SUPPLEMENTARY INFORMATION

GAFFlipid parameters

Atom types

The following atom types were created:

- g1, g2, g3 carbon atoms in the glycerol region of the lipid. These are exactly the same as the c3 GAFF atom type.
- a3, b3 carbon atoms in the sn-1 and sn-2 chain respectively. These are the same as the c3 GAFF atom type however with modified Lennard-Jones parameters (r=2.01Å, ε=0.055kcal/mol).
- hl hydrogen atom in the sn-1 and sn-2 chains. This is the same as the hc GAFF atom type however with modified Lennard-Jones parameters (r=1.34Å, ε=0.024kcal/mol).

Torsion parameters

Two torsion parameters were modified using Paramfit. All other torsions were taken from GAFF.

Sn-1 chain

```
a3-a3-a3-a3    1    -0.0866       180.0001          1.000       paramfit
a3-a3-a3-a3    1    -0.1109       180.0001          2.000       paramfit
a3-a3-a3-a3    1     0.1352         0.000           3.000       paramfit

c2-a3-a3-a3    1     0.2109         0.000           3.000       paramfit
```

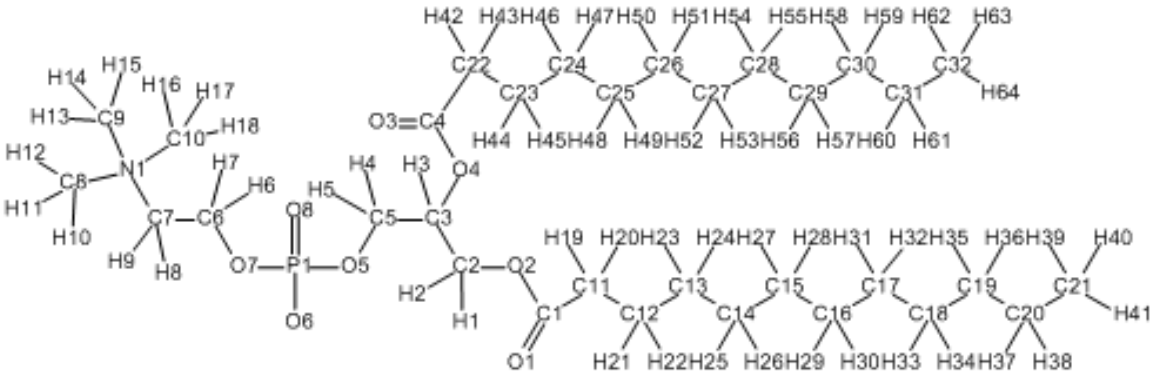
Sn-2 chain

```
b3-b3-b3-b3    1    -0.0866       180.0001          1.000       paramfit
b3-b3-b3-b3    1    -0.1109       180.0001          2.000       paramfit
b3-b3-b3-b3    1     0.1352         0.000           3.000       paramfit

c2-b3-b3-b3    1     0.2109         0.000           3.000       paramfit
```

Charges

DLPC

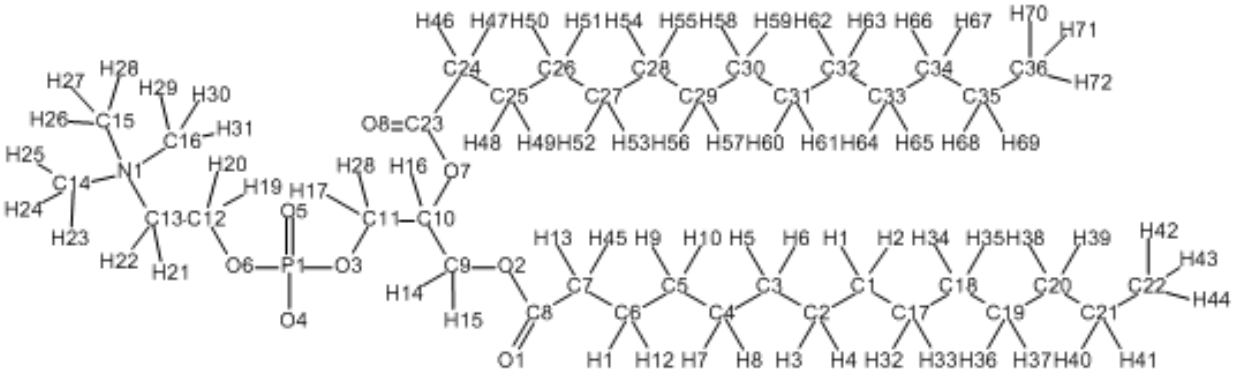


Atom name	Atom type	Charge
C20	a3	0.080314
H37	hl	-0.00909
H38	hl	-0.00909
C19	a3	-0.00809
H35	hl	0.005046
H36	hl	0.005046
C18	a3	-0.01611
H33	hl	0.000516
H34	hl	0.000516
C17	a3	0.007571
H31	hl	-0.00352
H32	hl	-0.00352
C16	a3	0.011731
H29	hl	-0.00425
H30	hl	-0.00425
C15	a3	0.009947
H27	hl	-0.00145
H28	hl	-0.00145
C14	a3	-0.01032
H25	hl	-0.00337
H26	hl	-0.00337
C13	a3	-0.00462
H23	hl	0.012983
H24	hl	0.012983
C12	a3	0.019156
H21	hl	0.004713
H22	hl	0.004713
C11	a3	-0.12468

H19	hl	0.052552
H20	hl	0.052552
C1	c	0.636392
O1	o	-0.53084
O2	os	-0.37352
C2	g1	0.012538
H1	hc	0.113642
H2	hc	0.113642
C3	g2	0.131093
H3	hc	0.137758
C5	g3	0.028727
H4	hc	0.107429
H5	hc	0.107429
O5	os	-0.43404
P1	p4	1.085275
O6	o	-0.72691
O8	o	-0.72691
O7	os	-0.40264
C6	c3	0.169293
H6	hc	0.042234
H7	hc	0.042234
C7	c3	0.045158
H8	hc	0.056736
H9	hc	0.056736
N1	n4	0.012316
C8	c3	-0.16168
H10	hc	0.117176
H11	hc	0.117176
H12	hc	0.117176
C9	c3	-0.16168
H13	hc	0.117176
H14	hc	0.117176
H15	hc	0.117176
C10	c3	-0.16168
H16	hc	0.117176
H17	hc	0.117176
H18	hc	0.117176
O4	os	-0.50751
C4	c	0.775678
O3	o	-0.58433
C22	b3	-0.04909
H42	hl	0.025767
H43	hl	0.025767
C23	b3	-0.00459

H44	hl	0.00586
H45	hl	0.00586
C24	b3	-0.00552
H46	hl	0.007891
H47	hl	0.007891
C25	b3	0.011518
H48	hl	-0.00352
H49	hl	-0.00352
C26	b3	0.012096
H50	hl	-0.00673
H51	hl	-0.00673
C27	b3	0.02615
H52	hl	-0.01045
H53	hl	-0.01045
C28	b3	0.022081
H54	hl	-0.01042
H55	hl	-0.01042
C29	b3	0.003037
H56	hl	-0.00617
H57	hl	-0.00617
C30	b3	0.004534
H58	hl	-0.00049
H59	hl	-0.00049
C31	b3	0.066338
H60	hl	-0.00942
H61	hl	-0.00942
C32	b3	-0.12472
H62	hl	0.025941
H63	hl	0.025941
H64	hl	0.025941
C21	a3	-0.15003
H39	hl	0.031811
H40	hl	0.031811
H41	hl	0.031811

DMPC



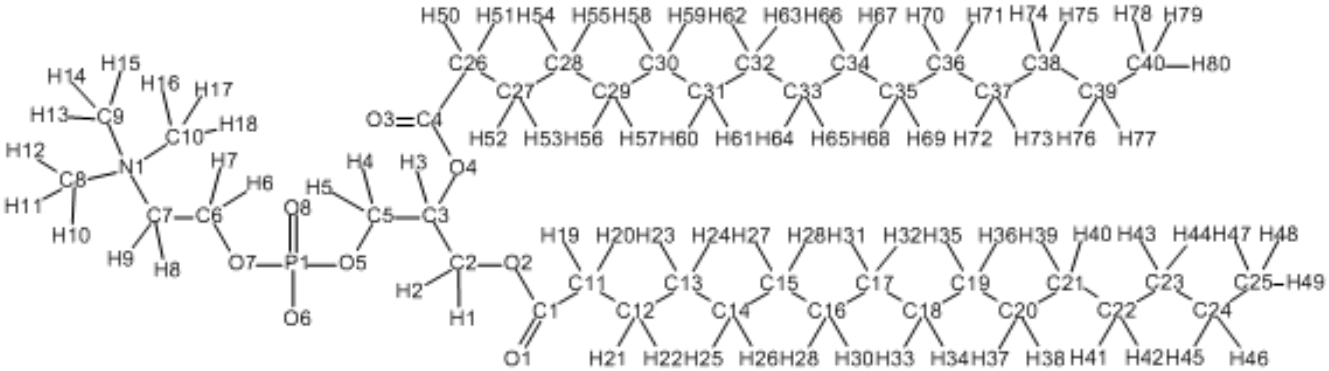
Atom name	Atom type	Charge
C22	a3	-0.13943
H42	hl	0.029884
H43	hl	0.029884
H44	hl	0.029884
C21	a3	0.066877
H40	hl	-0.00646
H41	hl	-0.00646
C20	a3	-0.00062
H38	hl	0.002479
H39	hl	0.002479
C19	a3	-0.00664
H36	hl	-0.00406
H37	hl	-0.00406
C18	a3	0.022612
H34	hl	-0.00936
H35	hl	-0.00936
C17	a3	0.02337
H32	hl	-0.00901
H33	hl	-0.00901
C1	a3	0.006657
H1	hl	-0.00713
H2	hl	-0.00713
C2	a3	0.038691
H3	hl	-0.01276
H4	hl	-0.01276
C3	a3	0.013952
H5	hl	-0.00986
H6	hl	-0.00986
C4	a3	0.007998
H7	hl	-0.00636

H8	hl	-0.00636
C5	a3	-0.0079
H9	hl	0.006894
H10	hl	0.006894
C6	a3	0.051298
H11	hl	0.010186
H12	hl	0.010186
C7	a3	-0.1626
H13	hl	0.04393
H45	hl	0.04393
C8	c	0.75978
O1	o	-0.60062
O2	os	-0.40425
C9	g1	-0.01542
H14	hc	0.120993
H15	hc	0.120993
C10	g2	0.087406
H16	hc	0.144396
C11	g3	0.044154
H17	hc	0.092393
H18	hc	0.092393
O3	os	-0.41455
P1	p4	1.109949
O4	o	-0.7226
O5	o	-0.7226
O6	os	-0.44469
C12	c3	0.168041
H19	hc	0.039679
H20	hc	0.039679
C13	c3	0.009524
H21	hc	0.080485
H22	hc	0.080485
N1	n4	0.021802
C14	c3	-0.15338
H23	hc	0.11381
H24	hc	0.11381
H25	hc	0.11381
C15	c3	-0.15338
H26	hc	0.11381
H27	hc	0.11381
H28	hc	0.11381
C16	c3	-0.15338
H29	hc	0.11381
H30	hc	0.11381

H31	hc	0.11381
O7	os	-0.41785
C23	c	0.718704
O8	o	-0.58227
C24	b3	-0.08952
H46	hl	0.045575
H47	hl	0.045575
C25	b3	0.003511
H48	hl	0.004379
H49	hl	0.004379
C26	b3	-0.00985
H50	hl	0.007371
H51	hl	0.007371
C27	b3	0.017463
H52	hl	-4.36E-05
H53	hl	-4.36E-05
C28	b3	-0.01348
H54	hl	0.000613
H55	hl	0.000613
C29	b3	0.012539
H56	hl	-0.00471
H57	hl	-0.00471
C30	b3	0.000625
H58	hl	-0.00049
H59	hl	-0.00049
C31	b3	0.007386
H60	hl	-0.00176
H61	hl	-0.00176
C32	b3	0.004726
H62	hl	-0.00142
H63	hl	-0.00142
C33	b3	-0.01026
H64	hl	-0.00026
H65	hl	-0.00026
C34	b3	-0.00287
H66	hl	0.002298
H67	hl	0.002298
C35	b3	0.069637
H68	hl	-0.00771
H69	hl	-0.00771
C36	b3	-0.13612
H70	hl	0.029142
H71	hl	0.029142
H72	hl	0.029142

Electronic Supplementary Material (ESI) for Soft Matter

DPPC



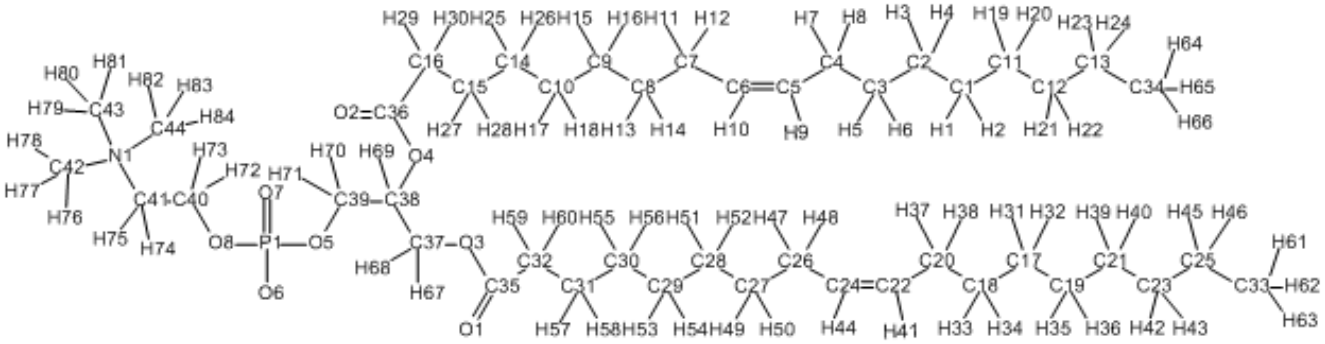
Atom name	Atom type	Charge
C23	a3	0.011053
H43	hl	-7.30E-05
H44	hl	-7.30E-05
C22	a3	-0.00628
H41	hl	-0.00585
H42	hl	-0.00585
C21	a3	0.029365
H39	hl	-0.01097
H40	hl	-0.01097
C20	a3	0.011198
H37	hl	-0.0053
H38	hl	-0.0053
C19	a3	0.018479
H35	hl	-0.00626
H36	hl	-0.00626
C18	a3	-0.00383
H33	hl	-0.00407
H34	hl	-0.00407
C17	a3	0.032267
H31	hl	-0.00891
H32	hl	-0.00891
C16	a3	-0.00442
H29	hl	-0.00325
H30	hl	-0.00325
C15	a3	0.016457
H27	hl	-0.0045
H28	hl	-0.0045
C14	a3	-0.00498
H25	hl	0.001204
H26	hl	0.001204
C13	a3	-0.00818

H23	hl	0.009148
H24	hl	0.009148
C12	a3	-0.01014
H21	hl	0.014958
H22	hl	0.014958
C11	a3	-0.0742
H19	hl	0.031168
H20	hl	0.031168
C1	c	0.727106
O1	o	-0.58459
O2	os	-0.41756
C2	g1	0.026457
H1	hc	0.115663
H2	hc	0.115663
C3	g2	0.043792
H3	hc	0.151315
C5	g3	0.038535
H4	hc	0.098733
H5	hc	0.098733
O5	os	-0.41372
P1	p4	1.09722
O6	o	-0.72048
O8	o	-0.72048
O7	os	-0.46394
C6	c3	0.285482
H6	hc	0.014201
H7	hc	0.014201
C7	c3	0.02128
H8	hc	0.041019
H9	hc	0.041019
N1	n4	0.055017
C8	c3	-0.09738
H10	hc	0.094534
H11	hc	0.094534
H12	hc	0.094534
C9	c3	-0.09738
H13	hc	0.094534
H14	hc	0.094534
H15	hc	0.094534
C10	c3	-0.09738
H16	hc	0.094534
H17	hc	0.094534
H18	hc	0.094534
O4	os	-0.42256

C4	c	0.772046
O3	o	-0.60003
C26	b3	-0.08457
H50	hl	0.031059
H51	hl	0.031059
C27	b3	0.022721
H52	hl	-0.00326
H53	hl	-0.00326
C28	b3	0.015214
H54	hl	0.001033
H55	hl	0.001033
C29	b3	0.013506
H56	hl	-0.00338
H57	hl	-0.00338
C30	b3	0.00482
H58	hl	-0.00897
H59	hl	-0.00897
C31	b3	0.030704
H60	hl	-0.01355
H61	hl	-0.01355
C32	b3	0.029241
H62	hl	-0.01183
H63	hl	-0.01183
C33	b3	0.021517
H64	hl	-0.01325
H65	hl	-0.01325
C34	b3	0.019405
H66	hl	-0.01159
H67	hl	-0.01159
C35	b3	0.037245
H68	hl	-0.01442
H69	hl	-0.01442
C36	b3	0.020266
H70	hl	-0.01133
H71	hl	-0.01133
C37	b3	0.008811
H72	hl	-0.01123
H73	hl	-0.01123
C38	b3	0.002328
H74	hl	-0.00031
H75	hl	-0.00031
C39	b3	0.084996
H76	hl	-0.0123
H77	hl	-0.0123

C40	b3	-0.1461
H78	hl	0.030144
H79	hl	0.030144
H80	hl	0.030144
C24	a3	0.064269
H45	hl	-0.00749
H46	hl	-0.00749
C25	a3	-0.13222
H47	hl	0.028289
H48	hl	0.028289
H49	hl	0.028289

DOPC



Atom name	Atom type	Charge
C33	a3	-0.13506
H61	hl	0.027797
H62	hl	0.027797
H63	hl	0.027797
C25	a3	0.084367
H45	hl	-0.01113
H46	hl	-0.01113
C23	a3	-0.0125
H42	hl	0.006459
H43	hl	0.006459
C21	a3	-0.03367
H39	hl	0.00963
H40	hl	0.00963
C19	a3	-0.01693
H35	hl	0.006705
H36	hl	0.006705
C17	a3	-0.00389
H31	hl	0.001535
H32	hl	0.001535
C18	a3	0.0072
H33	hl	0.007316
H34	hl	0.007316
C20	a3	0.04484
H37	hl	0.027339
H38	hl	0.027339
C22	c2	-0.23488
H41	hc	0.115649
C24	c2	-0.2079
H44	hc	0.117152
C26	a3	0.027135
H47	hl	0.028662
H48	hl	0.028662

C27	a3	-0.00621
H49	hl	0.006144
H50	hl	0.006144
C28	a3	0.00319
H51	hl	0.001425
H52	hl	0.001425
C29	a3	-0.01841
H53	hl	0.005691
H54	hl	0.005691
C30	a3	0.011864
H55	hl	0.005074
H56	hl	0.005074
C31	a3	0.016422
H57	hl	0.000663
H58	hl	0.000663
C32	a3	-0.06855
H59	hl	0.02545
H60	hl	0.02545
C35	c	0.70891
O1	o	-0.56898
O3	os	-0.39093
C37	g1	-0.03749
H67	hc	0.126461
H68	hc	0.126461
C38	g2	0.079998
H69	hc	0.136169
C39	g3	0.01006
H70	hc	0.107655
H71	hc	0.107655
O5	os	-0.40744
P1	p4	1.06745
O6	o	-0.71298
O7	o	-0.71298
O8	os	-0.40414
C40	c3	0.142683
H72	hc	0.057749
H73	hc	0.057749
C41	c3	-0.01483
H74	hc	0.073563
H75	hc	0.073563
N1	n4	0.019315
C42	c3	-0.14067
H76	hc	0.110461
H77	hc	0.110461

H78	hc	0.110461
C43	c3	-0.14067
H79	hc	0.110461
H80	hc	0.110461
H81	hc	0.110461
C44	c3	-0.14067
H82	hc	0.110461
H83	hc	0.110461
H84	hc	0.110461
O4	os	-0.42262
C36	c	0.746096
O2	o	-0.58309
C16	b3	-0.00459
H29	hl	0.007325
H30	hl	0.007325
C15	b3	-0.00432
H27	hl	0.010081
H28	hl	0.010081
C14	b3	-0.0249
H25	hl	0.008108
H26	hl	0.008108
C10	b3	-0.00403
H17	hl	0.001853
H18	hl	0.001853
C9	b3	0.009933
H15	hl	0.000202
H16	hl	0.000202
C8	b3	-0.02661
H13	hl	0.013481
H14	hl	0.013481
C7	b3	0.044251
H11	hl	0.035453
H12	hl	0.035453
C6	c2	-0.26316
H10	hc	0.131941
C5	c2	-0.17236
H9	hc	0.109585
C4	b3	-0.00395
H7	hl	0.029747
H8	hl	0.029747
C3	b3	-0.02355
H5	hl	0.015218
H6	hl	0.015218
C2	b3	0.019429

H3	hl	0.006465
H4	hl	0.006465
C1	b3	-0.03152
H1	hl	0.008452
H2	hl	0.008452
C11	b3	-0.02629
H19	hl	0.006927
H20	hl	0.006927
C12	b3	0.002474
H21	hl	0.000429
H22	hl	0.000429
C13	b3	0.083887
H23	hl	-0.01214
H24	hl	-0.01214
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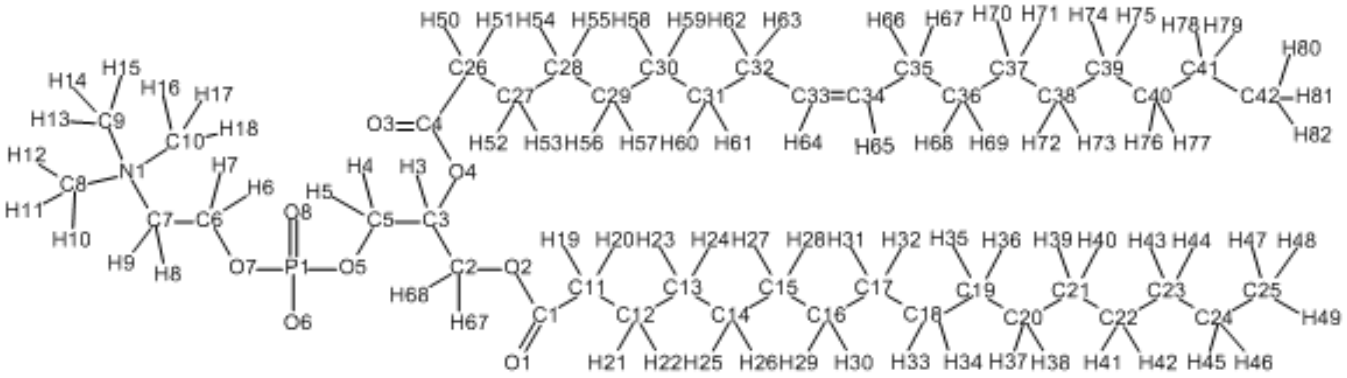
H64	hl	0.027621
H65	hl	0.027621
H66	hl	0.027621

POPC



Atom name	Atom type	Charge
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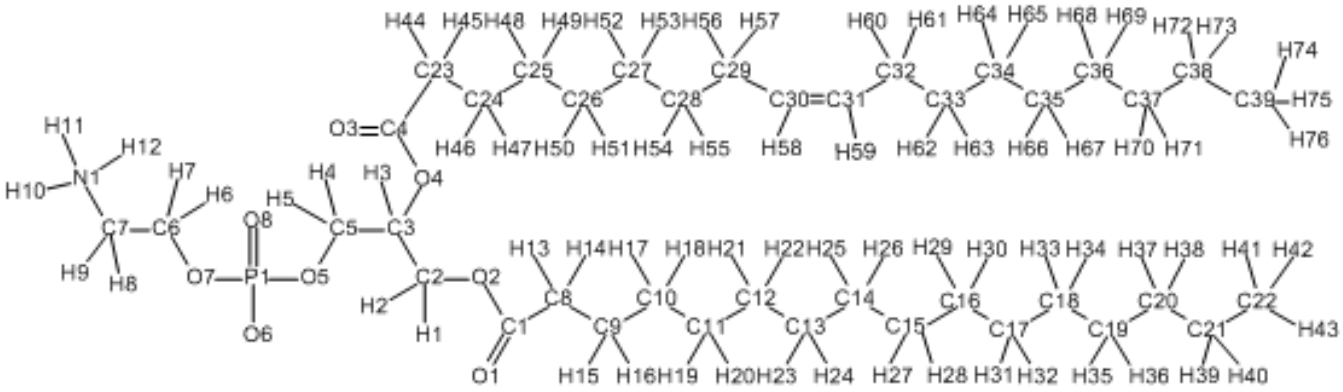
H46	hl	-0.00835
C23	a3	-0.01459
H43	hl	0.006652
H44	hl	0.006652
C22	a3	-0.03565
H41	hl	0.009043
H42	hl	0.009043
C21	a3	0.001865
H39	hl	0.000135
H40	hl	0.000135
C20	a3	-0.00408
H37	hl	0.003338
H38	hl	0.003338
C17	a3	0.034836
H31	hl	-0.01146
H32	hl	-0.01146
C16	a3	0.012557
H29	hl	-0.00821
H30	hl	-0.00821
C15	a3	0.008775
H27	hl	-0.00729
H28	hl	-0.00729
C14	a3	0.025596
H25	hl	-0.00435
H26	hl	-0.00435
C13	a3	-0.01667
H23	hl	0.009738
H24	hl	0.009738
C12	a3	0.007922

H21	hl	0.003758
H22	hl	0.003758
C11	a3	-0.10509
H19	hl	0.045089
H20	hl	0.045089
C1	c	0.705221
O1	o	-0.55615
O2	os	-0.38208
C2	g1	-0.04173
H1	hc	0.118845
H2	hc	0.118845
C3	g2	0.019264
H3	hc	0.177318
C5	g3	0.057992
H4	hc	0.086808
H5	hc	0.086808
O5	os	-0.40086
P1	p4	1.065607
O6	o	-0.72112
O8	o	-0.72112
O7	os	-0.4101
C6	c3	0.204228
H6	hc	0.038859
H7	hc	0.038859
C7	c3	-0.0012
H8	hc	0.061629
H9	hc	0.061629
N1	n4	0.039962
O4	os	-0.29866
C4	c	0.599571
O3	o	-0.56022
C26	b3	-0.06771
H50	hl	0.035157
H51	hl	0.035157
C27	b3	-0.00316
H52	hl	0.00613
H53	hl	0.00613
C28	b3	0.011064
H54	hl	0.010444
H55	hl	0.010444
C29	b3	-0.04101
H56	hl	0.015613
H57	hl	0.015613
C30	b3	-0.02854

H58	hl	0.009944
H59	hl	0.009944
C31	b3	-0.00611
H60	hl	0.012268
H61	hl	0.012268
C32	b3	0.03974
H62	hl	0.031876
H63	hl	0.031876
C33	c2	-0.24681
H64	hc	0.13018
C34	c2	-0.21727
H65	hc	0.116853
C35	b3	0.040954
H66	hl	0.023286
H67	hl	0.023286
C36	b3	-0.00524
H68	hl	0.008765
H69	hl	0.008765
C37	b3	-0.00641
H70	hl	0.002893
H71	hl	0.002893
C38	b3	0.028045
H72	hl	-0.00825
H73	hl	-0.00825
C39	b3	-0.00468
H74	hl	-0.00545
H75	hl	-0.00545
C40	b3	0.012184
H76	hl	-0.00322
H77	hl	-0.00322
C41	b3	0.07304
H78	hl	-0.01252
H79	hl	-0.01252
C42	b3	-0.11185
H80	hl	0.02185
H81	hl	0.02185
H82	hl	0.02185
C8	c3	-0.14247
H10	hc	0.110303
H11	hc	0.110303
H12	hc	0.110303
C9	c3	-0.14247
H13	hc	0.110303
H14	hc	0.110303

H15	hc	0.110303
C10	c3	-0.14247
H16	hc	0.110303
H17	hc	0.110303
H18	hc	0.110303
C25	a3	-0.15677
H47	hl	0.033342
H48	hl	0.033342
H49	hl	0.033342
C18	a3	-0.00184
H33	hl	-0.00459
H34	hl	-0.00459
C19	a3	0.005808
H35	hl	-0.00054
H36	hl	-0.00054

POPE



Atom name	Atom type	Charge
C21	a3	0.068212
H39	hl	-0.00581
H40	hl	-0.00581
C20	a3	-0.00229
H37	hl	0.00211
H38	hl	0.00211
C19	a3	-0.01816
H35	hl	0.003707
H36	hl	0.003707
C18	a3	-0.00203
H33	hl	-0.003
H34	hl	-0.003
C17	a3	0.026188
H31	hl	-0.00319
H32	hl	-0.00319
C14	a3	0.000409
H25	hl	0.003092
H26	hl	0.003092
C13	a3	-0.02069
H23	hl	0.008719
H24	hl	0.008719
C12	a3	-0.01513
H21	hl	0.006161
H22	hl	0.006161
C11	a3	-0.01524
H19	hl	0.012753
H20	hl	0.012753
C10	a3	-0.01161
H17	hl	0.005064

H18	hl	0.005064
C9	a3	0.033841
H15	hl	-0.00196
H16	hl	-0.00196
C8	a3	-0.11115
H13	hl	0.035876
H14	hl	0.035876
C1	c	0.814082
O1	o	-0.61169
O2	os	-0.45103
C2	g1	-0.00951
H1	hc	0.121089
H2	hc	0.121089
C3	g2	0.115804
H3	hc	0.126275
C5	g3	-0.01117
H4	hc	0.11539
H5	hc	0.11539
O5	os	-0.41802
P1	p4	1.106888
O6	o	-0.74652
O8	o	-0.74652
O7	os	-0.43418
C6	c3	0.116518
H6	hc	0.081046
H7	hc	0.081046
C7	c3	-0.05255
H8	hc	0.096704
H9	hc	0.096704
N1	n4	-0.18841
O4	os	-0.44335
C4	c	0.759345
O3	o	-0.59449
C23	b3	-0.07689
H44	hl	0.033063
H45	hl	0.033063
C24	b3	0.004715
H46	hl	0.010477
H47	hl	0.010477
C25	b3	-0.00538
H48	hl	0.006393
H49	hl	0.006393
C26	b3	-0.03601
H50	hl	0.014117

H51	hl	0.014117
C27	b3	0.004332
H52	hl	0.001935
H53	hl	0.001935
C28	b3	0.002666
H54	hl	0.010517
H55	hl	0.010517
C29	b3	0.013752
H56	hl	0.032774
H57	hl	0.032774
C30	c2	-0.24112
H58	hc	0.123854
C31	c2	-0.18126
H59	hc	0.111239
C32	b3	0.026943
H60	hl	0.027134
H61	hl	0.027134
C33	b3	-0.02653
H62	hl	0.009424
H63	hl	0.009424
C34	b3	0.013513
H64	hl	0.005807
H65	hl	0.005807
C35	b3	-0.02174
H66	hl	0.006199
H67	hl	0.006199
C36	b3	-0.01859
H68	hl	0.005803
H69	hl	0.005803
C37	b3	-0.01164
H70	hl	0.005805
H71	hl	0.005805
C38	b3	0.074161
H72	hl	-0.00952
H73	hl	-0.00952
C39	b3	-0.13151
H74	hl	0.027117
H75	hl	0.027117
H76	hl	0.027117
H10	hn	0.271742
H11	hn	0.271742
H12	hn	0.271742
C15	a3	-0.00916
H27	hl	0.004357

H28	hl	0.004357
C16	a3	-0.01841
H29	hl	0.00417
H30	hl	0.00417
C22	a3	-0.13812
H41	hl	0.029442
H42	hl	0.029442
H43	hl	0.029442