Supporting Information. Results from additional runs, Lipid14 force field parameters, residue atom names, atom types, atom partial charges.

LIPID14: The Amber Lipid Force Field

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Lipid14 results from additional runs

Table S1. Lipid bilayer structural results from additional simulations. A single 125ns production was extended to run out to 250ns. A production run was restarted using the standard heating protocol (run for 125ns with the first 25ns removed for equilibration). Two 50ns production runs were performed on CPUs using the same protocol as the GPU production runs (with 5ns equilibration time). See article text for detailed description of experimental terms.

Lipid system	Area per lipid A_L (Å^2)	Volume per lipid V_L (Å^3)	Isothermal area compressibility modulus K_A (mNm^{-1})	Bilayer thickness D_{HH} (Å)	Bilayer Luzzati thickness D_B (Å)
DLPC					
GPU extended	63.51	949.04	317.23	29.85	29.91
GPU cold restart	63.16	948.75	319.39	31.00	30.23
CPU run1	63.19	949.53	248.54	29.90	30.08
CPU run2	63.67	948.93	233.19	30.30	29.81
DMPC					
GPU extended	60.13	1048.58	234.00	34.20	34.90
GPU cold restart	59.29	1048.96	213.55	34.20	35.41
CPU run1	60.09	1051.35	172.20	34.35	35.01
CPU run2	59.70	1046.93	148.65	35.20	35.11
DPPC					
GPU extended	62.11	1178.51	346.35	37.90	37.97
GPU cold restart	61.42	1177.26	269.54	37.75	38.36
CPU run1	62.41	1177.94	463.88	37.75	37.77
CPU run2	62.47	1177.79	384.36	36.60	37.73
DOPC					
GPU extended	68.85	1249.61	457.15	36.85	36.31
GPU cold restart	69.04	1249.26	284.22	37.00	36.21
CPU run1	69.00	1249.72	466.65	37.05	36.24
CPU run2	68.94	1249.65	556.11	37.40	36.26
POPC					
GPU extended	65.27	1205.51	367.91	37.25	36.96
GPU cold restart	65.59	1205.61	235.21	36.75	36.79
CPU run1	65.27	1205.50	441.45	37.30	36.95
CPU run2	65.76	1205.73	266.54	37.60	36.69
POPE					
GPU extended	55.57	1138.84	294.59	41.70	41.01
GPU cold restart	55.74	1138.92	367.41	42.25	40.89
CPU run1	55.78	1139.16	286.61	42.25	40.87
CPU run2	55.97	1139.17	142.73	41.65	40.74

Lipid14 force field parameters

Please see http://ambermd.org for specific implementation details for AMBER. Please see http://ambermd.org/formats.html for the specifications of the AMBER force field parameter and topology files.

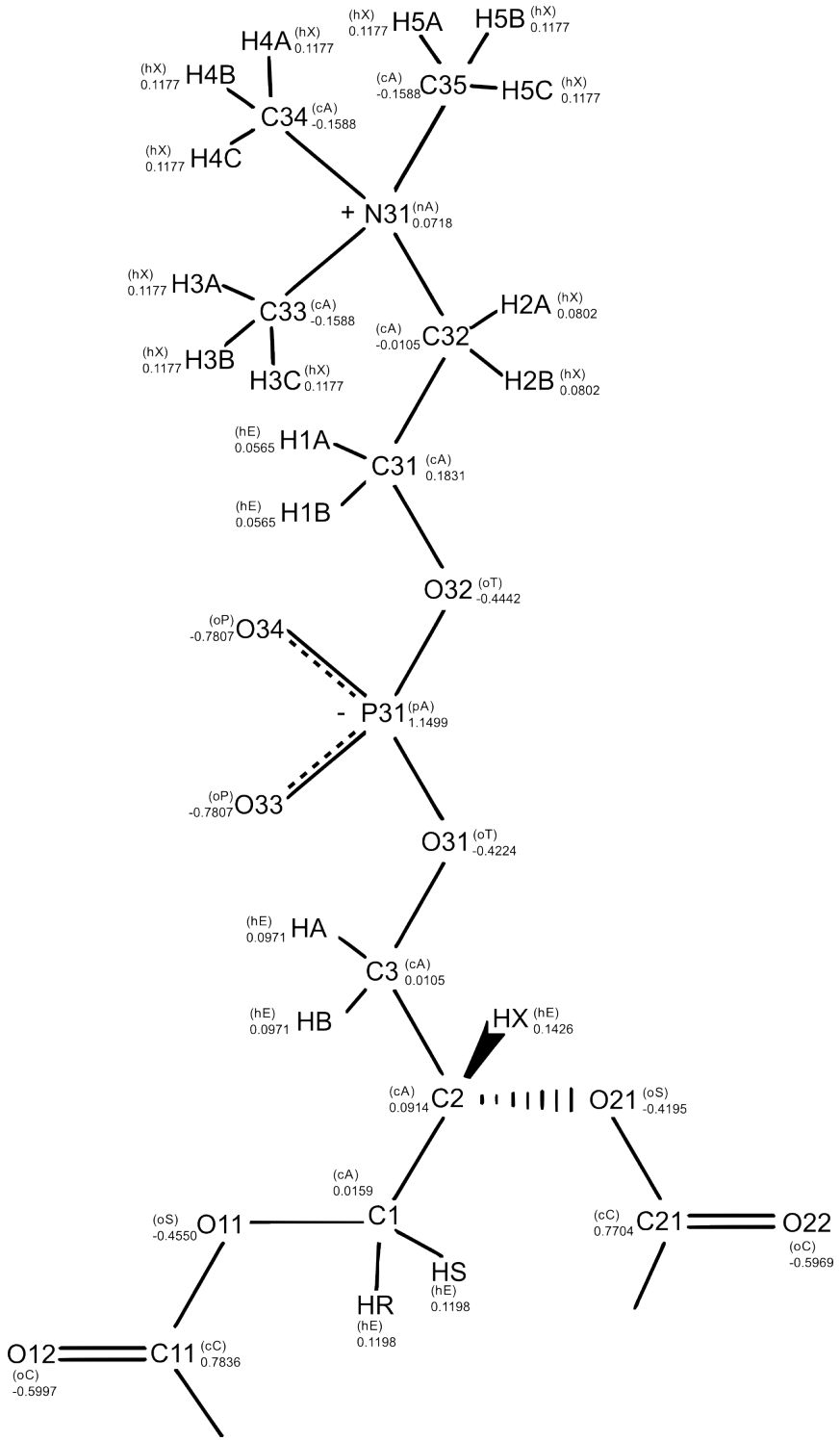

Figure S1. Atoms names, atom types (in parentheses) and atom charges in the Lipid14 phosphatidylcholine residue. The Lipid14 residue name is PC.

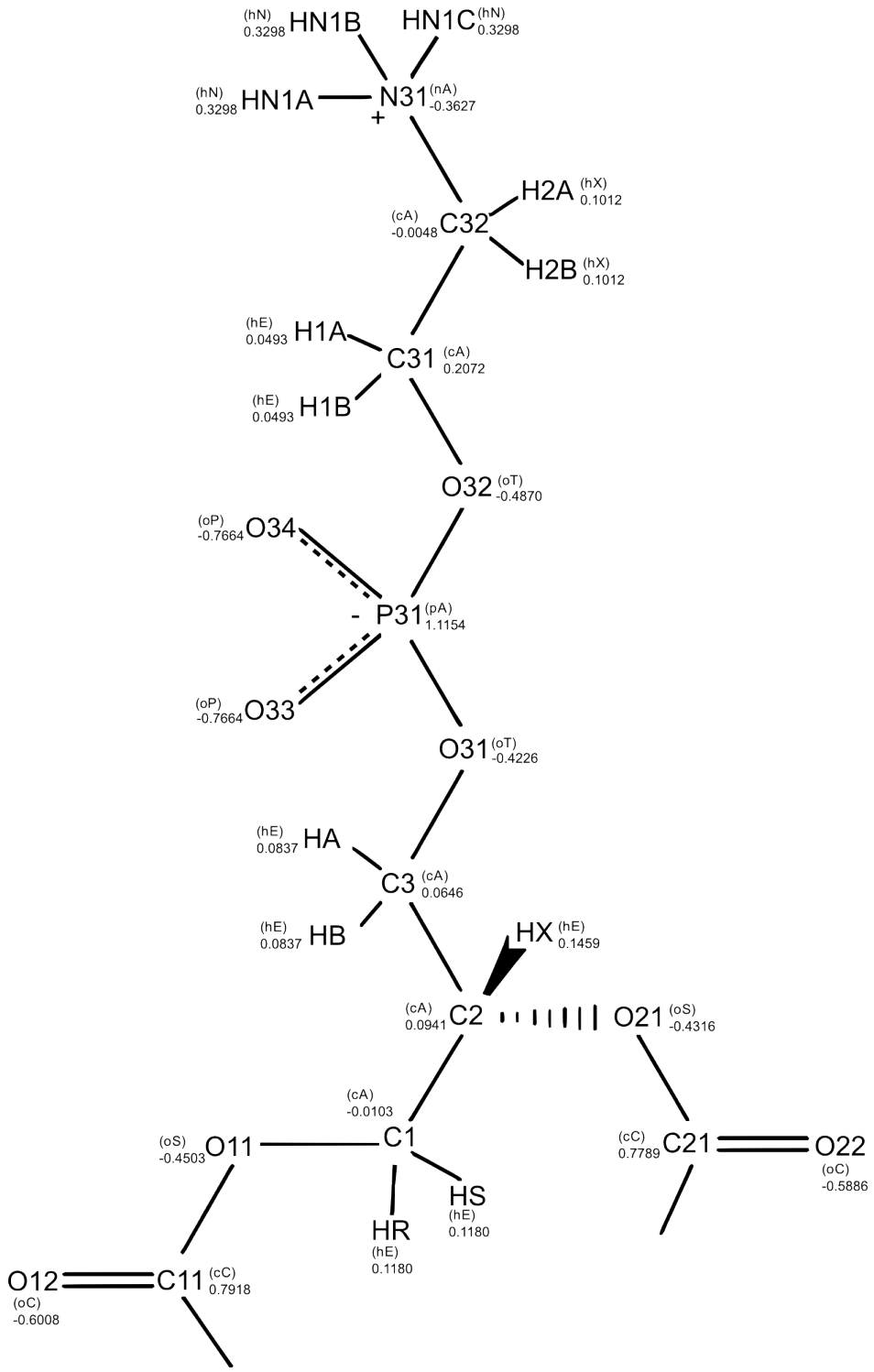

Figure S2. Atoms names, atom types (in parentheses) and atom charges in the Lipid14 phosphatidylethanolamine residue. The Lipid14 residue name is PE.

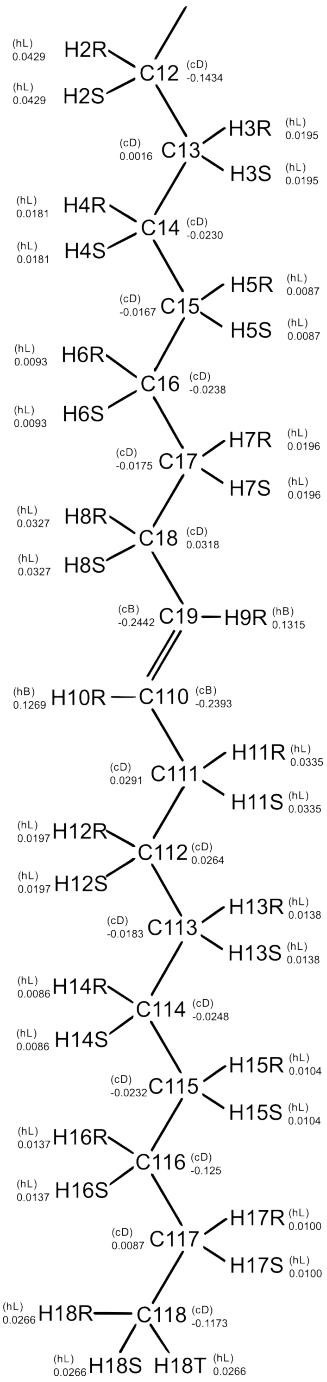

Figure S3. Atoms names, atom types (in parentheses) and atom charges in the Lipid14 oleoyl residue. The Lipid14 residue name is OL.

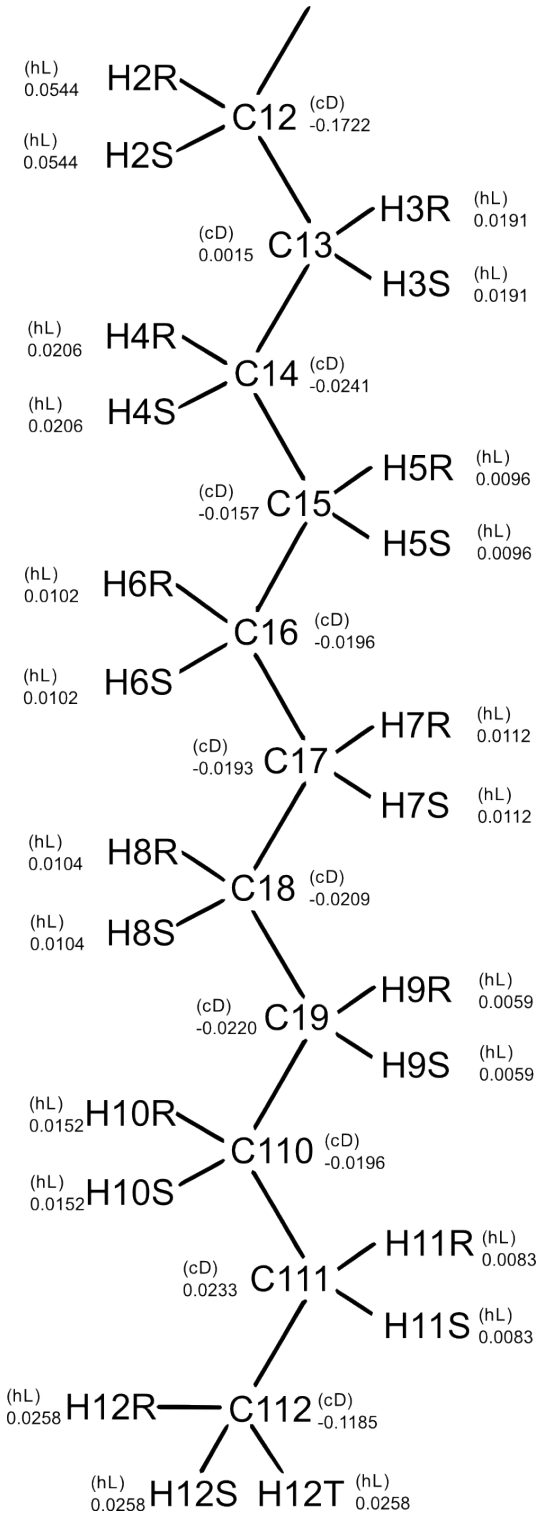

Figure S4. Atoms names, atom types (in parentheses) and atom charges in the Lipid14 lauroyl residue. The Lipid14 residue name is LA.

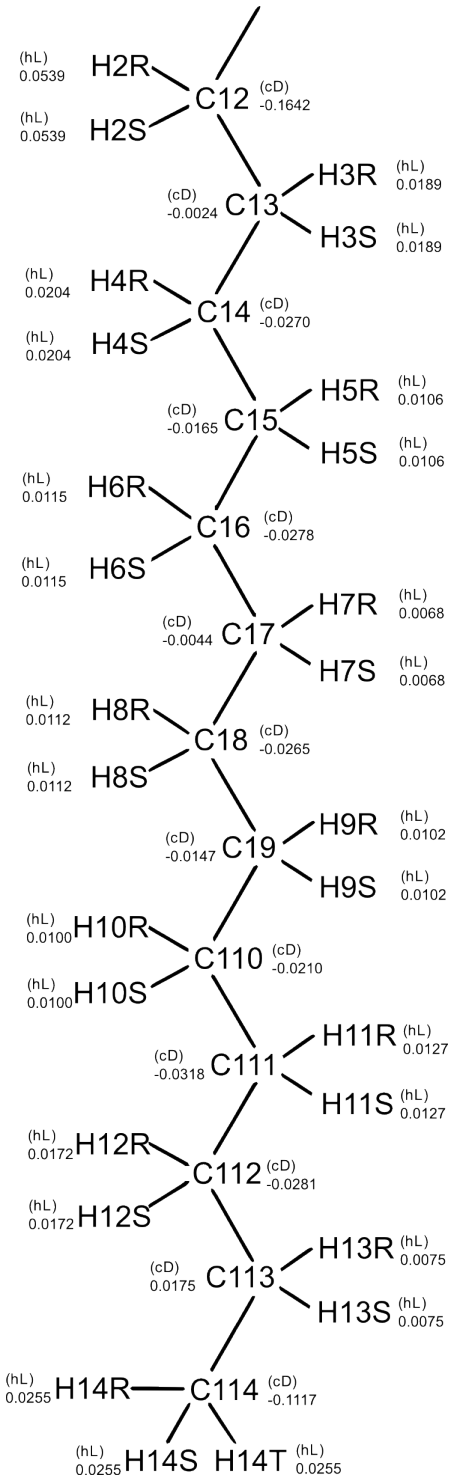

Figure S5. Atoms names, atom types (in parentheses) and atom charges in the Lipid14 myristoyl residue. The Lipid14 residue name is MY.

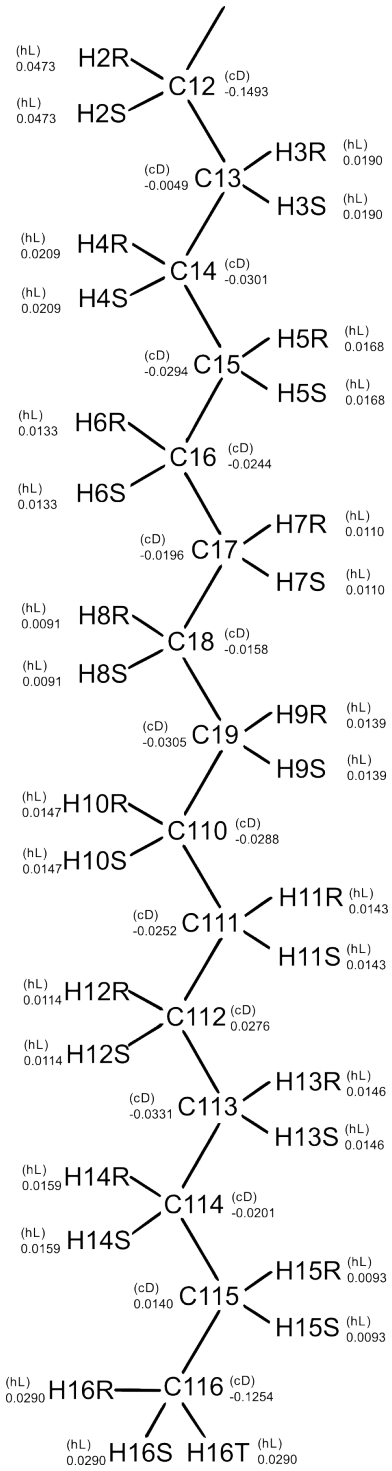

Figure S6. Atoms names, atom types (in parentheses) and atom charges in the Lipid14 palmitoyl residue. The Lipid14 residue name is PA.

Lipid14 force field parameter file (lipid14.dat)

This is the actual lipid14.dat file. Changes due to the introduction of new atom types (cD, hL) are italicized. New parameters are in bold text.

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AMBER Lipid14 Force Field, C. Dickson, B. Madej, A.Skjevik, K. Teigen, I.R. Gould, R.C. Walker*
cA 12.01                              sp3 carbon (GAFF c3-head,glycerol)
cB 12.01                              aliphatic sp2 carbon (GAFF c2-tail)
cC 12.01                              carbonyl sp2 carbon (GAFF c -head,glycerol)
cD 12.010                             sp3 carbon (GAFFlipid a3-tail)
oC 16.00                              sp2 oxygen with one connected atom (e.g C=O, COO-) (GAFF o -)
oS 16.00                              sp3 oxygen in ethers and esters (GAFF os-)
oP 16.00                              sp2 oxygen with one connected atom (e.g P-O) in phosphate group (GAFF o -)
oT 16.00                              sp3 oxygen bonded to carbon in phosphate group (GAFF os-)
nA 14.01                              sp3 N with four connected atoms (GAFF n4-)
pA 30.97                              phosphorus with four connected atoms, such as O=P(OH)3 (GAFF p5-)
hE 1.008                              H bonded to aliphatic carbon with 1 electrwd. group (GAFF h1-)
hX 1.008                              H bonded to C next to positively charged group (GAFF hx-)
hB 1.008                              H bonded to aromatic carbon (GAFF ha-)
hN 1.008                              H bonded to nitrogen (GAFF hn-)
hL 1.008                              H bonded to aliphatic carbon without electrwd. group (GAFFlipid h1-)

cA cB cC cD oC oS oP oT nA pA hE hX hB hN hL
cA-cA  303.1    1.5350       Lipid11  v1.0 (GAFF c3-c3)
cA-hE  335.9    1.0930       Lipid11  v1.0 (GAFF c3-h1)
cA-hX  338.7    1.0910       Lipid11  v1.0 (GAFF c3-hx)
cA-nA  293.6    1.4990       Lipid11  v1.0 (GAFF c3-n4)
cA-oS  301.5    1.4390       Lipid11  v1.0 (GAFF c3-os)
cA-oT  301.5    1.4390       Lipid11  v1.0 (GAFF c3-os)
cB-cB  589.7    1.3240       Lipid11  v1.0 (GAFF c2-c2)
cB-hB  344.3    1.0870       Lipid11  v1.0 (GAFF c2-ha)
cC-oC  648.0    1.2140       Lipid11  v1.0 (GAFF c -o )
cC-oS  411.3    1.3430       Lipid11  v1.0 (GAFF c -os)
cD-cB  328.3    1.5080       Lipid14  v2.0 (GAFF c3-c2)
cD-cC  328.3    1.5080       Lipid14  v2.0 (GAFF c3-c )
cD-cD  303.1    1.5350       Lipid14  v2.0 (GAFF c3-c3)
cD-hL  337.3    1.0920       Lipid14  v2.0 (GAFF c3-hc)
hN-nA  369.0    1.0330       Lipid11  v1.0 (GAFF hn-n4)
oP-pA  487.7    1.4810       Lipid11  v1.0 (GAFF o -p5)
oT-pA  342.5    1.6020       Lipid11  v1.0 (GAFF os-p5)


cA-cA-cA   63.210     110.630   Lipid11  v1.0 (GAFF c3-c3-c3)
cA-cA-hE   46.360     110.070   Lipid11  v1.0 (GAFF c3-c3-h1)
cA-cA-hX   46.020     111.740   Lipid11  v1.0 (GAFF c3-c3-hx)
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cA-nA-cA   62.840     110.640   Lipid11  v1.0 (GAFF c3-n4-c3)
cA-nA-hN   46.190     110.110   Lipid11  v1.0 (GAFF c3-n4-hn)
cA-oS-cC   63.630     115.140   Lipid11  v1.0 (GAFF c3-os-c )
cA-oT-pA   78.480     118.000   Lipid11  v1.0 (GAFF c3-os-p5)
cB-cB-hB   50.040     120.940   Lipid11  v1.0 (GAFF c2-c2-ha)
cB-cD-hL   47.030     110.490   Lipid14  v2.0 (GAFF c2-c3-hc)
cC-cD-hL   47.200     109.680   Lipid14  v2.0 (GAFF c -c3-hc)
cD-cB-cB   64.330     123.420   Lipid14  v2.0 (GAFF c3-c2-c2)
cD-cB-hB   45.660     117.300   Lipid14  v2.0 (GAFF c3-c2-ha)
cD-cC-oC   68.030     123.110   Lipid14  v2.0 (GAFF c3-c -o )
cD-cC-oS   69.260     111.960   Lipid14  v2.0 (GAFF c3-c -os)
cD-cD-cB   63.530     111.440   Lipid14  v2.0 (GAFF c3-c3-c2)
cD-cD-cC   63.790     110.530   Lipid14  v2.0 (GAFF c3-c3-c )
cD-cD-cD   63.210     110.630   Lipid14  v2.0 (GAFF c3-c3-c3)
cD-cD-hL   46.370     110.050   Lipid14  v2.0 (GAFF c3-c3-hc)
hE-cA-hE   39.180     109.550   Lipid11  v1.0 (GAFF h1-c3-h1)
hE-cA-oS   50.840     108.820   Lipid11  v1.0 (GAFF h1-c3-os)
hE-cA-oT   50.840     108.820   Lipid11  v1.0 (GAFF h1-c3-os)
hL-cD-hL   39.430     108.350   Lipid14  v2.0 (GAFF hc-c3-hc)
hN-nA-hN   40.520     108.110   Lipid11  v1.0 (GAFF hn-n4-hn)
hX-cA-hX   39.040     110.740   Lipid11  v1.0 (GAFF hx-c3-hx)
hX-cA-nA   49.020     107.910   Lipid11  v1.0 (GAFF hx-c3-n4)
oC-cC-oS   75.930     123.330   Lipid11  v1.0 (GAFF o -c -os)
oP-pA-oP   46.010     115.800   Lipid11  v1.0 (GAFF o -p5-o )
oP-pA-oT   44.010     116.090   Lipid11  v1.0 (GAFF o -p5-os)
oT-pA-oT   45.370     101.770   Lipid11  v1.0 (GAFF os-p5-os)

cA-cA-cA-hE   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
cA-cA-cA-oS   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
cA-cA-cA-oT   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
cA-cA-nA-cA   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-n4-X )
cA-cA-nA-hN   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-n4-X )
cA-cA-oT-pA   1    0.3833       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-os-X )
cA-nA-cA-hX   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-n4-X )
cA-oS-cC-oS   1    2.700      180.0          2.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c -os-X )
cA-oT-pA-oP   1    0.800        0.0          2.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -os-p5-X )
cA-oT-pA-oP   1    0.800        0.0          2.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -os-p5-X )
cA-oT-pA-oT   1    0.25         0.0         -3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF c3-os-p5-os)
cA-oT-pA-oT   1    1.20         0.0          2.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF c3-os-p5-os)
cB-cB-cD-cD   1    0.3464       0.000        1.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cB-cD-cD   1   -0.5577       0.000        2.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cB-cD-cD   1   -0.2920       0.000        3.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cB-cD-cD   1   -0.0943       0.000        4.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cB-cD-cD   1    0.0226       0.000        5.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cD-cD-cD   1    0.0251     180.000        1.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cD-cD-cD   1    0.0054     180.000        2.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cD-cD-cD   1    0.2007       0.000        3.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cD-cD-cD   1    0.2103       0.000        4.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cD-cD-cD   1    0.0811       0.000        5.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cB-cD-cD-hL   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF X -c3-c3-X )
cC-cD-cD-hL   1    0.1556       0.0          3.000    SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF X -c3-c3-X )
cC-oS-cA-cA   1    0.383        0.0         -3.000    SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF c3-c3-os-c )
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cC-oS-cA-cA   1    0.80        180.0          1.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF c3-c3-os-c )
cC-oS-cA-hE   1    0.3833        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-os-X )
cD-cB-cB-cD   1    0.3073      180.000        1.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cB-cB-cD   1    4.0051      180.000        2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cB-cB-cD   1    0.1990        0.000        3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cB-cB-cD   1    0.3242        0.000        4.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cB-cB-cD   1   -0.0415        0.000        5.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cB-cB-hB   1    6.650       180.0          2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF X -c2-c2-X )
cD-cC-oS-cA   1    2.700       180.000        2.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c -os-X )
cD-cD-cC-oC   1   -0.9110      180.000        1.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oC   1    0.7382      180.000        2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oC   1    0.3290        0.000        3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oC   1   -0.5864        0.000        4.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oC   1    0.1333        0.000        5.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oS   1   -0.1226      180.000        1.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oS   1   -0.2054      180.000        2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oS   1    0.1802        0.000        3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oS   1    0.5107        0.000        4.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cC-oS   1    0.1355        0.000        5.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cD-cC   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF )
cD-cD-cD-cD   1    0.3112      180.000        1.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cD-cD   1   -0.1233      180.000        2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cD-cD   1    0.1149        0.000        3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cD-cD   1   -0.2199        0.000        4.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cD-cD   1    0.2170        0.000        5.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.10 (paramfit)
cD-cD-cD-hL   1    0.16          0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF c3-c3-c3-hc)
hB-cB-cB-hB   1    6.650       180.0          2.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c2-c2-X )
hE-cA-cA-hE   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
hE-cA-cA-nA   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
hE-cA-cA-hX   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
hE-cA-cA-oS   1    0.00          0.0         -3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF h1-c3-c3-os)
hE-cA-cA-oS   1    0.25          0.0          1.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF h1-c3-c3-os)
hE-cA-cA-oT   1    0.00          0.0         -3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF h1-c3-c3-os)
hE-cA-cA-oT   1    0.25          0.0          1.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF h1-c3-c3-os)
hE-cA-oT-pA   1    0.3833        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-os-X )
hB-cB-cD-cD   1    0.000         0.0          2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF X -c3-c2-X )
hB-cB-cD-hL   1    0.000         0.0          2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF X -c3-c2-X )
hL-cD-cB-cB   1    0.38        180.0         -3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF hc-c3-c2-c2)
hL-cD-cB-cB   1    1.15          0.0          1.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF hc-c3-c2-c2)
hL-cD-cC-oC   1    0.80          0.0         -1.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF hc-c3-c -o )
hL-cD-cC-oC   1    0.08        180.0          3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF hc-c3-c -o )
hL-cD-cC-oS   1    0.000       180.0          2.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF X -c -c3-X )
hL-cD-cD-hL   1    0.15          0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid14  v2.0 (GAFF hc-c3-c3-hc)
hN-nA-cA-hX   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-n4-X )
hX-cA-cA-oT   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
nA-cA-cA-oT   1    0.1556        0.0          3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF X -c3-c3-X )
cA-oS-cC-oC   1    2.70        180.0         -2.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF c3-os-c -o )
cA-oS-cC-oC   1    1.40        180.0          1.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF c3-os-c -o )
oS-cA-cA-oS   1    0.144         0.0         -3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF os-c3-c3-os)
oS-cA-cA-oS   1    1.175         0.0          2.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF os-c3-c3-os)
oT-cA-cA-oS   1    0.144         0.0         -3.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF os-c3-c3-os)
oT-cA-cA-oS   1    1.175         0.0          2.000     SCEE=1.2 SCNB=2.0 Lipid11  v1.0 (GAFF os-c3-c3-os)
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cD-oC-cC-oS          10.5          180.0          2.0          Lipid14  v2.0 ester improper (GAFF X -X -c -o )
cB-cD-cB-hB          1.1           180.0          2.0          Lipid14  v2.0 aliphatic improper (GAFF c2-c3-c2-ha - default)

  hw  ow  0000.      0000.                                  4.  flag for fast water - Hack for no 10-12 terms


MOD4       RE
  cA           1.9080  0.1094            OPLS
  cB           1.9080  0.0860            Lipid14 v2.10
  cC           1.9080  0.0700            Lipid14 v2.10
  cD           1.9080  0.1094            OPLS
  oC           1.6500  0.1400            Lipid14 v2.10
  oS           1.6500  0.1200            Lipid14 v2.10
  oT           1.6500  0.1200            Lipid14 v2.10
  oP           1.6500  0.1400            Lipid14 v2.10
  nA           1.8240  0.1700            OPLS
  pA           2.1000  0.2000            JCC,7,(1986),230;
  hE           1.3870  0.0157            Veenstra et al JCC,8,(1992),963
  hX           1.1000  0.0157            Veenstra et al JCC,8,(1992),963
  hB           1.2500  0.0070            Lipid14 v2.10
  hN           0.6000  0.0157           !Ferguson base pair geom.
  hL           1.4600  0.0100            Lipid14 v2.10

END
```