -1.731615    -0.765816      23.47
 C       2.727844    -0.506076    -2.664284      94.33
 O       2.931866    -1.574571    -3.732431     240.02
 H       3.941234    -1.388469    -4.071967      22.59
 H       3.217168     0.319170    -3.165680      24.13
 H       1.617748    -0.160145    -2.897298      24.70
 C      -0.222979    -0.101517     1.327014      49.26
 H      -0.821914    -1.057469     1.632108      23.50
 C       0.162953     2.284896     1.007829      17.33
 H      -0.163119     3.303192     1.496159      22.63
 C       1.455580     1.927152     0.403631       1.34
 O       2.297201     2.898870    -0.127880     183.03
 C       1.746851     3.947620    -1.072578      70.89
 H       2.166161     3.776590    -2.068255      25.21
 H       0.437810     3.834073    -1.212107      24.06
 H       1.909149     4.862410    -0.604922      25.66
 C       1.755687     0.525441     0.115699      19.86
 O       3.023081     0.329930    -0.284074     105.52
 C       0.934883    -0.434860     0.534052      67.36
 H       1.234822    -1.417275     0.737405      25.38
 C      -0.788238     1.160087     1.335503       5.35
 C      -2.266831     1.532938     1.831701      91.23
 H      -2.739219     0.625383     2.283599      26.09
 O      -2.204607     2.656763     2.802716     250.44
 H      -2.310039     2.321887     3.711173      27.22
 C      -3.053486     1.769434     0.532874      85.83
 H      -2.542367     2.619518    -0.009114      26.42
 O      -3.074442     0.750211    -0.526290     192.22
 H      -2.133174     0.805418    -0.819742      31.48
 C      -4.479313     2.206032     0.835543     106.19
 O      -5.340092     2.607709    -0.182916     302.97
 H      -5.351338     3.455645    -0.611191      28.50
 H      -4.428911     2.654961     2.066576      22.95
 H      -4.991904     1.360492     1.272296      26.06
55
name = lig-etoh-Waterframe_963
 C       5.078211    -0.617642     1.588154      34.15
 H       5.251157     0.443535     1.622835      24.21
 C       4.754040    -2.931165     0.760375      57.89
 H       4.352948    -3.687551     0.112658      16.71
 C       4.903703    -3.400031     2.112798      -1.92
 O       5.016841    -4.815108     2.483621     298.85
 C       4.260980    -5.606774     1.539678     164.88
 H       3.218482    -5.422071     1.421020      27.98
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 H       4.337553    -6.671256     1.764465      26.89
 H       4.783375    -5.431637     0.525981      29.40
 C       5.132189    -2.510633     3.218694      15.12
 O       5.492125    -2.900534     4.474394     171.17
 H       5.214266    -3.862973     4.717578      24.15
 C       5.191406    -1.188591     2.978377      22.20
 H       5.552753    -0.385889     3.832405      18.57
 C       4.857587    -1.505848     0.489923      23.81
 C       4.704239    -1.219525    -0.981415      79.51
 H       5.140805    -2.060705    -1.633001      21.16
 O       5.583453    -0.226331    -1.490101     191.89
 H       5.272498     0.735049    -1.236619      25.30
 C       3.103544    -0.861367    -1.224746      83.46
 H       2.495434    -1.656820    -0.755497      23.79
 C       2.660357    -0.565888    -2.619757      87.13
 O       2.922117    -1.533662    -3.737218     256.78
 H       3.861435    -1.478665    -4.215100      24.27
 H       3.144705     0.429837    -2.707544      24.40
 H       1.468287    -0.670724    -2.497934      25.22
 C      -0.263292    -0.156647     1.253243      63.67
 H      -0.907694    -1.052140     1.671156      23.64
 C       0.130191     2.242724     0.975685      38.65
 H      -0.108095     3.311131     0.953598      22.84
 C       1.424702     1.987244     0.435672      -0.99
 O       2.311147     2.896975    -0.123466     192.76
 C       1.764077     3.942039    -1.127850      85.41
 H       2.468870     3.670205    -1.847000      26.21
 H       0.547801     3.894771    -1.268598      25.66
 H       2.066748     4.679984    -0.554826      26.18
 C       1.753086     0.590311     0.114518     -12.13
 O       3.057490     0.299320    -0.350054     145.25
 C       0.870065    -0.440939     0.573610      57.83
 H       1.377668    -1.495927     0.438298      22.13
 C      -0.683025     1.207069     1.386702      42.77
 C      -2.157797     1.535817     1.750658      96.11
 H      -2.657442     0.768822     2.281400      26.89
 O      -2.236554     2.691329     2.810710     244.69
 H      -2.300428     2.047348     3.505157      27.03
 C      -2.999551     1.868075     0.543143      97.86
 H      -2.736353     2.888844     0.077124      25.82
 O      -3.080383     0.904109    -0.463100     208.86
 H      -2.276381     0.754430    -1.020990      29.62
 C      -4.441187     2.189942     0.878111      89.80
 O      -5.400956     2.580038    -0.125662     276.01
 H      -5.174962     3.508205    -0.263061      29.00
 H      -4.584063     3.127046     1.647330      23.30
 H      -4.913000     1.197430     1.145408      25.62
55
name = lig-etoh-Waterframe_964
 C       5.070875    -0.695731     1.641083      58.84
 H       5.197165     0.273697     1.433413      25.54
 C       4.748565    -3.000448     0.750708      59.75
 H       4.439393    -3.568413    -0.091877      18.18
 C       4.877969    -3.405004     2.116871       6.02
 O       4.921068    -4.808397     2.547970     215.74
 C       4.335389    -5.603533     1.488673     115.58
 H       3.236090    -5.211880     1.723645      23.95
 H       4.291198    -6.551001     1.732992      27.05
 H       4.630791    -5.609244     0.258355      24.41
 C       5.227528    -2.526333     3.204307     -18.14
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 O       5.482022    -2.937303     4.487006     180.03
 H       5.455343    -3.989611     4.532792      24.10
 C       5.136918    -1.105534     2.946809      45.11
 H       5.531353    -0.506664     3.902839      19.46
 C       4.879801    -1.634989     0.519613      19.86
 C       4.665514    -1.277524    -1.059975      77.72
 H       4.961044    -2.326081    -1.444318      22.85
 O       5.570444    -0.152755    -1.482712     215.09
 H       5.292960     0.547765    -0.769550      25.55
 C       3.230511    -0.836974    -1.182889      98.71
 H       2.775970    -1.750125    -0.811733      22.98
 C       2.587883    -0.612409    -2.632994      94.41
 O       2.907814    -1.488748    -3.700348     278.97
 H       3.874681    -1.337621    -3.918667      26.79
 H       2.655003     0.491829    -2.896262      24.79
 H       1.485177    -0.636547    -2.464047      25.68
 C      -0.377926    -0.182229     1.186854      22.96
 H      -1.104456    -0.906662     1.658429      21.92
 C       0.172953     2.253685     0.908213      61.91
 H      -0.290541     3.134226     0.664895      23.21
 C       1.396636     1.965204     0.367588      29.78
 O       2.297867     2.900858    -0.106537     246.92
 C       1.862057     3.901864    -1.085559     107.80
 H       2.304288     3.924075    -2.137981      25.34
 H       0.908287     3.795485    -1.440363      29.42
 H       2.021977     5.139374    -0.906954      22.97
 C       1.775099     0.682289     0.186490      10.72
 O       3.009170     0.317129    -0.440483     168.71
 C       0.918047    -0.462293     0.607541      33.34
 H       1.005132    -1.678098     0.277927      18.53
 C      -0.656887     1.226569     1.453729      21.03
 C      -2.024257     1.563528     1.775843      82.51
 H      -2.416809     0.612419     2.113143      25.66
 O      -2.259353     2.648683     2.771008     263.88
 H      -2.293331     2.364249     3.706678      27.77
 C      -2.990695     2.138782     0.487529      67.27
 H      -2.375246     3.024523     0.182001      24.62
 O      -3.078779     0.978542    -0.450942     185.37
 H      -2.290141     0.884151    -1.051323      28.80
 C      -4.514067     2.160721     1.005428      93.90
 O      -5.437383     2.580818    -0.116035     301.61
 H      -5.279724     3.527963    -0.337891      28.77
 H      -4.380042     2.885253     1.639405      27.47
 H      -4.735248     1.147651     1.498896      25.69
55
name = lig-etoh-Waterframe_965
 C       5.057687    -0.756110     1.560650      50.22
 H       5.048458     0.221625     1.191870      22.03
 C       4.735523    -3.048234     0.837379      74.70
 H       4.748299    -3.722465     0.002585      22.84
 C       4.916296    -3.486332     2.173909      16.86
 O       4.868854    -4.755556     2.539119     265.78
 C       4.270320    -5.657723     1.508662      96.82
 H       3.059837    -5.426784     1.151577      20.35
 H       4.477744    -6.623612     1.926372      24.11
 H       4.966583    -5.369852     0.461203      22.50
 C       5.253307    -2.526711     3.160198      -3.86
 O       5.482968    -2.989716     4.490001     159.81
 H       5.401687    -4.057151     4.586095      23.11
 C       5.164528    -1.124943     2.954829      61.76
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 H       5.141070    -0.320294     3.694863      20.90
 C       4.902572    -1.690436     0.531838      41.30
 C       4.733096    -1.255686    -1.002143      93.29
 H       4.712720    -2.010053    -1.858184      20.13
 O       5.543539    -0.157513    -1.465126     261.46
 H       5.645045     0.702070    -0.865787      23.32
 C       3.274619    -0.943418    -1.230172      65.80
 H       2.674337    -1.685390    -0.723675      19.78
 C       2.484919    -0.572210    -2.619129      97.71
 O       2.916942    -1.468429    -3.650025     268.02
 H       3.842069    -1.361097    -3.898797      28.31
 H       2.588482     0.376110    -3.153749      22.86
 H       1.511288    -0.847599    -2.473999      25.91
 C      -0.386064    -0.107807     1.160157      60.28
 H      -1.065040    -0.891602     1.314865      23.14
 C       0.153680     2.275940     0.860665      53.98
 H      -0.294153     3.230566     0.818819      21.67
 C       1.422732     1.983394     0.261781     -15.97
 O       2.320690     2.972023    -0.123103     232.25
 C       1.944919     3.903010    -1.117948      63.47
 H       2.601926     3.590146    -2.077094      20.57
 H       0.953230     3.669924    -1.287333      28.14
 H       1.829732     5.122673    -0.561692      17.99
 C       1.805925     0.473764     0.246431       7.96
 O       2.946362     0.430017    -0.481879     135.45
 C       0.881252    -0.430153     0.630684      62.39
 H       1.162940    -1.539193     0.247656      19.61
 C      -0.615440     1.218274     1.419788      40.08
 C      -2.066077     1.628606     1.833876      72.65
 H      -2.638635     0.656608     2.012214      23.99
 O      -2.258244     2.613065     2.741434     288.66
 H      -2.219924     2.336534     3.687619      27.13
 C      -2.968308     2.206745     0.523365      68.75
 H      -2.672981     3.123494    -0.030300      24.91
 O      -3.058603     1.071701    -0.478236     189.45
 H      -2.196199     1.102876    -0.969698      27.75
 C      -4.507188     2.272898     1.052923      80.80
 O      -5.454526     2.539011    -0.056464     281.25
 H      -5.344619     3.458450    -0.431777      27.73
 H      -4.609307     2.824248     2.091072      24.29
 H      -4.857282     1.271678     1.488504      25.17
55
name = lig-etoh-Waterframe_966
 C       5.045035    -0.763476     1.463262      45.93
 H       4.914047     0.377624     1.373889      19.80
 C       4.768419    -3.089826     0.897434      72.79
 H       4.798651    -3.948634     0.221047      21.41
 C       4.974309    -3.462835     2.176580       9.39
 O       4.775013    -4.795133     2.530941     289.34
 C       4.262768    -5.696600     1.527075     113.00
 H       3.189349    -5.676682     1.119492      25.69
 H       4.448636    -6.807003     1.952052      22.85
 H       5.085898    -5.816011     0.799839      23.05
 C       5.238824    -2.542462     3.252250      10.49
 O       5.491907    -3.021181     4.469051     241.52
 H       5.132254    -4.004337     4.636017      24.93
 C       5.201932    -1.171041     2.876136      50.44
 H       4.984653    -0.502222     3.568575      22.53
 C       4.924634    -1.736678     0.460373      33.55
 C       4.769447    -1.196094    -0.951935     101.17
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 H       5.238643    -1.942673    -1.601182      20.35
 O       5.581328    -0.189537    -1.472628     232.29
 H       5.468747     0.794840    -1.027075      22.29
 C       3.149440    -0.883903    -1.245200      65.29
 H       2.599327    -1.714140    -0.754975      21.95
 C       2.470119    -0.583377    -2.598852      96.88
 O       2.926352    -1.522237    -3.634471     275.30
 H       3.814925    -1.388321    -3.949491      27.92
 H       2.628411     0.520087    -2.617005      23.42
 H       1.444029    -0.818779    -2.381982      25.84
 C      -0.341710    -0.068837     1.152504      43.87
 H      -1.075255    -0.791114     1.172599      22.52
 C       0.193993     2.292940     0.811284      49.10
 H       0.035512     3.362501     1.124016      20.72
 C       1.403754     1.936750     0.257904      -5.55
 O       2.386718     2.973273    -0.094437     196.39
 C       1.943353     3.903382    -1.165508      84.72
 H       2.806752     3.937690    -1.932064      22.16
 H       0.806033     3.728253    -1.530011      23.93
 H       2.214381     4.895372    -0.673001      21.65
 C       1.825198     0.536775     0.237335      -0.49
 O       2.941499     0.444713    -0.530739     130.06
 C       0.867946    -0.492239     0.610091      66.66
 H       1.056677    -1.533477     0.560586      22.32
 C      -0.715079     1.294680     1.344951      31.61
 C      -2.174473     1.646765     1.725416      88.44
 H      -2.812404     0.798887     2.188053      23.11
 O      -2.237645     2.656521     2.814365     278.48
 H      -2.163374     2.029491     3.576565      26.61
 C      -3.029325     2.139442     0.603608     102.91
 H      -2.843947     3.109382     0.157002      25.34
 O      -3.026886     1.202745    -0.498084     225.66
 H      -2.153294     1.135604    -0.957793      27.39
 C      -4.473636     2.369104     1.066588      83.51
 O      -5.459717     2.508962     0.031543     278.77
 H      -5.274973     3.433493    -0.352496      27.14
 H      -4.939062     3.239391     1.956585      21.10
 H      -4.700555     1.325808     1.152661      25.40
55
name = lig-etoh-Waterframe_967
 C       5.041465    -0.789446     1.502382      49.69
 H       4.912811     0.385846     1.245410      20.71
 C       4.856548    -3.086373     0.817223      64.91
 H       4.554492    -3.864453     0.064513      16.77
 C       4.994668    -3.462187     2.215724      13.97
 O       4.663333    -4.855217     2.565169     271.17
 C       4.350452    -5.842913     1.539034      95.46
 H       3.479082    -5.474307     1.228767      32.73
 H       4.025244    -6.773170     2.288508      22.51
 H       4.879725    -6.025254     0.748770      30.78
 C       5.206739    -2.569745     3.243873      -1.48
 O       5.496501    -3.030191     4.522717     280.31
 H       5.202521    -4.032563     4.569407      31.54
 C       5.209515    -1.213325     2.776715      71.92
 H       5.183982    -0.562973     3.595914      23.85
 C       4.933875    -1.700151     0.428972      26.20
 C       4.730636    -1.244456    -1.023827      85.73
 H       4.975910    -2.217990    -1.402719      22.39
 O       5.670660    -0.149626    -1.466486     225.11
 H       5.115529     0.773177    -1.286439      21.70
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 C       3.103407    -0.832921    -1.185324      84.89
 H       2.622775    -1.688602    -0.643860      20.89
 C       2.527269    -0.636948    -2.561937      92.67
 O       2.893713    -1.563844    -3.618559     262.67
 H       3.847036    -1.448760    -3.833228      26.50
 H       2.699039     0.462755    -2.908484      24.00
 H       1.347031    -0.615966    -2.609135      24.06
 C      -0.369079    -0.029699     1.136125      13.81
 H      -1.131094    -0.753065     1.447787      21.90
 C       0.191770     2.315332     0.862980      27.65
 H       0.207708     3.475491     1.083224      22.56
 C       1.439117     1.943101     0.308671      23.16
 O       2.397629     2.890964    -0.067193     194.27
 C       2.022896     3.950109    -1.166141      92.49
 H       2.595027     3.899072    -2.046421      25.86
 H       0.954890     3.852687    -1.837615      24.37
 H       1.976193     4.844083    -0.858272      27.03
 C       1.778257     0.639846     0.154768       7.16
 O       2.974810     0.377714    -0.562133     162.41
 C       0.933314    -0.493620     0.595860      49.08
 H       1.063658    -1.441575     0.675657      21.90
 C      -0.824993     1.371811     1.204500      -0.55
 C      -2.245384     1.662184     1.695938      84.49
 H      -2.497830     0.644892     2.062026      22.98
 O      -2.194578     2.686589     2.900946     227.19
 H      -2.263182     2.192911     3.785913      24.81
 C      -3.098681     2.209697     0.593436      98.06
 H      -2.427380     3.119328     0.509399      23.72
 O      -3.036649     1.306242    -0.517936     221.96
 H      -2.110322     1.257529    -0.857765      29.15
 C      -4.549717     2.314167     1.076745     100.65
 O      -5.466518     2.543529     0.052562     313.85
 H      -5.417110     3.467533    -0.386903      27.83
 H      -4.209890     3.224301     1.857857      22.15
 H      -4.759653     1.506954     1.819137      25.92
55
name = lig-etoh-Waterframe_968
 C       5.036569    -0.788045     1.487170      45.71
 H       5.115864     0.378428     1.250137      21.59
 C       4.940287    -3.049099     0.751874      64.27
 H       4.563092    -3.701096    -0.077241      19.11
 C       4.928961    -3.608052     2.112333      -2.44
 O       4.636609    -4.859437     2.613899     220.83
 C       4.318179    -5.946933     1.601500      96.05
 H       3.502753    -5.522492     1.008152      28.21
 H       3.978420    -6.903831     2.209954      24.60
 H       5.178202    -6.220196     0.801521      27.82
 C       5.208725    -2.615792     3.185568      -6.50
 O       5.477134    -3.003111     4.569556     137.60
 H       5.584648    -3.983179     4.728165      20.38
 C       5.213654    -1.249824     2.864738      46.98
 H       5.558827    -0.406794     3.579382      21.90
 C       4.931463    -1.679120     0.443780      34.16
 C       4.658226    -1.306991    -1.092879      85.18
 H       4.611035    -1.995333    -2.016439      22.08
 O       5.702366    -0.165666    -1.450621     142.95
 H       5.219270     0.805564    -1.595214      22.69
 C       3.195035    -0.912575    -1.148987      83.04
 H       2.591460    -1.655062    -0.587827      22.54
 C       2.569511    -0.634829    -2.632948      90.77
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 O       2.843535    -1.627907    -3.582755     250.63
 H       3.831685    -1.686484    -3.932769      24.17
 H       3.049219     0.210336    -3.131517      24.13
 H       1.365821    -0.679789    -2.471720      23.86
 C      -0.389692     0.035898     1.075528      46.62
 H      -0.902718    -0.779365     1.704602      21.62
 C       0.185631     2.373503     0.933130      55.84
 H      -0.199266     3.481550     0.927947      21.80
 C       1.437440     2.030287     0.362826      -9.49
 O       2.395463     2.874721    -0.108358     189.94
 C       2.082767     3.949015    -1.179597      72.10
 H       2.872512     3.721668    -1.815914      24.53
 H       1.066022     3.424117    -1.318321      24.99
 H       1.880583     4.990064    -0.679079      22.40
 C       1.752270     0.541709     0.041056       0.64
 O       2.986278     0.385311    -0.512078     155.11
 C       0.887443    -0.327797     0.641582      66.73
 H       1.312647    -1.348216     0.594280      22.18
 C      -0.816604     1.377737     1.079171      27.87
 C      -2.191465     1.649200     1.827066      72.69
 H      -2.668087     0.714064     2.090929      23.92
 O      -2.150187     2.670636     2.931636     256.87
 H      -2.456336     2.218547     3.803528      25.02
 C      -3.116411     2.265797     0.592335      76.02
 H      -2.824154     3.387186     0.241933      21.93
 O      -3.062434     1.402024    -0.557554     205.18
 H      -2.129744     1.332356    -0.878058      28.02
 C      -4.524973     2.342084     1.141743     111.60
 O      -5.527248     2.579662     0.056152     309.35
 H      -5.241197     3.555168    -0.197841      27.55
 H      -4.476215     3.181595     1.655259      27.39
 H      -5.148574     1.759135     1.903558      25.14
55
name = lig-etoh-Waterframe_969
 C       5.070284    -0.763002     1.532480      38.29
 H       5.248646     0.314805     1.387703      24.06
 C       4.944124    -3.130918     0.735202      78.22
 H       4.937271    -3.806530    -0.139378      24.84
 C       4.877958    -3.621176     2.027706       5.28
 O       4.633217    -4.913779     2.596807     135.48
 C       4.270975    -5.985881     1.644695     111.48
 H       3.470620    -5.920026     0.718421      23.51
 H       3.990378    -6.830319     2.196342      27.35
 H       5.489850    -6.286820     1.412285      23.68
 C       5.229015    -2.716401     3.180879     -15.46
 O       5.451644    -2.935059     4.530989     153.76
 H       5.495308    -3.875259     4.767610      20.79
 C       5.238099    -1.266631     2.871311      24.94
 H       5.648777    -0.556080     3.822184      20.62
 C       4.947899    -1.720920     0.383556      13.61
 C       4.651710    -1.261090    -1.098344      83.79
 H       5.007106    -2.093448    -1.891951      22.54
 O       5.680522    -0.253424    -1.451095     159.66
 H       5.354963     0.774533    -1.585865      24.17
 C       3.225763    -0.920711    -1.203699      83.06
 H       2.697758    -1.790762    -0.809947      26.22
 C       2.674023    -0.637147    -2.658242     105.85
 O       2.784657    -1.789292    -3.573507     251.87
 H       3.664786    -1.588552    -4.183606      22.55
 H       3.012052     0.363941    -2.797240      27.66
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 H       1.575391    -0.379974    -2.469278      27.23
 C      -0.403649     0.066586     1.054240      47.10
 H      -1.042716    -0.748477     1.598762      22.57
 C       0.163438     2.443849     0.898291      50.10
 H      -0.244135     3.454983     0.996330      22.64
 C       1.422431     2.020444     0.339713       9.90
 O       2.449833     2.906911    -0.120874     236.55
 C       2.067446     3.831621    -1.100077      95.95
 H       2.929918     4.006410    -1.829587      24.85
 H       1.183785     3.686844    -1.761340      26.98
 H       2.210585     5.085516    -0.603132      21.65
 C       1.706378     0.698565     0.032627      21.22
 O       2.996030     0.386111    -0.445728     126.42
 C       0.869728    -0.251542     0.634375      45.09
 H       1.144246    -1.482589     0.757521      22.47
 C      -0.799853     1.366233     1.146303      23.47
 C      -2.125104     1.724929     1.844971      89.06
 H      -2.704709     0.909554     2.229252      24.55
 O      -2.098275     2.614919     2.932577     279.64
 H      -2.491209     2.100028     3.733248      25.73
 C      -3.118332     2.266675     0.661137      87.39
 H      -3.062884     3.288765     0.265102      23.32
 O      -3.103522     1.481082    -0.584144     227.32
 H      -2.204333     1.361733    -0.965347      28.75
 C      -4.612910     2.476762     1.191453      86.72
 O      -5.573047     2.632282     0.081400     291.22
 H      -5.314101     3.504832    -0.484800      26.67
 H      -4.810070     3.380573     1.784020      25.10
 H      -4.832753     1.371174     1.524090      24.67
55
name = lig-etoh-Waterframe_970
 C       5.136976    -0.832581     1.552270      70.52
 H       5.159712     0.160434     1.379947      26.99
 C       4.909969    -3.195510     0.659695      51.65
 H       5.137260    -4.011195    -0.016087      19.41
 C       4.885435    -3.581076     2.141424     -13.57
 O       4.586232    -4.958766     2.512316     163.99
 C       4.333981    -6.081787     1.722019     128.11
 H       3.667796    -5.691354     0.743177      21.56
 H       3.829203    -6.659588     2.350891      28.27
 H       5.196306    -6.582210     1.015559      25.30
 C       5.212492    -2.683221     3.110996      36.18
 O       5.423096    -2.906285     4.460221     202.20
 H       5.084956    -3.750928     4.752164      24.30
 C       5.298258    -1.366373     2.806240      53.59
 H       5.337440    -0.695924     3.823025      22.39
 C       4.976385    -1.744356     0.439204      -9.11
 C       4.801306    -1.241848    -1.015383      91.67
 H       4.896567    -2.291850    -1.376325      22.50
 O       5.666889    -0.324133    -1.484081     219.49
 H       5.293184     0.653131    -1.196945      24.77
 C       3.169207    -0.879603    -1.278448      76.58
 H       2.664087    -1.739680    -0.864567      27.58
 C       2.736483    -0.615703    -2.627573     107.21
 O       2.735919    -1.869678    -3.557155     224.21
 H       3.564130    -1.767391    -4.232241      23.62
 H       3.294657     0.188024    -3.221792      25.76
 H       1.737129    -0.423499    -2.666446      29.14
 C      -0.426278     0.046672     1.088578      26.66
 H      -1.244542    -0.731503     1.218043      22.41
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 C       0.122241     2.436614     0.814113      65.93
 H       0.122578     3.436214     1.035868      21.74
 C       1.397573     2.129174     0.260655      14.20
 O       2.482015     2.899917    -0.086330     239.03
 C       2.113930     3.871237    -1.093355      89.32
 H       2.962207     3.921695    -1.919556      24.10
 H       1.286503     3.730821    -1.661674      29.36
 H       1.765093     4.869396    -0.470188      21.09
 C       1.713390     0.757066     0.105330       5.28
 O       2.998707     0.353174    -0.406676     132.49
 C       0.855011    -0.268106     0.577560      37.30
 H       1.210339    -1.504485     0.679818      22.23
 C      -0.760794     1.483385     1.310044      28.05
 C      -2.165227     1.782235     1.744969      89.82
 H      -2.400480     0.710159     2.042607      23.93
 O      -2.030776     2.601901     2.957471     266.84
 H      -2.282440     2.078078     3.825432      25.92
 C      -3.137807     2.381575     0.713640      84.46
 H      -2.465397     3.218341     0.610269      25.41
 O      -3.179988     1.529434    -0.557888     231.92
 H      -2.262618     1.476591    -0.909868      30.11
 C      -4.718107     2.507184     1.149914      90.20
 O      -5.622642     2.682473     0.100287     282.79
 H      -5.237439     3.476664    -0.482226      26.62
 H      -4.680927     3.076286     2.314421      23.50
 H      -4.862887     1.484035     1.578034      25.44
55
name = lig-etoh-Waterframe_971
 C       5.200116    -0.914566     1.490931      65.40
 H       5.057958     0.078123     1.335593      25.98
 C       4.895504    -3.190552     0.764769      86.01
 H       4.925478    -3.877819    -0.079002      25.65
 C       4.889807    -3.665595     2.053851      11.43
 O       4.597168    -4.933033     2.499809     211.72
 C       4.347733    -6.149505     1.653966     131.06
 H       3.563759    -5.783730     1.025016      25.47
 H       3.676633    -6.821388     2.282919      26.23
 H       5.116110    -6.746366     1.356256      30.18
 C       5.181860    -2.691722     3.121272       3.81
 O       5.378650    -2.915686     4.418425     214.11
 H       4.997424    -3.768123     4.726699      23.47
 C       5.352487    -1.343049     2.778682      55.71
 H       5.271901    -0.604050     3.571558      22.17
 C       5.002070    -1.814691     0.507753      62.27
 C       4.783800    -1.373333    -0.887436      90.44
 H       4.891918    -2.054381    -1.708320      25.89
 O       5.685994    -0.318512    -1.532816     122.44
 H       5.581328     0.569537    -0.964422      24.81
 C       3.235414    -0.866955    -1.192605      75.11
 H       2.518445    -1.630198    -0.848844      26.24
 C       2.752384    -0.605170    -2.773136      96.19
 O       2.700810    -1.873965    -3.508638     262.37
 H       3.619994    -1.922180    -3.973778      25.34
 H       3.583528    -0.095270    -3.374800      24.01
 H       1.801346    -0.191528    -2.753617      28.89
 C      -0.434938     0.126027     1.108909      48.95
 H      -1.166608    -0.649983     1.125620      23.84
 C       0.174469     2.511573     0.760577      55.80
 H      -0.007088     3.519320     1.033328      21.68
 C       1.399408     2.107474     0.201987       0.67
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 O       2.485995     2.921005    -0.060989     198.48
 C       2.123062     3.994339    -1.107584      94.70
 H       3.130928     4.121526    -1.628832      23.20
 H       1.335999     3.363469    -1.436718      26.80
 H       1.910837     4.852711    -0.724155      26.37
 C       1.756255     0.652007     0.172872       0.23
 O       2.983118     0.338552    -0.390216     159.73
 C       0.799677    -0.287683     0.543476      58.67
 H       1.211768    -1.285377     0.267470      23.74
 C      -0.718574     1.483332     1.344687      27.16
 C      -2.210133     1.721463     1.755490      68.86
 H      -2.738218     0.679805     1.975410      23.44
 O      -1.987655     2.622529     2.989222     238.25
 H      -2.125649     1.992778     3.813469      25.88
 C      -3.151060     2.500147     0.716118      77.92
 H      -2.685308     3.548476     0.432551      23.52
 O      -3.243232     1.605682    -0.468677     227.03
 H      -2.349066     1.573231    -0.881328      29.75
 C      -4.669983     2.416754     1.181105      84.78
 O      -5.669758     2.765046     0.120757     267.32
 H      -5.278275     3.601640    -0.223140      29.58
 H      -4.930659     3.335297     2.010386      23.73
 H      -5.098113     1.513616     1.458932      26.65
55
name = lig-etoh-Waterframe_972
 C       5.249811    -0.888058     1.438297      47.56
 H       5.165110     0.189946     1.167179      22.05
 C       4.886524    -3.226999     0.782728      59.75
 H       4.469418    -3.777783    -0.061433      21.69
 C       4.918764    -3.730159     2.066446      43.76
 O       4.637888    -4.983521     2.524438     244.95
 C       4.255266    -6.152175     1.608177     117.23
 H       3.745685    -6.089373     0.718072      28.97
 H       3.798090    -6.950473     2.457338      22.59
 H       5.201902    -6.508944     1.402888      27.86
 C       5.164186    -2.714978     3.087655      13.86
 O       5.314868    -2.946586     4.445234     146.71
 H       5.349694    -4.059334     4.694749      16.12
 C       5.368753    -1.290362     2.806763      38.41
 H       5.475520    -0.627653     3.508951      21.28
 C       5.039661    -1.904204     0.448397      46.24
 C       4.674738    -1.425360    -0.950761      92.79
 H       4.905658    -2.226190    -1.663063      26.38
 O       5.688885    -0.311062    -1.517046      74.90
 H       5.868694     0.567960    -1.006233      25.16
 C       3.279551    -0.869832    -1.112861      73.12
 H       2.600315    -1.723754    -0.852182      23.82
 C       2.851456    -0.608252    -2.853019      91.24
 O       2.689796    -1.847890    -3.455677     295.58
 H       3.525782    -1.937230    -3.966435      26.03
 H       3.604394     0.171081    -3.143141      24.72
 H       1.971576     0.103079    -2.848189      26.44
 C      -0.412248     0.151637     1.088405      47.61
 H      -1.151021    -0.497077     1.428311      22.85
 C       0.214421     2.532953     0.793077      37.52
 H      -0.181158     3.601582     0.750030      21.22
 C       1.459641     1.987932     0.236484      -8.95
 O       2.485293     2.993415    -0.052946     196.84
 C       2.163441     4.040125    -1.065716      98.08
 H       3.023917     4.287861    -1.704077      24.30
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 H       1.404654     3.687695    -2.137724      22.82
 H       1.815942     5.014680    -0.727887      25.40
 C       1.768756     0.619379     0.182825      26.84
 O       2.996393     0.347696    -0.383474     161.05
 C       0.780659    -0.310066     0.497854      70.16
 H       0.667053    -1.237688     0.268907      24.52
 C      -0.753917     1.481228     1.238035      14.04
 C      -2.182467     1.767337     1.827571      78.70
 H      -2.898430     0.973029     2.122352      22.87
 O      -1.990145     2.610411     3.003056     252.58
 H      -2.153897     2.055536     3.872273      25.29
 C      -3.189470     2.500303     0.732735      97.96
 H      -3.237092     3.543067     0.460694      22.54
 O      -3.263803     1.689851    -0.387526     253.79
 H      -2.427231     1.624437    -0.893792      28.58
 C      -4.669785     2.432028     1.209638      90.34
 O      -5.680417     2.843675     0.146898     294.13
 H      -5.391837     3.642210    -0.271362      32.20
 H      -4.778013     3.109685     1.993621      27.31
 H      -4.817325     1.401930     1.535310      27.35
55
name = lig-etoh-Waterframe_973
 C       5.292430    -0.890191     1.419089      52.64
 H       5.528673     0.214002     1.043877      21.85
 C       4.832733    -3.317152     0.681849      43.91
 H       4.293770    -4.071433     0.093497      15.77
 C       4.951769    -3.706319     2.170154      -2.65
 O       4.630446    -5.087203     2.519689     216.68
 C       4.260280    -6.140378     1.618550      86.52
 H       3.686847    -5.948425     0.673764      27.52
 H       3.668432    -6.988891     2.352103      22.53
 H       5.333356    -6.493642     1.148666      25.17
 C       5.200299    -2.680966     3.107042      -3.67
 O       5.260785    -2.976535     4.470213     147.11
 H       5.242810    -4.054138     4.638748      22.41
 C       5.348699    -1.314970     2.749319      57.57
 H       5.634139    -0.807456     3.599039      23.41
 C       5.066038    -1.853554     0.379905      20.26
 C       4.683330    -1.361212    -1.058924      95.91
 H       4.669921    -2.320344    -1.606164      23.74
 O       5.673548    -0.357416    -1.495956     151.18
 H       5.485794     0.436097    -0.869768      26.09
 C       3.215969    -0.881567    -1.182191      79.83
 H       2.573689    -1.686696    -0.752972      24.05
 C       2.980287    -0.499324    -2.688848      92.87
 O       2.724324    -1.793972    -3.458267     273.94
 H       3.432473    -1.922651    -4.065679      27.98
 H       3.854572    -0.121994    -3.241215      25.94
 H       1.859026    -0.112871    -2.883372      24.38
 C      -0.431555     0.146899     1.076774      29.64
 H      -1.032341    -0.587483     1.572161      21.57
 C       0.210860     2.405046     0.814037      65.86
 H       0.129797     3.531632     0.500629      19.79
 C       1.482559     2.058031     0.348648      -7.08
 O       2.456298     3.038657    -0.089496     205.51
 C       2.215404     4.074717    -1.081542      73.83
 H       3.216039     4.361348    -1.344595      22.91
 H       1.394447     3.751260    -2.077787      22.17
 H       1.524521     4.927690    -0.372700      18.88
 C       1.793731     0.603593     0.122250      -6.53
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 O       3.058158     0.344067    -0.381877     137.46
 C       0.727047    -0.365025     0.467871      54.03
 H       0.676775    -1.421393     0.274236      22.41
 C      -0.819109     1.568568     1.115785      31.31
 C      -2.166519     1.925456     1.864432      84.70
 H      -2.358367     0.892411     2.109500      22.57
 O      -2.001197     2.623424     3.038453     275.82
 H      -2.333058     2.069448     3.854560      24.78
 C      -3.259021     2.490735     0.834298      96.92
 H      -2.603248     3.429865     0.788982      22.36
 O      -3.253058     1.713005    -0.397598     246.52
 H      -2.359681     1.745435    -0.804019      28.70
 C      -4.708739     2.492184     1.249958      98.46
 O      -5.662669     2.866288     0.219702     318.13
 H      -5.150902     3.559765    -0.223326      30.67
 H      -4.708954     2.891621     2.226304      27.28
 H      -4.964414     1.359264     1.513798      24.43
55
name = lig-etoh-Waterframe_974
 C       5.357287    -0.959045     1.356313      47.11
 H       5.776967     0.154817     1.263363      22.12
 C       4.790566    -3.294946     0.758596      61.23
 H       4.571513    -4.040311    -0.048081      21.18
 C       4.922319    -3.705151     2.041280      12.55
 O       4.621406    -5.097232     2.543880     206.20
 C       4.321282    -6.119737     1.567305      97.71
 H       3.422887    -5.557802     1.096039      24.17
 H       3.759350    -6.895325     2.079985      24.91
 H       5.173704    -6.903833     1.051869      23.53
 C       5.223587    -2.715197     3.161093      -0.02
 O       5.218492    -2.952392     4.479016     114.66
 H       5.095126    -3.849791     4.675684      23.67
 C       5.358699    -1.380563     2.706328      48.02
 H       5.680876    -0.599621     3.566206      22.29
 C       5.005430    -1.893265     0.323601      38.86
 C       4.730414    -1.366843    -1.078719      98.07
 H       4.820110    -2.053971    -1.976765      22.57
 O       5.615235    -0.401690    -1.470180     196.74
 H       5.300472     0.501451    -1.164796      24.67
 C       3.201625    -0.861011    -1.244391      89.44
 H       2.447662    -1.607585    -0.980688      25.51
 C       3.014723    -0.493987    -2.580107      98.29
 O       2.763492    -1.721645    -3.470231     246.94
 H       3.632844    -1.774401    -3.918904      25.42
 H       3.889958     0.082067    -2.931298      26.24
 H       2.176637     0.396821    -2.669651      24.77
 C      -0.503956     0.180378     1.061700      28.21
 H      -1.179501    -0.643592     1.435606      21.63
 C       0.251669     2.413956     0.733648      53.39
 H      -0.017521     3.541701     0.920198      20.32
 C       1.555448     2.048609     0.381098      23.93
 O       2.435334     2.987212    -0.102466     218.01
 C       2.197960     4.112963    -1.021368      94.06
 H       3.125059     4.594721    -1.134251      26.21
 H       1.812227     3.628863    -1.809605      29.28
 H       1.572470     5.146804    -0.535343      22.61
 C       1.758972     0.648454     0.082467      -9.86
 O       3.098637     0.328193    -0.383342     130.76
 C       0.731743    -0.331791     0.429552      39.10
 H       1.226015    -1.444688     0.369021      20.58
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 C      -0.860604     1.544918     1.075773      27.47
 C      -2.167150     1.882494     1.842011      88.13
 H      -2.409955     0.864340     2.173027      22.66
 O      -2.006873     2.706675     3.117111     248.37
 H      -2.423300     2.075370     3.812092      25.13
 C      -3.209429     2.501183     0.939837      83.41
 H      -2.895251     3.608936     0.577626      22.31
 O      -3.217830     1.734155    -0.422657     191.76
 H      -2.275431     1.793208    -0.694395      28.58
 C      -4.748281     2.476574     1.349125      75.22
 O      -5.604496     2.919058     0.313197     275.42
 H      -5.192774     3.656876    -0.222335      28.91
 H      -5.034579     3.172676     2.459870      23.33
 H      -5.127042     1.371462     1.378326      23.59
55
name = lig-etoh-Waterframe_975
 C       5.424855    -1.083087     1.312979      45.54
 H       5.639475    -0.016720     0.997486      23.03
 C       4.756042    -3.213326     0.733238      77.50
 H       4.830426    -3.924002    -0.126404      23.66
 C       4.882134    -3.750867     2.086232      26.34
 O       4.675842    -5.032004     2.541613     214.44
 C       4.264947    -6.099983     1.554322     117.60
 H       3.579553    -5.739147     0.634383      24.38
 H       3.897848    -6.730874     2.163652      27.26
 H       5.155939    -6.286261     0.849036      25.61
 C       5.182766    -2.781425     3.066439      15.23
 O       5.183251    -2.915180     4.509497     156.07
 H       5.217409    -3.937567     4.745889      20.30
 C       5.428229    -1.454578     2.686100      42.99
 H       5.516063    -0.420107     3.389505      21.76
 C       4.952563    -1.946047     0.342028      41.81
 C       4.677502    -1.476718    -1.080535      74.79
 H       4.929659    -2.336673    -1.785105      22.50
 O       5.600312    -0.333925    -1.456648     130.55
 H       5.436986     0.584335    -1.370010      25.83
 C       3.253848    -0.894620    -1.146157      80.73
 H       2.554474    -1.694846    -0.977618      25.33
 C       2.999683    -0.402170    -2.678146     102.74
 O       2.818200    -1.572059    -3.465644     282.37
 H       3.752765    -1.789828    -3.855921      23.96
 H       3.916383     0.103933    -2.880387      25.18
 H       2.161169     0.299677    -2.697827      26.53
 C      -0.501300     0.115557     0.955215      32.93
 H      -1.409366    -0.546282     1.231367      19.88
 C       0.196320     2.498987     0.715760      66.05
 H       0.059570     3.517927     1.110575      19.03
 C       1.525646     2.036718     0.290749       8.53
 O       2.506942     2.934623    -0.068766     201.04
 C       2.175852     4.158894    -0.916899     104.64
 H       3.154724     4.566636    -1.212968      24.82
 H       1.946717     3.834376    -1.923213      27.89
 H       1.331680     4.763678    -0.665195      28.22
 C       1.756788     0.673763     0.072179      28.54
 O       3.063095     0.312772    -0.367519     170.92
 C       0.787520    -0.186653     0.435184      54.71
 H       0.993584    -1.406770     0.660484      20.47
 C      -0.782285     1.487972     1.109232      21.75
 C      -2.155227     1.806071     1.874466      79.85
 H      -2.879546     1.056058     2.218489      21.58
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 O      -2.013696     2.767128     3.130641     247.69
 H      -2.199670     2.260700     3.976439      26.89
 C      -3.216900     2.525621     0.924549      81.77
 H      -3.298673     3.611590     0.779670      21.71
 O      -3.175925     1.782028    -0.383877     226.90
 H      -2.257417     1.701727    -0.716927      28.06
 C      -4.752314     2.433304     1.448270      80.51
 O      -5.562950     3.000513     0.359877     252.98
 H      -5.196222     3.900854     0.024716      28.61
 H      -4.972777     3.208031     2.448352      24.56
 H      -4.960218     1.432210     1.800804      27.39
55
name = lig-etoh-Waterframe_976
 C       5.467357    -1.107153     1.313118      84.64
 H       5.562345    -0.145685     0.949315      26.02
 C       4.732539    -3.341744     0.698451      58.56
 H       4.562817    -4.123033    -0.070017      20.86
 C       4.841413    -3.721441     2.110440      18.91
 O       4.705383    -5.009693     2.480125     215.96
 C       4.260359    -5.993217     1.506707     134.40
 H       3.361499    -5.805131     0.822469      25.14
 H       4.039164    -6.931297     2.094173      25.71
 H       5.161178    -6.187298     1.135606      28.94
 C       5.140465    -2.767574     3.097426       5.60
 O       5.152480    -2.912262     4.482473     166.60
 H       5.233822    -3.983917     4.816668      18.78
 C       5.504619    -1.481228     2.599459      52.02
 H       5.557181    -0.856685     3.621615      21.05
 C       4.953652    -1.943742     0.353312      28.26
 C       4.657811    -1.463066    -1.019381      97.41
 H       4.657512    -2.365856    -1.647472      24.14
 O       5.632689    -0.316434    -1.469649     136.94
 H       5.210235     0.412710    -1.080768      28.46
 C       3.229978    -0.923760    -1.170881      69.38
 H       2.565769    -1.679251    -0.742497      22.90
 C       3.003790    -0.312010    -2.686756     103.78
 O       2.868065    -1.447980    -3.503902     278.68
 H       3.730540    -1.647246    -4.094232      24.21
 H       3.824715     0.240566    -3.154185      25.03
 H       2.091023     0.043676    -2.823378      27.65
 C      -0.494431     0.136216     0.823188      46.60
 H      -1.125722    -0.819740     0.993173      21.09
 C       0.160660     2.496708     0.781634      61.85
 H       0.098666     3.511087     0.936358      21.24
 C       1.382123     2.121567     0.157276      -0.87
 O       2.595473     2.943884    -0.051843     173.52
 C       2.182286     4.110280    -0.851744      87.81
 H       3.090443     4.887786    -0.658517      22.82
 H       1.792713     3.798988    -2.123803      21.94
 H       1.453418     4.481654    -0.332528      27.17
 C       1.812776     0.703523     0.062580       1.79
 O       3.025640     0.292559    -0.314488     154.36
 C       0.772199    -0.217445     0.514242      42.68
 H       1.040963    -1.367222     0.347336      20.85
 C      -0.747583     1.479508     1.215026      32.87
 C      -2.185886     1.885717     1.939736      68.19
 H      -2.467478     0.768422     2.240009      22.16
 O      -2.003536     2.785770     3.068452     296.33
 H      -1.994537     2.215301     3.851023      28.11
 C      -3.265739     2.530506     0.909155      90.94
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 H      -2.778958     3.475722     0.896517      26.14
 O      -3.163872     1.845428    -0.317198     247.76
 H      -2.220147     1.743797    -0.563829      28.67
 C      -4.685123     2.453485     1.504165     111.83
 O      -5.553079     3.047739     0.419698     255.47
 H      -4.981634     3.883297     0.311170      29.92
 H      -4.534679     2.953203     2.339192      30.20
 H      -5.147681     1.542120     1.694052      28.46
55
name = lig-etoh-Waterframe_977
 C       5.475355    -1.029731     1.283712      26.33
 H       5.744607    -0.049762     1.220125      21.78
 C       4.724375    -3.428794     0.707108      69.81
 H       4.220464    -4.124289     0.062457      17.81
 C       4.797035    -3.671011     2.029477      11.56
 O       4.680293    -5.037565     2.469103     200.45
 C       4.310006    -5.943490     1.487058     114.63
 H       3.381885    -5.582067     1.157722      29.39
 H       4.042657    -7.044597     2.108557      24.05
 H       5.059262    -6.301877     0.690202      28.36
 C       5.124163    -2.722812     3.121449      27.12
 O       5.136661    -2.937902     4.447813     157.81
 H       4.782927    -3.961742     4.710341      18.79
 C       5.565258    -1.520407     2.701817      43.39
 H       6.010102    -0.792859     3.348474      23.24
 C       4.974436    -2.063701     0.348033      17.41
 C       4.669427    -1.381876    -1.006873     125.15
 H       4.727300    -2.040170    -1.851926      26.33
 O       5.615187    -0.379079    -1.459340     174.64
 H       5.429762     0.431053    -0.948898      26.73
 C       3.186931    -0.832286    -1.242291      74.22
 H       2.408708    -1.655407    -1.114085      23.99
 C       2.982429    -0.299760    -2.633992      99.51
 O       2.899466    -1.421822    -3.623884     266.46
 H       3.826618    -1.413359    -4.133912      23.07
 H       3.617817     0.650721    -2.798067      23.99
 H       1.979693     0.292625    -2.567332      25.74
 C      -0.515096     0.172209     0.795605      15.53
 H      -1.262750    -0.638347     0.945186      21.67
 C       0.186620     2.475334     0.846609      43.06
 H      -0.173198     3.451563     0.912999      22.38
 C       1.407729     2.101100     0.069557       8.93
 O       2.591146     2.947704    -0.061424     166.97
 C       2.219214     4.102600    -0.727163     102.92
 H       2.864113     5.083157    -0.673103      24.38
 H       1.958951     3.767319    -2.002284      22.63
 H       1.277836     4.524294    -0.201295      23.31
 C       1.707170     0.736556     0.107485       2.69
 O       3.045212     0.287376    -0.255484     142.77
 C       0.875967    -0.288916     0.467113      50.75
 H       1.030203    -1.272787     0.191663      21.64
 C      -0.821075     1.542030     1.282758      16.42
 C      -2.154995     1.885811     1.958406      96.64
 H      -2.389291     0.876149     2.491245      21.88
 O      -1.987141     2.784139     2.996977     312.17
 H      -2.013077     2.253067     3.791002      28.18
 C      -3.181609     2.468341     0.993659      88.45
 H      -2.825985     3.558881     0.807287      23.43
 O      -3.172154     1.885558    -0.301252     248.69
 H      -2.200154     1.819303    -0.439080      28.80
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 C      -4.612014     2.513217     1.470758     100.82
 O      -5.524504     3.113438     0.544926     277.99
 H      -5.209324     3.920712    -0.046450      28.39
 H      -4.588298     2.997306     2.465725      26.55
 H      -5.000170     1.467487     1.494185      25.75
55
name = lig-etoh-Waterframe_978
 C       5.456370    -1.134610     1.364373      59.61
 H       5.821404    -0.153776     1.013398      23.55
 C       4.692849    -3.349800     0.665806      51.20
 H       4.229599    -3.993472    -0.053937      21.63
 C       4.779794    -3.724448     2.101860      13.53
 O       4.695616    -5.018588     2.512138     212.86
 C       4.302306    -5.996876     1.457201      98.75
 H       3.333113    -5.713915     1.108505      28.07
 H       4.095099    -6.993303     2.206644      23.20
 H       4.773117    -5.872893     0.340437      25.14
 C       5.109500    -2.751892     3.057740     -10.26
 O       5.101330    -3.003186     4.449119     144.04
 H       4.646562    -3.938279     4.693614      20.39
 C       5.649519    -1.409319     2.679280      75.89
 H       6.246490    -0.870589     3.281947      25.55
 C       5.020827    -2.003959     0.322531      29.55
 C       4.640730    -1.366671    -1.093490      96.15
 H       4.846171    -2.158531    -1.836869      22.92
 O       5.609140    -0.412405    -1.418840     200.37
 H       5.740417     0.473059    -1.108685      26.17
 C       3.195340    -0.752626    -1.230990      78.02
 H       2.475722    -1.621397    -1.190801      25.86
 C       2.897987    -0.240661    -2.616169      84.08
 O       2.924149    -1.335431    -3.713355     257.82
 H       3.821189    -1.571297    -4.176141      22.53
 H       3.794962     0.474843    -2.846961      24.08
 H       1.712828     0.176730    -2.567003      25.67
 C      -0.488293     0.169893     0.879193      60.15
 H      -1.360071    -0.366826     0.939201      24.63
 C       0.214429     2.479735     0.859394      53.47
 H      -0.048081     3.571150     0.999496      24.62
 C       1.447588     2.082168     0.172066      -2.19
 O       2.537542     2.905137    -0.053468     211.87
 C       2.181895     4.215109    -0.653061     123.79
 H       3.117781     4.730087    -0.650533      25.24
 H       2.164334     4.085940    -1.610079      29.85
 H       1.032021     4.570978    -0.560103      22.88
 C       1.751432     0.687090     0.090262       9.33
 O       3.030306     0.300418    -0.213180     148.84
 C       0.733201    -0.285187     0.401584      66.51
 H       0.995467    -1.213623     0.273926      27.27
 C      -0.768790     1.503802     1.195873      27.12
 C      -2.099636     1.780102     1.967930     105.59
 H      -2.744411     1.011520     2.289124      25.27
 O      -1.947937     2.829874     3.002887     290.72
 H      -2.177603     2.481930     3.858524      29.24
 C      -3.079689     2.502526     1.036387      91.18
 H      -2.952687     3.639407     0.963488      23.24
 O      -3.161596     1.880448    -0.317731     218.01
 H      -2.301420     1.748826    -0.785790      29.97
 C      -4.559584     2.548116     1.448947      81.23
 O      -5.531225     3.209742     0.642713     251.97
 H      -5.040326     3.776634    -0.109513      27.38
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 H      -4.930714     2.988277     2.614004      23.46
 H      -4.763970     1.378361     1.573697      24.49
55
name = lig-etoh-Waterframe_979
 C       5.494667    -1.155804     1.313089      56.56
 H       5.876058    -0.177864     0.822178      21.65
 C       4.650571    -3.221846     0.691010      54.77
 H       4.455389    -3.889733    -0.137965      22.08
 C       4.785746    -3.712406     2.061695       1.32
 O       4.710382    -5.050555     2.536657     223.55
 C       4.190463    -6.004852     1.455566     143.63
 H       3.087211    -5.966609     1.285663      24.14
 H       4.582826    -6.980960     1.671309      26.23
 H       5.166255    -5.946846     0.786340      25.42
 C       5.152757    -2.729523     3.084695      -3.93
 O       5.060352    -3.050217     4.419913     143.36
 H       4.943115    -4.029373     4.651183      19.53
 C       5.671672    -1.467659     2.693687      72.47
 H       6.136642    -0.979100     3.421114      25.41
 C       4.969100    -1.931264     0.305672      44.94
 C       4.632119    -1.382863    -1.095070      82.16
 H       4.571582    -2.299188    -1.763766      21.41
 O       5.700128    -0.397792    -1.456017     173.06
 H       5.239729     0.380694    -0.918553      22.69
 C       3.214267    -0.792920    -1.189739      79.39
 H       2.588102    -1.535309    -0.706377      23.44
 C       2.879886    -0.203213    -2.700422      90.97
 O       2.898931    -1.233843    -3.740948     287.67
 H       3.830438    -1.355460    -4.036130      24.89
 H       3.513659     0.611594    -3.130995      25.37
 H       1.793485     0.183482    -2.953796      24.51
 C      -0.538726     0.120746     0.980727      50.63
 H      -1.228421    -0.652518     1.112797      22.63
 C       0.247896     2.486773     0.835642      65.70
 H       0.289865     3.610958     1.179883      20.01
 C       1.459723     2.024272     0.378105      12.68
 O       2.446913     2.906872    -0.045972     188.19
 C       2.198745     4.289626    -0.671990     104.07
 H       2.884303     4.841733    -0.118901      26.35
 H       2.235618     4.177524    -1.749206      25.80
 H       1.316731     4.894687    -0.028814      22.60
 C       1.729903     0.622336     0.090463       6.19
 O       3.034992     0.292098    -0.211733     157.72
 C       0.636957    -0.262606     0.308461      49.54
 H       0.782042    -1.341969     0.366577      24.31
 C      -0.695776     1.490186     1.147591      25.50
 C      -2.079528     1.794499     1.944586      77.11
 H      -2.425731     0.811176     2.223286      23.91
 O      -1.883366     2.852754     3.038011     260.85
 H      -2.287125     2.448669     3.793801      29.02
 C      -3.042940     2.635450     0.965942      84.24
 H      -2.368768     3.504029     0.881734      24.30
 O      -3.165642     1.863531    -0.331964     221.27
 H      -2.359467     1.927805    -0.902453      29.48
 C      -4.566701     2.487450     1.522618      73.58
 O      -5.527602     3.309552     0.688365     248.76
 H      -4.831435     3.729150     0.025143      26.55
 H      -4.347481     2.964741     2.682160      24.57
 H      -5.022827     1.445645     1.418224      24.24
55
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name = lig-etoh-Waterframe_980
 C       5.599933    -1.030811     1.233853      33.26
 H       6.041065     0.038375     1.262257      19.25
 C       4.597846    -3.229421     0.741012      68.27
 H       4.481445    -4.015949    -0.022597      21.93
 C       4.809779    -3.636845     2.005100      17.09
 O       4.666188    -5.093485     2.505916     259.47
 C       4.252098    -6.025603     1.515647     128.87
 H       3.103874    -5.987437     1.232944      26.56
 H       4.525770    -6.927287     1.806261      25.11
 H       4.538727    -5.673479     0.446221      24.68
 C       5.178371    -2.798185     3.101541      18.53
 O       5.043996    -3.084429     4.404369     198.82
 H       5.131153    -3.978731     4.543492      21.17
 C       5.660230    -1.580972     2.688874      35.34
 H       5.911846    -0.823118     3.416247      21.09
 C       4.877543    -1.871256     0.334263      41.31
 C       4.674293    -1.407405    -1.059429      70.85
 H       4.665485    -2.168633    -1.903044      22.15
 O       5.724829    -0.396746    -1.496145     106.80
 H       5.374905     0.657345    -1.208680      17.16
 C       3.202051    -0.798369    -1.179299      67.43
 H       2.515785    -1.653383    -1.013004      23.10
 C       2.844487    -0.192026    -2.796323     107.50
 O       2.883121    -1.171465    -3.760359     299.11
 H       3.765209    -1.314657    -4.134151      26.42
 H       3.427794     0.673640    -2.800858      25.68
 H       1.902387     0.190786    -2.580385      26.71
 C      -0.560768     0.085825     0.990588      22.37
 H      -1.185555    -0.698859     1.516999      20.63
 C       0.275096     2.444531     0.871055      54.27
 H       0.049459     3.540114     1.230749      19.18
 C       1.515285     1.972296     0.468067      19.78
 O       2.399161     2.947369    -0.056021     175.67
 C       2.239734     4.323777    -0.526969      89.46
 H       3.090478     4.991205    -0.162045      24.61
 H       2.133471     4.515915    -1.877738      22.55
 H       1.183059     4.715099    -0.294138      24.51
 C       1.649522     0.602578     0.134419       7.31
 O       3.050375     0.287494    -0.238930     145.14
 C       0.638536    -0.324728     0.268677      48.85
 H       0.705012    -1.505211     0.019695      19.76
 C      -0.787069     1.534473     1.252460      14.46
 C      -2.014595     1.929321     1.870480     102.26
 H      -2.259540     0.982996     2.448355      20.99
 O      -1.818822     2.799256     3.057887     271.32
 H      -2.154246     2.341270     3.813416      29.00
 C      -3.038643     2.575354     0.885225      88.45
 H      -2.719525     3.626701     0.634235      24.35
 O      -3.169231     1.868773    -0.349254     246.01
 H      -2.392384     2.210592    -0.846831      28.04
 C      -4.503799     2.550279     1.542438      98.13
 O      -5.466457     3.386871     0.761899     271.54
 H      -5.011372     4.090446     0.117373      27.98
 H      -4.481938     2.763832     2.555332      28.95
 H      -4.808427     1.530806     1.519892      27.86
55
name = lig-etoh-Waterframe_981
 C       5.648177    -1.017858     1.359584      55.78
 H       5.893609     0.049129     1.064085      19.40
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 C       4.565895    -3.221574     0.724497      45.04
 H       4.190305    -3.949052    -0.053591      16.06
 C       4.806383    -3.751263     2.074463      26.16
 O       4.622543    -5.030444     2.433792     278.11
 C       4.272748    -6.016213     1.478004     117.47
 H       3.119359    -6.081973     1.744164      26.40
 H       4.525125    -7.038254     1.938651      23.21
 H       4.390554    -5.917286     0.470739      31.77
 C       5.203935    -2.851161     3.048065       5.44
 O       5.047400    -3.120394     4.428219     143.07
 H       5.026490    -4.113514     4.680719      23.17
 C       5.657851    -1.542798     2.568410      82.39
 H       5.802024    -0.788106     3.490658      23.12
 C       4.905307    -1.798995     0.396379      59.15
 C       4.680619    -1.320703    -1.093687      96.92
 H       4.958969    -2.181152    -1.724779      22.87
 O       5.692039    -0.418814    -1.538119     170.02
 H       5.774683     0.646557    -1.288837      22.58
 C       3.207260    -0.797968    -1.286138      80.82
 H       2.486120    -1.636041    -1.287061      22.18
 C       2.829164    -0.155961    -2.663703      99.85
 O       2.866797    -1.150543    -3.823882     268.60
 H       3.743576    -1.354119    -4.145807      27.16
 H       3.601923     0.585466    -2.881036      24.59
 H       1.827743     0.040813    -2.569108      27.16
 C      -0.532560     0.135925     0.980676      62.92
 H      -1.343005    -0.548987     1.506050      21.49
 C       0.211776     2.375922     1.000751      66.63
 H       0.007129     3.463607     0.930230      22.28
 C       1.501338     2.045178     0.436815      -1.84
 O       2.456766     2.948866    -0.070684     195.27
 C       2.186933     4.362784    -0.386367     104.11
 H       3.197019     4.855374    -0.180304      21.64
 H       2.377690     4.208935    -1.668669      20.72
 H       1.268717     4.696885    -0.182106      26.42
 C       1.729791     0.588531     0.147126     -18.26
 O       2.975245     0.265394    -0.278475     136.34
 C       0.573124    -0.401446     0.328952      50.75
 H       0.888930    -1.358121    -0.324396      18.96
 C      -0.727066     1.450434     1.295248      49.92
 C      -2.021806     2.034467     1.915268      91.57
 H      -2.830250     1.179043     2.120113      22.68
 O      -1.744165     2.772880     3.068070     293.59
 H      -1.980335     2.229092     3.810584      27.76
 C      -3.106857     2.551470     0.873526      98.65
 H      -3.093835     3.624064     0.660857      24.30
 O      -3.148974     1.865969    -0.391854     239.31
 H      -2.508324     2.210926    -1.046550      27.73
 C      -4.430572     2.644403     1.493549     117.55
 O      -5.397071     3.440556     0.853252     253.04
 H      -4.961621     4.328916     0.505473      29.24
 H      -4.514691     2.938908     2.466420      28.70
 H      -4.789547     1.644973     1.439914      29.07
55
name = lig-etoh-Waterframe_982
 C       5.569204    -1.036370     1.330986      61.68
 H       5.838248    -0.005161     1.081427      22.24
 C       4.576396    -3.132598     0.731072      62.30
 H       3.940881    -3.575463    -0.070995      15.56
 C       4.793354    -3.757567     1.986484      30.00
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 O       4.610700    -5.015766     2.394405     251.02
 C       4.149167    -6.085554     1.497429     123.01
 H       3.083389    -6.335279     1.676841      27.62
 H       5.062146    -6.951852     1.793988      23.54
 H       4.580474    -5.990419     0.539774      32.10
 C       5.241936    -2.826782     3.021158      22.54
 O       5.081271    -3.121487     4.428680      23.77
 H       5.042620    -4.213379     4.585656      19.00
 C       5.641254    -1.541686     2.713907      64.99
 H       6.099236    -0.861158     3.630371      24.14
 C       4.968235    -1.837243     0.421964      43.74
 C       4.681329    -1.249473    -1.078376     114.47
 H       4.714507    -2.194390    -1.584773      25.14
 O       5.702580    -0.414444    -1.616801     208.24
 H       5.427017     0.349140    -0.916549      24.77
 C       3.221512    -0.831355    -1.395268      92.45
 H       2.625446    -1.679840    -1.029780      20.61
 C       2.872898    -0.157164    -2.604718     106.98
 O       2.839750    -1.137362    -3.853064     260.71
 H       3.760931    -1.358998    -3.894189      26.93
 H       3.421145     0.749011    -3.011522      24.35
 H       1.890801     0.212776    -2.777937      26.52
 C      -0.559158     0.054198     1.004657      35.03
 H      -1.499115    -0.648562     0.893187      21.09
 C       0.297241     2.420677     1.036139      67.61
 H      -0.111406     3.384618     1.016643      25.02
 C       1.437867     2.037855     0.368110       4.82
 O       2.517415     2.899173    -0.032030     188.11
 C       2.203821     4.318723    -0.352814     133.60
 H       2.835843     4.999717     0.308842      24.81
 H       2.124493     4.456587    -1.338795      28.81
 H       1.406677     4.812255     0.134070      26.00
 C       1.686568     0.597955     0.181686      24.82
 O       2.913902     0.220293    -0.339415     146.99
 C       0.692767    -0.312498     0.359131      49.75
 H       0.478670    -1.424024     0.083055      21.17
 C      -0.722618     1.416004     1.353687      -0.86
 C      -2.122989     1.965837     1.904222      79.13
 H      -2.579088     0.979055     2.275723      22.86
 O      -1.682762     2.787819     3.100404     241.80
 H      -1.940344     2.255809     3.862265      26.78
 C      -3.076218     2.737429     0.831339      82.21
 H      -2.573452     3.685788     0.577330      25.32
 O      -3.136353     1.831672    -0.423257     199.33
 H      -2.530534     2.233815    -1.077440      28.42
 C      -4.470226     2.635115     1.502256      82.80
 O      -5.367508     3.532945     0.893317     212.18
 H      -4.872170     4.431954     0.741850      29.17
 H      -4.008109     3.052555     2.704778      22.76
 H      -5.062322     1.669629     1.515030      25.42
55
name = lig-etoh-Waterframe_983
 C       5.507355    -1.017460     1.426835      65.18
 H       5.868219    -0.052716     1.277897      24.51
 C       4.538229    -3.103789     0.683817      32.20
 H       3.937564    -3.707690    -0.006763      21.61
 C       4.804627    -3.601126     1.917782      15.36
 O       4.564638    -5.069132     2.382239     244.48
 C       4.141628    -6.169803     1.510270      85.71
 H       3.173684    -6.522901     1.447439      30.01
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 H       4.797892    -7.163072     1.909652      22.62
 H       4.205886    -5.678893     0.395417      26.34
 C       5.241027    -2.833338     3.058210      19.12
 O       5.138694    -3.120965     4.370357      36.91
 H       5.309362    -4.231695     4.501929      19.85
 C       5.645621    -1.517322     2.810341      59.56
 H       6.212455    -1.006579     3.738594      22.92
 C       4.995263    -1.810559     0.329685      54.94
 C       4.687040    -1.361466    -1.071030      92.62
 H       4.713686    -2.165937    -1.816709      22.62
 O       5.669245    -0.364403    -1.634001     202.04
 H       5.750415     0.594723    -1.204269      22.78
 C       3.217703    -0.853729    -1.276114      68.00
 H       2.588674    -1.807436    -1.228000      21.08
 C       2.862086    -0.162050    -2.815262      97.31
 O       2.850443    -1.111869    -3.821567     281.18
 H       3.700595    -1.524808    -3.987167      26.89
 H       3.665037     0.687158    -2.699966      21.87
 H       1.805312     0.201933    -2.432308      23.86
 C      -0.572341     0.030840     0.983567      53.52
 H      -1.346446    -0.669433     0.679346      21.55
 C       0.292514     2.436981     1.049715      51.06
 H       0.134448     3.426324     1.340927      23.36
 C       1.456188     1.992237     0.312709       8.80
 O       2.528893     2.856631     0.014844     176.67
 C       2.206419     4.292249    -0.235747      99.91
 H       3.159824     4.800131     0.165063      23.84
 H       2.099820     4.756192    -1.211031      26.15
 H       1.054990     4.333835     0.261485      20.13
 C       1.684537     0.623977     0.137779      24.39
 O       2.902406     0.223352    -0.382489     151.71
 C       0.645934    -0.291514     0.459659      47.23
 H       1.034051    -1.328114     0.287872      21.81
 C      -0.780632     1.434527     1.374359       6.26
 C      -2.084705     1.837434     1.885863      90.89
 H      -2.606103     1.096189     2.419593      23.59
 O      -1.670238     2.792388     3.108078     198.35
 H      -2.062690     2.437466     3.935077      27.26
 C      -2.987909     2.735092     0.799654      73.73
 H      -2.506492     3.736951     0.579244      24.80
 O      -3.118204     1.851043    -0.399475     212.27
 H      -2.509457     2.151201    -1.103505      27.55
 C      -4.447262     2.735218     1.535033      74.73
 O      -5.386674     3.651230     0.928230     221.72
 H      -4.878038     4.515228     0.639970      28.12
 H      -4.297920     2.893655     2.816088      24.12
 H      -4.777328     1.600511     1.588105      24.61
55
name = lig-etoh-Waterframe_984
 C       5.485717    -0.979919     1.542831      62.92
 H       5.833911    -0.030034     1.323919      25.05
 C       4.502561    -3.103540     0.596564      56.97
 H       4.212098    -3.881714    -0.083237      23.14
 C       4.768869    -3.652662     2.002533       2.08
 O       4.502766    -5.045173     2.371395     226.72
 C       4.142745    -6.178563     1.479375     120.07
 H       3.094474    -6.295053     1.801179      25.02
 H       4.671760    -7.054563     1.577707      26.02
 H       4.317368    -6.076654     0.231058      25.56
 C       5.217884    -2.802555     3.043006      21.62
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 O       5.232701    -3.178393     4.340813     194.90
 H       5.094976    -4.232030     4.660222      21.39
 C       5.648009    -1.498568     2.768347      59.95
 H       6.036317    -0.884092     3.558949      21.99
 C       5.003978    -1.763641     0.327017      23.65
 C       4.703453    -1.367844    -1.128493      82.95
 H       5.048459    -2.187308    -1.820989      19.73
 O       5.640949    -0.327416    -1.656049     195.21
 H       5.496232     0.605163    -1.196529      22.85
 C       3.177497    -0.865813    -1.236174      65.45
 H       2.375357    -1.642692    -1.193652      21.99
 C       2.913383    -0.202127    -2.795471      73.51
 O       2.855448    -1.129178    -3.840364     266.32
 H       3.760440    -1.371851    -4.126358      25.67
 H       3.734026     0.580324    -3.108513      22.18
 H       1.719162     0.203017    -2.786611      23.34
 C      -0.614021     0.107892     0.945991      56.99
 H      -1.375863    -0.554545     1.196273      23.02
 C       0.230385     2.342990     1.061149      58.89
 H       0.391814     3.244714     1.609828      20.91
 C       1.461484     2.007372     0.332191       3.38
 O       2.524485     2.831784     0.014211     172.37
 C       2.212908     4.227478    -0.082185      89.44
 H       3.054008     4.799726     0.375520      24.91
 H       2.182998     4.417828    -1.422162      21.17
 H       1.093407     4.638978     0.528694      20.14
 C       1.672719     0.606765     0.064479       0.86
 O       2.926823     0.252916    -0.386873     171.87
 C       0.712606    -0.349988     0.524241      51.84
 H       1.076519    -1.289882     0.423085      22.23
 C      -0.745279     1.414396     1.288601      41.22
 C      -2.036966     1.874134     1.960602      96.66
 H      -2.724097     1.097348     2.146068      24.96
 O      -1.690746     2.778835     3.069925     289.51
 H      -2.258461     2.456864     3.813894      26.84
 C      -2.938391     2.581184     0.888084      90.37
 H      -2.604443     3.624419     0.631732      24.04
 O      -3.114809     1.908970    -0.348334     247.21
 H      -2.439029     2.072519    -1.025318      27.57
 C      -4.354085     2.862985     1.549023     103.41
 O      -5.403011     3.740498     0.970981     286.70
 H      -4.923715     4.407758     0.328056      28.27
 H      -4.432691     3.107871     2.451385      29.78
 H      -4.823615     1.880982     1.207614      25.09
55
name = lig-etoh-Waterframe_985
 C       5.450728    -0.927338     1.401450      52.02
 H       5.728091     0.129151     1.305562      21.58
 C       4.585537    -3.138572     0.684580      70.81
 H       4.494309    -3.643324    -0.264753      23.75
 C       4.679100    -3.736073     1.947124      24.27
 O       4.479301    -4.993846     2.353451     236.03
 C       4.108093    -6.127506     1.438585     132.15
 H       3.000702    -6.333319     1.784626      24.71
 H       4.771808    -6.853962     1.762958      25.28
 H       4.234872    -5.943031     0.320238      26.77
 C       5.172220    -2.849278     3.020892       5.12
 O       5.339803    -3.244400     4.380724     251.41
 H       4.966357    -4.154760     4.442201      25.37
 C       5.626185    -1.492942     2.759006      36.27
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 H       5.866278    -0.886861     3.489022      20.02
 C       4.961225    -1.787263     0.439227      27.74
 C       4.738311    -1.268741    -1.151356      71.41
 H       4.788786    -2.285577    -1.662203      22.05
 O       5.595502    -0.283494    -1.668555     242.69
 H       5.241361     0.440243    -1.176942      27.39
 C       3.148268    -0.838384    -1.380575      77.37
 H       2.499570    -1.591269    -0.958653      23.55
 C       2.951900    -0.243021    -2.705408     109.35
 O       2.873516    -1.229061    -3.905704     271.70
 H       3.784594    -1.276989    -4.268628      25.49
 H       3.606879     0.551622    -2.969094      25.63
 H       2.041666     0.417120    -2.894338      25.18
 C      -0.575261     0.048653     0.919537      33.68
 H      -1.183408    -0.515873     1.572288      21.77
 C       0.336761     2.312534     1.042732      69.45
 H       0.107238     3.235153     1.683654      22.19
 C       1.422855     1.947637     0.380938      25.57
 O       2.488634     2.798552     0.048651     187.23
 C       2.243064     4.221945     0.023713     111.22
 H       2.986115     4.778253     0.474358      26.82
 H       2.074972     4.437491    -1.220550      23.22
 H       1.335049     4.680669     0.512375      24.82
 C       1.635615     0.581236     0.034110      12.73
 O       2.979665     0.291399    -0.364898     127.17
 C       0.764596    -0.389638     0.531498      49.86
 H       0.746356    -1.366783     0.527500      23.15
 C      -0.772999     1.430429     1.234642      10.14
 C      -2.021831     1.920856     1.981435      98.18
 H      -2.399221     0.892381     2.382774      22.56
 O      -1.743741     2.742350     3.037364     273.11
 H      -2.291567     2.462451     3.819320      26.89
 C      -2.930490     2.628313     0.999350      89.57
 H      -2.268925     3.490846     0.777871      24.65
 O      -3.138852     1.922338    -0.304520     223.62
 H      -2.277978     2.093713    -0.721108      29.62
 C      -4.344346     2.897014     1.469512      99.61
 O      -5.355980     3.848661     0.957724     301.71
 H      -5.089925     4.311560     0.105253      28.05
 H      -4.162101     3.130042     2.593137      25.88
 H      -4.919580     1.986583     1.593668      25.63
55
name = lig-etoh-Waterframe_986
 C       5.431409    -0.913793     1.372519      54.88
 H       5.546042     0.191246     1.071085      22.25
 C       4.703182    -3.152011     0.697705      76.81
 H       4.459756    -3.790562    -0.182005      19.57
 C       4.649193    -3.697299     1.957512      27.89
 O       4.443912    -5.001942     2.331780     248.57
 C       4.059351    -6.032444     1.447875     138.15
 H       3.005770    -6.578722     1.371300      27.44
 H       4.814646    -6.932617     1.867621      23.87
 H       4.222113    -5.700131     0.539031      33.84
 C       5.164623    -2.849797     3.036159      -0.19
 O       5.426338    -3.290601     4.346763     231.90
 H       5.171341    -4.157019     4.626365      22.35
 C       5.531075    -1.519524     2.681274      60.97
 H       5.831381    -1.016808     3.553389      24.21
 C       4.891797    -1.757402     0.409044      41.42
 C       4.665987    -1.277081    -1.073947      84.14
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 H       4.806237    -2.093364    -1.855421      23.96
 O       5.548967    -0.237520    -1.656987     193.81
 H       5.537107     0.628743    -1.332099      27.74
 C       3.216243    -0.806584    -1.380040      72.19
 H       2.641830    -1.726406    -1.214074      24.69
 C       2.941580    -0.243406    -2.802588     116.08
 O       2.903958    -1.304105    -3.902143     281.23
 H       3.778040    -1.524849    -4.354765      24.85
 H       3.827808     0.281533    -2.744131      24.63
 H       2.037851     0.178777    -2.629580      27.95
 C      -0.489975     0.022936     0.997921      52.44
 H      -1.098433    -0.895535     1.343671      21.81
 C       0.280350     2.337034     1.102066      51.62
 H       0.205980     3.532274     1.227685      21.02
 C       1.483495     1.877578     0.372477       3.78
 O       2.456862     2.768009     0.120750     201.33
 C       2.251548     4.262033     0.069061     128.09
 H       3.209994     4.555635     0.372706      23.79
 H       2.190783     4.746305    -0.789798      28.18
 H       1.480562     4.378587     0.553585      30.63
 C       1.700751     0.521853     0.035945      18.04
 O       2.992256     0.311901    -0.373329     140.15
 C       0.684073    -0.423915     0.493379      50.27
 H       1.013307    -1.514224     0.353194      21.89
 C      -0.753122     1.421719     1.198597      33.47
 C      -2.024203     1.785847     1.942825      89.75
 H      -2.491480     0.900849     2.573618      21.80
 O      -1.766156     2.766410     3.086272     196.64
 H      -2.216099     2.383347     3.904409      26.02
 C      -2.979036     2.724439     0.978875      81.16
 H      -2.433874     3.664027     0.876763      24.21
 O      -3.128245     1.939991    -0.247483     214.93
 H      -2.276303     1.835258    -0.719540      29.12
 C      -4.414049     2.927985     1.513518      83.79
 O      -5.266039     3.931366     0.919315     307.48
 H      -4.829770     4.324295     0.118618      26.72
 H      -3.993725     3.477166     2.722617      22.44
 H      -4.781358     1.953146     1.746354      26.13
55
name = lig-etoh-Waterframe_987
 C       5.350774    -0.953668     1.412601      54.85
 H       5.604974     0.183849     1.267899      22.62
 C       4.748085    -3.141117     0.594906      59.96
 H       4.358649    -3.958582    -0.034004      15.63
 C       4.688970    -3.638162     2.044210       9.83
 O       4.376649    -5.007715     2.375854     292.22
 C       4.054462    -5.997497     1.406839     110.85
 H       2.924293    -6.039662     1.573931      26.81
 H       4.682111    -7.112808     1.325663      25.00
 H       4.425092    -5.766514     0.425959      29.45
 C       5.166552    -2.859248     3.037827      13.07
 O       5.510258    -3.294476     4.283868     221.57
 H       5.221801    -4.186793     4.469457      23.02
 C       5.440006    -1.518249     2.655854      52.73
 H       5.994958    -0.887434     3.506724      22.83
 C       4.868632    -1.756038     0.291631      40.57
 C       4.608665    -1.267944    -1.048732     104.14
 H       4.938572    -2.066307    -1.694185      23.78
 O       5.557159    -0.213050    -1.646275     141.38
 H       5.535153     0.613943    -1.093377      25.92
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 C       3.261068    -0.843112    -1.286781      83.07
 H       2.473399    -1.601426    -1.238675      23.72
 C       2.991401    -0.299362    -2.914479      83.87
 O       2.904338    -1.348303    -3.841227     266.41
 H       3.882716    -1.617229    -4.073271      22.37
 H       3.789301     0.514416    -3.333323      23.34
 H       2.028200     0.124783    -2.952851      26.64
 C      -0.450941    -0.024462     1.108289      41.29
 H      -1.463380    -0.682549     1.015019      21.67
 C       0.272365     2.318519     1.030545      62.43
 H       0.010188     3.472013     1.030699      21.20
 C       1.428552     1.881163     0.426935      14.52
 O       2.499399     2.783355     0.135007     167.93
 C       2.308148     4.245975     0.130784     104.97
 H       3.271781     4.628226     0.715535      23.89
 H       2.114322     4.627334    -0.843446      26.68
 H       1.558264     4.645356     1.015638      22.42
 C       1.727183     0.492474     0.117772      20.53
 O       2.982653     0.257388    -0.440729     147.27
 C       0.755723    -0.440059     0.364407      44.87
 H       1.060059    -1.669915     0.213590      19.98
 C      -0.756511     1.347220     1.285919      11.29
 C      -2.086768     1.779294     1.958228      72.17
 H      -2.792900     0.886987     2.011085      24.26
 O      -1.759354     2.769528     3.136039     200.11
 H      -2.063707     2.219336     3.952735      24.52
 C      -3.020073     2.704184     0.955403      89.08
 H      -2.680830     3.718035     0.725312      25.24
 O      -3.133389     1.968259    -0.232170     211.75
 H      -2.297087     1.646437    -0.610839      29.25
 C      -4.385767     3.020522     1.656783      92.83
 O      -5.168912     3.947698     0.865547     287.10
 H      -4.644548     4.447765     0.246963      29.10
 H      -4.444539     3.528388     2.739048      23.99
 H      -5.061964     2.111150     1.622587      25.15
55
name = lig-etoh-Waterframe_988
 C       5.211546    -1.000498     1.394135      61.56
 H       5.611013     0.044573     1.403039      23.11
 C       4.689846    -3.184769     0.630375      47.46
 H       4.419352    -3.725977    -0.299872      14.61
 C       4.726900    -3.678677     1.916987      32.91
 O       4.372083    -4.965757     2.446204     304.04
 C       4.025412    -5.967365     1.287571     126.12
 H       2.965301    -5.977355     1.297777      31.25
 H       4.384008    -6.867717     1.824145      25.06
 H       4.276626    -5.597243     0.145074      28.19
 C       5.200012    -2.808531     3.041692       9.63
 O       5.586966    -3.304922     4.255625     239.98
 H       5.167458    -4.211241     4.227072      31.00
 C       5.413104    -1.487247     2.726371      45.25
 H       6.008695    -0.700372     3.495091      21.64
 C       4.930837    -1.801844     0.324916      45.72
 C       4.718731    -1.277736    -1.151126      95.21
 H       4.712692    -2.190568    -1.709329      22.49
 O       5.582609    -0.209637    -1.595060     280.51
 H       5.292582     0.548173    -0.951326      23.37
 C       3.150365    -0.816154    -1.382718      71.56
 H       2.470299    -1.655682    -1.064332      19.21
 C       3.036741    -0.326078    -2.938540      84.30
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 O       2.919493    -1.453886    -3.787803     273.14
 H       3.892437    -1.786210    -4.090955      23.25
 H       3.619455     0.609793    -3.448280      21.22
 H       1.966849     0.197034    -3.050587      23.16
 C      -0.439434    -0.074163     1.090290      33.72
 H      -1.395292    -0.758974     1.149142      20.21
 C       0.185730     2.265205     0.924834      59.83
 H      -0.110448     3.291240     1.113998      20.12
 C       1.472715     1.933765     0.466323       7.61
 O       2.529442     2.788285     0.146246     181.81
 C       2.385447     4.208697     0.288043      75.49
 H       3.504957     4.813733     0.366356      20.71
 H       1.999882     4.472789    -0.859419      21.97
 H       1.437352     4.835206     1.063747      19.15
 C       1.765748     0.514812     0.186502       6.83
 O       2.953106     0.249504    -0.472861     162.26
 C       0.769654    -0.461972     0.333804      45.76
 H       0.734642    -1.664037    -0.046497      17.75
 C      -0.752164     1.274835     1.439554      15.36
 C      -2.140862     1.917324     1.927321      95.79
 H      -2.722908     1.058400     2.226302      24.24
 O      -1.778551     2.667774     3.149193     242.26
 H      -1.979381     2.177339     4.036488      25.31
 C      -3.006360     2.692227     1.045439      85.18
 H      -2.423934     3.581512     0.701401      23.59
 O      -3.201860     1.963312    -0.271700     199.81
 H      -2.251722     1.695932    -0.304664      28.87
 C      -4.401306     3.088117     1.733521      96.79
 O      -5.101891     3.936909     0.816101     316.66
 H      -4.678673     4.534515     0.184595      27.11
 H      -4.229849     3.254402     2.658702      28.75
 H      -5.131934     2.159461     1.817772      24.37
55
name = lig-etoh-Waterframe_989
 C       5.149647    -0.958921     1.448280      76.07
 H       5.271405     0.004672     1.015660      23.25
 C       4.596125    -3.207283     0.602694      78.29
 H       4.449027    -3.855016    -0.283310      22.52
 C       4.773528    -3.724938     1.916347       6.82
 O       4.392576    -4.909367     2.386077     259.85
 C       3.931522    -5.905475     1.287572     127.20
 H       2.951047    -6.046748     1.029057      28.16
 H       4.238042    -6.750729     1.689580      23.97
 H       4.753178    -5.674374     0.313557      25.33
 C       5.240508    -2.787388     2.965263      21.07
 O       5.628995    -3.349878     4.225074     208.93
 H       5.321680    -4.319192     4.485452      26.64
 C       5.407621    -1.422195     2.758417      55.10
 H       5.734076    -0.755594     3.719486      19.58
 C       4.972535    -1.854245     0.340105      13.95
 C       4.751891    -1.330663    -1.216483      74.16
 H       4.973051    -2.043710    -2.067774      19.66
 O       5.607455    -0.249005    -1.518881     286.77
 H       5.379740     0.775464    -1.208911      19.62
 C       3.145039    -0.790562    -1.517708      62.11
 H       2.538211    -1.729269    -1.377181      16.57
 C       2.947390    -0.312446    -2.914011      94.35
 O       2.940515    -1.603447    -3.752315     237.63
 H       3.920374    -1.689152    -4.120492      24.58
 H       3.948852     0.154237    -2.913759      16.79
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 H       1.837295     0.126188    -2.878879      21.11
 C      -0.484590    -0.112610     1.033512      60.94
 H      -0.927792    -1.000630     1.349198      20.82
 C       0.105602     2.229853     0.901632      61.27
 H      -0.061827     3.195539     1.068547      19.38
 C       1.533500     1.913737     0.491530      -2.22
 O       2.551283     2.777248     0.205668     161.61
 C       2.420791     4.246571     0.327519      68.96
 H       3.526921     4.559220     0.314244      21.55
 H       1.865714     4.793398    -0.654905      21.48
 H       1.778030     4.215903     1.324264      21.04
 C       1.766879     0.532733     0.186253       2.89
 O       2.932067     0.312560    -0.480090     158.84
 C       0.674211    -0.433346     0.407848      51.16
 H       0.816799    -1.326906    -0.216420      17.91
 C      -0.731125     1.257394     1.463137      32.22
 C      -2.101516     1.852903     2.032671      96.87
 H      -2.671797     1.081749     2.470271      21.71
 O      -1.788907     2.598847     3.166165     255.74
 H      -2.260569     1.990467     3.870802      22.57
 C      -3.030235     2.744920     1.066247      75.13
 H      -2.455294     3.706522     0.911607      21.79
 O      -3.252075     1.958228    -0.249675     191.55
 H      -2.388263     1.553470    -0.566075      26.26
 C      -4.363469     3.090870     1.674325      89.03
 O      -5.108978     3.914988     0.820274     311.85
 H      -4.486916     4.392094     0.171490      26.77
 H      -3.944100     3.668078     2.761881      22.92
 H      -4.861375     2.116401     1.935016      24.87
55
name = lig-etoh-Waterframe_990
 C       5.150067    -0.894212     1.411655      51.82
 H       5.005551     0.149226     1.252048      19.80
 C       4.571799    -3.217050     0.564766      40.89
 H       4.271099    -4.028659    -0.087262      18.56
 C       4.799288    -3.637141     1.933599      14.04
 O       4.367715    -4.947365     2.275339     322.96
 C       3.956889    -5.856948     1.347977     124.40
 H       2.913497    -5.606826     1.085290      25.41
 H       4.103328    -6.906435     1.641223      23.51
 H       4.739381    -5.913261     0.486137      28.50
 C       5.297310    -2.876678     2.944483       4.45
 O       5.664543    -3.364564     4.188792     315.71
 H       5.175704    -4.353527     4.236934      24.66
 C       5.380146    -1.376663     2.752016      54.15
 H       5.421982    -0.776167     3.634721      22.07
 C       4.908382    -1.893793     0.289946      25.35
 C       4.691139    -1.324586    -1.185328     108.76
 H       5.148170    -2.160183    -1.825548      18.74
 O       5.688295    -0.262225    -1.491897     180.70
 H       5.242370     0.653376    -1.037110      19.35
 C       3.218134    -0.871713    -1.476491      75.10
 H       2.437948    -1.629908    -1.297907      19.02
 C       2.899196    -0.382064    -2.879576     106.54
 O       2.920719    -1.658049    -3.698075     256.87
 H       3.881283    -1.801517    -3.894004      25.06
 H       3.649966     0.243057    -3.314008      23.31
 H       2.135636     0.341498    -3.271884      23.16
 C      -0.575018    -0.121884     1.070743      40.72
 H      -1.171620    -0.849176     1.471707      21.02
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 C       0.212754     2.235545     0.930119      69.74
 H      -0.092656     3.229341     0.970277      19.30
 C       1.442624     1.874265     0.532574       5.79
 O       2.576563     2.765445     0.235263     194.09
 C       2.428604     4.216603     0.401632     142.78
 H       3.313323     4.637557     0.535024      26.62
 H       1.730069     4.765797    -0.223836      27.48
 H       2.258195     4.495439     1.309503      29.97
 C       1.682484     0.542506     0.147091      15.36
 O       2.938549     0.324863    -0.533390     147.90
 C       0.733903    -0.365024     0.392023      66.57
 H       0.844069    -1.272618     0.073545      21.55
 C      -0.800005     1.238249     1.367706      23.87
 C      -2.058405     1.672156     2.097594      69.76
 H      -2.752692     0.787463     2.121031      22.35
 O      -1.784516     2.574132     3.259327     228.44
 H      -2.358677     2.324495     4.117993      25.17
 C      -2.954830     2.695906     1.013774      79.05
 H      -2.500907     3.680482     0.705933      21.60
 O      -3.299202     1.984843    -0.174321     222.74
 H      -2.517359     1.632004    -0.679171      25.83
 C      -4.249265     3.072351     1.663335      94.91
 O      -5.166190     3.883038     0.818014     264.07
 H      -4.570860     4.398890     0.136141      28.16
 H      -4.231316     4.020732     2.535871      21.10
 H      -4.861886     2.295724     2.037663      25.80
55
name = lig-etoh-Waterframe_991
 C       5.138912    -0.934739     1.359339      48.88
 H       5.024378     0.129371     1.426845      21.57
 C       4.608238    -3.195005     0.601086      60.86
 H       4.165139    -3.793040    -0.179525      18.54
 C       4.752744    -3.646004     1.865982      27.08
 O       4.415934    -4.945351     2.288828     257.39
 C       3.989261    -5.892842     1.306105      96.88
 H       2.916577    -5.471809     0.987769      26.62
 H       3.607014    -6.817844     2.068323      24.01
 H       4.422472    -5.966883     0.447557      32.62
 C       5.380386    -2.798043     2.962817       3.78
 O       5.671516    -3.392069     4.145298     204.04
 H       5.196420    -4.384734     4.323446      20.97
 C       5.318549    -1.452917     2.668443      63.39
 H       5.335283    -0.790653     3.378038      24.98
 C       4.790943    -1.788538     0.271483      46.62
 C       4.698434    -1.318282    -1.105064      99.27
 H       4.655571    -2.262811    -1.713479      23.35
 O       5.716223    -0.288516    -1.471770     173.55
 H       5.574658     0.645460    -0.929147      21.62
 C       3.212186    -0.888114    -1.357934      65.65
 H       2.617431    -1.712398    -0.968237      21.27
 C       2.960827    -0.450064    -2.968292     102.79
 O       2.855369    -1.648487    -3.636774     291.72
 H       3.702322    -2.022209    -3.830434      27.42
 H       3.654136     0.205994    -3.466752      26.70
 H       1.908816    -0.103823    -2.920427      25.16
 C      -0.554285    -0.076167     1.100372      42.94
 H      -1.388870    -0.744766     1.290099      21.17
 C       0.196613     2.262255     1.045658      68.44
 H      -0.019657     3.392967     1.067958      20.38
 C       1.482510     1.922277     0.499176       6.74
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 O       2.540641     2.745599     0.271754     199.79
 C       2.437982     4.190398     0.547143     100.62
 H       3.359150     4.603099     0.046372      23.10
 H       1.708405     4.479961    -0.097043      27.94
 H       2.132189     4.582274     1.660486      23.43
 C       1.713641     0.548914     0.043462       0.95
 O       2.921851     0.312562    -0.575715     128.52
 C       0.672893    -0.452955     0.398433      55.10
 H       0.940240    -1.466610     0.379226      22.01
 C      -0.834015     1.258197     1.272022      32.90
 C      -2.069791     1.648756     2.040461      66.05
 H      -2.707270     0.685299     2.369844      21.45
 O      -1.771288     2.520218     3.326781     182.40
 H      -2.392132     2.235253     4.148346      23.83
 C      -2.842340     2.603436     1.023080      92.62
 H      -2.096022     3.346813     0.688746      24.27
 O      -3.357937     1.972294    -0.137109     239.75
 H      -2.491288     1.855934    -0.630511      27.67
 C      -4.241014     3.171495     1.696489      91.05
 O      -5.223604     3.818830     0.768443     263.42
 H      -4.840678     4.571189     0.134860      26.91
 H      -3.763486     3.544019     2.653390      25.58
 H      -4.768373     2.323310     2.060757      27.31
55
name = lig-etoh-Waterframe_992
 C       5.090205    -0.961240     1.353597      72.30
 H       5.258905     0.092265     1.072951      23.55
 C       4.610598    -3.097543     0.563563      69.35
 H       4.259626    -3.685542    -0.275014      20.03
 C       4.772449    -3.678079     1.904992      25.47
 O       4.534558    -4.922010     2.333242     193.08
 C       3.876259    -5.911781     1.299555      90.93
 H       2.827495    -5.555375     0.943776      24.85
 H       3.700017    -6.984655     2.003665      24.59
 H       4.627015    -6.285360     0.546177      27.09
 C       5.333860    -2.865805     2.875248       7.37
 O       5.689968    -3.392163     4.138411     211.44
 H       5.206268    -4.337168     4.376098      23.20
 C       5.292882    -1.473259     2.621455      63.83
 H       5.553162    -0.764369     3.381274      22.83
 C       4.737091    -1.733901     0.352024      50.25
 C       4.657606    -1.266338    -1.070047     103.01
 H       4.869905    -1.979612    -1.857316      24.16
 O       5.717606    -0.364072    -1.476879     159.77
 H       5.607139     0.526152    -0.948765      25.82
 C       3.233862    -0.805733    -1.309237      87.25
 H       2.642646    -1.700307    -1.125832      25.11
 C       2.941975    -0.516394    -2.897878     114.99
 O       2.780799    -1.715008    -3.654967     268.77
 H       3.655330    -1.970360    -4.016260      25.91
 H       3.779600     0.215202    -3.087710      26.29
 H       1.957659    -0.217135    -2.666401      27.34
 C      -0.473008    -0.058003     1.038818      48.43
 H      -1.259027    -0.918604     1.129270      22.51
 C       0.193924     2.283279     1.113873      54.56
 H       0.044340     3.406460     1.561858      20.72
 C       1.466642     1.890661     0.444124       2.33
 O       2.531355     2.743298     0.336677     184.74
 C       2.418164     4.189286     0.615873      68.95
 H       3.336068     4.560004    -0.115249      21.97
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 H       1.464694     4.497460     0.157026      25.39
 H       2.327536     4.179381     1.967099      21.10
 C       1.653099     0.519619     0.006014       4.09
 O       2.897823     0.319401    -0.592802     162.10
 C       0.653575    -0.513062     0.424438      45.66
 H       1.003357    -1.645628     0.394583      21.67
 C      -0.795470     1.343733     1.284947      21.66
 C      -2.112577     1.717930     2.003534      88.87
 H      -2.608766     0.814897     2.514825      22.13
 O      -1.747511     2.445263     3.307182     226.83
 H      -2.243821     1.781209     3.899745      23.61
 C      -2.881837     2.585131     1.108818      99.75
 H      -2.094619     3.296326     0.912094      25.40
 O      -3.360659     1.900525    -0.149917     214.17
 H      -2.736348     1.836406    -0.940072      28.56
 C      -4.168889     3.233579     1.702840     106.28
 O      -5.237070     3.753341     0.760261     267.37
 H      -4.707996     4.548134     0.316842      26.76
 H      -3.972131     3.842911     2.480027      28.66
 H      -4.684453     2.269724     1.946576      25.91
55
name = lig-etoh-Waterframe_993
 C       5.073259    -0.838299     1.424882      49.02
 H       5.500885     0.179059     1.183051      21.41
 C       4.555391    -3.137595     0.575107      61.35
 H       4.454889    -3.851638    -0.242912      21.99
 C       4.798855    -3.674398     1.816114      21.95
 O       4.598469    -5.029711     2.305556     215.27
 C       3.835037    -5.944829     1.404225     110.02
 H       2.865054    -5.483388     1.128801      25.36
 H       3.695238    -6.871212     1.983872      24.67
 H       4.767133    -6.200486     0.597205      23.28
 C       5.255509    -2.911569     2.894764       2.47
 O       5.705413    -3.349641     4.115180     243.47
 H       5.222780    -4.224410     4.381581      25.40
 C       5.340493    -1.451040     2.670047      25.89
 H       5.909461    -0.911674     3.595346      20.08
 C       4.727520    -1.792717     0.315531      25.04
 C       4.644988    -1.231548    -1.089881     108.41
 H       4.832657    -2.167717    -1.610643      23.22
 O       5.716251    -0.385296    -1.478453     223.29
 H       5.583545     0.528197    -1.113312      26.71
 C       3.228358    -0.813222    -1.381580     100.35
 H       2.531570    -1.623501    -1.061917      23.34
 C       2.863213    -0.546096    -2.695708     104.71
 O       2.749239    -1.768133    -3.707787     236.93
 H       3.625871    -1.839331    -4.216388      23.95
 H       3.594512     0.174947    -3.315609      23.59
 H       2.095776     0.169445    -3.020059      25.37
 C      -0.488638    -0.027148     0.965050      32.10
 H      -1.269389    -0.845921     1.363937      22.12
 C       0.295714     2.288054     1.125515      59.62
 H       0.237192     3.233842     1.818478      19.76
 C       1.344984     1.854465     0.450701      14.42
 O       2.545448     2.718559     0.371869     190.13
 C       2.346111     4.108456     0.661017     125.76
 H       3.210998     4.924311     0.446403      23.40
 H       1.397077     4.740326     0.703847      26.25
 H       2.842163     4.383359     1.666933      24.80
 C       1.564328     0.499748     0.025768      26.49
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 O       2.858709     0.376078    -0.564983     143.54
 C       0.790041    -0.474030     0.406284      63.09
 H       0.792555    -1.669366     0.015945      20.02
 C      -0.758611     1.303907     1.352374      16.26
 C      -2.070386     1.715629     2.049210      89.96
 H      -2.689654     0.834684     1.981706      25.62
 O      -1.735169     2.370217     3.225127     292.95
 H      -2.000120     1.988615     4.119405      26.75
 C      -2.959750     2.679432     1.063075      84.90
 H      -2.481146     3.581098     0.672527      25.25
 O      -3.353107     1.807515    -0.136707     207.12
 H      -2.717493     2.051210    -0.895346      26.82
 C      -4.200083     3.207245     1.694906     107.65
 O      -5.166672     3.707823     0.772717     280.19
 H      -4.848438     4.462656     0.107779      27.50
 H      -4.217030     4.090200     2.301224      25.73
 H      -4.760712     2.446041     2.425668      26.09
55
name = lig-etoh-Waterframe_994
 C       5.095134    -0.852114     1.463503      59.09
 H       5.340214     0.253451     1.451584      22.62
 C       4.504291    -3.239712     0.548514      62.55
 H       4.429693    -3.929817    -0.316913      24.55
 C       4.794255    -3.779521     1.847576      -8.27
 O       4.647639    -5.123077     2.243682     269.49
 C       3.896974    -5.976810     1.524697     119.90
 H       2.983596    -5.538329     1.320220      30.20
 H       3.647104    -6.737077     2.026691      25.78
 H       4.069419    -6.139602     0.338284      23.48
 C       5.198200    -2.782626     2.929101      19.19
 O       5.701777    -3.323039     4.100836     226.44
 H       5.339902    -4.150696     4.397621      24.72
 C       5.431864    -1.485172     2.733259      42.27
 H       5.967285    -0.844114     3.663507      20.27
 C       4.770857    -1.697143     0.380258      15.58
 C       4.660094    -1.317723    -1.098618      79.10
 H       4.607659    -2.210648    -1.763693      19.99
 O       5.715794    -0.351018    -1.489658     261.94
 H       5.465371     0.492412    -1.160203      27.85
 C       3.121629    -0.857128    -1.315847      67.44
 H       2.640182    -1.734536    -0.820723      17.75
 C       2.798235    -0.498162    -2.865282      82.43
 O       2.719900    -1.717584    -3.700653     253.19
 H       3.676895    -1.834045    -4.120176      23.40
 H       3.835591    -0.116491    -3.189793      20.10
 H       1.686833     0.047007    -2.891437      21.87
 C      -0.512309    -0.030906     0.944938      55.02
 H      -1.316040    -0.782784     1.271725      21.57
 C       0.256609     2.237932     1.220092      66.77
 H       0.425612     3.228021     1.647794      18.62
 C       1.415604     1.904682     0.454522      13.05
 O       2.505899     2.690151     0.362133     206.87
 C       2.396625     4.141782     0.837464      88.27
 H       2.743644     4.514463    -0.156952      23.48
 H       1.207585     4.370359     0.757817      22.53
 H       2.625486     4.071192     1.771918      28.47
 C       1.662717     0.574285    -0.001598      13.35
 O       2.834668     0.433514    -0.546639     141.68
 C       0.706427    -0.481045     0.394517      56.29
 H       0.898385    -1.529497    -0.211309      17.95
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 C      -0.703699     1.251889     1.396476      44.27
 C      -2.036958     1.696547     1.954898      76.66
 H      -2.751484     0.904065     2.062744      24.07
 O      -1.709583     2.357495     3.197538     265.08
 H      -2.278663     2.047781     3.975104      26.05
 C      -2.987684     2.725874     0.973369      63.12
 H      -2.535342     3.604520     0.416913      24.04
 O      -3.330451     1.741948    -0.088226     255.73
 H      -2.706588     2.156853    -0.762493      25.41
 C      -4.323748     3.230028     1.756090      95.14
 O      -5.167888     3.655262     0.723045     279.97
 H      -4.590475     4.254584     0.065586      28.07
 H      -3.639798     3.955427     2.474147      25.00
 H      -4.847722     2.540038     2.518408      26.44
55
name = lig-etoh-Waterframe_995
 C       5.163729    -0.933012     1.519260      64.01
 H       5.038463     0.146701     1.309002      22.17
 C       4.547065    -3.211363     0.612816      32.49
 H       4.233889    -3.739236    -0.315341      17.74
 C       4.753597    -3.781613     1.899341      13.80
 O       4.794175    -5.124738     2.233916     309.19
 C       3.787739    -6.022784     1.508147     130.27
 H       2.881764    -5.582676     1.715861      27.19
 H       3.851121    -7.031323     2.116554      23.59
 H       4.195264    -6.406066     0.565630      26.01
 C       5.167884    -2.860707     2.937983      14.69
 O       5.695598    -3.309184     4.131320     320.81
 H       5.306813    -4.127033     4.297180      31.08
 C       5.484743    -1.433962     2.722876      45.52
 H       5.789552    -0.758522     3.636500      20.38
 C       4.796460    -1.771023     0.434173      20.56
 C       4.607483    -1.321795    -1.070735      87.25
 H       4.926245    -2.095417    -1.832899      21.27
 O       5.661177    -0.335871    -1.512888     229.62
 H       5.492529     0.433279    -1.038646      29.15
 C       3.076976    -0.853044    -1.253342      63.11
 H       2.373604    -1.653686    -0.910802      16.70
 C       2.792876    -0.510231    -2.994738      87.77
 O       2.703711    -1.638143    -3.690917     257.41
 H       3.660996    -1.987334    -4.020254      22.45
 H       3.430488     0.340797    -3.127419      23.64
 H       1.710496     0.014257    -2.899184      22.65
 C      -0.540129    -0.122136     0.960612      38.64
 H      -1.323594    -0.828585     0.889306      19.96
 C       0.312327     2.202234     1.271493      78.20
 H      -0.095543     3.094477     1.638030      20.02
 C       1.456977     1.899977     0.536341      15.33
 O       2.511832     2.727778     0.342684     213.36
 C       2.381376     4.090727     0.892721      82.59
 H       2.812572     4.722086     0.073720      24.44
 H       1.227668     4.295648     0.951130      23.22
 H       2.806761     4.220681     1.980729      23.49
 C       1.618162     0.598656     0.058640      13.97
 O       2.912244     0.405272    -0.609051     167.75
 C       0.655358    -0.395827     0.276017      70.42
 H       0.734166    -1.473383     0.079069      18.20
 C      -0.734845     1.248404     1.411113      28.31
 C      -2.067994     1.753873     1.849857      90.52
 H      -2.621035     0.900034     2.268816      21.40
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 O      -1.700743     2.386413     3.216255     232.17
 H      -2.485945     2.041880     3.668358      25.77
 C      -3.007996     2.610348     0.978634      89.80
 H      -2.406506     3.517836     0.650879      22.26
 O      -3.306262     1.717552    -0.060472     289.29
 H      -2.937912     1.728879    -0.995734      24.16
 C      -4.269747     3.206101     1.773068      91.07
 O      -5.211880     3.647939     0.673503     266.96
 H      -4.586452     4.239952     0.095234      28.53
 H      -3.992356     4.128264     2.637692      23.25
 H      -4.875728     2.424308     2.159955      26.33
55
name = lig-etoh-Waterframe_996
 C       5.197714    -0.966054     1.446478      40.80
 H       5.173819     0.112479     1.278444      16.48
 C       4.604715    -3.147442     0.698603      63.89
 H       4.158118    -3.798282    -0.074894      10.75
 C       4.737650    -3.714692     1.951292      73.53
 O       4.910535    -5.133381     2.195799     314.82
 C       3.747261    -6.095511     1.565749     118.16
 H       2.701661    -5.705041     1.558068      24.19
 H       4.091313    -7.096091     2.302022      26.11
 H       4.047149    -6.139192     0.573369      33.77
 C       5.250654    -2.896458     2.958215       6.82
 O       5.661415    -3.325686     4.187235     273.46
 H       5.259172    -4.281235     4.453727      24.60
 C       5.455176    -1.497073     2.761474      39.18
 H       5.650193    -0.884206     3.569936      20.37
 C       4.803703    -1.889344     0.402170      45.93
 C       4.566736    -1.285354    -1.009757     133.27
 H       4.739761    -2.270034    -1.542729      26.10
 O       5.545189    -0.315248    -1.505895     195.66
 H       5.648958     0.438707    -0.961836      29.84
 C       3.117904    -0.823574    -1.376358      90.55
 H       2.315545    -1.515276    -1.119225      21.11
 C       2.763075    -0.411749    -2.843166      99.82
 O       2.734924    -1.632552    -3.764525     231.82
 H       3.737792    -1.869078    -4.050304      24.48
 H       3.247213     0.340476    -3.436565      25.11
 H       1.727594    -0.170492    -3.025551      24.64
 C      -0.593734    -0.116545     0.958986      49.60
 H      -1.315760    -0.807261     0.824996      20.57
 C       0.279291     2.171644     1.320230      63.40
 H       0.001388     3.147205     1.568953      20.41
 C       1.480946     1.879945     0.667237      -2.18
 O       2.562590     2.807821     0.333088     201.96
 C       2.343215     4.069255     0.909903     129.61
 H       2.887921     4.904148     0.593668      25.67
 H       1.424720     4.505756     1.188879      26.63
 H       3.153891     4.240705     1.903090      21.86
 C       1.654907     0.565272     0.077818       2.27
 O       2.920972     0.368321    -0.626473     165.26
 C       0.609819    -0.363114     0.178431      77.27
 H       0.844962    -1.290437    -0.013319      20.39
 C      -0.775576     1.184062     1.334491      31.57
 C      -2.083704     1.757968     1.948865      82.45
 H      -2.689625     0.760981     1.998005      21.33
 O      -1.743563     2.441951     3.196336     272.11
 H      -2.313991     2.305620     3.973697      26.88
 C      -2.935267     2.550108     1.029973      97.86
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 H      -2.359126     3.421832     0.642724      22.89
 O      -3.356409     1.641424    -0.063282     266.13
 H      -3.001075     1.929995    -0.975304      24.51
 C      -4.253946     3.120518     1.667388     107.09
 O      -5.211413     3.668516     0.654500     287.50
 H      -4.939706     4.448167     0.108901      29.91
 H      -4.335530     3.944552     2.393023      25.36
 H      -4.705575     2.302159     2.124219      29.09
55
name = lig-etoh-Water-frame_997
 C       5.232375    -1.014272     1.424069      58.81
 H       5.520054     0.005864     1.338560      19.71
 C       4.569619    -3.259375     0.719133      22.48
 H       4.292714    -4.004911    -0.039102      14.91
 C       4.806024    -3.746878     2.032604      16.45
 O       4.905493    -5.133163     2.118774     292.03
 C       3.878479    -6.084138     1.639245     103.78
 H       2.750336    -5.716007     1.769332      22.56
 H       3.775727    -7.236166     2.151390      23.12
 H       3.962901    -6.238641     0.592202      29.21
 C       5.364888    -2.886557     3.043001     -11.34
 O       5.639241    -3.341347     4.274794     213.64
 H       5.069826    -4.387837     4.476845      24.07
 C       5.381280    -1.542825     2.725639      74.81
 H       5.644924    -1.010080     3.504170      26.33
 C       4.816435    -1.740358     0.367502      42.52
 C       4.530128    -1.325903    -1.016949     130.93
 H       4.595407    -2.139547    -1.763095      23.99
 O       5.441685    -0.313276    -1.496937     235.36
 H       5.427803     0.424639    -0.847214      26.47
 C       3.154585    -0.791465    -1.489021      86.13
 H       2.602285    -1.703233    -1.270208      19.34
 C       2.703461    -0.368462    -2.799713     101.60
 O       2.798564    -1.615084    -3.820815     194.01
 H       3.791381    -1.754273    -4.086893      24.20
 H       3.499933     0.293621    -3.257617      22.84
 H       1.722281    -0.144797    -2.606690      24.24
 C      -0.602368    -0.109267     0.838594      32.88
 H      -1.399370    -0.806686     1.053267      19.07
 C       0.237912     2.143805     1.321006      67.17
 H       0.287240     3.130516     1.643141      18.98
 C       1.568415     1.848220     0.721634      -8.87
 O       2.522000     2.848252     0.334961     192.57
 C       2.448363     4.179725     1.046649      92.92
 H       2.832175     4.802613     0.077544      20.97
 H       1.462449     4.379554     1.209977      28.54
 H       2.697418     3.733142     2.023216      25.77
 C       1.731940     0.570740     0.082934      18.49
 O       2.851998     0.389483    -0.571876     141.59
 C       0.601689    -0.391644     0.147433      50.03
 H       0.772824    -1.283577    -0.361666      19.32
 C      -0.829479     1.237237     1.340970      32.64
 C      -2.082939     1.618645     2.101558      75.50
 H      -2.865109     0.824746     2.406849      20.93
 O      -1.793037     2.523704     3.174794     275.92
 H      -2.193422     2.182441     3.988709      26.70
 C      -2.898079     2.590548     1.015363      85.33
 H      -2.316865     3.302822     0.438705      23.96
 O      -3.399586     1.569418    -0.062478     239.23
 H      -3.184265     2.249296    -0.767992      23.90
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C	-4.290028	3.056759	1.522513	104.76
O	-5.221420	3.652403	0.635323	332.13
H	-4.732199	4.450861	0.398628	31.56
H	-3.939292	3.620693	2.293057	27.17
H	-4.800995	2.194261	2.011090	27.67