SUPPORTING INFORMATION
FOR *J. PHYS.CHEM. B*
Hyvönen & Kovanen

Molecular Dynamics Simulation of Sphingomyelin Bilayer

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Table S1. The atom types and atomic charges of sphingomyelin (16:0) molecule for CHARMM force field.

```
GROUP                 !          H15B
ATOM N    NTL   -0.60 !           |
ATOM C13  CTL5  -0.35 !      H15A-C15-H15C
ATOM H13A HL     0.25 !           |
ATOM H13B HL     0.25 !    H13B   |    H14A
ATOM H13C HL     0.25 !      |    |     |
ATOM C14  CTL5  -0.35 !H13A-C13----N----C14-H14B     (+)
ATOM H14A HL     0.25 !      |    |     |
ATOM H14B HL     0.25 !    H13C   |    H14C
ATOM H14C HL     0.25 !           |
ATOM C15  CTL5  -0.35 !           |
ATOM H15A HL     0.25 !           |
ATOM H15B HL     0.25 !           |
ATOM H15C HL     0.25 !           |
ATOM C12  CTL2  -0.10 !     H12A--C12---H12B
ATOM H12A HL     0.25 !           |
ATOM H12B HL     0.25 !           |
GROUP                 !
ATOM C11  CTL2  -0.08 !           |
ATOM H11A HAL2   0.09 !     H11A--C11---H11B
ATOM H11B HAL2   0.09 !           |
ATOM P    PL     1.50 !       O13  O12
ATOM O13  O2L   -0.80 !        \\ /
ATOM O14  O2L   -0.80 !    (-)   P
ATOM O11  OSL   -0.55 !        // \
ATOM O12  OSL   -0.55 !       O14  O11
ATOM C1   CTL2  -0.08 !           |
ATOM HA   HAL2   0.09 !       HA---C1---HB
ATOM HB   HAL2   0.09 !           |
GROUP                 !           |
ATOM C2   CTL1   0.02 !      HS---C2- - - - - - -
ATOM HS   HAL1   0.09 !           |         |
ATOM N21  NH1   -0.50 !          N21-HN
ATOM HN   HL     0.28 !      O22  |
ATOM C21  CL     0.55 !       \\ /          |
ATOM O22  OBL   -0.54 !         C21
ATOM C22  CTL2  -0.08 !         |           |
ATOM H2R  HAL2   0.09 !  H2R---C22---H2S
ATOM H2S  HAL2   0.09 !         |           |
GROUP                 !
ATOM C3   CTL1  -0.04 !         |           |
ATOM HX   HAL1   0.09 !                HX---C3---O3--HO
ATOM O3   OHL   -0.60 !         |           |
ATOM HO   HOL    0.43 !                     |
ATOM C34  CEL1  -0.14 !                    C34---H4X
ATOM H4X  HEL1   0.15 !         |          //
ATOM C35  CEL1  -0.14 !                  C35---H5X
ATOM H5X  HEL1   0.15 !
ATOM C36  CTL2  -0.08 !                  |
ATOM H6X  HAL2   0.09 !             H6X---C36---H6Y
ATOM H6Y  HAL2   0.09 !         |          |
GROUP                 !
ATOM C23  CTL2  -0.18 !         |          |
ATOM H3R  HAL2   0.09 !  H3R ---C23---H3S
ATOM H3S  HAL2   0.09 !         |          |
...                                    . . .
GROUP                 !
ATOM C215 CTL2  -0.18 !         |          |
ATOM H15R HAL2   0.09 !  H15R---C215--H15S
ATOM H15S HAL2   0.09 !         |          |
GROUP                 !
ATOM C216 CTL3  -0.27 !         |
ATOM H16R HAL3   0.09 !  H16R---C216--H16S|
ATOM H16S HAL3   0.09 !         |
ATOM H16T HAL3   0.09 !        H16T        |
GROUP                 !
ATOM C37  CTL2  -0.18 !                    |
```

```
ATOM H7X  HAL2    0.09 !           H7X---C37---H7Y
ATOM H7Y  HAL2    0.09 !                  |
GROUP                  !
ATOM C38  CTL2   -0.18 !                  |
ATOM H8X  HAL2    0.09 !           H8X---C38---H8Y
ATOM H8Y  HAL2    0.09 !                  |
...                                        . . .
GROUP                  !
ATOM C317 CTL2   -0.18 !                  |
ATOM H17X HAL2    0.09 !           H17X---C317--H17Y
ATOM H17Y HAL2    0.09 !                  |
GROUP                  !
ATOM C318 CTL3   -0.27 !                  |
ATOM H18X HAL3    0.09 !           H18X---C318--H18Y
ATOM H18Y HAL3    0.09 !                  |
ATOM H18Z HAL3    0.09 !                 H18Z
```

Table S2. The bonded and Lennard-Jones parameters of sphingomyelin (16:0) molecule for CHARMM force field.

```
BONDS
!V(bond) = Kb(b - b0)**2
!Kb: kcal/mole/A**2
!b0: A
!atom type    Kb          b0
NH1   CL    370.000     1.3450  ! from protein NH1 C
NH1   CTL1  320.000     1.4300  ! from protein NH1 CT1
NH1   HL    440.000     0.9970  ! from protein NH1 H
CTL1  CEL1  365.000     1.502

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
CTL1 NH1  CL     50.0      120.00   ! from protein CT1 NH1 C
HL   NH1  CL     34.0      123.00   ! from protein H NH1 C
HL   NH1  CTL1   35.0      117.00   ! from protein H NH1 CT1
NH1  CL   CTL2   80.000    116.5000 ! from protein NH1 C CT2
OBL  CL   NH1    80.0      122.5    ! from protein O C NH1
CTL2 CTL1 NH1    70.0      113.5    ! from protein NH1 CT1 CT2
HAL1 CTL1 NH1    48.0      108.0    ! from protein NH1 CT1 HB
NH1  CTL1 CTL1   70.0      113.5    ! from protein NH1 CT1 CT1
CTL1 CTL1 OHL    75.700    110.10
CTL1 CTL1 CEL1   32.00     112.20
HAL1 CTL1 CEL1   45.00     111.50
OHL  CTL1 CEL1   75.700    110.10
CTL1 CEL1 HEL1   40.00     116.00
CTL1 CEL1 CEL1   48.00     123.50

DIHEDRALS
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!atom types             Kchi    n   delta
X    CTL2 CEL1 X        1.2  3  180.0
CTL2 CEL1 CEL1 CTL2     0.36 1    0.0
CTL2 CEL1 CEL1 CTL2     3.55 2  180.0
HEL1 CEL1 CEL1 CTL2     3.45 2  180.0
X    CEL1 CEL1 X        3.55 2  180.0
CTL2 X    X    CEL1    70.0  0    0.0
CEL1 X    X    CEL1   150.0  0    0.0
HEL1 X    X    CEL1    75.0  0    0.0
HAL2 X    X    CEL1    75.0  0    0.0
CL   CTL1 NH1  CL       0.2  1  180.0
CL   CTL2 NH1  CL       0.2  1  180.0
CTL1 CL   NH1  CTL1     1.6  1    0.0
CTL1 CL   NH1  CTL1     2.5  2  180.0
CTL1 CTL1 NH1  CTL1     1.8  1    0.0
```

```
CTL2 CL   NH1  CTL1     1.6  1    0.0
CTL2 CL   NH1  CTL1     2.5  2  180.0
CTL2 CL   NH1  CTL2     1.6  1    0.0
CTL2 CL   NH1  CTL2     2.5  2  180.0
CTL2 CTL1 NH1  CL       1.8  1    0.0
CTL2 NH1  CL   CTL1     1.6  1    0.0
CTL2 NH1  CL   CTL1     2.5  2  180.0
HL   NH1  CL   CTL1     2.5  2  180.0
HL   NH1  CL   CTL2     2.5  2  180.0
HL   NH1  CTL1 CTL1     0.0  1    0.0
HAL1 CTL2 NH1  CL       0.0  3    0.0
HAL1 CTL2 NH1  HL       0.0  3    0.0
HAL2 CTL2 NH1  CL       0.0  3    0.0
HAL2 CTL2 NH1  HL       0.0  3    0.0
NH1  CL   CTL2 CTL2     0.0  1    0.0
OBL  CL   NH1  CTL1     2.5  2  180.0
OBL  CL   NH1  HL       2.5  2  180.0
CTL2 CTL1 NH1  HL       0.0  1    0.0
CTL1 NH1  CL   OBL      2.5  2  180.0
CTL1 CTL1 CEL1 HEL1     0.12 3    0.00
CTL1 CTL1 CEL1 CEL1     0.4  3    0.00
HAL1 CTL1 NH1  HL       0.0  3    0.00
HAL1 CTL1 NH1  CL       0.0  3    0.00
CL   NH1  CTL1 CTL1     1.8  1    0.0
HAL1 CTL1 CEL1 HEL1     0.87 3    0.00
HAL1 CTL1 CEL1 CEL1     0.12 3    0.00
OHL  CTL1 CEL1 HEL1     0.87 3    0.00
OHL  CTL1 CEL1 CEL1     0.03 3    0.00

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
OBL  X    X    CL         100.00    0     0.00 ! acetic acid
HEL2 HEL2 CEL2 CEL2         3.00    0     0.00 ! ethene, yin,adm jr., 12/95
OCL  X    X    CL          96.00    0     0.00 ! acetate
NH1  X    X    HL          20.00    0     0.00

!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
HOL      0.0       -0.046     0.2245
OBL      0.0       -0.12      1.70  0.0 -0.12 1.4
OCL      0.0       -0.12      1.70
OHL      0.0       -0.1521    1.77
OSL      0.0       -0.1521    1.77
NTL      0.0       -0.20      1.85  ! as all other nitrogens
NH1      0.0       -0.20      1.85  0.0 -0.20 1.55
```