Supplementary Material

CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature

Richard M. Venable,[1] Alex Sodt,[1] Brent Rogaski,[2] Huan Rui,[3] Elizabeth Hatcher,[4] Alexander D. MacKerell, Jr.,[4,*] Richard W. Pastor,[1,*] and Jeffery B. Klauda[2,*]

1) Laboratory of Computational Biology, National Heart, Lung, and Blood Institute, National Institutes of Health, Bethesda, MD 20892

2) Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742

3) Center for Bioinformatics and Department of Molecular Biosciences, The University of Kansas, 2030 Becker Drive, Lawrence KS 66047, USA

4) Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, 20 Penn Street, Baltimore, Maryland 21201

*Corresponding authors: alex@outerbanks.umaryland.edu, pastorr@nhlbi.nih.gov, jbklauda@umd.edu

Table S1. CHelpG charges at the MP2/cc-pVDZ model chemistry for conformations C3 through C6 of the CER6 model for SM. Atom names correspond to Figure 2. Also shown are the charges used in unoptimized CHARMM36 (C36u) and charge optimized C36.

	C3	C4	C5	C6	C36u	C36
C3	+0.601	+0.490	+0.509	+0.421	+0.05	+0.50
H3	-0.090	+0.001	-0.087	-0.035	+0.09	-0.11
O3	-0.744	-0.655	-0.693	-0.646	-0.45	-0.69
HO	+0.429	+0.348	+0.424	+0.348	+0.31	+0.30
C2	+0.220	+0.140	+0.157	+0.284	+0.07	+0.30
H2	-0.002	+0.044	+0.013	+0.048	+0.09	+0.05
N	-0.749	-0.801	-0.776	-0.754	-0.47	-0.70
H	+0.334	+0.443	+0.351	+0.351	+0.31	+0.35
CF	+0.675	+0.743	+0.738	+0.702	+0.51	+0.55
OF	-0.515	-0.592	-0.556	-0.540	-0.51	-0.60

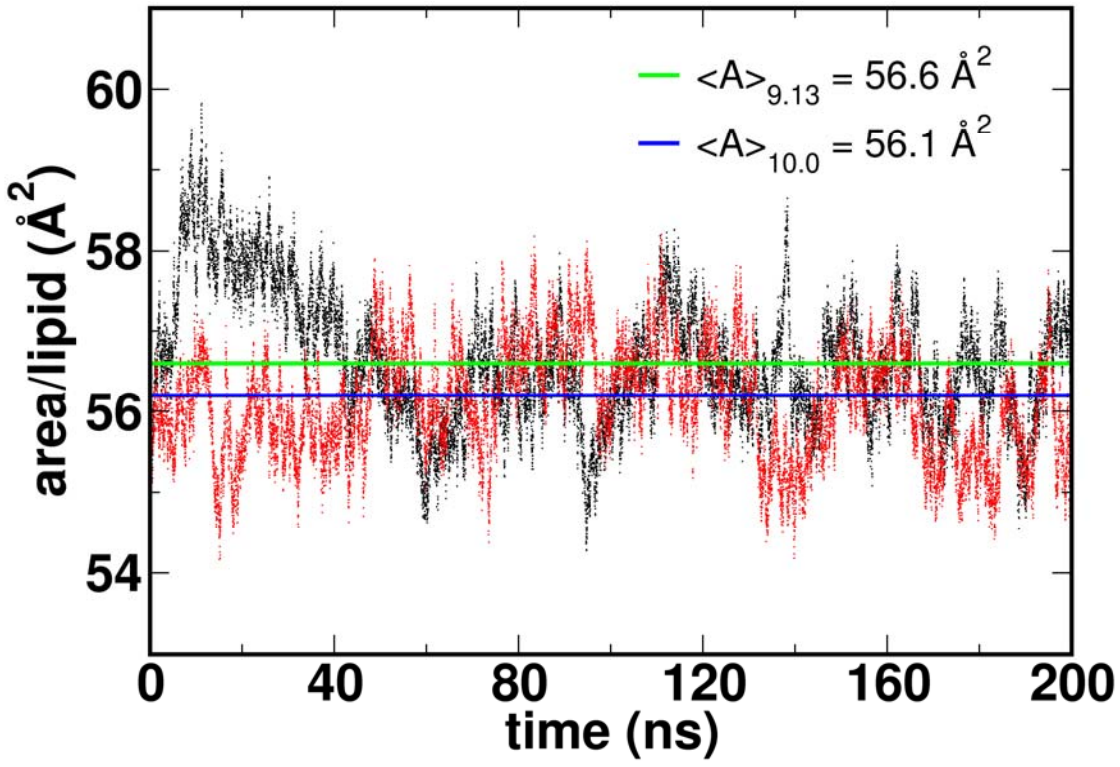

Figure S1. Effect of Anton short range nonbonded interaction cutoff on the area/lipid, A; the blue line is the average for the red time series (R_{cut} = 10.0 Å), and green is the average for the black time series (R_{cut} = 9.13 Å).

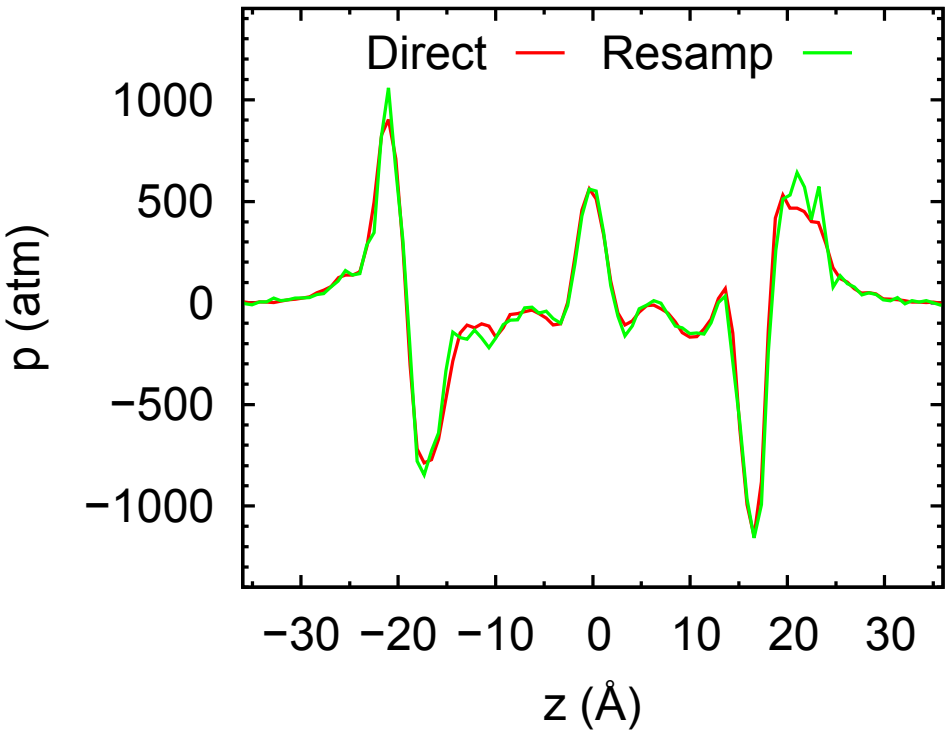

Figure S2. Comparison of pressure profiles from a 100 ns PSM simulation with full sampling (Direct) or via the 10% resampling (Resamp) of 100 ps intervals spaced 1 ns apart, using restart files from the fully sampled simulation. The $\overline{F}'(0)$ values and standard errors obtained are -0.190 ± 0.009 and -0.192 ± 0.004 for the fully sampled and resampled data, respectively.

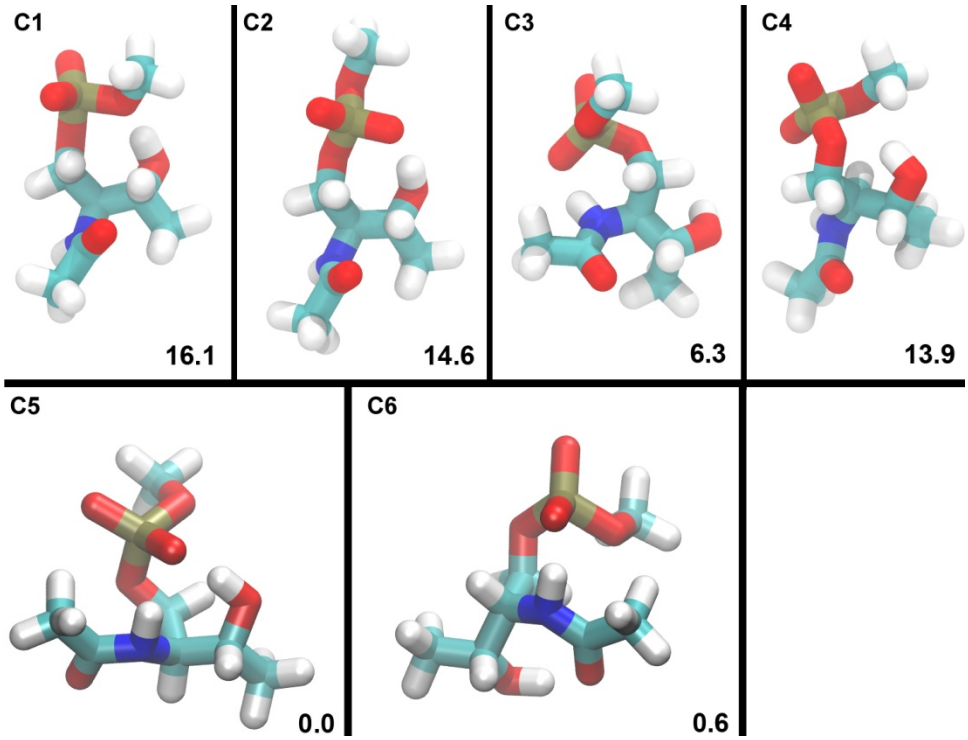

Figure S3. Conformations of local minima calculated at the MP2/cc-pVDZ model chemistry for the CER6 molecule. The energies relative to the global minima are shown in the bottom right corner in kcal/mol.

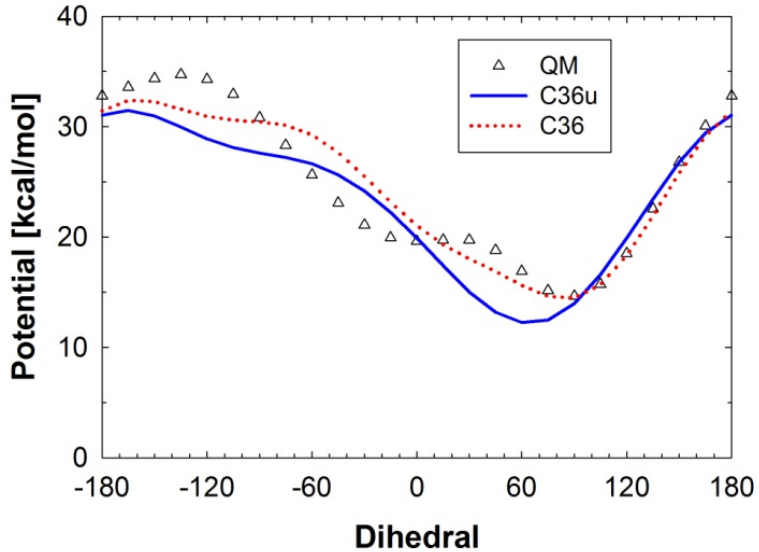

Figure S4. The torsional energy of the tOH (H-O3-C3-C2) torsion of CER6 from QM (MP2/cc-pVDZ) and C36u and C36 relative to the minima of t4. Constraints were included to maintain the C2 conformation in Figure S3.

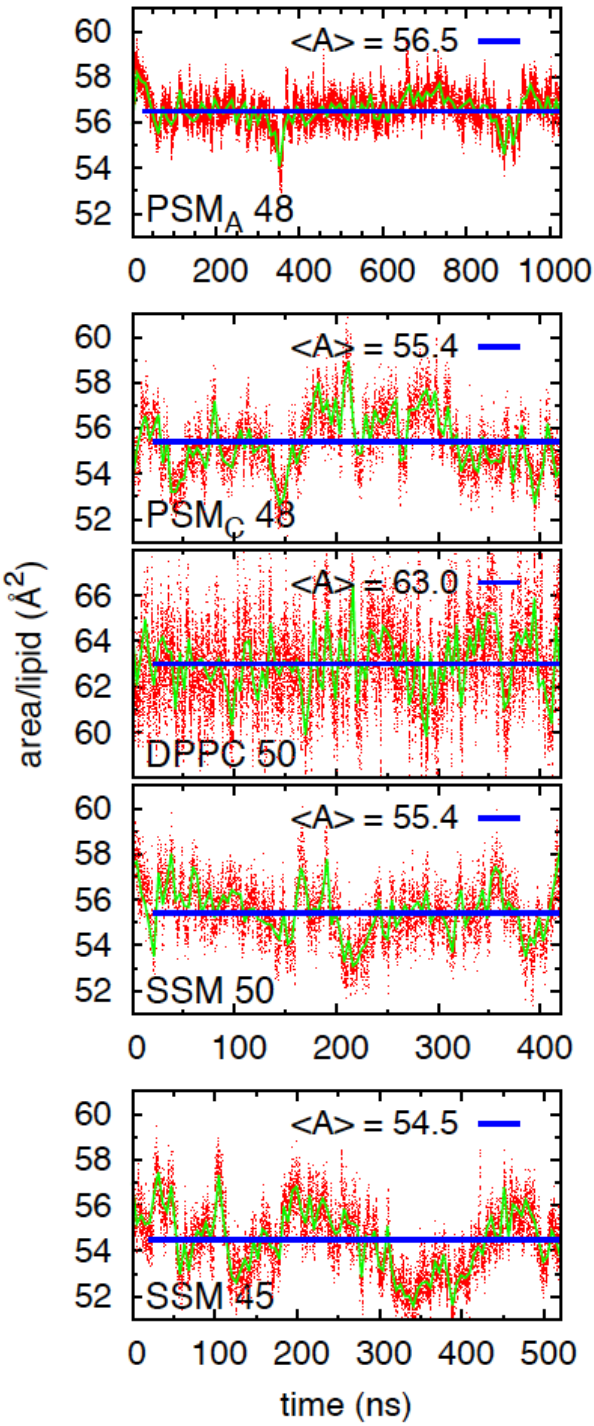

Figure S5. Area/lipid time series from CHARMM and Anton (PSM_A) simulations; red dots are snapshot values, the green line is a smoothed local average, and the heavy blue line is the average over the interval indicated by the line endpoints.

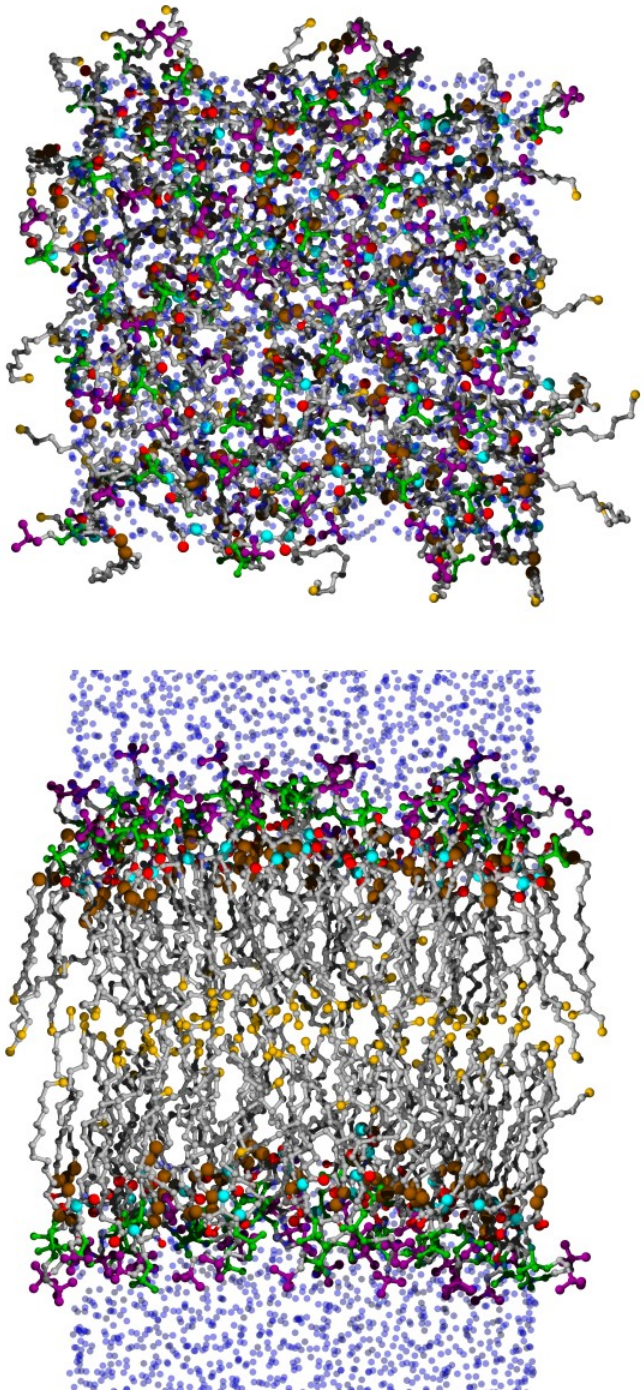

Figure S6. Molecular image snapshot at 200 ns from the PSM simulation run with CHARMM, top and side views. Colors: water is transparent blue, the choline group is purple, the phosphate group is green, amide N is cyan, amide O is orange, hydroxyl O is red, vinyl C=C atoms are brown, chain ends are yellow; all other C atoms are gray.

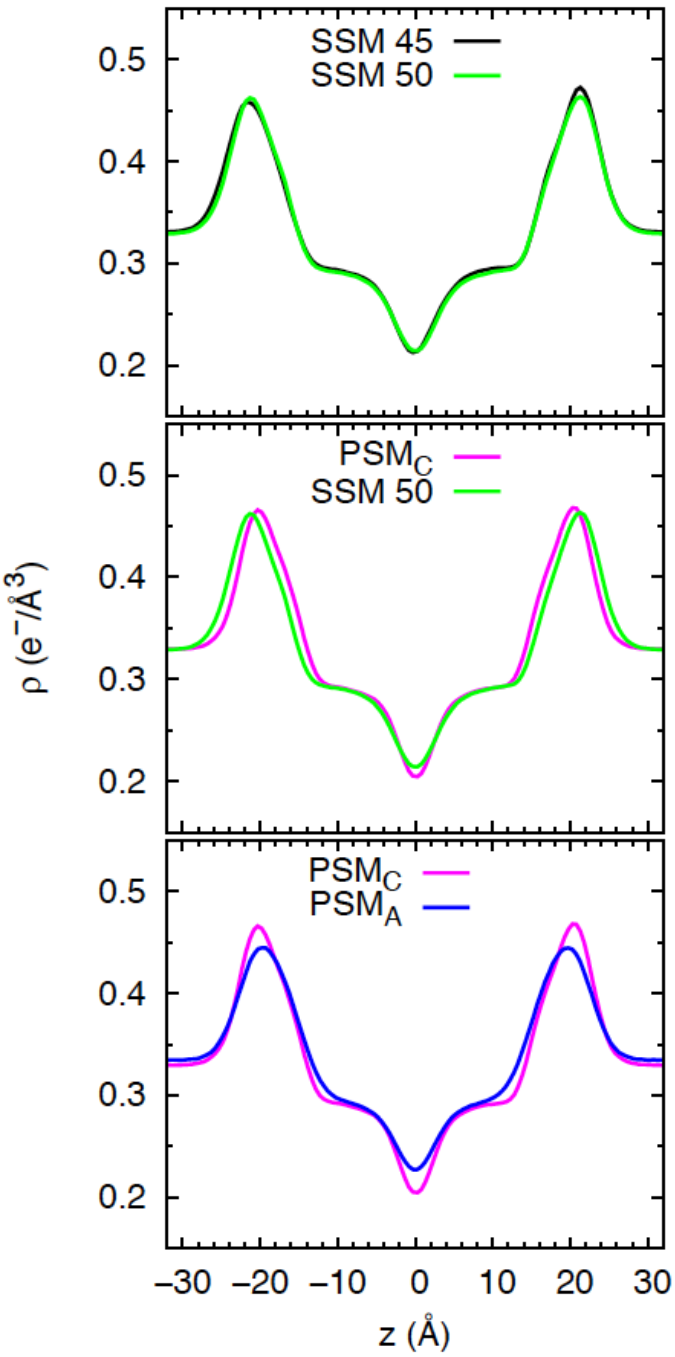

Figure S7. Electron density *z* profiles for all atoms. Top panel: comparison of SSM at 45 and 50°C; they are nearly identical. Middle panel: CHARMM simulations of SSM at 50°C and PSM at 48°C; the expected smaller $d_{P\text{-}P}$ is observed for PSM. Bottom panel: PSM simulations from CHARMM (PSM_C) and Anton (PSM_A); the difference is most likely due to the different VDW methods and cutoffs.

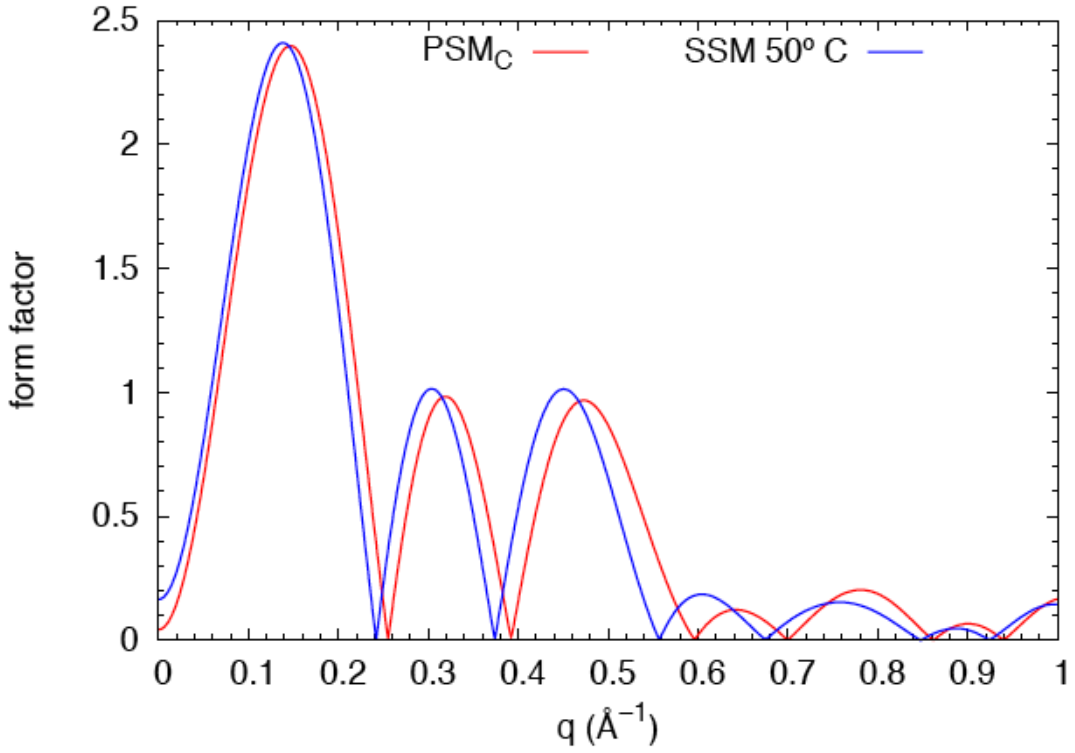

Figure S8. Calculated x-ray scattering form factors from the MD simulations.

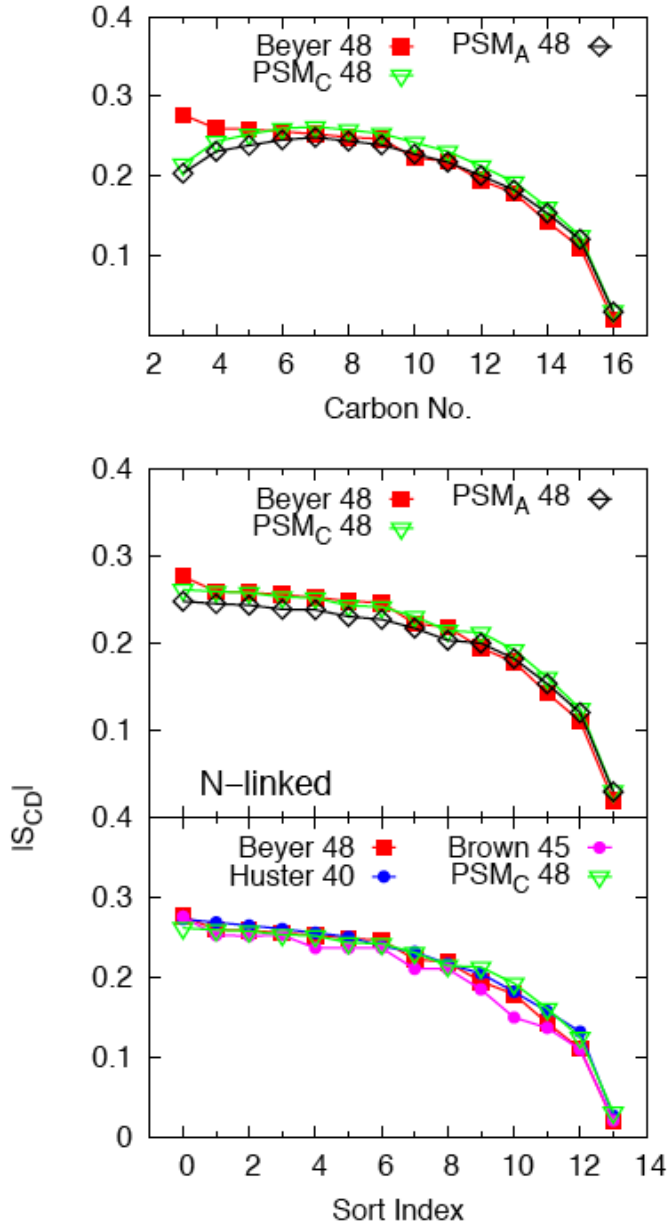

Figure S9. Order parameter profiles based on chain position (top panel) and value-sorted order (lower 2 panels). Labels: PSM_C = PSM simulated with CHARMM; PSM_A = PSM simulated with Anton; Beyer (7), Huster (8), and Brown (9) are the last authors of the respective PSM-d31 NMR papers; the temperature from experiment or simulation is listed in each label. The top panel shows an apparent discrepancy, which is resolved by value sorting the simulation values, as shown in the middle panel. The lower panel compares the sorted S_{CD} profile from the CHARMM simulation to the profiles from all three NMR papers.

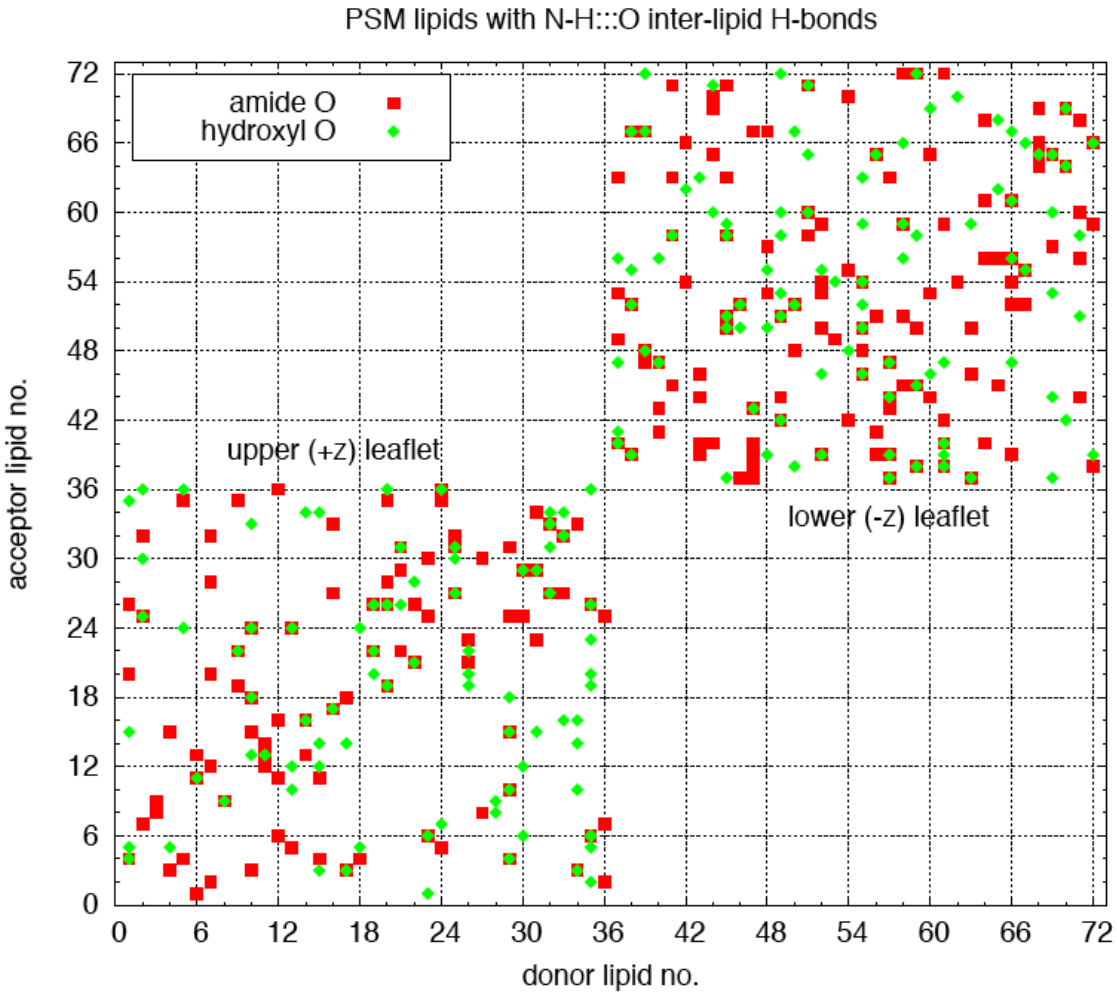

Figure S10. Observed inter-lipid H-bonds with an occupancy of 0.1% or above.

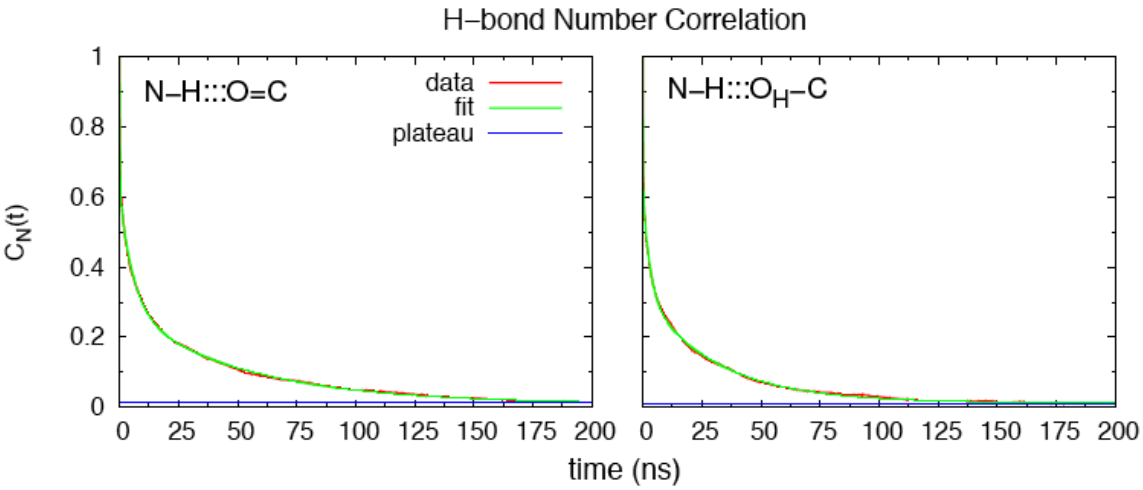

Figure S11. Hydrogen bond number correlation functions and fits for PSM, using the pairs shown in Figure S10; see Table S2 below for fit data.

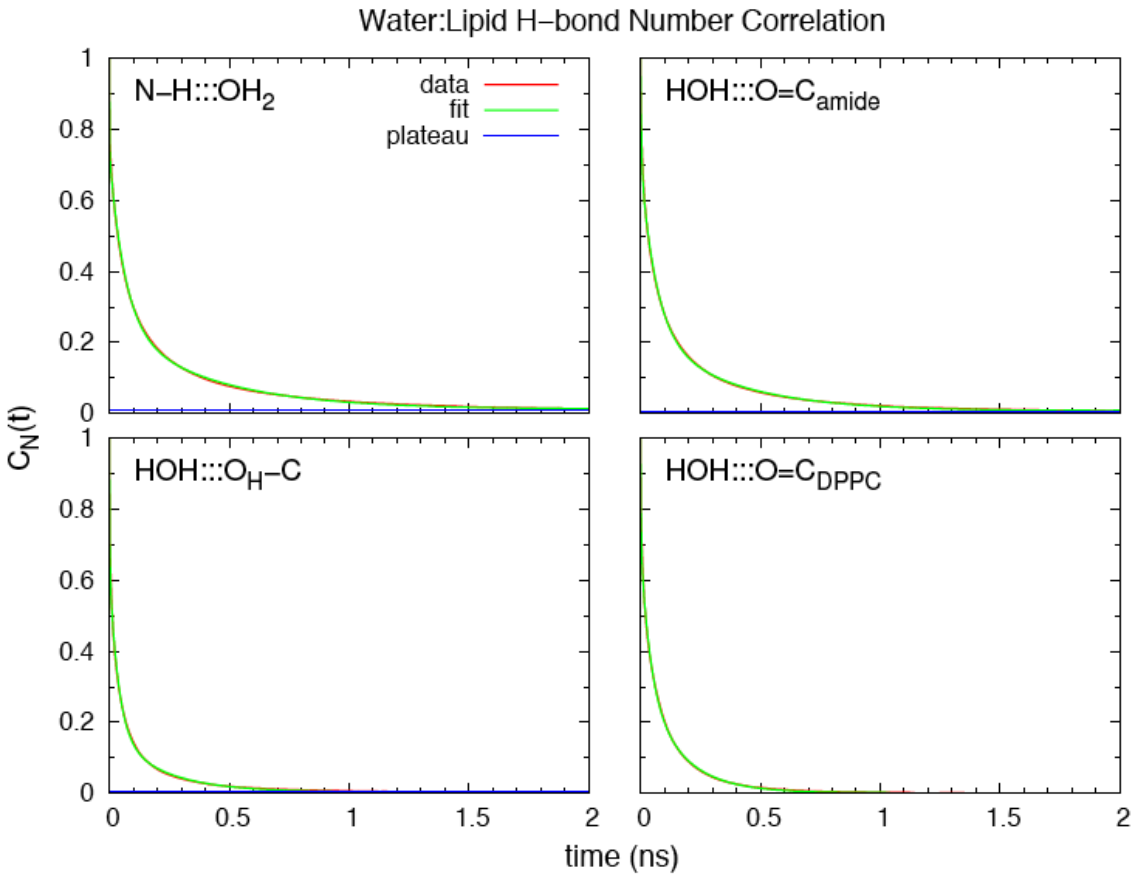

Figure S12. Number correlation functions for water-lipid hydrogen bonds. Correlation functions were evaluated from twenty 5 ns intervals, spaced 20 ns apart; the lower right panel is for the DPPC ester carbonyl O as the acceptor, the other 3 panels represent water:PSM interactions, with the amide H as a donor in the top left panel.

Table S2. Fit coefficients (a) and relaxation times (τ, ns) from 3 exponential fits.

$C_N(t)$	a_1	τ_1	a_2	τ_2	a_3	τ_3	plateau[a]
N-H:::OH_2	0.268	0.001	0.480	0.064	0.240	0.401	0.011
HOH:::O=C_{amide}	0.291	0.004	0.474	0.065	0.229	0.350	0.006
HOH:::O_H-C	0.363	0.002	0.465	0.037	0.168	0.210	0.003
HOH:::O=C_{DPPC}	0.299	0.003	0.382	0.040	0.318	0.155	0.001

[a] The plateau values were free parameters in the three exponential fit, which was constrained by the expression $a_1 + a_2 + a_3 + \text{plateau} = 1.0$.

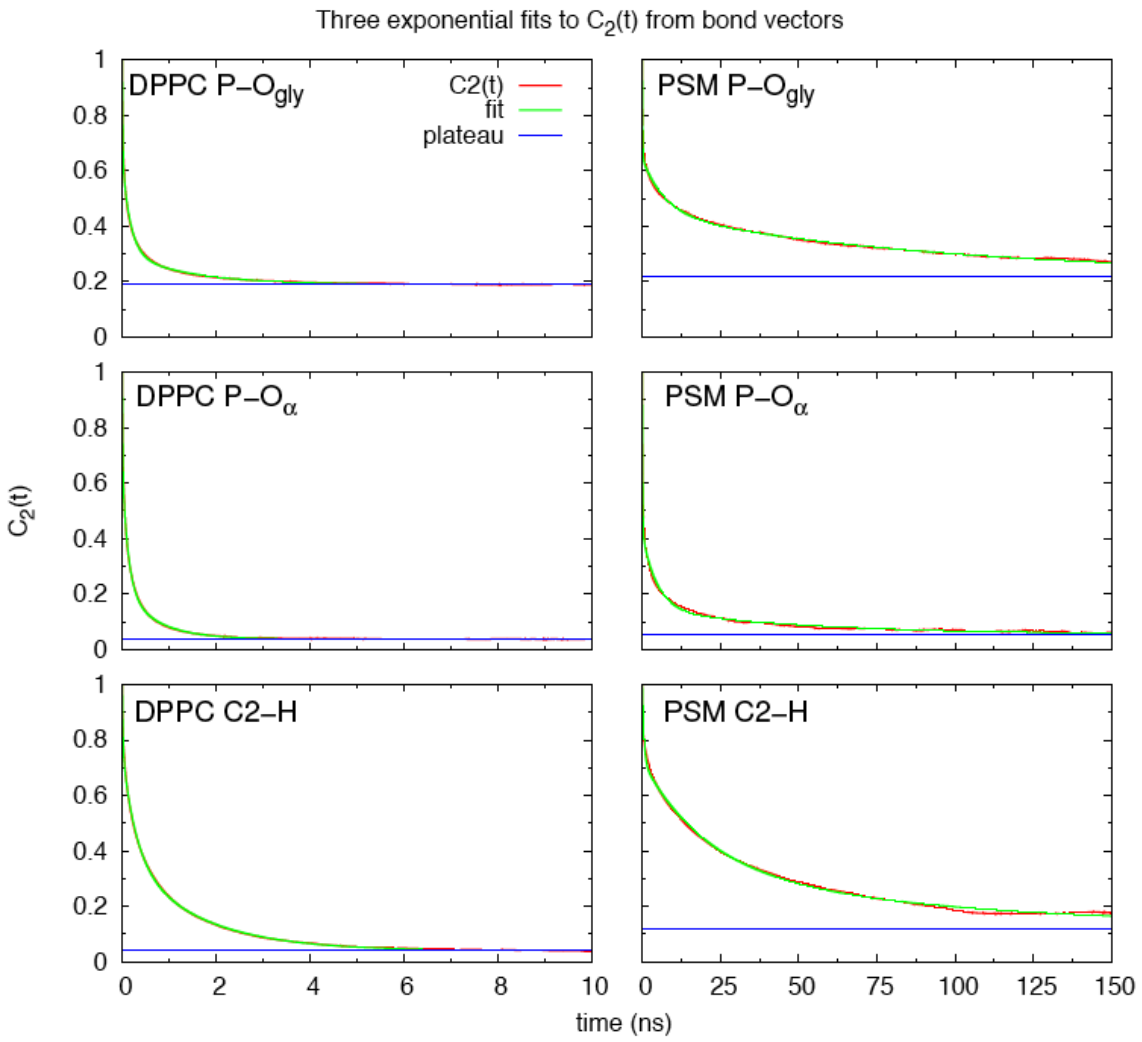

Figure S13. Second rank reorientational correlation functions $C_2(t) = \langle P_2(\hat{\mu}(0) \cdot \hat{\mu}(t)) \rangle$ selected bonds of DPPC (left) and PSM (right).

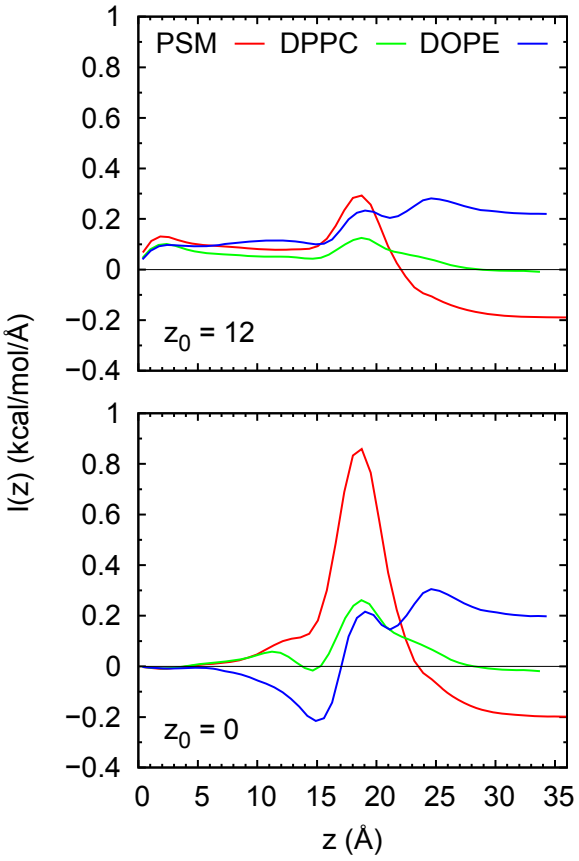

Figure S14. Evaluation of $\bar{F}'(0)$ from integration of the pressure profiles. Equation (2) in the main text can be written more generally as

$$\bar{F}'(0) = -\int_0^{L_z/2} (z - z_0)[p_T(z) - p_N(z)]dz$$

where z_0 is an arbitrary plane in the bilayer. The lower panel of the figure shows the integral

$$I(z) = -\int_0^{z} (z' - z_0)[p_T(z') - p_N(z')]dz'$$

when z_0 =0 (the bilayer midplane). It is evident that values for z ≈ 35 Å, which approximate $\bar{F}'(0)$, are quite distinct, lending increased confidence to the result that $\bar{F}'(0)$ for PSM is approximately equal in magnitude to that of DOPE but opposite in sign; i.e., a bilayer of pure PSM has positive curvature. This result does not depend on the value of z_0: as shown in the top panel for z_0 = 12 Å, the intermediate values of $I(z)$ differ for those of z_0 = 0, but $\bar{F}'(0)$ is the same.

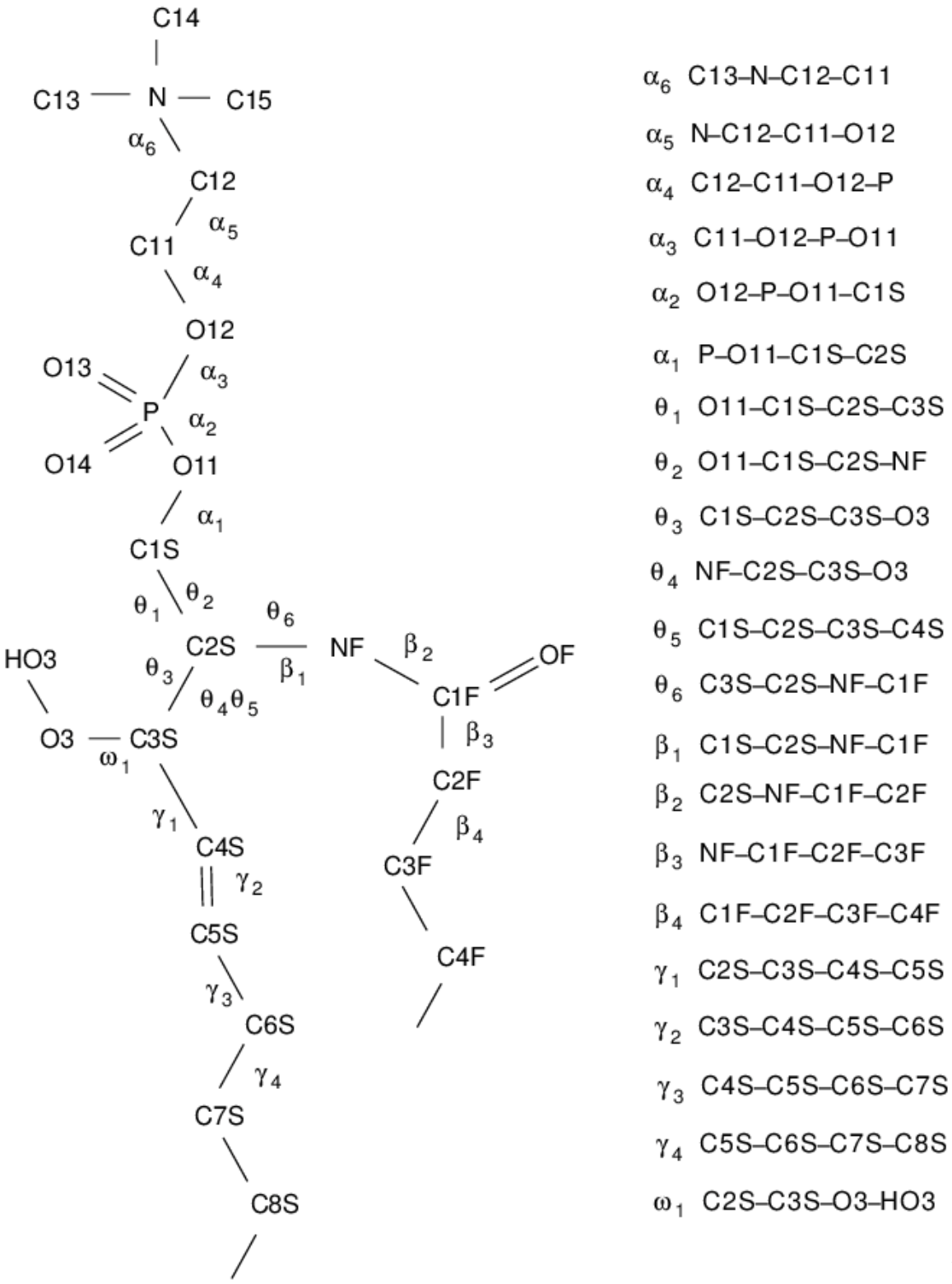

Figure S15. Atom names, and dihedral labels and definitions used for head group conformational analysis, and for the plots in Figure S16.

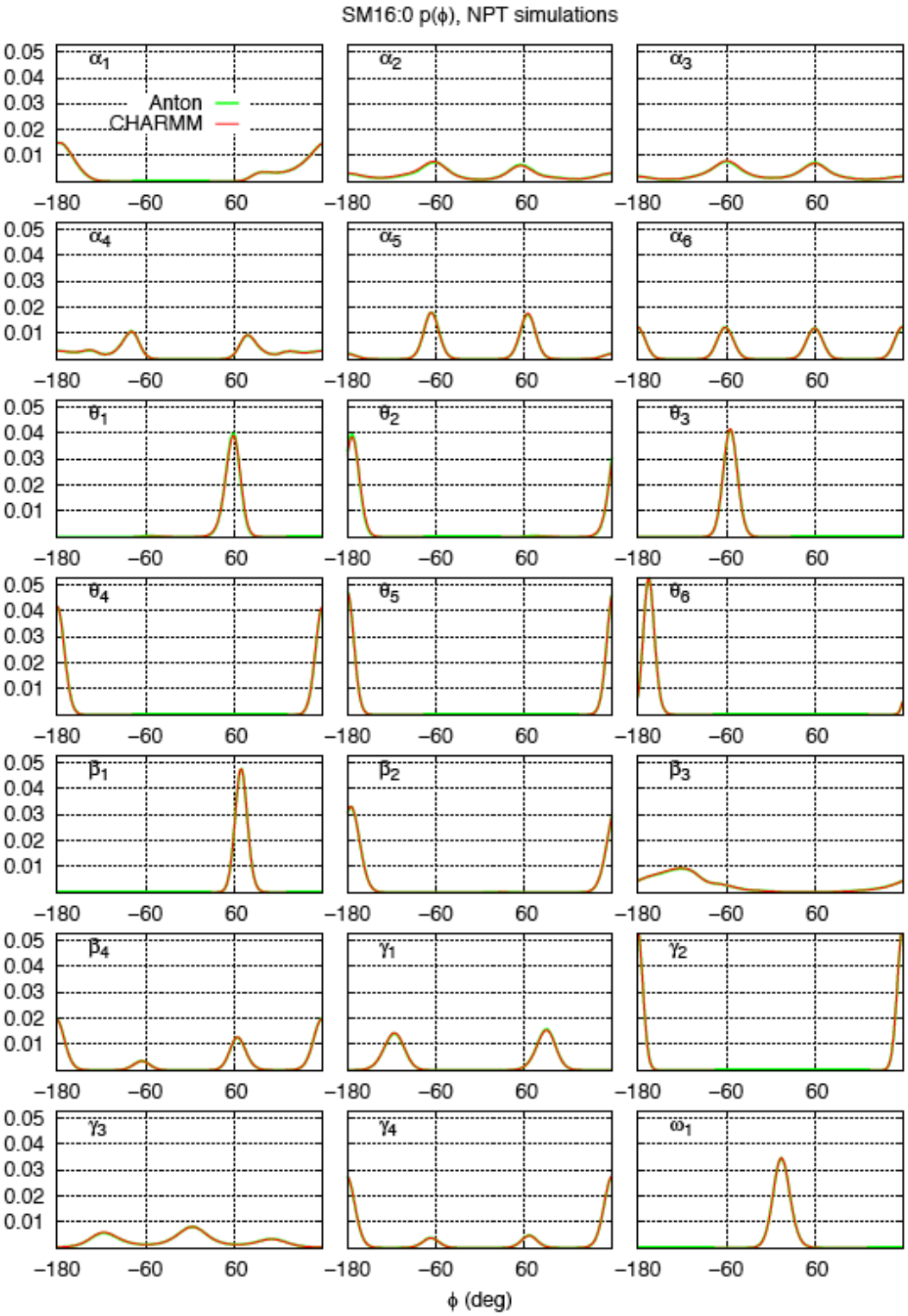

Figure S16. PSM head group dihedral distributions from both CHARMM and ANTON simulations.

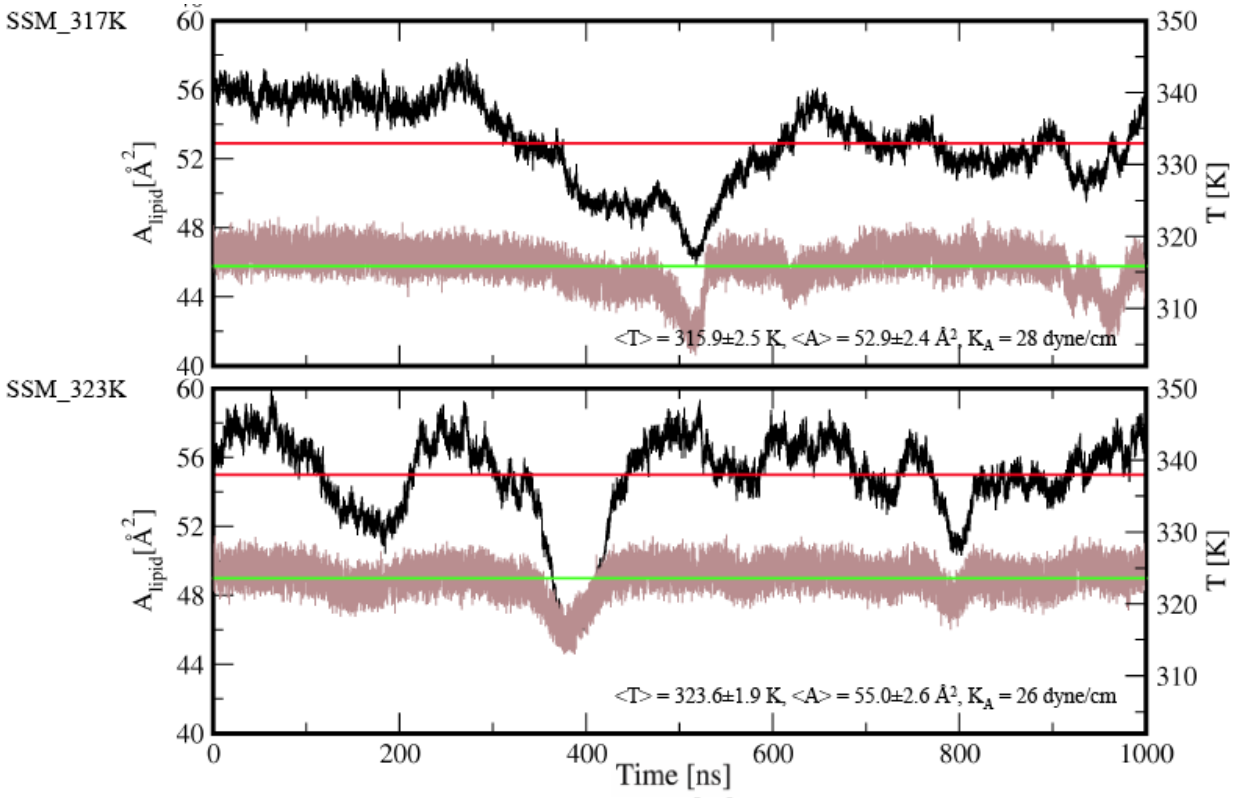

Figure S17. Temperature and area/lipid anomalies observed for SSM on ANTON. The black and red lines are the respective area/lipid time series and averages (left axis); the brown and green lines are time series and averages for the temperature (right axis).

Topology and parameter stream file input for CHARMM.

The following pages are the complete listing of the file with the new molecules and parameters added for sphingomyelins, in CHARMM input format. While complete, using cut-and-paste of these listings to obtain the inputs is inadvisable, due to line wrap issues. The file can be downloaded from http://terpconnect.umd.edu/~jbklauda/research/download.html .

```
* Toppar stream for ceramides and spingomyelins; requires flex format files
* Lipid:   top_all36_lipid.rtf and par_all36_lipid.prm
* Protein: top_all36_prot.rtf and par_all36_prot.prm
*

! REFERENCES
!
! PSM and SSM Lipids
!
! Venable, R.M., B. Rogaski, H. Rui, L. Hatcher, A.D. MacKerell, Jr., R.W. Pastor,
! & J.B. Klauda. CHARMM All-Atom Additive Force Field for Sphingomyelin:
! Elucidation of Hydrogen Bonding and of Positive Curvature. In prep. (2014).
!
! Ceramide
!
! Submited by Sam Tonddast-Navaei of U. Cincinnati. Advised by Russell Devane
!

set nat ?NATC
set app
!We're exploiting what is arguably a bug in the parser. On the left hand side,
!the quotes have proirity, so NAT is correctly substituted. On the right hand
!side, the ? has priority and NATC" (sic) is not a valid substitution...
if "@NAT" ne "?NATC" if @nat ne 0 set app append

read rtf card @app
* cer/sm residues
*
36  1

! Ceramides

MASS   165 NHL   14.00700 N !
MASS   166 CTO1  12.01100 C !
MASS   167 CEL3  12.01100 C !
MASS   168 CTO2  12.01100 C !


RESI PSM          0.00 !   sphingomyelin d18:1/16:0
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ATOM N    NTL    -0.60 !                   H15B
ATOM C15  CTL5   -0.35 !                    |
ATOM H15A HL      0.25 !             H15A-C15-H15C
ATOM H15B HL      0.25 !                    |
ATOM H15C HL      0.25 !             H13C   |   H14C
ATOM C14  CTL5   -0.35 !              |     |   |
ATOM H14A HL      0.25 !        H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !              |     |   |
ATOM H14C HL      0.25 !             H13B   |   H14B
ATOM C13  CTL5   -0.35 !                    |
ATOM H13A HL      0.25 !                    |
ATOM H13B HL      0.25 !                    |
ATOM H13C HL      0.25 !              H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                    |
ATOM H12A HL      0.25 !                    |
ATOM H12B HL      0.25 !              H11A-C11-H11B
GROUP                  !                    |
ATOM C11  CTL2   -0.08 !                    |
ATOM H11A HAL2    0.09 !                    |
ATOM H11B HAL2    0.09 !         (-) O13  O12
```

```
ATOM P    PL      1.50 !               \ /
ATOM O13  O2L    -0.78 !                P  (+)
ATOM O14  O2L    -0.78 !               / \
ATOM O11  OSLP    -0.57 !         (-) O14  O11
ATOM O12  OSLP    -0.57 !                  |
ATOM C1S  CTL2   -0.08 !                  |
ATOM H1S  HAL2    0.09 !             H1S---C1S---H1T
ATOM H1T  HAL2    0.09 !                  |
GROUP                  !             H2S---C2S-------------NF--HNF
ATOM NF   NHL    -0.70 !                  |                |
ATOM HNF  H       0.35 !                  |                |
ATOM C2S  CTL1    0.30 !                  |                |
ATOM H2S  HAL1    0.05 !                  |                |
GROUP                  !                  |                |
ATOM C3S  CTO1    0.50 !                  |                C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                  |                |
ATOM O3   OHL    -0.69 !                  |                |
ATOM HO3  HOL     0.30 !                  |       H2F----C2F---H2G
GROUP                  !                  |                |
ATOM C4S  CEL3   -0.15 !                  |            [(CH2)3F (C3F,C4F...C15F)
ATOM H4S  HEL1    0.15 !                  |                |
GROUP                  !                  |       H16F---C16F---H16G
ATOM C5S  CEL3   -0.15 !                  |                |
ATOM H5S  HEL1    0.15 !                  |               H16H
GROUP                  !            H3S----C3S--O3--HO3
ATOM C6S  CTL2   -0.18 !                  |
ATOM H6S  HAL2    0.09 !                C4S--H4S
ATOM H6T  HAL2    0.09 !                ||
GROUP                  !                C5S--H5S
ATOM C7S  CTL2   -0.18 !                  |
ATOM H7S  HAL2    0.09 !                  |
ATOM H7T  HAL2    0.09 !               [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                  |
ATOM C8S  CTL2   -0.18 !           H18S---C18S---H18U
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ATOM H8T  HAL2    0.09 !                H18T
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ATOM H9T  HAL2    0.09 !
GROUP                  !
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ATOM H10T HAL2    0.09 !
GROUP
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ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
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ATOM H12T HAL2    0.09 !
GROUP
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ATOM H13T  HAL2   0.09 !
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ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
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ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
```
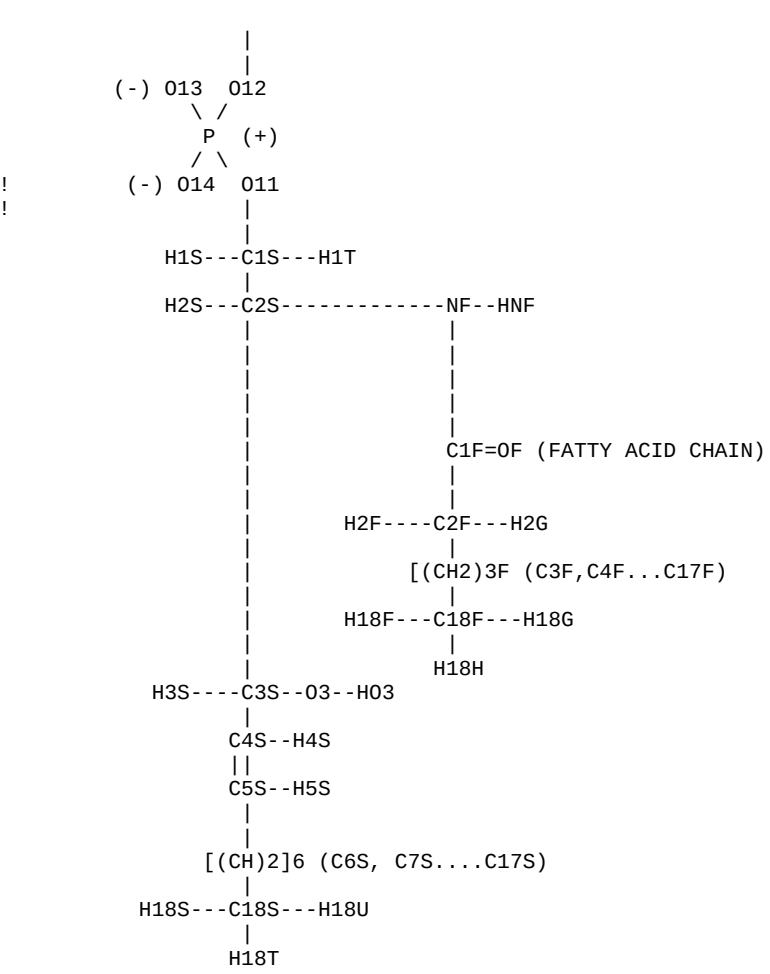

```
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                  !
ATOM C16F CTL3   -0.27 !
ATOM H16F HAL3    0.09 !
ATOM H16G HAL3    0.09 !
ATOM H16H HAL3    0.09 !

!SPHINGOSINE CHAIN
```

```
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F H16H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
 IC   C8S      C7S     C6S     C5S        1.5354  112.41 -179.61  111.46   1.5077
 IC   C7S      C6S     C5S     C4S        1.5391  111.46 -117.13  124.77   1.3444
 IC   C6S      C5S     C4S     C3S        1.5077  124.77  179.01  124.28   1.5009
 IC   C5S      C4S     C3S     C2S        1.3444  124.28  -84.24  110.14   1.5343
 IC   C5S      C4S     C3S     O3         1.3444  124.28  156.07  107.64   1.4235
 IC   C13      C12    *N       C14        1.4967  109.68  116.91  107.30   1.5040
 IC   C13      C12    *N       C15        1.4967  109.68 -123.42  110.88   1.4938
 IC   C12      N       C15     H15A       1.5212  110.88 -177.15  111.31   1.0816
 IC   H15A     N      *C15     H15B       1.0816  111.31  118.98  109.44   1.0875
 IC   H15A     N      *C15     H15C       1.0816  111.31 -122.11  111.46   1.0818
 IC   C12      N       C14     H14A       1.5212  107.30 -178.89  114.23   1.0739
```

```
IC   H14A     N      *C14     H14B       1.0739  114.23  123.44  110.21   1.0968
IC   H14A     N      *C14     H14C       1.0739  114.23 -124.43  111.41   1.0948
IC   C12      N       C13     H13A       1.5212  109.68  176.44  111.15   1.0822
IC   H13A     N      *C13     H13B       1.0822  111.15  121.89  111.75   1.0814
IC   H13A     N      *C13     H13C       1.0822  111.15 -118.50  109.57   1.0892
IC   C13      N       C12     C11        1.4967  109.68 -178.83  116.30   1.5392
IC   C11      N      *C12     H12A       1.5392  116.30  117.04  108.30   1.0985
IC   C11      N      *C12     H12B       1.5392  116.30 -126.61  112.36   1.0787
IC   N        C12     C11     O12        1.5212  116.30  126.79  107.85   1.4239
IC   O12      C12    *C11     H11A       1.4239  107.85  118.10  109.30   1.1131
IC   O12      C12    *C11     H11B       1.4239  107.85 -123.12  113.16   1.1140
IC   C12      C11     O12     P          1.5392  107.85  -68.29  118.09   1.5886
IC   C11      O12     P       O11        1.4239  118.09 -167.58  104.18   1.5725
IC   O11      O12    *P       O13        1.5725  104.18  116.57  107.05   1.4823
IC   O11      O12    *P       O14        1.5725  104.18 -118.73  106.98   1.4805
IC   O12      P       O11     C1S        1.5886  104.18   51.85  121.69   1.4327
IC   P        O11     C1S     C2S        1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O11    *C1S     H1S        1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O11    *C1S     H1T        1.5586  111.21 -123.25  112.85   1.1152
IC   C2S      C3S     O3      HO3        1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S        1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S        1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S        1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S        1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S        1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S        1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T        1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S        1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S        1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T        1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S        1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S        1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T        1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S       1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S        1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T        1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S       1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S       1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T       1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S       1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S       1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T       1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S       1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S       1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T       1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S       1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S       1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T       1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S       1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S       1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T       1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S       1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S       1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T       1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S       1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S       1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T       1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S       1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S       1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T       1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S       1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T       1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U       1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F        1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF         1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F        1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F        1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G        1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F        1.4964  111.92  179.54  112.84   1.5310
IC   C4F      C2F    *C3F     H3F        1.5310  112.84 -121.63  109.37   1.1145
IC   H3F      C2F    *C3F     H3G        1.1145  109.37 -117.07  109.08   1.1157
```

```
 IC   C2F      C3F     C4F     C5F        1.5434  112.23  174.86  112.58   1.5342
 IC   C5F      C3F    *C4F     H4F        1.5342  112.58 -120.18  108.65   1.1140
 IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
 IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
 IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
 IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
 IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
 IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
 IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
 IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
 IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
 IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
 IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
 IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
 IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    H16F       1.5334  113.16  -59.91  110.49   1.1113
 IC   H16F     C15F   *C16F    H16G       1.1113  110.49  119.86  110.41   1.1115
 IC   H16F     C15F   *C16F    H16H       1.1113  110.49 -120.11  110.63   1.1112
 IC   C4S      C2S    *C3S     O3         1.5009  110.14  118.36  109.80   1.4235 ! OH chirality (ch
 IC   C4S      C2S    *C3S     H3S        1.5009  110.14 -121.14  110.10   1.1140 ! OH chirality (ch
 IC   O11      C1S     C2S     C3S        1.4327  111.21  175.67  114.25   1.5343 ! assume ok
 IC   C1F      C2S    *NF      HNF        1.3364  124.85 -157.81  113.39   1.0062 ! assume ok
! IC   C1S      C2S     C3S     C4S        1.5586  114.25  -70.50  110.14   1.5009! assume redundent
! SWAPPED
 IC   C4S      C3S     C2S     C1S        1.5009  110.14  160.94  114.25   1.5586
 IC   C1S      C2S     NF      C1F        1.5586  111.52  -70.50  124.85   1.3364
! SWAPPED
 IC   C3S      C1S    *C2S     NF         1.5343  114.25  120.00  111.52   1.4406
 IC   C3S      C1S    *C2S     H2S        1.5343  114.25 -120.00  105.03   1.1194
PATCH FIRST NONE LAST NONE

RESI SSM          0.00 !   sphingomyelin d18:1/18:0
GROUP                  !
ATOM N    NTL    -0.60 !                    H15B
ATOM C15  CTL5   -0.35 !                     |
ATOM H15A HL      0.25 !              H15A-C15-H15C
ATOM H15B HL      0.25 !                     |
ATOM H15C HL      0.25 !              H13C   |   H14C
ATOM C14  CTL5   -0.35 !               |     |   |
ATOM H14A HL      0.25 !         H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !               |     |   |
ATOM H14C HL      0.25 !              H13B   |   H14B
ATOM C13  CTL5   -0.35 !                     |
ATOM H13A HL      0.25 !                     |
ATOM H13B HL      0.25 !                     |
ATOM H13C HL      0.25 !               H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                     |
ATOM H12A HL      0.25 !                     |
ATOM H12B HL      0.25 !               H11A-C11-H11B
GROUP                  !                     |
```

```
ATOM C11  CTL2   -0.08 !
ATOM H11A HAL2    0.09 !
ATOM H11B HAL2    0.09 !
ATOM P    PL      1.50 !
ATOM O13  O2L    -0.78 !
ATOM O14  O2L    -0.78 !
ATOM O11  OSLP    -0.57 !
ATOM O12  OSLP    -0.57 !
ATOM C1S  CTL2   -0.08 !
ATOM H1S  HAL2    0.09 !
ATOM H1T  HAL2    0.09 !
GROUP                  !
ATOM NF   NHL    -0.70 !
ATOM HNF  H       0.35 !
ATOM C2S  CTL1    0.30 !
ATOM H2S  HAL1    0.05 !
GROUP                  !
ATOM C3S  CTO1    0.50 !
ATOM H3S  HAL1   -0.11 !
ATOM O3   OHL    -0.69 !
ATOM HO3  HOL     0.30 !
GROUP                  !
ATOM C4S  CEL3   -0.15 !
ATOM H4S  HEL1    0.15 !
GROUP                  !
ATOM C5S  CEL3   -0.15 !
ATOM H5S  HEL1    0.15 !
GROUP                  !
ATOM C6S  CTL2   -0.18 !
ATOM H6S  HAL2    0.09 !
ATOM H6T  HAL2    0.09 !
GROUP                  !
ATOM C7S  CTL2   -0.18 !
ATOM H7S  HAL2    0.09 !
ATOM H7T  HAL2    0.09 !
GROUP                  !
ATOM C8S  CTL2   -0.18 !
ATOM H8S  HAL2    0.09 !
ATOM H8T  HAL2    0.09 !
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
```



```
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                  !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
```

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GROUP                   !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                   !
ATOM C18F CTL3   -0.27 !
ATOM H18F HAL3    0.09 !
ATOM H18G HAL3    0.09 !
ATOM H18H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F H18H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C13      C12    *N       C14        1.4967  109.68  116.91  107.30   1.5040
 IC   C13      C12    *N       C15        1.4967  109.68 -123.42  110.88   1.4938
 IC   C12      N       C15     H15A       1.5212  110.88 -177.15  111.31   1.0816
 IC   H15A     N      *C15     H15B       1.0816  111.31  118.98  109.44   1.0875
 IC   H15A     N      *C15     H15C       1.0816  111.31 -122.11  111.46   1.0818
 IC   C12      N       C14     H14A       1.5212  107.30 -178.89  114.23   1.0739
 IC   H14A     N      *C14     H14B       1.0739  114.23  123.44  110.21   1.0968
 IC   H14A     N      *C14     H14C       1.0739  114.23 -124.43  111.41   1.0948
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IC   C12      N       C13     H13A       1.5212  109.68  176.44  111.15   1.0822
IC   H13A     N      *C13     H13B       1.0822  111.15  121.89  111.75   1.0814
IC   H13A     N      *C13     H13C       1.0822  111.15 -118.50  109.57   1.0892
IC   C13      N       C12     C11        1.4967  109.68 -178.83  116.30   1.5392
IC   C11      N      *C12     H12A       1.5392  116.30  117.04  108.30   1.0985
IC   C11      N      *C12     H12B       1.5392  116.30 -126.61  112.36   1.0787
IC   N        C12     C11     O12        1.5212  116.30  126.79  107.85   1.4239
IC   O12      C12    *C11     H11A       1.4239  107.85  118.10  109.30   1.1131
IC   O12      C12    *C11     H11B       1.4239  107.85 -123.12  113.16   1.1140
IC   C12      C11     O12     P          1.5392  107.85  -68.29  118.09   1.5886
IC   C11      O12     P       O11        1.4239  118.09 -167.58  104.18   1.5725
IC   O11      O12    *P       O13        1.5725  104.18  116.57  107.05   1.4823
IC   O11      O12    *P       O14        1.5725  104.18 -118.73  106.98   1.4805
IC   O12      P       O11     C1S        1.5886  104.18   51.85  121.69   1.4327
IC   P        O11     C1S     C2S        1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O11    *C1S     H1S        1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O11    *C1S     H1T        1.5586  111.21 -123.25  112.85   1.1152
IC   O11      C1S     C2S     C3S        1.4327  111.21  175.67  114.25   1.5343
IC   C3S      C1S    *C2S     NF         1.5343  114.25  120.00  111.52   1.4406
IC   C3S      C1S    *C2S     H2S        1.5343  114.25 -120.00  105.03   1.1194
IC   C1S      C2S     NF      C1F        1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF        1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S        1.5586  114.25  170.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3         1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S        1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3        1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S        1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S        1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S        1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S        1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S        1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S        1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T        1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S        1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S        1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T        1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S        1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S        1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T        1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S       1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S        1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T        1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S       1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S       1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T       1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S       1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S       1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T       1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S       1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S       1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T       1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S       1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S       1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T       1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S       1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S       1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T       1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S       1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S       1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T       1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S       1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S       1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T       1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S       1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S       1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T       1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S       1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T       1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U       1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F        1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF         1.4964  114.97  162.54  122.11   1.2268
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 IC   NF       C1F     C2F     C3F        1.3364  114.97  146.57  111.92   1.5432
 IC   C3F      C1F    *C2F     H2F        1.5432  111.92 -120.83  107.93   1.1115
 IC   H2F      C1F    *C2F     H2G        1.1115  107.93 -117.30  109.04   1.1113
 IC   C1F      C2F     C3F     C4F        1.4964  111.92   59.54  112.84   1.5310
 IC   C4F      C2F    *C3F     H3F        1.5310  112.84 -121.63  109.37   1.1145
 IC   H3F      C2F    *C3F     H3G        1.1145  109.37 -117.07  109.08   1.1157
 IC   C2F      C3F     C4F     C5F        1.5434  112.23  174.86  112.58   1.5342
 IC   C5F      C3F    *C4F     H4F        1.5342  112.58 -120.18  108.65   1.1140
 IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
 IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
 IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
 IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
 IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
 IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
 IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
 IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
 IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
 IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
 IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
 IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
 IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    H18F       1.5334  113.16  -59.91  110.49   1.1113
 IC   H18F     C17F   *C18F    H18G       1.1113  110.49  119.86  110.41   1.1115
 IC   H18F     C17F   *C18F    H18H       1.1113  110.49 -120.11  110.63   1.1112
PATCH FIRST NONE LAST NONE

RESI OSM          0.00 !   sphingomyelin d18:1/18:1 (w/oleic acid)
GROUP                  !
ATOM N    NTL    -0.60 !                   H15B
ATOM C15  CTL5   -0.35 !                   |
ATOM H15A HL      0.25 !              H15A-C15-H15C
ATOM H15B HL      0.25 !                   |
ATOM H15C HL      0.25 !              H13C  |   H14C
ATOM C14  CTL5   -0.35 !               |    |   |
ATOM H14A HL      0.25 !         H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !               |    |   |
ATOM H14C HL      0.25 !              H13B  |   H14B
ATOM C13  CTL5   -0.35 !                   |
ATOM H13A HL      0.25 !                   |
ATOM H13B HL      0.25 !                   |
ATOM H13C HL      0.25 !               H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                   |
ATOM H12A HL      0.25 !                   |
ATOM H12B HL      0.25 !              H11A-C11-H11B
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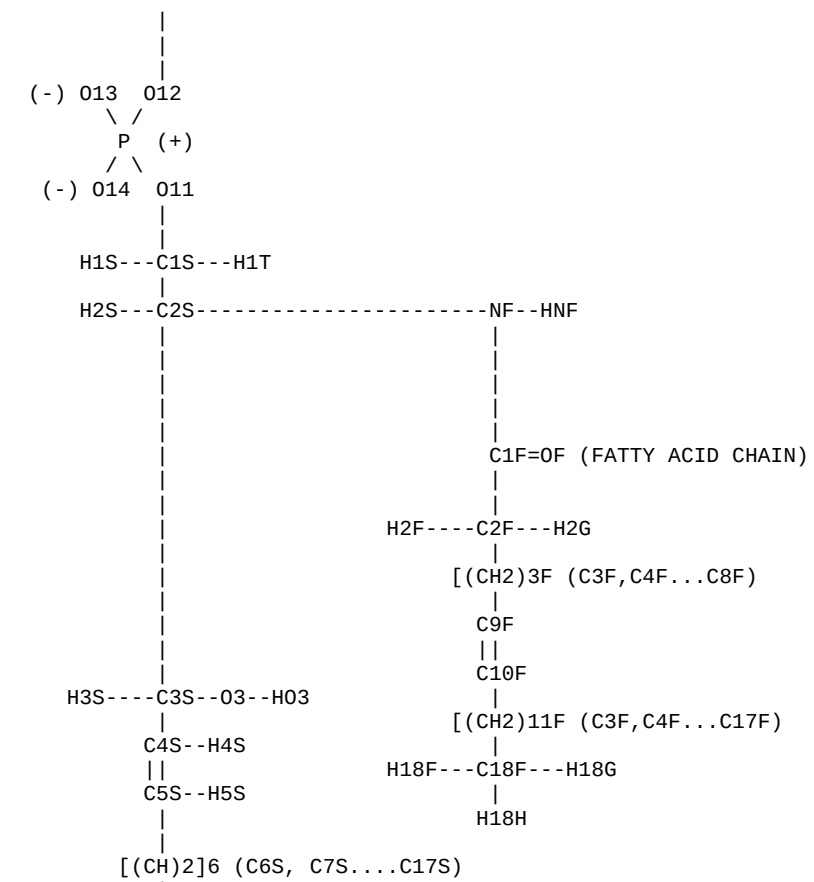
GROUP                 !
ATOM C11  CTL2   -0.08 !
ATOM H11A HAL2    0.09 !
ATOM H11B HAL2    0.09 !
ATOM P    PL      1.50 !
ATOM O13  O2L    -0.78 !
ATOM O14  O2L    -0.78 !
ATOM O11  OSLP    -0.57 !
ATOM O12  OSLP    -0.57 !
ATOM C1S  CTL2   -0.08 !
ATOM H1S  HAL2    0.09 !
ATOM H1T  HAL2    0.09 !
GROUP                 !
ATOM NF   NHL    -0.70 !
ATOM HNF  H       0.35 !
ATOM C2S  CTL1    0.30 !
ATOM H2S  HAL1    0.05 !
GROUP                 !
ATOM C3S  CTO1    0.50 !
ATOM H3S  HAL1   -0.11 !
ATOM O3   OHL    -0.69 !
ATOM HO3  HOL     0.30 !
GROUP                 !
ATOM C4S  CEL3   -0.15 !
ATOM H4S  HEL1    0.15 !
GROUP                 !
ATOM C5S  CEL3   -0.15 !
ATOM H5S  HEL1    0.15 !
GROUP                 !
ATOM C6S  CTL2   -0.18 !
ATOM H6S  HAL2    0.09 !
ATOM H6T  HAL2    0.09 !
GROUP                 !
ATOM C7S  CTL2   -0.18 !
ATOM H7S  HAL2    0.09 !
ATOM H7T  HAL2    0.09 !
GROUP                 !
ATOM C8S  CTL2   -0.18 !
ATOM H8S  HAL2    0.09 !
ATOM H8T  HAL2    0.09 !
GROUP                 !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                 !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
```



```
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CEL1   -0.15 !
ATOM H9F  HEL1    0.15 !
GROUP                  !
ATOM C10F CEL1   -0.15 !
ATOM H10F HEL1    0.15 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                  !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
GROUP                  !
```

```
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                  !
ATOM C18F CTL3   -0.27 !
ATOM H18F HAL3    0.09 !
ATOM H18G HAL3    0.09 !
ATOM H18H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F
BOND  C10F H10F
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F H18H

DOUBLE C4S  C5S
DOUBLE C9F  C10F
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
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IC   C10S     C9S     C8S     C7S       1.5344  112.66 -179.89  112.50   1.5354
IC   C9S      C8S     C7S     C6S       1.5345  112.50 -179.79  112.41   1.5391
IC   C8S      C7S     C6S     C5S       1.5354  112.41 -179.61  111.46   1.5077
IC   C7S      C6S     C5S     C4S       1.5391  111.46 -117.13  124.77   1.3444
IC   C6S      C5S     C4S     C3S       1.5077  124.77  179.01  124.28   1.5009
IC   C5S      C4S     C3S     C2S       1.3444  124.28  -84.24  110.14   1.5343
IC   C5S      C4S     C3S     O3        1.3444  124.28  156.07  107.64   1.4235
IC   C4S      C3S     C2S     C1S       1.5009  110.14  -70.50  114.25   1.5586
IC   C13      C12    *N       C14       1.4967  109.68  116.91  107.30   1.5040
IC   C13      C12    *N       C15       1.4967  109.68 -123.42  110.88   1.4938
IC   C12      N       C15     H15A      1.5212  110.88 -177.15  111.31   1.0816
IC   H15A     N      *C15     H15B      1.0816  111.31  118.98  109.44   1.0875
IC   H15A     N      *C15     H15C      1.0816  111.31 -122.11  111.46   1.0818
IC   C12      N       C14     H14A      1.5212  107.30 -178.89  114.23   1.0739
IC   H14A     N      *C14     H14B      1.0739  114.23  123.44  110.21   1.0968
IC   H14A     N      *C14     H14C      1.0739  114.23 -124.43  111.41   1.0948
IC   C12      N       C13     H13A      1.5212  109.68  176.44  111.15   1.0822
IC   H13A     N      *C13     H13B      1.0822  111.15  121.89  111.75   1.0814
IC   H13A     N      *C13     H13C      1.0822  111.15 -118.50  109.57   1.0892
IC   C13      N       C12     C11       1.4967  109.68 -178.83  116.30   1.5392
IC   C11      N      *C12     H12A      1.5392  116.30  117.04  108.30   1.0985
IC   C11      N      *C12     H12B      1.5392  116.30 -126.61  112.36   1.0787
IC   N        C12     C11     O12       1.5212  116.30  126.79  107.85   1.4239
IC   O12      C12    *C11     H11A      1.4239  107.85  118.10  109.30   1.1131
IC   O12      C12    *C11     H11B      1.4239  107.85 -123.12  113.16   1.1140
IC   C12      C11     O12     P         1.5392  107.85  -68.29  118.09   1.5886
IC   C11      O12     P       O11       1.4239  118.09 -167.58  104.18   1.5725
IC   O11      O12    *P       O13       1.5725  104.18  116.57  107.05   1.4823
IC   O11      O12    *P       O14       1.5725  104.18 -118.73  106.98   1.4805
IC   O12      P       O11     C1S       1.5886  104.18   51.85  121.69   1.4327
IC   P        O11     C1S     C2S       1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O11    *C1S     H1S       1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O11    *C1S     H1T       1.5586  111.21 -123.25  112.85   1.1152
IC   O11      C1S     C2S     C3S       1.4327  111.21  175.67  114.25   1.5343
IC   C3S      C1S    *C2S     NF        1.5343  114.25  120.00  111.52   1.4406
IC   C3S      C1S    *C2S     H2S       1.5343  114.25 -120.00  105.03   1.1194
IC   C1S      C2S     NF      C1F       1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF       1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S       1.5586  114.25  -70.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3        1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S       1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3       1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S       1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S       1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S       1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S       1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S       1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S       1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T       1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S       1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S       1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T       1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S       1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S       1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T       1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S      1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S       1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T       1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S      1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S      1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T      1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S      1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S      1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T      1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S      1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S      1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T      1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S      1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S      1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T      1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S      1.5345  112.58 -179.99  112.58   1.5345
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 IC   C15S     C13S   *C14S    H14S       1.5345  112.58  121.30  109.12   1.1133
 IC   C15S     C13S   *C14S    H14T       1.5345  112.58 -121.31  109.12   1.1133
 IC   C13S     C14S    C15S    C16S       1.5345  112.58  180.00  112.58   1.5346
 IC   C16S     C14S   *C15S    H15S       1.5346  112.58  121.30  109.11   1.1133
 IC   C16S     C14S   *C15S    H15T       1.5346  112.58 -121.30  109.11   1.1133
 IC   C14S     C15S    C16S    C17S       1.5345  112.58  180.00  112.64   1.5337
 IC   C17S     C15S   *C16S    H16S       1.5337  112.64  121.32  109.14   1.1133
 IC   C17S     C15S   *C16S    H16T       1.5337  112.64 -121.32  109.14   1.1133
 IC   C15S     C16S    C17S    C18S       1.5346  112.64  180.00  113.23   1.5309
 IC   C18S     C16S   *C17S    H17S       1.5309  113.23  121.67  108.77   1.1142
 IC   C18S     C16S   *C17S    H17T       1.5309  113.23 -121.67  108.77   1.1142
 IC   C16S     C17S    C18S    H18S       1.5337  113.23  180.00  110.63   1.1113
 IC   H18S     C17S   *C18S    H18T       1.1113  110.63  120.07  110.47   1.1114
 IC   H18S     C17S   *C18S    H18U       1.1113  110.63 -120.07  110.47   1.1114
 IC   C2S      NF      C1F     C2F        1.4406  124.85 -156.83  114.97   1.4964
 IC   C2F      NF     *C1F     OF         1.4964  114.97  162.54  122.11   1.2268
 IC   NF       C1F     C2F     C3F        1.3364  114.97 -146.57  111.92   1.5432
 IC   C3F      C1F    *C2F     H2F        1.5432  111.92 -120.83  107.93   1.1115
 IC   H2F      C1F    *C2F     H2G        1.1115  107.93 -117.30  109.04   1.1113
 IC   C1F      C2F     C3F     C4F        1.4964  111.92  179.54  112.84   1.5310
 IC   C4F      C2F    *C3F     H3F        1.5310  112.84 -121.63  109.37   1.1145
 IC   H3F      C2F    *C3F     H3G        1.1145  109.37 -117.07  109.08   1.1157
 IC   C2F      C3F     C4F     C5F        1.5434  112.23  174.86  112.58   1.5342
 IC   C5F      C3F    *C4F     H4F        1.5342  112.58 -120.18  108.65   1.1140
 IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
 IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
 IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
 IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
 IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
 IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
 IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
 IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
 IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
 IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
 IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
 IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   C8F      C9F     C10F    C11F       1.5340  112.34    0.00  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  180.00  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38    0.00  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    H18F       1.5334  113.16  -59.91  110.49   1.1113
 IC   H18F     C17F   *C18F    H18G       1.1113  110.49  119.86  110.41   1.1115
 IC   H18F     C17F   *C18F    H18H       1.1113  110.49 -120.11  110.63   1.1112
PATCH FIRST NONE LAST NONE

RESI ASM          0.00 !   sphingomyelin d18:1/20:0
GROUP                  !
ATOM N    NTL    -0.60 !                   H15B
ATOM C15  CTL5   -0.35 !                   |
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ATOM H15A HL      0.25 !             H15A-C15-H15C
ATOM H15B HL      0.25 !                   |
ATOM H15C HL      0.25 !             H13C  |   H14C
ATOM C14  CTL5   -0.35 !              |    |   |
ATOM H14A HL      0.25 !        H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !              |    |   |
ATOM H14C HL      0.25 !             H13B  |   H14B
ATOM C13  CTL5   -0.35 !                   |
ATOM H13A HL      0.25 !                   |
ATOM H13B HL      0.25 !                   |
ATOM H13C HL      0.25 !              H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                   |
ATOM H12A HL      0.25 !                   |
ATOM H12B HL      0.25 !              H11A-C11-H11B
GROUP                  !                   |
ATOM C11  CTL2   -0.08 !                   |
ATOM H11A HAL2    0.09 !                   |
ATOM H11B HAL2    0.09 !         (-) O13  O12
ATOM P    PL      1.50 !               \ /
ATOM O13  O2L    -0.78 !                P  (+)
ATOM O14  O2L    -0.78 !               / \
ATOM O11  OSLP    -0.57 !         (-) O14  O11
ATOM O12  OSLP    -0.57 !                   |
ATOM C1S  CTL2   -0.08 !                   |
ATOM H1S  HAL2    0.09 !             H1S---C1S---H1T
ATOM H1T  HAL2    0.09 !                   |
GROUP                  !             H2S---C2S-------------NF--HNF
ATOM NF   NHL    -0.70 !                   |               |
ATOM HNF  H       0.35 !                   |               |
ATOM C2S  CTL1    0.30 !                   |               |
ATOM H2S  HAL1    0.05 !                   |               |
GROUP                  !                   |               |
ATOM C3S  CTO1    0.50 !                   |               C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                   |               |
ATOM O3   OHL    -0.69 !                   |               |
ATOM HO3  HOL     0.30 !                   |       H2F----C2F---H2G
GROUP                  !                   |               |
ATOM C4S  CEL3   -0.15 !                   |            [(CH2)3F (C3F,C4F...C19F)
ATOM H4S  HEL1    0.15 !                   |               |
GROUP                  !                   |       H20F---C20F---H20G
ATOM C5S  CEL3   -0.15 !                   |               |
ATOM H5S  HEL1    0.15 !                   |              H20H
GROUP                  !            H3S----C3S--O3--HO3
ATOM C6S  CTL2   -0.18 !                   |
ATOM H6S  HAL2    0.09 !                 C4S--H4S
ATOM H6T  HAL2    0.09 !                 ||
GROUP                  !                 C5S--H5S
ATOM C7S  CTL2   -0.18 !                   |
ATOM H7S  HAL2    0.09 !                   |
ATOM H7T  HAL2    0.09 !               [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                   |
ATOM C8S  CTL2   -0.18 !          H18S---C18S---H18U
ATOM H8S  HAL2    0.09 !                   |
ATOM H8T  HAL2    0.09 !                 H18T
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
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```
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
```

```
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                  !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
GROUP                  !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                  !
ATOM C18F CTL2   -0.18 !
ATOM H18F HAL2    0.09 !
ATOM H18G HAL2    0.09 !
GROUP                  !
ATOM C19F CTL2   -0.18 !
ATOM H19F HAL2    0.09 !
ATOM H19G HAL2    0.09 !
GROUP                  !
ATOM C20F CTL3   -0.27 !
ATOM H20F HAL3    0.09 !
ATOM H20G HAL3    0.09 !
ATOM H20H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
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BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F C19F C19F H19F  C19F H19G
BOND  C19F C20F C20F H20F  C20F H20G
BOND  C20F H20H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
 IC   C8S      C7S     C6S     C5S        1.5354  112.41 -179.61  111.46   1.5077
 IC   C7S      C6S     C5S     C4S        1.5391  111.46 -117.13  124.77   1.3444
 IC   C6S      C5S     C4S     C3S        1.5077  124.77  179.01  124.28   1.5009
 IC   C5S      C4S     C3S     C2S        1.3444  124.28  -84.24  110.14   1.5343
 IC   C5S      C4S     C3S     O3         1.3444  124.28  156.07  107.64   1.4235
 IC   C4S      C3S     C2S     C1S        1.5009  110.14  -70.50  114.25   1.5586
 IC   C13      C12    *N       C14        1.4967  109.68  116.91  107.30   1.5040
 IC   C13      C12    *N       C15        1.4967  109.68 -123.42  110.88   1.4938
 IC   C12      N       C15     H15A       1.5212  110.88 -177.15  111.31   1.0816
 IC   H15A     N      *C15     H15B       1.0816  111.31  118.98  109.44   1.0875
 IC   H15A     N      *C15     H15C       1.0816  111.31 -122.11  111.46   1.0818
 IC   C12      N       C14     H14A       1.5212  107.30 -178.89  114.23   1.0739
 IC   H14A     N      *C14     H14B       1.0739  114.23  123.44  110.21   1.0968
 IC   H14A     N      *C14     H14C       1.0739  114.23 -124.43  111.41   1.0948
 IC   C12      N       C13     H13A       1.5212  109.68  176.44  111.15   1.0822
 IC   H13A     N      *C13     H13B       1.0822  111.15  121.89  111.75   1.0814
 IC   H13A     N      *C13     H13C       1.0822  111.15 -118.50  109.57   1.0892
 IC   C13      N       C12     C11        1.4967  109.68 -178.83  116.30   1.5392
 IC   C11      N      *C12     H12A       1.5392  116.30  117.04  108.30   1.0985
 IC   C11      N      *C12     H12B       1.5392  116.30 -126.61  112.36   1.0787
 IC   N        C12     C11     O12        1.5212  116.30  126.79  107.85   1.4239
 IC   O12      C12    *C11     H11A       1.4239  107.85  118.10  109.30   1.1131
 IC   O12      C12    *C11     H11B       1.4239  107.85 -123.12  113.16   1.1140
 IC   C12      C11     O12     P          1.5392  107.85  -68.29  118.09   1.5886
 IC   C11      O12     P       O11        1.4239  118.09 -167.58  104.18   1.5725
 IC   O11      O12    *P       O13        1.5725  104.18  116.57  107.05   1.4823
 IC   O11      O12    *P       O14        1.5725  104.18 -118.73  106.98   1.4805
 IC   O12      P       O11     C1S        1.5886  104.18   51.85  121.69   1.4327
 IC   P        O11     C1S     C2S        1.5725  121.69  103.66  111.21   1.5586
 IC   C2S      O11    *C1S     H1S        1.5586  111.21  118.79  108.35   1.1121
 IC   C2S      O11    *C1S     H1T        1.5586  111.21 -123.25  112.85   1.1152
 IC   O11      C1S     C2S     C3S        1.4327  111.21  175.67  114.25   1.5343
 IC   C3S      C1S    *C2S     NF         1.5343  114.25  120.00  111.52   1.4406
 IC   C3S      C1S    *C2S     H2S        1.5343  114.25 -120.00  105.03   1.1194
 IC   C1S      C2S     NF      C1F        1.5586  111.52  160.94  124.85   1.3364
 IC   C1F      C2S    *NF      HNF        1.3364  124.85 -157.81  113.39   1.0062
 IC   C1S      C2S     C3S     C4S        1.5586  114.25  -70.50  110.14   1.5009
 IC   C4S      C2S    *C3S     O3         1.5009  110.14  118.36  109.80   1.4235
 IC   C4S      C2S    *C3S     H3S        1.5009  110.14 -121.14  110.10   1.1140
 IC   C2S      C3S     O3      HO3        1.5343  109.80   46.50  104.54   0.9610
 IC   C2S      C3S     C4S     C5S        1.5343  110.14  -84.24  124.28   1.3444
 IC   C5S      C3S    *C4S     H4S        1.3444  124.28  178.79  115.93   1.1003
 IC   C3S      C4S     C5S     C6S        1.5009  124.28  179.01  124.77   1.5077
 IC   C6S      C4S    *C5S     H5S        1.5077  124.77 -178.18  119.00   1.1029
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IC   C4S      C5S     C6S     C7S        1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S        1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T        1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S        1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S        1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T        1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S        1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S        1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T        1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S       1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S        1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T        1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S       1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S       1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T       1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S       1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S       1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T       1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S       1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S       1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T       1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S       1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S       1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T       1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S       1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S       1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T       1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S       1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S       1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T       1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S       1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S       1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T       1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S       1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S       1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T       1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S       1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T       1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U       1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F        1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF         1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F        1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F        1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G        1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F        1.4964  111.92  179.54  112.84   1.5310
IC   C4F      C2F    *C3F     H3F        1.5310  112.84 -121.63  109.37   1.1145
IC   H3F      C2F    *C3F     H3G        1.1145  109.37 -117.07  109.08   1.1157
IC   C2F      C3F     C4F     C5F        1.5434  112.23  174.86  112.58   1.5342
IC   C5F      C3F    *C4F     H4F        1.5342  112.58 -120.18  108.65   1.1140
IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
```

```
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    C19F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C19F     C17F   *C18F    H18F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H18F     C17F   *C18F    H18G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C17F     C18F    C19F    C20F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C20F     C18F   *C19F    H19F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H19F     C18F   *C19F    H19G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C18F     C19F    C20F    H20F       1.5334  113.16  -59.91  110.49   1.1113
 IC   H20F     C19F   *C20F    H20G       1.1113  110.49  119.86  110.41   1.1115
 IC   H20F     C19F   *C20F    H20H       1.1113  110.49 -120.11  110.63   1.1112
PATCH FIRST NONE LAST NONE

RESI BSM          0.00 !   sphingomyelin d18:1/22:0
GROUP                  !
ATOM N    NTL    -0.60 !                   H15B
ATOM C15  CTL5   -0.35 !                    |
ATOM H15A HL      0.25 !             H15A-C15-H15C
ATOM H15B HL      0.25 !                    |
ATOM H15C HL      0.25 !             H13C   |   H14C
ATOM C14  CTL5   -0.35 !              |     |    |
ATOM H14A HL      0.25 !        H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !              |     |    |
ATOM H14C HL      0.25 !             H13B   |   H14B
ATOM C13  CTL5   -0.35 !                    |
ATOM H13A HL      0.25 !                    |
ATOM H13B HL      0.25 !                    |
ATOM H13C HL      0.25 !               H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                    |
ATOM H12A HL      0.25 !                    |
ATOM H12B HL      0.25 !               H11A-C11-H11B
GROUP                  !                    |
ATOM C11  CTL2   -0.08 !                    |
ATOM H11A HAL2    0.09 !                    |
ATOM H11B HAL2    0.09 !         (-) O13  O12
ATOM P    PL      1.50 !               \ /
ATOM O13  O2L    -0.78 !                P  (+)
ATOM O14  O2L    -0.78 !               / \
ATOM O11  OSLP    -0.57 !          (-) O14  O11
ATOM O12  OSLP    -0.57 !                   |
ATOM C1S  CTL2   -0.08 !                   |
ATOM H1S  HAL2    0.09 !             H1S---C1S---H1T
ATOM H1T  HAL2    0.09 !                   |
GROUP                  !             H2S---C2S------------NF--HNF
ATOM NF   NHL    -0.70 !                   |               |
ATOM HNF  H       0.35 !                   |               |
ATOM C2S  CTL1    0.30 !                   |               |
ATOM H2S  HAL1    0.05 !                   |               |
GROUP                  !                   |               |
ATOM C3S  CTO1    0.50 !                   |              C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                   |               |
ATOM O3   OHL    -0.69 !                   |               |
ATOM HO3  HOL     0.30 !                   |       H2F----C2F---H2G
GROUP                  !                   |               |
ATOM C4S  CEL3   -0.15 !                   |           [(CH2)3F (C3F,C4F...C21F)
```

```
ATOM H4S  HEL1    0.15 !                    |               |
GROUP                  !                    |       H22F---C22F---H22G
ATOM C5S  CEL3   -0.15 !                    |               |
ATOM H5S  HEL1    0.15 !                    |              H22H
GROUP                  !            H3S----C3S--O3--HO3
ATOM C6S  CTL2   -0.18 !                    |
ATOM H6S  HAL2    0.09 !                  C4S--H4S
ATOM H6T  HAL2    0.09 !                  ||
GROUP                  !                  C5S--H5S
ATOM C7S  CTL2   -0.18 !                    |
ATOM H7S  HAL2    0.09 !                    |
ATOM H7T  HAL2    0.09 !                [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                    |
ATOM C8S  CTL2   -0.18 !           H18S---C18S---H18U
ATOM H8S  HAL2    0.09 !                    |
ATOM H8T  HAL2    0.09 !                  H18T
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
```

```
GROUP                   !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                   !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                   !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                   !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                   !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                   !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                   !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                   !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                   !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                   !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                   !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                   !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
GROUP                   !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                   !
ATOM C18F CTL2   -0.18 !
ATOM H18F HAL2    0.09 !
ATOM H18G HAL2    0.09 !
GROUP                   !
ATOM C19F CTL2   -0.18 !
ATOM H19F HAL2    0.09 !
ATOM H19G HAL2    0.09 !
GROUP                   !
ATOM C20F CTL2   -0.18 !
ATOM H20F HAL2    0.09 !
ATOM H20G HAL2    0.09 !
GROUP                   !
ATOM C21F CTL2   -0.18 !
ATOM H21F HAL2    0.09 !
ATOM H21G HAL2    0.09 !
GROUP                   !
ATOM C22F CTL3   -0.27 !
ATOM H22F HAL3    0.09 !
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ATOM H22G HAL3    0.09 !
ATOM H22H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F C19F C19F H19F  C19F H19G
BOND  C19F C20F C20F H20F  C20F H20G
BOND  C20F C21F C21F H21F  C21F H21G
BOND  C21F C22F C22F H22F  C22F H22G
BOND  C22F H22H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
 IC   C8S      C7S     C6S     C5S        1.5354  112.41 -179.61  111.46   1.5077
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IC   C7S      C6S     C5S     C4S       1.5391  111.46 -117.13  124.77   1.3444
IC   C6S      C5S     C4S     C3S       1.5077  124.77  179.01  124.28   1.5009
IC   C5S      C4S     C3S     C2S       1.3444  124.28  -84.24  110.14   1.5343
IC   C5S      C4S     C3S     O3        1.3444  124.28  156.07  107.64   1.4235
IC   C4S      C3S     C2S     C1S       1.5009  110.14  -70.50  114.25   1.5586
IC   C13      C12    *N       C14       1.4967  109.68  116.91  107.30   1.5040
IC   C13      C12    *N       C15       1.4967  109.68 -123.42  110.88   1.4938
IC   C12      N       C15     H15A      1.5212  110.88 -177.15  111.31   1.0816
IC   H15A     N      *C15     H15B      1.0816  111.31  118.98  109.44   1.0875
IC   H15A     N      *C15     H15C      1.0816  111.31 -122.11  111.46   1.0818
IC   C12      N       C14     H14A      1.5212  107.30 -178.89  114.23   1.0739
IC   H14A     N      *C14     H14B      1.0739  114.23  123.44  110.21   1.0968
IC   H14A     N      *C14     H14C      1.0739  114.23 -124.43  111.41   1.0948
IC   C12      N       C13     H13A      1.5212  109.68  176.44  111.15   1.0822
IC   H13A     N      *C13     H13B      1.0822  111.15  121.89  111.75   1.0814
IC   H13A     N      *C13     H13C      1.0822  111.15 -118.50  109.57   1.0892
IC   C13      N       C12     C11       1.4967  109.68 -178.83  116.30   1.5392
IC   C11      N      *C12     H12A      1.5392  116.30  117.04  108.30   1.0985
IC   C11      N      *C12     H12B      1.5392  116.30 -126.61  112.36   1.0787
IC   N        C12     C11     O12       1.5212  116.30  126.79  107.85   1.4239
IC   O12      C12    *C11     H11A      1.4239  107.85  118.10  109.30   1.1131
IC   O12      C12    *C11     H11B      1.4239  107.85 -123.12  113.16   1.1140
IC   C12      C11     O12     P         1.5392  107.85  -68.29  118.09   1.5886
IC   C11      O12     P       O11       1.4239  118.09 -167.58  104.18   1.5725
IC   O11      O12    *P       O13       1.5725  104.18  116.57  107.05   1.4823
IC   O11      O12    *P       O14       1.5725  104.18 -118.73  106.98   1.4805
IC   O12      P       O11     C1S       1.5886  104.18   51.85  121.69   1.4327
IC   P        O11     C1S     C2S       1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O11    *C1S     H1S       1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O11    *C1S     H1T       1.5586  111.21 -123.25  112.85   1.1152
IC   O11      C1S     C2S     C3S       1.4327  111.21  175.67  114.25   1.5343
IC   C3S      C1S    *C2S     NF        1.5343  114.25  120.00  111.52   1.4406
IC   C3S      C1S    *C2S     H2S       1.5343  114.25 -120.00  105.03   1.1194
IC   C1S      C2S     NF      C1F       1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF       1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S       1.5586  114.25  -70.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3        1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S       1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3       1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S       1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S       1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S       1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S       1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S       1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S       1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T       1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S       1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S       1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T       1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S       1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S       1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T       1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S      1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S       1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T       1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S      1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S      1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T      1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S      1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S      1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T      1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S      1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S      1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T      1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S      1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S      1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T      1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S      1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S      1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T      1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S      1.5345  112.58  180.00  112.58   1.5346
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IC   C16S     C14S   *C15S    H15S       1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T       1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S       1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S       1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T       1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S       1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S       1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T       1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S       1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T       1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U       1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F        1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF         1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F        1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F        1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G        1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F        1.4964  111.92  179.54  112.84   1.5310
IC   C4F      C2F    *C3F     H3F        1.5310  112.84 -121.63  109.37   1.1145
IC   H3F      C2F    *C3F     H3G        1.1145  109.37 -117.07  109.08   1.1157
IC   C2F      C3F     C4F     C5F        1.5434  112.23  174.86  112.58   1.5342
IC   C5F      C3F    *C4F     H4F        1.5342  112.58 -120.18  108.65   1.1140
IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
IC   C16F     C17F    C18F    C19F       1.5345  112.68 -178.23  113.16   1.5306
IC   C19F     C17F   *C18F    H18F       1.5306  113.16 -121.86  108.84   1.1140
IC   H18F     C17F   *C18F    H18G       1.1140  108.84 -116.70  108.76   1.1144
IC   C17F     C18F    C19F    C20F       1.5344  112.57  179.80  112.59   1.5346
IC   C20F     C18F   *C19F    H19F       1.5346  112.59 -121.28  109.10   1.1133
IC   H19F     C18F   *C19F    H19G       1.1133  109.10 -117.38  109.12   1.1133
IC   C18F     C19F    C20F    C21F       1.5345  112.59 -179.89  112.63   1.5337
IC   C21F     C19F   *C20F    H20F       1.5337  112.63 -121.33  109.16   1.1133
IC   H20F     C19F   *C20F    H20G       1.1133  109.16 -117.38  109.14   1.1133
IC   C19F     C20F    C21F    C22F       1.5346  112.63  179.93  113.24   1.5309
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 IC   C22F     C20F   *C21F    H21F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H21F     C20F   *C21F    H21G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C20F     C21F    C22F    H22F       1.5337  113.24  -59.91  110.47   1.1114
 IC   H22F     C21F   *C22F    H22G       1.1114  110.47  119.87  110.48   1.1113
 IC   H22F     C21F   *C22F    H22H       1.1114  110.47 -120.06  110.63   1.1113
PATCH FIRST NONE LAST NONE

RESI 23SM         0.00 !   sphingomyelin d18:1/23:0
GROUP                  !
ATOM N    NTL    -0.60 !                  H15B
ATOM C15  CTL5   -0.35 !                   |
ATOM H15A HL      0.25 !             H15A-C15-H15C
ATOM H15B HL      0.25 !                   |
ATOM H15C HL      0.25 !             H13C  |   H14C
ATOM C14  CTL5   -0.35 !              |    |   |
ATOM H14A HL      0.25 !        H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !              |    |   |
ATOM H14C HL      0.25 !             H13B  |   H14B
ATOM C13  CTL5   -0.35 !                   |
ATOM H13A HL      0.25 !                   |
ATOM H13B HL      0.25 !                   |
ATOM H13C HL      0.25 !              H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                   |
ATOM H12A HL      0.25 !                   |
ATOM H12B HL      0.25 !              H11A-C11-H11B
GROUP                  !                   |
ATOM C11  CTL2   -0.08 !                   |
ATOM H11A HAL2    0.09 !                   |
ATOM H11B HAL2    0.09 !         (-) O13  O12
ATOM P    PL      1.50 !               \ /
ATOM O13  O2L    -0.78 !                P  (+)
ATOM O14  O2L    -0.78 !               / \
ATOM O11  OSLP    -0.57 !         (-) O14  O11
ATOM O12  OSLP    -0.57 !                   |
ATOM C1S  CTL2   -0.08 !                   |
ATOM H1S  HAL2    0.09 !             H1S---C1S---H1T
ATOM H1T  HAL2    0.09 !                   |
GROUP                  !             H2S---C2S-------------NF--HNF
ATOM NF   NHL    -0.70 !                   |               |
ATOM HNF  H       0.35 !                   |               |
ATOM C2S  CTL1    0.30 !                   |               |
ATOM H2S  HAL1    0.05 !                   |               |
GROUP                  !                   |               |
ATOM C3S  CTO1    0.50 !                   |               C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                   |               |
ATOM O3   OHL    -0.69 !                   |               |
ATOM HO3  HOL     0.30 !                   |       H2F----C2F---H2G
GROUP                  !                   |               |
ATOM C4S  CEL3   -0.15 !                   |            [(CH2)3F (C3F,C4F...C22F)
ATOM H4S  HEL1    0.15 !                   |               |
GROUP                  !                   |       H23F---C23F---H23G
ATOM C5S  CEL3   -0.15 !                   |               |
ATOM H5S  HEL1    0.15 !                   |              H23H
GROUP                  !            H3S----C3S--O3--HO3
ATOM C6S  CTL2   -0.18 !                   |
ATOM H6S  HAL2    0.09 !                 C4S--H4S
ATOM H6T  HAL2    0.09 !                 ||
GROUP                  !                 C5S--H5S
ATOM C7S  CTL2   -0.18 !                   |
ATOM H7S  HAL2    0.09 !                   |
ATOM H7T  HAL2    0.09 !                [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                   |
ATOM C8S  CTL2   -0.18 !           H18S---C18S---H18U
ATOM H8S  HAL2    0.09 !                   |
ATOM H8T  HAL2    0.09 !                 H18T
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
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ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
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ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                  !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
GROUP                  !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                  !
ATOM C18F CTL2   -0.18 !
ATOM H18F HAL2    0.09 !
ATOM H18G HAL2    0.09 !
GROUP                  !
ATOM C19F CTL2   -0.18 !
ATOM H19F HAL2    0.09 !
ATOM H19G HAL2    0.09 !
GROUP                  !
ATOM C20F CTL2   -0.18 !
ATOM H20F HAL2    0.09 !
ATOM H20G HAL2    0.09 !
GROUP                  !
ATOM C21F CTL2   -0.18 !
ATOM H21F HAL2    0.09 !
ATOM H21G HAL2    0.09 !
GROUP                  !
ATOM C22F CTL2   -0.18 !
ATOM H22F HAL2    0.09 !
ATOM H22G HAL2    0.09 !
GROUP                  !
ATOM C23F CTL3   -0.27 !
ATOM H23F HAL3    0.09 !
ATOM H23G HAL3    0.09 !
ATOM H23H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
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BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F C19F C19F H19F  C19F H19G
BOND  C19F C20F C20F H20F  C20F H20G
BOND  C20F C21F C21F H21F  C21F H21G
BOND  C21F C22F C22F H22F  C22F H22G
BOND  C22F C23F C23F H23F  C23F H23G
BOND  C23F H23H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
 IC   C8S      C7S     C6S     C5S        1.5354  112.41 -179.61  111.46   1.5077
 IC   C7S      C6S     C5S     C4S        1.5391  111.46 -117.13  124.77   1.3444
 IC   C6S      C5S     C4S     C3S        1.5077  124.77  179.01  124.28   1.5009
 IC   C5S      C4S     C3S     C2S        1.3444  124.28  -84.24  110.14   1.5343
 IC   C5S      C4S     C3S     O3         1.3444  124.28  156.07  107.64   1.4235
 IC   C4S      C3S     C2S     C1S        1.5009  110.14  -70.50  114.25   1.5586
 IC   C13      C12    *N       C14        1.4967  109.68  116.91  107.30   1.5040
 IC   C13      C12    *N       C15        1.4967  109.68 -123.42  110.88   1.4938
 IC   C12      N       C15     H15A       1.5212  110.88 -177.15  111.31   1.0816
 IC   H15A     N      *C15     H15B       1.0816  111.31  118.98  109.44   1.0875
 IC   H15A     N      *C15     H15C       1.0816  111.31 -122.11  111.46   1.0818
 IC   C12      N       C14     H14A       1.5212  107.30 -178.89  114.23   1.0739
 IC   H14A     N      *C14     H14B       1.0739  114.23  123.44  110.21   1.0968
 IC   H14A     N      *C14     H14C       1.0739  114.23 -124.43  111.41   1.0948
 IC   C12      N       C13     H13A       1.5212  109.68  176.44  111.15   1.0822
 IC   H13A     N      *C13     H13B       1.0822  111.15  121.89  111.75   1.0814
 IC   H13A     N      *C13     H13C       1.0822  111.15 -118.50  109.57   1.0892
 IC   C13      N       C12     C11        1.4967  109.68 -178.83  116.30   1.5392
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IC   C11      N      *C12     H12A       1.5392  116.30  117.04  108.30   1.0985
IC   C11      N      *C12     H12B       1.5392  116.30 -126.61  112.36   1.0787
IC   N        C12     C11     O12        1.5212  116.30  126.79  107.85   1.4239
IC   O12      C12    *C11     H11A       1.4239  107.85  118.10  109.30   1.1131
IC   O12      C12    *C11     H11B       1.4239  107.85 -123.12  113.16   1.1140
IC   C12      C11     O12     P          1.5392  107.85  -68.29  118.09   1.5886
IC   C11      O12     P       O11        1.4239  118.09 -167.58  104.18   1.5725
IC   O11      O12    *P       O13        1.5725  104.18  116.57  107.05   1.4823
IC   O11      O12    *P       O14        1.5725  104.18 -118.73  106.98   1.4805
IC   O12      P       O11     C1S        1.5886  104.18   51.85  121.69   1.4327
IC   P        O11     C1S     C2S        1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O11    *C1S     H1S        1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O11    *C1S     H1T        1.5586  111.21 -123.25  112.85   1.1152
IC   O11      C1S     C2S     C3S        1.4327  111.21  175.67  114.25   1.5343
IC   C3S      C1S    *C2S     NF         1.5343  114.25  120.00  111.52   1.4406
IC   C3S      C1S    *C2S     H2S        1.5343  114.25 -120.00  105.03   1.1194
IC   C1S      C2S     NF      C1F        1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF        1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S        1.5586  114.25  -70.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3         1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S        1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3        1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S        1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S        1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S        1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S        1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S        1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S        1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T        1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S        1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S        1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T        1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S        1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S        1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T        1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S       1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S        1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T        1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S       1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S       1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T       1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S       1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S       1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T       1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S       1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S       1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T       1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S       1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S       1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T       1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S       1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S       1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T       1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S       1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S       1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T       1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S       1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S       1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T       1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S       1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S       1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T       1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S       1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T       1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U       1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F        1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF         1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F        1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F        1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G        1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F        1.4964  111.92  179.54  112.84   1.5310
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 IC   C4F      C2F    *C3F     H3F        1.5310  112.84 -121.63  109.37   1.1145
 IC   H3F      C2F    *C3F     H3G        1.1145  109.37 -117.07  109.08   1.1157
 IC   C2F      C3F     C4F     C5F        1.5434  112.23  174.86  112.58   1.5342
 IC   C5F      C3F    *C4F     H4F        1.5342  112.58 -120.18  108.65   1.1140
 IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
 IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
 IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
 IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
 IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
 IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
 IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
 IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
 IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
 IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
 IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
 IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
 IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    C19F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C19F     C17F   *C18F    H18F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H18F     C17F   *C18F    H18G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C17F     C18F    C19F    C20F       1.5344  112.57  179.80  112.59   1.5346
 IC   C20F     C18F   *C19F    H19F       1.5346  112.59 -121.28  109.10   1.1133
 IC   H19F     C18F   *C19F    H19G       1.1133  109.10 -117.38  109.12   1.1133
 IC   C18F     C19F    C20F    C21F       1.5345  112.59 -179.89  112.63   1.5337
 IC   C21F     C19F   *C20F    H20F       1.5337  112.63 -121.33  109.16   1.1133
 IC   H20F     C19F   *C20F    H20G       1.1133  109.16 -117.38  109.14   1.1133
 IC   C19F     C20F    C21F    C22F       1.5346  112.63  179.93  113.24   1.5309
 IC   C22F     C20F   *C21F    H21F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H21F     C20F   *C21F    H21G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C20F     C21F    C22F    C23F       1.5346  112.63  179.93  113.24   1.5309
 IC   C23F     C21F   *C22F    H22F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H22F     C21F   *C22F    H22G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C21F     C22F    C23F    H23F       1.5337  113.24  -59.91  110.47   1.1114
 IC   H23F     C22F   *C23F    H23G       1.1114  110.47  119.87  110.48   1.1113
 IC   H23F     C22F   *C23F    H23H       1.1114  110.47 -120.06  110.63   1.1113
PATCH FIRST NONE LAST NONE

RESI LSM          0.00 !   sphingomyelin d18:1/24:0
GROUP                  !
ATOM N    NTL    -0.60 !                   H15B
ATOM C15  CTL5   -0.35 !                   |
ATOM H15A HL      0.25 !             H15A-C15-H15C
ATOM H15B HL      0.25 !                   |
ATOM H15C HL      0.25 !             H13C  |   H14C
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ATOM C14  CTL5   -0.35 !              |    |   |
ATOM H14A HL      0.25 !        H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !              |    |   |
ATOM H14C HL      0.25 !           H13B  |   H14B
ATOM C13  CTL5   -0.35 !                 |
ATOM H13A HL      0.25 !                 |
ATOM H13B HL      0.25 !                 |
ATOM H13C HL      0.25 !              H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                 |
ATOM H12A HL      0.25 !                 |
ATOM H12B HL      0.25 !              H11A-C11-H11B
GROUP                  !                 |
ATOM C11  CTL2   -0.08 !                 |
ATOM H11A HAL2    0.09 !                 |
ATOM H11B HAL2    0.09 !         (-) O13  O12
ATOM P    PL      1.50 !               \ /
ATOM O13  O2L    -0.78 !                P  (+)
ATOM O14  O2L    -0.78 !               / \
ATOM O11  OSLP    -0.57 !          (-) O14  O11
ATOM O12  OSLP    -0.57 !                 |
ATOM C1S  CTL2   -0.08 !                 |
ATOM H1S  HAL2    0.09 !             H1S---C1S---H1T
ATOM H1T  HAL2    0.09 !                 |
GROUP                  !             H2S---C2S-------------NF--HNF
ATOM NF   NHL    -0.70 !                 |               |
ATOM HNF  H       0.35 !                 |               |
ATOM C2S  CTL1    0.30 !                 |               |
ATOM H2S  HAL1    0.05 !                 |               |
GROUP                  !                 |               |
ATOM C3S  CTO1    0.50 !                 |               C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                 |               |
ATOM O3   OHL    -0.69 !                 |               |
ATOM HO3  HOL     0.30 !                 |       H2F----C2F---H2G
GROUP                  !                 |               |
ATOM C4S  CEL3   -0.15 !                 |            [(CH2)3F (C3F,C4F...C23F)
ATOM H4S  HEL1    0.15 !                 |               |
GROUP                  !                 |       H24F---C24F---H24G
ATOM C5S  CEL3   -0.15 !                 |               |
ATOM H5S  HEL1    0.15 !                 |              H24H
GROUP                  !            H3S----C3S--O3--HO3
ATOM C6S  CTL2   -0.18 !                 |
ATOM H6S  HAL2    0.09 !                C4S--H4S
ATOM H6T  HAL2    0.09 !                ||
GROUP                  !                C5S--H5S
ATOM C7S  CTL2   -0.18 !                 |
ATOM H7S  HAL2    0.09 !                 |
ATOM H7T  HAL2    0.09 !               [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                 |
ATOM C8S  CTL2   -0.18 !           H18S---C18S---H18U
ATOM H8S  HAL2    0.09 !                 |
ATOM H8T  HAL2    0.09 !                H18T
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
```

```
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
```

```
GROUP                   !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                   !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                   !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
GROUP                   !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                   !
ATOM C18F CTL2   -0.18 !
ATOM H18F HAL2    0.09 !
ATOM H18G HAL2    0.09 !
GROUP                   !
ATOM C19F CTL2   -0.18 !
ATOM H19F HAL2    0.09 !
ATOM H19G HAL2    0.09 !
GROUP                   !
ATOM C20F CTL2   -0.18 !
ATOM H20F HAL2    0.09 !
ATOM H20G HAL2    0.09 !
GROUP                   !
ATOM C21F CTL2   -0.18 !
ATOM H21F HAL2    0.09 !
ATOM H21G HAL2    0.09 !
GROUP                   !
ATOM C22F CTL2   -0.18 !
ATOM H22F HAL2    0.09 !
ATOM H22G HAL2    0.09 !
GROUP                   !
ATOM C23F CTL2   -0.18 !
ATOM H23F HAL2    0.09 !
ATOM H23G HAL2    0.09 !
GROUP                   !
ATOM C24F CTL3   -0.27 !
ATOM H24F HAL3    0.09 !
ATOM H24G HAL3    0.09 !
ATOM H24H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
```

```
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F C19F C19F H19F  C19F H19G
BOND  C19F C20F C20F H20F  C20F H20G
BOND  C20F C21F C21F H21F  C21F H21G
BOND  C21F C22F C22F H22F  C22F H22G
BOND  C22F C23F C23F H23F  C23F H23G
BOND  C23F C24F C24F H24F  C24F H24G
BOND  C24F H24H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
 IC   C8S      C7S     C6S     C5S        1.5354  112.41 -179.61  111.46   1.5077
 IC   C7S      C6S     C5S     C4S        1.5391  111.46 -117.13  124.77   1.3444
 IC   C6S      C5S     C4S     C3S        1.5077  124.77  179.01  124.28   1.5009
 IC   C5S      C4S     C3S     C2S        1.3444  124.28  -84.24  110.14   1.5343
 IC   C5S      C4S     C3S     O3         1.3444  124.28  156.07  107.64   1.4235
 IC   C4S      C3S     C2S     C1S        1.5009  110.14  -70.50  114.25   1.5586
 IC   C13      C12    *N       C14        1.4967  109.68  116.91  107.30   1.5040
 IC   C13      C12    *N       C15        1.4967  109.68 -123.42  110.88   1.4938
 IC   C12      N       C15     H15A       1.5212  110.88 -177.15  111.31   1.0816
 IC   H15A     N      *C15     H15B       1.0816  111.31  118.98  109.44   1.0875
 IC   H15A     N      *C15     H15C       1.0816  111.31 -122.11  111.46   1.0818
 IC   C12      N       C14     H14A       1.5212  107.30 -178.89  114.23   1.0739
 IC   H14A     N      *C14     H14B       1.0739  114.23  123.44  110.21   1.0968
 IC   H14A     N      *C14     H14C       1.0739  114.23 -124.43  111.41   1.0948
 IC   C12      N       C13     H13A       1.5212  109.68  176.44  111.15   1.0822
 IC   H13A     N      *C13     H13B       1.0822  111.15  121.89  111.75   1.0814
 IC   H13A     N      *C13     H13C       1.0822  111.15 -118.50  109.57   1.0892
 IC   C13      N       C12     C11        1.4967  109.68 -178.83  116.30   1.5392
 IC   C11      N      *C12     H12A       1.5392  116.30  117.04  108.30   1.0985
 IC   C11      N      *C12     H12B       1.5392  116.30 -126.61  112.36   1.0787
 IC   N        C12     C11     O12        1.5212  116.30  126.79  107.85   1.4239
 IC   O12      C12    *C11     H11A       1.4239  107.85  118.10  109.30   1.1131
 IC   O12      C12    *C11     H11B       1.4239  107.85 -123.12  113.16   1.1140
 IC   C12      C11     O12     P          1.5392  107.85  -68.29  118.09   1.5886
 IC   C11      O12     P       O11        1.4239  118.09 -167.58  104.18   1.5725
 IC   O11      O12    *P       O13        1.5725  104.18  116.57  107.05   1.4823
 IC   O11      O12    *P       O14        1.5725  104.18 -118.73  106.98   1.4805
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IC   O12      P       O11     C1S       1.5886  104.18   51.85  121.69   1.4327
IC   P        O11     C1S     C2S       1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O11    *C1S     H1S       1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O11    *C1S     H1T       1.5586  111.21 -123.25  112.85   1.1152
IC   O11      C1S     C2S     C3S       1.4327  111.21  175.67  114.25   1.5343
IC   C3S      C1S    *C2S     NF        1.5343  114.25  120.00  111.52   1.4406
IC   C3S      C1S    *C2S     H2S       1.5343  114.25 -120.00  105.03   1.1194
IC   C1S      C2S     NF      C1F       1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF       1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S       1.5586  114.25  -70.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3        1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S       1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3       1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S       1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S       1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S       1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S       1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S       1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S       1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T       1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S       1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S       1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T       1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S       1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S       1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T       1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S      1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S       1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T       1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S      1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S      1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T      1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S      1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S      1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T      1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S      1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S      1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T      1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S      1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S      1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T      1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S      1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S      1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T      1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S      1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S      1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T      1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S      1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S      1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T      1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S      1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S      1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T      1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S      1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T      1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U      1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F       1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF        1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F       1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F       1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G       1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F       1.4964  111.92  179.54  112.84   1.5310
IC   C4F      C2F    *C3F     H3F       1.5310  112.84 -121.63  109.37   1.1145
IC   H3F      C2F    *C3F     H3G       1.1145  109.37 -117.07  109.08   1.1157
IC   C2F      C3F     C4F     C5F       1.5434  112.23  174.86  112.58   1.5342
IC   C5F      C3F    *C4F     H4F       1.5342  112.58 -120.18  108.65   1.1140
IC   H4F      C3F    *C4F     H4G       1.1140  108.65 -117.52  109.62   1.1127
IC   C3F      C4F     C5F     C6F       1.5340  112.58 -174.06  112.39   1.5340
IC   C6F      C4F    *C5F     H5F       1.5340  112.39 -122.01  109.38   1.1130
IC   H5F      C4F    *C5F     H5G       1.1130  109.38 -117.34  108.92   1.1134
IC   C4F      C5F     C6F     C7F       1.5342  112.39  178.27  112.75   1.5340
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 IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
 IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
 IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
 IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
 IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
 IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
 IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
 IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    C19F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C19F     C17F   *C18F    H18F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H18F     C17F   *C18F    H18G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C17F     C18F    C19F    C20F       1.5344  112.57  179.80  112.59   1.5346
 IC   C20F     C18F   *C19F    H19F       1.5346  112.59 -121.28  109.10   1.1133
 IC   H19F     C18F   *C19F    H19G       1.1133  109.10 -117.38  109.12   1.1133
 IC   C18F     C19F    C20F    C21F       1.5345  112.59 -179.89  112.63   1.5337
 IC   C21F     C19F   *C20F    H20F       1.5337  112.63 -121.33  109.16   1.1133
 IC   H20F     C19F   *C20F    H20G       1.1133  109.16 -117.38  109.14   1.1133
 IC   C19F     C20F    C21F    C22F       1.5346  112.63  179.93  113.24   1.5309
 IC   C22F     C20F   *C21F    H21F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H21F     C20F   *C21F    H21G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C20F     C21F    C22F    C23F       1.5346  112.63  179.93  113.24   1.5309
 IC   C23F     C21F   *C22F    H22F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H22F     C21F   *C22F    H22G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C21F     C22F    C23F    C24F       1.5346  112.63  179.93  113.24   1.5309
 IC   C24F     C22F   *C23F    H23F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H23F     C22F   *C23F    H23G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C22F     C23F    C24F    H24F       1.5337  113.24  -59.91  110.47   1.1114
 IC   H24F     C23F   *C24F    H24G       1.1114  110.47  119.87  110.48   1.1113
 IC   H24F     C23F   *C24F    H24H       1.1114  110.47 -120.06  110.63   1.1113
PATCH FIRST NONE LAST NONE

RESI NSM          0.00 !   sphingomyelin d18:1/24:1 (w/nervonic acid)
GROUP                  !
ATOM N    NTL    -0.60 !                   H15B
ATOM C15  CTL5   -0.35 !                   |
ATOM H15A HL      0.25 !             H15A-C15-H15C
ATOM H15B HL      0.25 !                   |
ATOM H15C HL      0.25 !             H13C  |   H14C
ATOM C14  CTL5   -0.35 !              |    |   |
ATOM H14A HL      0.25 !        H13A-C13---N--C14-H14A   (+)
ATOM H14B HL      0.25 !              |    |   |
ATOM H14C HL      0.25 !             H13B  |   H14B
ATOM C13  CTL5   -0.35 !                   |
ATOM H13A HL      0.25 !                   |
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ATOM H13B HL      0.25 !                  |
ATOM H13C HL      0.25 !              H12A-C12-H12B
ATOM C12  CTL2   -0.10 !                  |
ATOM H12A HL      0.25 !                  |
ATOM H12B HL      0.25 !              H11A-C11-H11B
GROUP                  !                  |
ATOM C11  CTL2   -0.08 !                  |
ATOM H11A HAL2    0.09 !                  |
ATOM H11B HAL2    0.09 !         (-) O13  O12
ATOM P    PL      1.50 !               \ /
ATOM O13  O2L    -0.78 !                P  (+)
ATOM O14  O2L    -0.78 !               / \
ATOM O11  OSLP    -0.57 !         (-) O14  O11
ATOM O12  OSLP    -0.57 !                  |
ATOM C1S  CTL2   -0.08 !                  |
ATOM H1S  HAL2    0.09 !            H1S---C1S---H1T
ATOM H1T  HAL2    0.09 !                  |
GROUP                  !            H2S---C2S-------------------------NF--HNF
ATOM NF   NHL    -0.70 !                  |                            |
ATOM HNF  H       0.35 !                  |                            |
ATOM C2S  CTL1    0.30 !                  |                            |
ATOM H2S  HAL1    0.05 !                  |                            |
GROUP                  !                  |                            |
ATOM C3S  CTO1    0.50 !                  |                          C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                  |                            |
ATOM O3   OHL    -0.69 !                  |                            |
ATOM HO3  HOL     0.30 !                  |                   H2F----C2F---H2G
GROUP                  !                  |                            |
ATOM C4S  CEL3   -0.15 !                  |                       [(CH2)3F (C3F,C4F...C14F)
ATOM H4S  HEL1    0.15 !                  |                            |
GROUP                  !                  |                   H15F---C15F
ATOM C5S  CEL3   -0.15 !                  |                          ||
ATOM H5S  HEL1    0.15 !                  |                   H16F---C16F
GROUP                  !           H3S----C3S--O3--HO3                 |
ATOM C6S  CTL2   -0.18 !                  |                       [(CH2)17F (C17F,C4F...C23F)
ATOM H6S  HAL2    0.09 !                C4S--H4S                      |
ATOM H6T  HAL2    0.09 !                ||                  H24F---C24F---H24H
GROUP                  !                C5S--H5S                      |
ATOM C7S  CTL2   -0.18 !                  |                         H24G
ATOM H7S  HAL2    0.09 !                  |
ATOM H7T  HAL2    0.09 !              [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                  |
ATOM C8S  CTL2   -0.18 !          H18S---C18S---H18U
ATOM H8S  HAL2    0.09 !                  |
ATOM H8T  HAL2    0.09 !                H18T
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
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```
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CEL1   -0.15 !
```

```
ATOM H15F HEL1    0.15 !
GROUP                  !
ATOM C16F CEL1   -0.15 !
ATOM H16F HEL1    0.15 !
GROUP                  !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                  !
ATOM C18F CTL2   -0.18 !
ATOM H18F HAL2    0.09 !
ATOM H18G HAL2    0.09 !
GROUP                  !
ATOM C19F CTL2   -0.18 !
ATOM H19F HAL2    0.09 !
ATOM H19G HAL2    0.09 !
GROUP                  !
ATOM C20F CTL2   -0.18 !
ATOM H20F HAL2    0.09 !
ATOM H20G HAL2    0.09 !
GROUP                  !
ATOM C21F CTL2   -0.18 !
ATOM H21F HAL2    0.09 !
ATOM H21G HAL2    0.09 !
GROUP                  !
ATOM C22F CTL2   -0.18 !
ATOM H22F HAL2    0.09 !
ATOM H22G HAL2    0.09 !
GROUP                  !
ATOM C23F CTL2   -0.18 !
ATOM H23F HAL2    0.09 !
ATOM H23G HAL2    0.09 !
GROUP                  !
ATOM C24F CTL3   -0.27 !
ATOM H24F HAL3    0.09 !
ATOM H24G HAL3    0.09 !
ATOM H24H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O11
!PHOSLPHOCHOLINE
BOND  O11  P    O12  P     O13  P     O14  P
BOND  O12  C11  C11  H11A  C11  H11B
BOND  C11  C12  C12  H12A  C12  H12B
BOND  C12  N    N    C13   N    C14   N    C15
BOND  C13  H13A C13  H13B  C13  H13C
BOND  C14  H14A C14  H14B  C14  H14C
BOND  C15  H15A C15  H15B  C15  H15C
!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
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BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F
BOND  C16F H16F
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F C19F C19F H19F  C19F H19G
BOND  C19F C20F C20F H20F  C20F H20G
BOND  C20F C21F C21F H21F  C21F H21G
BOND  C21F C22F C22F H22F  C22F H22G
BOND  C22F C23F C23F H23F  C23F H23G
BOND  C23F C24F C24F H24F  C24F H24G
BOND  C24F H24H

DOUBLE C4S  C5S
DOUBLE C15F C16F
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
 IC   C8S      C7S     C6S     C5S        1.5354  112.41 -179.61  111.46   1.5077
 IC   C7S      C6S     C5S     C4S        1.5391  111.46 -117.13  124.77   1.3444
 IC   C6S      C5S     C4S     C3S        1.5077  124.77  179.01  124.28   1.5009
 IC   C5S      C4S     C3S     C2S        1.3444  124.28  -84.24  110.14   1.5343
 IC   C5S      C4S     C3S     O3         1.3444  124.28  156.07  107.64   1.4235
 IC   C4S      C3S     C2S     C1S        1.5009  110.14  -70.50  114.25   1.5586
 IC   C13      C12    *N       C14        1.4967  109.68  116.91  107.30   1.5040
 IC   C13      C12    *N       C15        1.4967  109.68 -123.42  110.88   1.4938
 IC   C12      N       C15     H15A       1.5212  110.88 -177.15  111.31   1.0816
 IC   H15A     N      *C15     H15B       1.0816  111.31  118.98  109.44   1.0875
 IC   H15A     N      *C15     H15C       1.0816  111.31 -122.11  111.46   1.0818
 IC   C12      N       C14     H14A       1.5212  107.30 -178.89  114.23   1.0739
 IC   H14A     N      *C14     H14B       1.0739  114.23  123.44  110.21   1.0968
 IC   H14A     N      *C14     H14C       1.0739  114.23 -124.43  111.41   1.0948
 IC   C12      N       C13     H13A       1.5212  109.68  176.44  111.15   1.0822
 IC   H13A     N      *C13     H13B       1.0822  111.15  121.89  111.75   1.0814
 IC   H13A     N      *C13     H13C       1.0822  111.15 -118.50  109.57   1.0892
 IC   C13      N       C12     C11        1.4967  109.68 -178.83  116.30   1.5392
 IC   C11      N      *C12     H12A       1.5392  116.30  117.04  108.30   1.0985
 IC   C11      N      *C12     H12B       1.5392  116.30 -126.61  112.36   1.0787
 IC   N        C12     C11     O12        1.5212  116.30  126.79  107.85   1.4239
 IC   O12      C12    *C11     H11A       1.4239  107.85  118.10  109.30   1.1131
 IC   O12      C12    *C11     H11B       1.4239  107.85 -123.12  113.16   1.1140
 IC   C12      C11     O12     P          1.5392  107.85  -68.29  118.09   1.5886
 IC   C11      O12     P       O11        1.4239  118.09 -167.58  104.18   1.5725
 IC   O11      O12    *P       O13        1.5725  104.18  116.57  107.05   1.4823
 IC   O11      O12    *P       O14        1.5725  104.18 -118.73  106.98   1.4805
 IC   O12      P       O11     C1S        1.5886  104.18   51.85  121.69   1.4327
 IC   P        O11     C1S     C2S        1.5725  121.69  103.66  111.21   1.5586
 IC   C2S      O11    *C1S     H1S        1.5586  111.21  118.79  108.35   1.1121
 IC   C2S      O11    *C1S     H1T        1.5586  111.21 -123.25  112.85   1.1152
 IC   O11      C1S     C2S     C3S        1.4327  111.21  175.67  114.25   1.5343
 IC   C3S      C1S    *C2S     NF         1.5343  114.25  120.00  111.52   1.4406
 IC   C3S      C1S    *C2S     H2S        1.5343  114.25 -120.00  105.03   1.1194
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IC   C1S      C2S     NF      C1F       1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF       1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S       1.5586  114.25  -70.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3        1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S       1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3       1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S       1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S       1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S       1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S       1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S       1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S       1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T       1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S       1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S       1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T       1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S       1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S       1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T       1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S      1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S       1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T       1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S      1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S      1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T      1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S      1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S      1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T      1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S      1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S      1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T      1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S      1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S      1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T      1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S      1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S      1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T      1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S      1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S      1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T      1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S      1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S      1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T      1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S      1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S      1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T      1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S      1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T      1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U      1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F       1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF        1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F       1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F       1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G       1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F       1.4964  111.92  179.54  112.84   1.5310
IC   C4F      C2F    *C3F     H3F       1.5310  112.84 -121.63  109.37   1.1145
IC   H3F      C2F    *C3F     H3G       1.1145  109.37 -117.07  109.08   1.1157
IC   C2F      C3F     C4F     C5F       1.5434  112.23  174.86  112.58   1.5342
IC   C5F      C3F    *C4F     H4F       1.5342  112.58 -120.18  108.65   1.1140
IC   H4F      C3F    *C4F     H4G       1.1140  108.65 -117.52  109.62   1.1127
IC   C3F      C4F     C5F     C6F       1.5340  112.58 -174.06  112.39   1.5340
IC   C6F      C4F    *C5F     H5F       1.5340  112.39 -122.01  109.38   1.1130
IC   H5F      C4F    *C5F     H5G       1.1130  109.38 -117.34  108.92   1.1134
IC   C4F      C5F     C6F     C7F       1.5342  112.39  178.27  112.75   1.5340
IC   C7F      C5F    *C6F     H6F       1.5340  112.75 -120.93  108.96   1.1137
IC   H6F      C5F    *C6F     H6G       1.1137  108.96 -117.41  109.22   1.1131
IC   C5F      C6F     C7F     C8F       1.5340  112.75 -178.89  112.33   1.5342
IC   C8F      C6F    *C7F     H7F       1.5342  112.33 -121.40  109.26   1.1132
IC   H7F      C6F    *C7F     H7G       1.1132  109.26 -117.45  109.12   1.1130
IC   C6F      C7F     C8F     C9F       1.5340  112.33  179.09  112.77   1.5340
IC   C9F      C7F    *C8F     H8F       1.5340  112.77 -121.23  109.16   1.1134
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 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
 IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   C14F     C15F    C16F    C17F       1.5345  112.68    0.00  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    C19F       1.5345  112.68    0.00  113.16   1.5306
 IC   C19F     C17F   *C18F    H18F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H18F     C17F   *C18F    H18G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C17F     C18F    C19F    C20F       1.5344  112.57  180.00  112.59   1.5346
 IC   C20F     C18F   *C19F    H19F       1.5346  112.59 -121.28  109.10   1.1133
 IC   H19F     C18F   *C19F    H19G       1.1133  109.10 -117.38  109.12   1.1133
 IC   C18F     C19F    C20F    C21F       1.5345  112.59 -179.89  112.63   1.5337
 IC   C21F     C19F   *C20F    H20F       1.5337  112.63 -121.33  109.16   1.1133
 IC   H20F     C19F   *C20F    H20G       1.1133  109.16 -117.38  109.14   1.1133
 IC   C19F     C20F    C21F    C22F       1.5346  112.63  179.93  113.24   1.5309
 IC   C22F     C20F   *C21F    H21F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H21F     C20F   *C21F    H21G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C20F     C21F    C22F    C23F       1.5346  112.63  179.93  113.24   1.5309
 IC   C23F     C21F   *C22F    H22F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H22F     C21F   *C22F    H22G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C21F     C22F    C23F    C24F       1.5346  112.63  179.93  113.24   1.5309
 IC   C24F     C22F   *C23F    H23F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H23F     C22F   *C23F    H23G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C22F     C23F    C24F    H24F       1.5337  113.24  -59.91  110.47   1.1114
 IC   H24F     C23F   *C24F    H24G       1.1114  110.47  119.87  110.48   1.1113
 IC   H24F     C23F   *C24F    H24H       1.1114  110.47 -120.06  110.63   1.1113
PATCH FIRST NONE LAST NONE

RESI CER2    0.00      !  CERAMIDE by by Sam Tonddast-Navaei (U. Cin/Russel Lab)
                       !
GROUP                  !                HO1
ATOM O1  OHL -0.69     !                  \
ATOM HO1 HOL  0.30     !                   O1
ATOM C1S  CTO2    0.49 !                   |
ATOM H1S  HAL2   -0.05 !             H1S---C1S---H1T
ATOM H1T  HAL2   -0.05 !                   |
GROUP                  !             H2S---C2S-------------NF--HNF
ATOM NF   NHL    -0.70 !                   |               |
ATOM HNF  H       0.35 !                   |               |
ATOM C2S  CTL1    0.30 !                   |               |
ATOM H2S  HAL1    0.05 !                   |               |
GROUP                  !                   |               |
ATOM C3S  CTO1    0.50 !                   |               C1F=OF (FATTY ACID CHAIN)
ATOM H3S  HAL1   -0.11 !                   |               |
ATOM O3   OHL    -0.69 !                   |               |
ATOM HO3  HOL     0.30 !                   |       H2F----C2F---H2G
GROUP                  !                   |               |
ATOM C4S  CEL3   -0.15 !                   |            [(CH2)3F (C3F,C4F...C23F)
ATOM H4S  HEL1    0.15 !                   |               |
GROUP                  !                   |       H24F---C24F---H24G
```

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ATOM C5S  CEL3   -0.15 !                    |               |
ATOM H5S  HEL1    0.15 !                    |              H24H
GROUP                  !            H3S----C3S--O3--HO3
ATOM C6S  CTL2   -0.18 !                    |
ATOM H6S  HAL2    0.09 !                   C4S--H4S
ATOM H6T  HAL2    0.09 !                   ||
GROUP                  !                   C5S--H5S
ATOM C7S  CTL2   -0.18 !                    |
ATOM H7S  HAL2    0.09 !                    |
ATOM H7T  HAL2    0.09 !                [(CH)2]6 (C6S, C7S....C17S)
GROUP                  !                   |
ATOM C8S  CTL2   -0.18 !           H18S---C18S---H18U
ATOM H8S  HAL2    0.09 !                   |
ATOM H8T  HAL2    0.09 !                  H18T
GROUP                  !
ATOM C9S  CTL2   -0.18 !
ATOM H9S  HAL2    0.09 !
ATOM H9T  HAL2    0.09 !
GROUP                  !
ATOM C10S CTL2   -0.18 !
ATOM H10S HAL2    0.09 !
ATOM H10T HAL2    0.09 !
GROUP
ATOM C11S CTL2   -0.18 !
ATOM H11S HAL2    0.09 !
ATOM H11T HAL2    0.09 !
GROUP
ATOM C12S CTL2   -0.18 !
ATOM H12S HAL2    0.09 !
ATOM H12T HAL2    0.09 !
GROUP
ATOM C13S  CTL2  -0.18 !
ATOM H13S  HAL2   0.09 !
ATOM H13T  HAL2   0.09 !
GROUP
ATOM C14S  CTL2  -0.18 !
ATOM H14S  HAL2   0.09 !
ATOM H14T  HAL2   0.09 !
GROUP
ATOM C15S CTL2   -0.18 !
ATOM H15S HAL2    0.09 !
ATOM H15T HAL2    0.09 !
GROUP
ATOM C16S CTL2   -0.18 !
ATOM H16S HAL2    0.09 !
ATOM H16T HAL2    0.09 !
GROUP
ATOM C17S CTL2   -0.18 !
ATOM H17S HAL2    0.09 !
ATOM H17T HAL2    0.09 !
GROUP                  !
ATOM C18S CTL3   -0.27 !
ATOM H18S HAL3    0.09 !
ATOM H18T HAL3    0.09 !
ATOM H18U HAL3    0.09 !
GROUP                  !FATTY ACID CHAIN
ATOM C1F  C       0.55 !
ATOM OF   O      -0.60 !
ATOM C2F  CTL2   -0.07 !
ATOM H2F  HAL2    0.06 !
ATOM H2G  HAL2    0.06 !
GROUP                  !
ATOM C3F  CTL2   -0.18 !
ATOM H3F  HAL2    0.09 !
ATOM H3G  HAL2    0.09 !
GROUP                  !
ATOM C4F  CTL2   -0.18 !
ATOM H4F  HAL2    0.09 !
ATOM H4G  HAL2    0.09 !
GROUP                  !
ATOM C5F  CTL2   -0.18 !
```

```
ATOM H5F  HAL2    0.09 !
ATOM H5G  HAL2    0.09 !
GROUP                  !
ATOM C6F  CTL2   -0.18 !
ATOM H6F  HAL2    0.09 !
ATOM H6G  HAL2    0.09 !
GROUP                  !
ATOM C7F  CTL2   -0.18 !
ATOM H7F  HAL2    0.09 !
ATOM H7G  HAL2    0.09 !
GROUP                  !
ATOM C8F  CTL2   -0.18 !
ATOM H8F  HAL2    0.09 !
ATOM H8G  HAL2    0.09 !
GROUP                  !
ATOM C9F  CTL2   -0.18 !
ATOM H9F  HAL2    0.09 !
ATOM H9G  HAL2    0.09 !
GROUP                  !
ATOM C10F CTL2   -0.18 !
ATOM H10F HAL2    0.09 !
ATOM H10G HAL2    0.09 !
GROUP                  !
ATOM C11F CTL2   -0.18 !
ATOM H11F HAL2    0.09 !
ATOM H11G HAL2    0.09 !
GROUP                  !
ATOM C12F CTL2   -0.18 !
ATOM H12F HAL2    0.09 !
ATOM H12G HAL2    0.09 !
GROUP                  !
ATOM C13F CTL2   -0.18 !
ATOM H13F HAL2    0.09 !
ATOM H13G HAL2    0.09 !
GROUP                  !
ATOM C14F CTL2   -0.18 !
ATOM H14F HAL2    0.09 !
ATOM H14G HAL2    0.09 !
GROUP                  !
ATOM C15F CTL2   -0.18 !
ATOM H15F HAL2    0.09 !
ATOM H15G HAL2    0.09 !
GROUP                  !
ATOM C16F CTL2   -0.18 !
ATOM H16F HAL2    0.09 !
ATOM H16G HAL2    0.09 !
GROUP                  !
ATOM C17F CTL2   -0.18 !
ATOM H17F HAL2    0.09 !
ATOM H17G HAL2    0.09 !
GROUP                  !
ATOM C18F CTL2   -0.18 !
ATOM H18F HAL2    0.09 !
ATOM H18G HAL2    0.09 !
GROUP                  !
ATOM C19F CTL2   -0.18 !
ATOM H19F HAL2    0.09 !
ATOM H19G HAL2    0.09 !
GROUP                  !
ATOM C20F CTL2   -0.18 !
ATOM H20F HAL2    0.09 !
ATOM H20G HAL2    0.09 !
GROUP                  !
ATOM C21F CTL2   -0.18 !
ATOM H21F HAL2    0.09 !
ATOM H21G HAL2    0.09 !
GROUP                  !
ATOM C22F CTL2   -0.18 !
ATOM H22F HAL2    0.09 !
ATOM H22G HAL2    0.09 !
GROUP                  !
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ATOM C23F CTL2   -0.18 !
ATOM H23F HAL2    0.09 !
ATOM H23G HAL2    0.09 !
GROUP                  !
ATOM C24F CTL3   -0.27 !
ATOM H24F HAL3    0.09 !
ATOM H24G HAL3    0.09 !
ATOM H24H HAL3    0.09 !

!SPHINGOSINE CHAIN
BOND  C18S H18S C18S H18T  C18S H18U
BOND  C18S C17S C17S H17S  C17S H17T
BOND  C17S C16S C16S H16S  C16S H16T
BOND  C16S C15S C15S H15S  C15S H15T
BOND  C15S C14S C14S H14S  C14S H14T
BOND  C14S C13S C13S H13S  C13S H13T
BOND  C13S C12S C12S H12S  C12S H12T
BOND  C12S C11S C11S H11S  C11S H11T
BOND  C11S C10S C10S H10S  C10S H10T
BOND  C10S C9S  C9S  H9S   C9S  H9T
BOND  C9S  C8S  C8S  H8S   C8S  H8T
BOND  C8S  C7S  C7S  H7S   C7S  H7T
BOND  C7S  C6S  C6S  H6S   C6S  H6T
BOND  C6S  C5S  C5S  H5S   C4S  H4S
BOND  C4S  C3S  C3S  H3S   C3S  O3
BOND  O3   HO3
BOND  C3S  C2S  C2S  H2S
BOND  C2S  C1S  C1S  H1S   C1S  H1T
BOND  C1S  O1   O1   HO1

!FATTY ACID CHAIN
BOND  C2S  NF   NF   HNF   NF   C1F
BOND  C1F  C2F  C2F  H2F   C2F  H2G
BOND  C2F  C3F  C3F  H3F   C3F  H3G
BOND  C3F  C4F  C4F  H4F   C4F  H4G
BOND  C4F  C5F  C5F  H5F   C5F  H5G
BOND  C5F  C6F  C6F  H6F   C6F  H6G
BOND  C6F  C7F  C7F  H7F   C7F  H7G
BOND  C7F  C8F  C8F  H8F   C8F  H8G
BOND  C8F  C9F  C9F  H9F   C9F  H9G
BOND  C9F  C10F C10F H10F  C10F H10G
BOND  C10F C11F C11F H11F  C11F H11G
BOND  C11F C12F C12F H12F  C12F H12G
BOND  C12F C13F C13F H13F  C13F H13G
BOND  C13F C14F C14F H14F  C14F H14G
BOND  C14F C15F C15F H15F  C15F H15G
BOND  C15F C16F C16F H16F  C16F H16G
BOND  C16F C17F C17F H17F  C17F H17G
BOND  C17F C18F C18F H18F  C18F H18G
BOND  C18F C19F C19F H19F  C19F H19G
BOND  C19F C20F C20F H20F  C20F H20G
BOND  C20F C21F C21F H21F  C21F H21G
BOND  C21F C22F C22F H22F  C22F H22G
BOND  C22F C23F C23F H23F  C23F H23G
BOND  C23F C24F C24F H24F  C24F H24G
BOND  C24F H24H

DOUBLE C4S  C5S
DOUBLE C1F  OF
IMPR   C1F C2F NF OF  NF C1F C2S HNF

 IC   C18S     C17S    C16S    C15S       1.5309  113.23  180.00  112.64   1.5346
 IC   C17S     C16S    C15S    C14S       1.5337  112.64  180.00  112.58   1.5345
 IC   C16S     C15S    C14S    C13S       1.5346  112.58  180.00  112.58   1.5345
 IC   C15S     C14S    C13S    C12S       1.5345  112.58 -179.99  112.58   1.5345
 IC   C14S     C13S    C12S    C11S       1.5345  112.58  179.97  112.58   1.5344
 IC   C13S     C12S    C11S    C10S       1.5345  112.58 -179.96  112.61   1.5345
 IC   C12S     C11S    C10S    C9S        1.5344  112.61  179.97  112.54   1.5344
 IC   C11S     C10S    C9S     C8S        1.5345  112.54 -179.87  112.66   1.5345
 IC   C10S     C9S     C8S     C7S        1.5344  112.66 -179.89  112.50   1.5354
 IC   C9S      C8S     C7S     C6S        1.5345  112.50 -179.79  112.41   1.5391
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IC   C8S      C7S     C6S     C5S       1.5354  112.41 -179.61  111.46   1.5077
IC   C7S      C6S     C5S     C4S       1.5391  111.46 -117.13  124.77   1.3444
IC   C6S      C5S     C4S     C3S       1.5077  124.77  179.01  124.28   1.5009
IC   C5S      C4S     C3S     C2S       1.3444  124.28  -84.24  110.14   1.5343
IC   C5S      C4S     C3S     O3        1.3444  124.28  156.07  107.64   1.4235
IC   C4S      C3S     C2S     C1S       1.5009  110.14  -70.50  114.25   1.5586
IC   HO1      O1      C1S     C2S       1.5725  121.69  103.66  111.21   1.5586
IC   C2S      O1     *C1S     H1S       1.5586  111.21  118.79  108.35   1.1121
IC   C2S      O1     *C1S     H1T       1.5586  111.21 -123.25  112.85   1.1152
IC   O1       C1S     C2S     C3S       1.4327  111.21  175.67  114.25   1.5343
IC   C3S      C1S    *C2S     NF        1.5343  114.25  120.00  111.52   1.4406
IC   C3S      C1S    *C2S     H2S       1.5343  114.25 -120.00  105.03   1.1194
IC   C1S      C2S     NF      C1F       1.5586  111.52  160.94  124.85   1.3364
IC   C1F      C2S    *NF      HNF       1.3364  124.85 -157.81  113.39   1.0062
IC   C1S      C2S     C3S     C4S       1.5586  114.25  -70.50  110.14   1.5009
IC   C4S      C2S    *C3S     O3        1.5009  110.14  118.36  109.80   1.4235
IC   C4S      C2S    *C3S     H3S       1.5009  110.14 -121.14  110.10   1.1140
IC   C2S      C3S     O3      HO3       1.5343  109.80   46.50  104.54   0.9610
IC   C2S      C3S     C4S     C5S       1.5343  110.14  -84.24  124.28   1.3444
IC   C5S      C3S    *C4S     H4S       1.3444  124.28  178.79  115.93   1.1003
IC   C3S      C4S     C5S     C6S       1.5009  124.28  179.01  124.77   1.5077
IC   C6S      C4S    *C5S     H5S       1.5077  124.77 -178.18  119.00   1.1029
IC   C4S      C5S     C6S     C7S       1.3444  124.77 -117.13  111.46   1.5391
IC   C7S      C5S    *C6S     H6S       1.5391  111.46  120.98  111.41   1.1142
IC   C7S      C5S    *C6S     H6T       1.5391  111.46 -120.60  109.91   1.1125
IC   C5S      C6S     C7S     C8S       1.5077  111.46 -179.61  112.41   1.5354
IC   C8S      C6S    *C7S     H7S       1.5354  112.41  121.26  109.74   1.1138
IC   C8S      C6S    *C7S     H7T       1.5354  112.41 -120.99  109.40   1.1147
IC   C6S      C7S     C8S     C9S       1.5391  112.41 -179.79  112.50   1.5345
IC   C9S      C7S    *C8S     H8S       1.5345  112.50  121.20  108.97   1.1132
IC   C9S      C7S    *C8S     H8T       1.5345  112.50 -121.38  109.07   1.1129
IC   C7S      C8S     C9S     C10S      1.5354  112.50 -179.89  112.66   1.5344
IC   C10S     C8S    *C9S     H9S       1.5344  112.66  121.49  109.05   1.1133
IC   C10S     C8S    *C9S     H9T       1.5344  112.66 -121.38  108.96   1.1136
IC   C8S      C9S     C10S    C11S      1.5345  112.66 -179.87  112.54   1.5345
IC   C11S     C9S    *C10S    H10S      1.5345  112.54  121.27  109.07   1.1133
IC   C11S     C9S    *C10S    H10T      1.5345  112.54 -121.34  109.11   1.1132
IC   C9S      C10S    C11S    C12S      1.5344  112.54  179.97  112.61   1.5344
IC   C12S     C10S   *C11S    H11S      1.5344  112.61  121.36  109.09   1.1133
IC   C12S     C10S   *C11S    H11T      1.5344  112.61 -121.33  109.07   1.1134
IC   C10S     C11S    C12S    C13S      1.5345  112.61 -179.96  112.58   1.5345
IC   C13S     C11S   *C12S    H12S      1.5345  112.58  121.29  109.12   1.1133
IC   C13S     C11S   *C12S    H12T      1.5345  112.58 -121.31  109.15   1.1133
IC   C11S     C12S    C13S    C14S      1.5344  112.58  179.97  112.58   1.5345
IC   C14S     C12S   *C13S    H13S      1.5345  112.58  121.30  109.13   1.1133
IC   C14S     C12S   *C13S    H13T      1.5345  112.58 -121.30  109.13   1.1133
IC   C12S     C13S    C14S    C15S      1.5345  112.58 -179.99  112.58   1.5345
IC   C15S     C13S   *C14S    H14S      1.5345  112.58  121.30  109.12   1.1133
IC   C15S     C13S   *C14S    H14T      1.5345  112.58 -121.31  109.12   1.1133
IC   C13S     C14S    C15S    C16S      1.5345  112.58  180.00  112.58   1.5346
IC   C16S     C14S   *C15S    H15S      1.5346  112.58  121.30  109.11   1.1133
IC   C16S     C14S   *C15S    H15T      1.5346  112.58 -121.30  109.11   1.1133
IC   C14S     C15S    C16S    C17S      1.5345  112.58  180.00  112.64   1.5337
IC   C17S     C15S   *C16S    H16S      1.5337  112.64  121.32  109.14   1.1133
IC   C17S     C15S   *C16S    H16T      1.5337  112.64 -121.32  109.14   1.1133
IC   C15S     C16S    C17S    C18S      1.5346  112.64  180.00  113.23   1.5309
IC   C18S     C16S   *C17S    H17S      1.5309  113.23  121.67  108.77   1.1142
IC   C18S     C16S   *C17S    H17T      1.5309  113.23 -121.67  108.77   1.1142
IC   C16S     C17S    C18S    H18S      1.5337  113.23  180.00  110.63   1.1113
IC   H18S     C17S   *C18S    H18T      1.1113  110.63  120.07  110.47   1.1114
IC   H18S     C17S   *C18S    H18U      1.1113  110.63 -120.07  110.47   1.1114
IC   C2S      NF      C1F     C2F       1.4406  124.85 -156.83  114.97   1.4964
IC   C2F      NF     *C1F     OF        1.4964  114.97  162.54  122.11   1.2268
IC   NF       C1F     C2F     C3F       1.3364  114.97 -146.57  111.92   1.5432
IC   C3F      C1F    *C2F     H2F       1.5432  111.92 -120.83  107.93   1.1115
IC   H2F      C1F    *C2F     H2G       1.1115  107.93 -117.30  109.04   1.1113
IC   C1F      C2F     C3F     C4F       1.4964  111.92  179.54  112.84   1.5310
IC   C4F      C2F    *C3F     H3F       1.5310  112.84 -121.63  109.37   1.1145
IC   H3F      C2F    *C3F     H3G       1.1145  109.37 -117.07  109.08   1.1157
IC   C2F      C3F     C4F     C5F       1.5434  112.23  174.86  112.58   1.5342
IC   C5F      C3F    *C4F     H4F       1.5342  112.58 -120.18  108.65   1.1140
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 IC   H4F      C3F    *C4F     H4G        1.1140  108.65 -117.52  109.62   1.1127
 IC   C3F      C4F     C5F     C6F        1.5340  112.58 -174.06  112.39   1.5340
 IC   C6F      C4F    *C5F     H5F        1.5340  112.39 -122.01  109.38   1.1130
 IC   H5F      C4F    *C5F     H5G        1.1130  109.38 -117.34  108.92   1.1134
 IC   C4F      C5F     C6F     C7F        1.5342  112.39  178.27  112.75   1.5340
 IC   C7F      C5F    *C6F     H6F        1.5340  112.75 -120.93  108.96   1.1137
 IC   H6F      C5F    *C6F     H6G        1.1137  108.96 -117.41  109.22   1.1131
 IC   C5F      C6F     C7F     C8F        1.5340  112.75 -178.89  112.33   1.5342
 IC   C8F      C6F    *C7F     H7F        1.5342  112.33 -121.40  109.26   1.1132
 IC   H7F      C6F    *C7F     H7G        1.1132  109.26 -117.45  109.12   1.1130
 IC   C6F      C7F     C8F     C9F        1.5340  112.33  179.09  112.77   1.5340
 IC   C9F      C7F    *C8F     H8F        1.5340  112.77 -121.23  109.16   1.1134
 IC   H8F      C7F    *C8F     H8G        1.1134  109.16 -117.38  109.08   1.1133
 IC   C7F      C8F     C9F     C10F       1.5342  112.77  179.02  112.34   1.5343
 IC   C10F     C8F    *C9F     H9F        1.5343  112.34 -121.27  109.27   1.1132
 IC   H9F      C8F    *C9F     H9G        1.1132  109.27 -117.45  109.10   1.1130
 IC   C8F      C9F     C10F    C11F       1.5340  112.34  178.16  112.74   1.5340
 IC   C11F     C9F    *C10F    H10F       1.5340  112.74 -121.18  109.16   1.1134
 IC   H10F     C9F    *C10F    H10G       1.1134  109.16 -117.35  109.10   1.1132
 IC   C9F      C10F    C11F    C12F       1.5343  112.74  178.91  112.38   1.5343
 IC   C12F     C10F   *C11F    H11F       1.5343  112.38 -121.39  109.34   1.1131
 IC   H11F     C10F   *C11F    H11G       1.1131  109.34 -117.43  108.98   1.1132
 IC   C10F     C11F    C12F    C13F       1.5340  112.38  176.93  112.68   1.5340
 IC   C13F     C11F   *C12F    H12F       1.5340  112.68 -121.02  109.05   1.1134
 IC   H12F     C11F   *C12F    H12G       1.1134  109.05 -117.34  109.20   1.1131
 IC   C11F     C12F    C13F    C14F       1.5343  112.68 -179.93  112.45   1.5345
 IC   C14F     C12F   *C13F    H13F       1.5345  112.45 -121.60  109.42   1.1129
 IC   H13F     C12F   *C13F    H13G       1.1129  109.42 -117.40  108.85   1.1134
 IC   C12F     C13F    C14F    C15F       1.5340  112.45  175.93  112.68   1.5334
 IC   C15F     C13F   *C14F    H14F       1.5334  112.68 -121.00  109.06   1.1131
 IC   H14F     C13F   *C14F    H14G       1.1131  109.06 -117.24  109.28   1.1130
 IC   C13F     C14F    C15F    C16F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C16F     C14F   *C15F    H15F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H15F     C14F   *C15F    H15G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C14F     C15F    C16F    C17F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C17F     C15F   *C16F    H16F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H16F     C15F   *C16F    H16G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C15F     C16F    C17F    C18F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C18F     C16F   *C17F    H17F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H17F     C16F   *C17F    H17G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C16F     C17F    C18F    C19F       1.5345  112.68 -178.23  113.16   1.5306
 IC   C19F     C17F   *C18F    H18F       1.5306  113.16 -121.86  108.84   1.1140
 IC   H18F     C17F   *C18F    H18G       1.1140  108.84 -116.70  108.76   1.1144
 IC   C17F     C18F    C19F    C20F       1.5344  112.57  179.80  112.59   1.5346
 IC   C20F     C18F   *C19F    H19F       1.5346  112.59 -121.28  109.10   1.1133
 IC   H19F     C18F   *C19F    H19G       1.1133  109.10 -117.38  109.12   1.1133
 IC   C18F     C19F    C20F    C21F       1.5345  112.59 -179.89  112.63   1.5337
 IC   C21F     C19F   *C20F    H20F       1.5337  112.63 -121.33  109.16   1.1133
 IC   H20F     C19F   *C20F    H20G       1.1133  109.16 -117.38  109.14   1.1133
 IC   C19F     C20F    C21F    C22F       1.5346  112.63  179.93  113.24   1.5309
 IC   C22F     C20F   *C21F    H21F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H21F     C20F   *C21F    H21G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C20F     C21F    C22F    C23F       1.5346  112.63  179.93  113.24   1.5309
 IC   C23F     C21F   *C22F    H22F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H22F     C21F   *C22F    H22G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C21F     C22F    C23F    C24F       1.5346  112.63  179.93  113.24   1.5309
 IC   C24F     C22F   *C23F    H23F       1.5309  113.24 -121.66  108.77   1.1142
 IC   H23F     C22F   *C23F    H23G       1.1142  108.77 -116.65  108.78   1.1142
 IC   C22F     C23F    C24F    H24F       1.5337  113.24  -59.91  110.47   1.1114
 IC   H24F     C23F   *C24F    H24G       1.1114  110.47  119.87  110.48   1.1113
 IC   H24F     C23F   *C24F    H24H       1.1114  110.47 -120.06  110.63   1.1113
PATCH FIRST NONE LAST NONE

end

read para card flex @app
* new parameters
*

ATOMS
MASS   165 NHL   14.00700 !N !
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MASS   166 CTO1  12.01100 !C !
MASS   167 CEL3  12.01100 !C !
MASS   168 CTO2  12.01100 !C !


BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
! Cyclopropane Moeity Addition
!

! Ceramides
! CC
CTL1  CEL3  250.000     1.490  ! prot22; Ala Dipeptide ab initio calc's (LK) fixed from 10/90 (5/91); CT1-C
CTO1  CEL3  250.000     1.490  ! prot22; Ala Dipeptide ab initio calc's (LK) fixed from 10/90 (5/91) ; CT1-C
CTO1  CTL1  222.500     1.500  ! lip36; alkanes, 3/92; CTL1-CTL1
CTO1  CTL3  222.500     1.538  ! lip36; alkanes, 3/92; CTL1-CTL3
CEL3  CTL2  365.000     1.502  ! lip36; butene; from propene, yin,adm jr., 12/95; CEL1-CTL2
CEL3  CEL3  440.000     1.340  ! lip36; butene, yin,adm jr., 12/95; CEL1-CEL1
CTL2  C     250.000     1.490  ! prot22; Ala Dipeptide ab initio calc's (LK) fixed from 10/90 (5/91); CT2-C
CTL3  C     250.000     1.490  ! prot22; Ala Dipeptide ab initio calc's (LK) fixed from 10/90 (5/91); CT3-C
CTO1  OHL   428.000     1.420  ! lip36; glycerol; OHL-CTL1
CTO1  OSL   340.000     1.430  ! lipid ester; rmv nov 2009
CTO1  HAL1  309.000     1.111  ! lip36; alkanes, 3/92; CTL1-HAL1
HEL1  CEL3  360.500     1.100  ! lip36; propene, yin,adm jr., 12/95; HEL1-CEL1
NHL   H     440.000     0.997  ! prot22; Alanine Dipeptide ab initio calc's (LK); NH1-H
NHL   CTL3  320.000     1.430  ! prot22; NMA Gas & Liquid Phase IR Spectra (LK); NH1-CT3
NHL   C     370.000     1.345  ! prot22; Alanine Dipeptide ab initio calc's (LK); NH1-C
NHL   CTL1  320.000     1.430  ! prot22; NMA Gas & Liquid Phase IR Spectra (LK); NH1-CT1
CTO2  HAL2  309.000     1.111  ! lip36; alkanes, 4/98
CTO2  CTL1  222.500     1.538  ! lip36; alkanes, 3/92
CTO2  OHL   428.000     1.420  ! glycerol


ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
! Ceramides
!CCC
CTL3   CTL1   CEL3    52.000   108.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); CT3-CT1-C
CTL3   CTO1   CEL3    52.000   108.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); CT3-CT1-C
CTL1   CEL3   CEL3    48.00    123.50   ! lip36; 2-butene,from 2-butene, yin,adm jr., 12/95; CEL1-CEL1-CTL2
CTO1   CEL3   CEL3    48.00    123.50   ! lip36; 2-butene,from 2-butene, yin,adm jr., 12/95; CEL1-CEL1-CTL2
CTL1   CTL1   CEL3    52.000   108.00   ! prot22; Alanine Dipeptide ab inition calc's (LK); CT1 CT1 C
CTL1   CTO1   CEL3    52.000   108.00   ! prot22; Alanine Dipeptide ab inition calc's (LK); CT1 CT1 C
C      CTL2   CTL2    52.000   108.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); CT3-CT1-C
CTL2   CTL1   CTO1    58.350   113.50   11.16   2.561  ! lip36; glycerol; CTL1-CTL1-CTL2
CEL3   CEL3   CTL2    48.000   123.50   ! lip36; 2-butene,from 2-butene, yin,adm jr., 12/95; CEL1-CEL1-CTL2
CEL3   CTL2   CTL3    32.00    112.20   ! lip36; 1-butene; from propene, yin,adm jr., 12/95; CEL1-CTL2-CTL3
CEL3   CTL2   CTL2    32.00    112.20   ! lip36; 1-butene; from propene, yin,adm jr., 12/95; CEL1-CTL2-CTL2
CTL3   CTL2   C       52.000   108.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); CT3-CT1-C
OHL    CTL1   CEL3    75.700   110.10   ! prot22; MeOH, EMB, 10/10/89; OH1-CT1-CT1
OHL    CTO1   CEL3    75.700   110.10   ! prot22; MeOH, EMB, 10/10/89; OH1-CT1-CT1
OHL    CTL1   CTL3    75.700   110.10   ! prot22; MeOH, EMB, 10/10/89; OH1 CT1 CT3
OHL    CTO1   CTL3    75.700   110.10   ! prot22; MeOH, EMB, 10/10/89; OH1 CT1 CT3
OHL    CTO1   CTL1    75.700   110.10   ! prot22; MeOH, EMB, 10/10/89; OH1 CT1 CT1
O      C      CTL2    80.000   121.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); O-C-CT2
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O      C      CTL3    80.000   121.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); O C CT3
OSL    CTO1   CTL1    75.700   110.10   ! analog for acetyl at sphingosine O3; rmv nov 2009
OSL    CTO1   CEL3    75.700   110.10   ! analog for acetyl at sphingosine O3; rmv nov 2009
CL     OSL    CTO1    40.00    109.60    30.0   2.2651 ! analog for acetyl at sphingosine O3; rmv nov 2009
CTL1   CEL3   HEL1    40.00    116.00   ! lip36; 1-butene, from propene,yin.adm jr.,12/95; HEL1-CEL1-CTL2
CTO1   CEL3   HEL1    40.00    116.00   ! lip36; 1-butene, from propene,yin.adm jr.,12/95; HEL1-CEL1-CTL2
HAL1    CTL1    CEL3     33.000    109.50   30.00    2.16300 ! prot22; alanine dipeptide, LK, replaced, adm jr.,
5/09/91; HA-CT1-C (Protein)
HAL1    CTO1    CEL3     33.000    109.50   30.00    2.16300 ! prot22; alanine dipeptide, LK, replaced, adm jr.,
5/09/91; HA-CT1-C (Protein)
HAL1   CTO1   CTL3    34.500   110.10   22.53   2.179  ! lip36; alkane, 3/92; HAL1-CTL1-CTL3
HAL1   CTO1   CTL1    34.500   110.10   22.53   2.179  ! lip36; alkane, 3/92; HAL1-CTL1-CTL1
HAL1   CTL1   CTO1    34.500   110.10   22.53   2.179  ! lip36; alkane, 3/92; HAL1-CTL1-CTL1
HAL3   CTL3   CTO1    33.430   110.10   22.53   2.179  ! lip36; alkane, 4/98; HAL3-CTL3-CTL
HEL1   CEL3   CEL3    52.00    119.50   ! lip36; 2-butene, yin,adm jr., 12/95; HEL1-CEL1-CEL1
HEL1   CEL3   CTL2    40.00    116.00   ! lip36; 1-butene; from propene, yin,adm jr., 12/95; HEL1-CEL1-CTL2
CEL3   CTL2   HAL2    45.00    111.50   ! lip36; 1-butene; from propene, yin,adm jr., 12/95; HAL2-CTL2-CEL1
HAL2    CTL2    C        33.000    109.50   30.00    2.16300 ! prot22; alanine dipeptide, LK, replaced, adm jr.,
5/09/91; HA-CT2-C
HAL3    CTL3    C        33.000    109.50   30.00    2.16300 ! prot22; alanine dipeptide, LK, replaced, adm jr.,
5/09/91; C CT3 HA
NHL    CTL1   OSL     80.000   122.50   ! prot22; NMA Vib Modes (LK); O-C-NH1
O      C      NHL     80.000   122.50   ! prot22; NMA Vib Modes (LK); O-C-NH1
HOL    OHL    CTO1    57.500   106.00   ! lip36; glycerol; HOL-OHL-CTL1
OHL    CTO1   HAL1    45.900   108.89   ! lip36; glycerol; OHL-CTL1-HAL1
OSL    CTO1   HAL1    45.900   108.89   ! lip36; glycerol; OHL-CTL1-HAL1; rmv nov 2009
NHL    CTL1   CTO1    70.000   113.50   ! prot22; Alanine Dipeptide ab initio calc's (LK); NH1-CT1-CT1
NHL    C      CTL2    80.000   116.50   ! prot22; NMA Vib Modes (LK);  NH1-C-CT2
NHL    CTL1   CTL2    70.000   113.50   ! prot22; Alanine Dipeptide ab initio calc's (LK); NH1-CT1-CT2
NHL    CTL1   CTL3    70.000   113.50   ! prot22;
NHL    CTL1   CTL1    70.000   113.50   ! prot22; Alanine Dipeptide ab initio calc's (LK); NH1-CT1-CT1
NHL    C      CTL3    80.000   116.50   ! prot22; NMA Vib Modes (LK); NH1-C-CT3
H      NHL    CTL3    35.000   117.00   ! prot22; NMA Vibrational Modes (LK); H-NH1-CT3
H      NHL    C       34.000   123.00   ! prot22; NMA Vib Modes (LK); H-NH1-C
H      NHL    CTL1    35.000   117.00   ! prot22; NMA Vibrational Modes (LK); H-NH1-CT1
CTL3   NHL    C       50.000   120.00   ! prot22; NMA Vib Modes (LK); CT3-NH1-C
CTL1   NHL    C       50.000   120.00   ! prot22; NMA Vib Modes (LK); CT1 NH1 C
NHL    CTL3   HAL3    51.500   109.50   ! prot22; NMA crystal (JCS); NH1-CT3-HA
NHL    CTL1   HAL1    48.000   108.00   ! prot22; Alanine Dipeptide ab initio calc's (LK); NH1-CT1-HB
HOL    OHL    CTO2    57.500   106.00   ! lip36; glycerol; HOL-OHL-CTL2
OHL    CTO2   HAL2    45.900   108.89   ! lip36; glycerol; OHL-CTL2-HAL1
HAL2   CTO2   CTL1    26.500   110.10   22.53   2.179  ! lip36; alkane, 4/98; HAL2-CTL2-CTL1
HAL1   CTL1   CTO2    34.500   110.10   22.53   2.179  ! lip36; alkane, 3/92; HAL1-CTL1-CTL2
NHL    CTL1   CTO2    70.000   113.50   ! prot22; Alanine Dipeptide ab initio calc's(LK);NH1-CT1-CTO2
CTO2   CTL1   CTO1    58.350   113.50   11.16   2.561  ! lip36; glycerol; CTL1-CTL1-CTL2
HAL2   CTO2   HAL2    35.500   109.00    5.40   1.80200 ! alkane, 3/92 HAL2-CLT2-HAL2
OHL    CTO2   CTL1    75.700   110.10   ! prot22; MeOH, EMB, 10/10/89; OH1 CT2 CT2


!
DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta

! Ceramides
!CCCC
CTL3 CTL1 CEL3 CEL3     0.9000  1   180.00 ! lip36; 2-pentene and 3-heptene; CEL1 CEL1 CTL2 CTL3
CEL3 CEL3 CTL2 CTL3     0.9100  1   180.00 ! lip36; 2-hexene, adm jr., 11/09
CEL3 CEL3 CTL2 CTL3     0.1800  2   180.00 !
CEL3 CEL3 CTL2 CTL3     0.1700  3   180.00 ! ""
CEL3 CEL3 CTL2 CTL2     0.9100  1   180.00 ! lip36; 2-hexene, adm jr., 11/09
CEL3 CEL3 CTL2 CTL2     0.1800  2   180.00 !
CEL3 CEL3 CTL2 CTL2     0.1700  3   180.00 ! ""
CTL1 CEL3 CEL3 CTL2     0.4500  1   180.00 ! lip36; 2-butene, adm jr., 4/04; X CEL1 CEL1 X
CTL1 CEL3 CEL3 CTL2     8.5000  2   180.00 ! lip36; 2-butene, adm jr., 4/04; X CEL1 CEL1 X
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CTO1 CEL3 CEL3 CTL2     0.1500  1     0.00 ! prot27; 2-butene, adm jr., 2/00 update; X CEL1 CEL1 X
CTO1 CEL3 CEL3 CTL2     8.5000  2   180.00 ! prot27; 2-butene, adm jr., 2/00 update; X CEL1 CEL1 X
CTL1 CTL1 CEL3 CEL3     0.6000  1   180.00 ! lip36; 2-hexene; CEL1 CEL1 CTL2 CTL2
!CCCO
O    C    CTL2 CTL3     1.400   1     0.00 ! prot22; lactams, adm jr; O C CT2 CT2/O C CT1 CT3
O    C    CTL2 CTL2     1.400   1     0.00 ! prot22; lactams, adm jr; O C CT2 CT2/O C CT1 CT3
OHL  CTL1 CEL3 CEL3     0.600   1   180.00 ! lip36; 2-hexene; CEL3 CEL3 CTL2 CTL2
OSL  CTO1 CEL3 CEL3     1.280   1    180.0 ! torsfit MP2/ccpVTZ, cer1 model, erh 8/09
OSL  CTO1 CEL3 CEL3     0.560   2    180.0 ! ""  analogy fot TACSPH, rmv nov 2009
OSL  CTO1 CEL3 CEL3     0.860   3      0.0 ! ""
CTL2 CTL1 CTO1 OHL      0.200   3     0.00 ! lip36; alkane, 3/92, X CTL1 CTL1 X
CTO1 CTL1 CTL2 OSL      0.390   1   180.00 ! torsfit MP2/ccpVTZ, sph model, erh 8/09; transferred from cer4
CTO1 CTL1 CTL2 OSL      0.510   2   180.00 ! ""
CTO1 CTL1 CTL2 OSL      0.870   3   180.00 ! ""
CTL2 CTL1 CTO1 OSL      0.390   1   180.00 ! torsfit MP2/ccpVTZ, sph model, erh 8/09; transferred from cer4
CTL2 CTL1 CTO1 OSL      0.510   2   180.00 ! ""       analogy for TACSPH, rmv nov 2009
CTL2 CTL1 CTO1 OSL      0.870   3   180.00 ! ""
!HCOH
HAL1 CTO1 OHL  HOL      0.140   3    0.00  ! lip36; glycerol, X CTL1 OHL  X
!COCC
CL   OSL  CTO1 CTL1     0.000   4     0.00 ! glycerol, beta1 6/07; from lip36 for TACSPH, rmv nov 2009
CL   OSL  CTO1 CTL1     0.150   3   180.00 ! glycerol, beta1 6/07
CL   OSL  CTO1 CTL1     1.453   2   180.00 ! glycerol, beta1 6/07
CL   OSL  CTO1 CTL1     0.837   1   180.00 ! glycerol, beta1 6/07
CEL3 CTO1 OSL  CL       0.220   1     0.00 ! og OMeTHP compounds 2 and 3; rmv nov 2009
CEL3 CTO1 OSL  CL       0.280   2   180.00 !  MCSA fit
CEL3 CTO1 OSL  CL       0.890   3     0.00 !  MP2/cc-pVTZ//MP2/6-31G*
!COCH
HAL1 CTO1 OSL  CL       0.00    3     0.00 ! lip36, X CT1 OSL X; TACCSPH, rmv nov 2009
!CCCH
HEL1 CEL3 CTL1 CTL3     0.1200  3     0.00 ! prot22; for butene, yin/adm jr., 12/95; HE1 CE1 CT2 CT3
HEL1 CEL3 CTO1 CTL3     0.1200  3     0.00 ! prot22; for butene, yin/adm jr., 12/95; HE1 CE1 CT2 CT3
HEL1 CEL3 CTL2 CTL2     0.1200  3     0.00 ! prot22; for butene, yin/adm jr., 12/95; HE1 CE1 CT2 CT3
HAL1 CTL1 CEL3 CEL3     0.0300  3     0.00 ! prot22;for butene, yin/adm jr., 12/95; CE1 CE1 CT3 HA
HAL1 CTO1 CEL3 CEL3     0.0300  3     0.00 ! prot22;for butene, yin/adm jr., 12/95; CE1 CE1 CT3 HA
CTL1 CTL1 CEL3 HEL1     0.1200  3     0.00 ! lip36; butene, yin, adm. jr; CTL2 CTL2 CEL1 HEL1
HAL1 CTL3 CTO1 CEL3     0.2000  3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL3 X
CTL2 CTL1 CTO1 HAL1     0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL3 X
CTL1 CTO1 CEL3 HEL1     0.1200  3     0.00 ! lip36  butene, yin, adm. jr; CTL2 CTL2 CEL1 HEL1
HAL1 CTL1 CTO1 CEL3     0.200   3     0.00 ! lip36; alkane, 3/92: X CTL1 CTL3 X
CTO1 CEL3 CEL3 HEL1     0.1500  1   180.00 ! lip36; 2-butene, adm jr., 2/00 update; X CEL1 CEL1 X
CTO1 CEL3 CEL3 HEL1     8.5000  2   180.00 ! lip36; 2-butene, adm jr., 2/00 update; X CEL1 CEL1 X
CEL3 CEL3 CTL2 HAL2     0.3000  3   180.00 ! lip36; 2-butene, adm jr., 4/04; CEL1 CEL1 CTL2 HAL2
HEL1 CEL3 CEL3 CTL2     0.1500  1   180.00 ! lip36; 2-butene, adm jr., 2/00 update; X CEL1 CEL1 X
HEL1 CEL3 CEL3 CTL2     8.5000  2   180.00 ! lip36; 2-butene, adm jr., 2/00 update; X CEL1 CEL1 X
HEL1 CEL3 CTL2 CTL3     0.1200  3     0.00 ! lip36; butene, yin,adm jr., 12/95; HEL1 CEL1 CTL2 CTL3
!HCCH
HEL1 CEL3 CTL1 HAL1     0.000   3     0.00 ! prot22; butene, adm jr., 2/00 update; HE1 CE1 CT2 HA
HEL1 CEL3 CTO1 HAL1     0.000   3     0.00 ! prot22; butene, adm jr., 2/00 update; HE1 CE1 CT2 HA
HAL3 CTL3 CTO1 HAL1     0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL3 X
HAL1 CTL1 CTO1 HAL1     0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL1 X
HEL1 CEL3 CEL3 HEL1     1.000   2   180.00 ! lip36; 2-butene, adm jr., 8/98 update; HEL1 CEL1 CEL1 HEL1
HEL1 CEL3 CTL2 HAL2     0.000   3     0.00 ! lip36; butene, adm jr., 2/00 update; HEL1 CEL1 CTL2 HAL2
!OCCH
OHL  CTL1 CEL3 HEL1     0.120   3   180.00 ! lip36; butene, yin, adm jr., 12/95; HEL1 CEL1 CTL1 CTL3
OHL  CTO1 CEL3 HEL1     0.120   3   180.00 ! lip36; butene, yin, adm jr., 12/95; HEL1 CEL1 CTL1 CTL3
OSL  CTO1 CEL3 HEL1     0.120   3   180.00 ! lip36; butene, yin, adm jr., 12/95; HEL1 CEL1 CTL1 CTL3 rmv nov
2009
O    C    CTL2 HAL2     0.000   3   180.00 ! prot22; adm jr., 8/13/90 acetamide geometry and vibrations; O C
CT2 HA
O    C    CTL3 HAL3     0.000   3   180.00 ! prot22; adm jr., 8/13/90 acetamide geometry and vibrations; O C
CT3 HA
HAL3 CTL3 CTO1 OHL      0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL3 X
HAL1 CTL1 CTO1 OHL      0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL1 X
HAL1 CTL1 CTO1 OSL      0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL1 X; rmv nov 2009
!NCCC
NHL  CTL1 CTL1 CTL3     0.260   1   180.00 ! torsfit MP2/ccpVTZ, cer3 model, erh 8/09
NHL  CTL1 CTL1 CTL3     0.390   2   180.00 ! ""
NHL  CTL1 CTL1 CTL3     0.120   3   180.00 ! ""
!NCCH
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NHL   C     CTL2 HAL2      0.000    3      0.00 ! prot22; LK for autogenerate dihe, sp2-methyl, no dihedral
potential; NH1 C CT2 HA
NHL   C     CTL3 HAL3      0.000    3      0.00 ! prot22; LK for autogenerate dihe, sp2-methyl, no dihedral
potential; NH1 C CT3 HA
NHL  CTL1 CTO1 HAL1     0.200   3     0.00 ! lip36; alkane, 3/92; X CTL1 CTL1 X
!HNCH
HAL3 CTL3 NHL   H          0.000    3      0.00 ! prot22; LK for autogenerate dihe, sp2-methyl, no dihedral
potential;  HA CT3 NH1 H
HAL1 CTL1 NHL   H        0.000   1     0.00 ! prot22; Alanine Dipeptide ab initio calc's (LK); HB CT1 NH1 H
!OCNH HNCC for NMA/CERN cis/trans barrier
H    NHL  C    O        0.530   1     0.00 ! fit to cern QM profile, jbk 10/12
H    NHL  C    O        1.270   2   180.00 ! fit to cern QM profile, jbk 10/12
H    NHL  C    O        0.140   3     0.00 ! fit to cern QM profile, jbk 10/12
H    NHL  C    O        0.780   4     0.00 ! fit to cern QM profile, jbk 10/12
H     NHL  C     CTL2     2.500   2   180.00 ! prot22;,Gives appropriate NMA cis/trans barrier. (LK); H NH1 C
CT2
H    NHL  CTL1 CTL2     0.000   1     0.00 ! prot22; Alanine Dipeptide ab initio calc's (LK); H NH1 CT1 CT2
H    NHL  CTL1 CTL1     0.000   1     0.00 ! prot22; Alanine Dipeptide ab initio calc's (LK); H NH1 CT1 CT1
H     NHL  C     CTL3     2.500   2   180.00 ! prot22; Gives appropriate NMA cis/trans barrier. (LK); H NH1 C
CT3
H    NHL  CTL1 CTL3     2.500   2   180.00 ! prot22;
H    NHL  CTL1 CTO1     0.000   1     0.00 ! prot22; Alanine Dipeptide ab initio calc's (LK); H NH1 CT1 CT1
!OCNC
O    C     NHL  CTL3     2.500   2   180.00 ! prot22; Gives appropriate NMA cis/trans barrier. (LK); O C NH1
CT3
O    C     NHL  CTL1     2.500   2   180.00 ! prot22; Gives appropriate NMA cis/trans barrier. (LK); O  C NH1
CT1
!CCNC
CTL1 NHL  C    CTL2     0.000   1     0.00 ! set to zero in fits
CTL1 NHL  C    CTL3     0.000   1     0.00 ! set to zero in fits
! torsion 4 and OH torsion
CTL2 C    NHL  CTL3     1.600   1     0.00 ! prot22; from CT2  C    NH1  CT2, adm jr. 10/21/96; CT2 C NH1 CT3
CTL3 C    NHL  CTL3     1.600   1     0.00 ! prot22; from CT2  C    NH1  CT2, adm jr. 10/21/96; CT2 C NH1 CT3
CTL1 CTL1 NHL  C        0.000   1     0.00 ! set to zero in fit
CTL2 CTL1 NHL  C        0.000   1     0.00 ! set to zero in fit
CTL3 CTL1 NHL  C        0.000   1     0.00 ! set to zero in fit
C    NHL  CTL1 CTO1     4.080   1     0.00 ! torsion fit to cer6 qm, jbk 10/12
C    NHL  CTL1 CTO1     1.560   2   180.00 ! torsion fit to cer6 qm, jbk 10/12
C    NHL  CTL1 CTO1     1.800   3     0.00 ! torsion fit to cer6 qm, jbk 10/12
CTL1 CTO1 OHL  HOL      5.000   1   180.00 ! torsion fit to cer6 qm, jbk 10/12
CTL1 CTO1 OHL  HOL      0.220   2     0.00 ! torsion fit to cer6 qm, jbk 10/12
CTL1 CTO1 OHL  HOL      1.110   3   180.00 ! torsion fit to cer6 qm, jbk 10/12
HOL   OHL  CTL1 CEL3      1.330    1      0.00 ! prot22; 2-propanol OH hf/6-31g* torsional surface, adm jr.,
3/2/93; H OH1 CT1 CT1
HOL   OHL  CTO1 CEL3      1.330    1      0.00 ! prot22; 2-propanol OH hf/6-31g* torsional surface, adm jr.,
3/2/93; H OH1 CT1 CT1
HOL  OHL  CTO1 CTL3     0.000   3     0.00 ! torsion fit to cer6 qm, jbk 9/12
!HCNC
HAL3 CTL3 NHL   C          0.000    3      0.00 ! prot22; LK for autogenerate dihe, sp2-methyl, no dihedral
potential; HA CT3 NH1 C
HAL1 CTL1 NHL  C        0.000   1     0.00 ! prot22; Alanine Dipeptide ab initio calc's (LK); HB CT1 NH1 C
!NCCO
NHL  CTL1 CTL2 OSL      1.630   1   180.00 ! torsfit MP2/ccpVTZ, cer3 model, erh 8/09; transferred
NHL  CTL1 CTL2 OSL      0.490   2     0.00 ! ""
NHL  CTL1 CTL2 OSL      0.570   3     0.00 ! ""
NHL  CTL1 CTO1 OSL      1.630   1   180.00 ! torsfit MP2/ccpVTZ, cer3 model, erh 8/09; transferred
NHL  CTL1 CTO1 OSL      0.490   2     0.00 ! ""         analogy for TACSPH, rmv nov 2009
NHL  CTL1 CTO1 OSL      0.570   3     0.00 ! ""
!OPOC
OSL  PL   OSL  CTL2     1.200   1   180.00 ! lip36; phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL2     0.100   2   180.00 ! lip36; phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL2     0.100   3   180.00 ! lip36; phosphate, new NA, 4/98, adm jr.
!torsion1
CEL3 CTO1 CTL1 NHL      0.940   1     0.00 ! torfit to cer4 qm, jbk 5/13
CEL3 CTO1 CTL1 NHL      0.880   2   180.00 ! torfit to cer4 qm, jbk 5/13
CEL3 CTO1 CTL1 NHL      2.090   3     0.00 ! torfit to cer4 qm, jbk 5/13
NHL  CTL1 CTO1 OHL      0.420   1     0.00 ! torfit to cer4 qm, jbk 5/13
NHL  CTL1 CTO1 OHL      1.530   2   180.00 ! torfit to cer4 qm, jbk 5/13
NHL  CTL1 CTO1 OHL      1.580   3   180.00 ! torfit to cer4 qm, jbk 5/13
CEL3 CTO1 CTL1 CTL2     0.000   1     0.00 ! torfit to cer4 qm, jbk 10/12
!torsion2
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CEL3 CEL3 CTO1 CTL1     0.860   1     0.00 ! torfit to cer4 qm w/adj, jbk 5/13
CEL3 CEL3 CTO1 CTL1     1.910   2     0.00 ! torfit to cer4 qm w/adj, jbk 5/13
CEL3 CEL3 CTO1 CTL1     1.520   3   180.00 ! torfit to cer4 qm w/adj, jbk 5/13
CEL3 CEL3 CTO1 OHL      1.380   1   180.00 ! torfit to cer4 qm w/adj, jbk 5/13
CEL3 CEL3 CTO1 OHL      0.580   2     0.00 ! torfit to cer4 qm w/adj, jbk 5/13
CEL3 CEL3 CTO1 OHL      1.030   3     0.00 ! torfit to cer4 qm w/adj, jbk 5/13
!torsion3
NHL  CTL1 CTL2 OSLP     1.370   1     0.00 ! torfit to cer3 qm, jbk 5/13
NHL  CTL1 CTL2 OSLP     0.340   2     0.00 ! torfit to cer3 qm, jbk 5/13
NHL  CTL1 CTL2 OSLP     0.200   3   180.00 ! torfit to cer3 qm, jbk 5/13
NHL  CTL1 CTL2 OSLP     0.020   4   180.00 ! torfit to cer3 qm, jbk 5/13
NHL  CTL1 CTL2 OSLP     0.140   5     0.00 ! torfit to cer3 qm, jbk 5/13
NHL  CTL1 CTL2 OSLP     0.060   6     0.00 ! torfit to cer3 qm, jbk 5/13
CTL1 CTL1 CTL2 OSLP     0.000   1     0.00 ! torfit to cer3 qm, jbk 5/13
!torsion5
CTL3 CTL2 C    NHL      1.990   1     0.00 ! torfit to cer2 qm, jbk 10/12
CTL3 CTL2 C    NHL      0.640   2   180.00 ! torfit to cer2 qm, jbk 10/12
CTL3 CTL2 C    NHL      0.280   3   180.00 ! torfit to cer2 qm, jbk 10/12
CTL2 CTL2 C    NHL      1.990   1     0.00 ! torfit to cer2 qm, jbk 10/12
CTL2 CTL2 C    NHL      0.640   2   180.00 ! torfit to cer2 qm, jbk 10/12
CTL2 CTL2 C    NHL      0.280   3   180.00 ! torfit to cer2 qm, jbk 10/12
X    CTL1 CTO1 X        0.200   3     0.00 ! alkane, 3/92
X    CTO1 CTL3 X        0.200   3     0.00 ! alkane, 3/92
!Added by STN for CER24, 3/13
NHL  CTL1 CTO2 OHL      0.550   1     0.00 ! jbk; NHL CTL1 CTO1 OHL
NHL  CTL1 CTO2 OHL      1.630   2   180.00 ! jbk; NHL CTL1 CTO1 OHL
NHL  CTL1 CTO2 OHL      1.430   3   180.00 ! jbk; NHL CTL1 CTO1 OHL
C    NHL  CTL1 CTO2     4.080   1     0.00 ! jbk; C   NHL CTL1 CTO1
C    NHL  CTL1 CTO2     1.560   2   180.00 ! jbk; C   NHL CTL1 CTO1
C    NHL  CTL1 CTO2     1.800   3     0.00 ! jbk; C   NHL CTL1 CTO1
X    CTL1 CTO2 X        0.200   3     0.00 ! alkane, 3/92; X CTL1 CTL2 X
X    CTO2 OHL  X        0.140   3     0.00 ! glycerol; X CTL2 OHL X
CTO2 CTL1 CTO1 OHL      0.200   3     0.00 ! lip36; alkane, 3/92, X CTL1 CTL1 X
H    NHL  CTL1 CTO2     0.000   1     0.00 ! prot22; Alanine Dipeptide ab initio calc's (LK); H NH1 CT1 CT2
CEL3 CTO1 CTL1 CTO2     0.000   1     0.00 ! torfit to cer4 qm, jbk 10/12

!
IMPROPER
!
!V(improper) = Kpsi(psi - psi0)**2
!
!Kpsi: kcal/mole/rad**2
!psi0: degrees
!note that the second column of numbers (0) is ignored
!
!atom types           Kpsi                   psi0
!
! Ceramides
NHL  X   X   H        20.       0     0.00   ! amide, from peptide; rmv nov 2009


NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
                !adm jr., 5/08/91, suggested cutoff scheme
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   eps,1-4       Rmin/2,1-4
! Ceramides
NHL      0.0       -0.2000    1.850 0.0 -0.20 1.55 ! ALLOW   PEP POL ARO
            ! This 1,4 vdW allows the C5 dipeptide minimum to exist.(LK) - TAKEN FROM NH1
CTO1     0.0       -0.0200    2.275 0.0 -0.01 1.9 ! alkane, 3/92
            ! Transferred from CTL1; lip36
CEL3     0.0       -0.0680    2.090   ! alkene, yin,adm jr., 12/95
            ! Transferred from CEL1; lip36! Added my STN for CER24
CTO2     0.0       -0.0560    2.010 0.0 -0.01 1.9 ! STN, 3/13
```

```
end

return
```