Supplementary Information

for

Predicting Partition Coefficients Of Neutral And Charged Solutes In The Mixed SLES-fatty Acids In Micellar System

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Calculation of micelle/water partition coefficients, $K_{mic,A}$

Log $K_{mic,A}$(mole/mol) for caprate ion was derived using data relative to the concentration of the monomer in water and in the micelle phase from Table A.1 of Tzocheva *et al*[1] using equation 26 of the same paper:

$$K_{mic/w} = \frac{\gamma_z y_z}{c_z} \qquad \text{Eq. 1}$$

In which γ_z and y_z are the activity coefficient and the molar fraction of caprate in the micellar phase and c_z is the concentration of caprate in the water phase. Free energy value was then calculated as: $\Delta G_{transf} = -2.303RT \text{ Log } K_{mic/w}$.

Convergence analysis for caprate PMF with the polarizable and the non-polarizable force fields

Figure S1 shows the convergence of the PMF for caprate at four different time portions of the windows (i.e. 0-2.5 ns, 0-5 ns, 0-7.5 ns and 0-10ns) when the non-polarizable force field (a) and the polarizable force field (b) are employed. As can be seen, in both cases the free energy surfaces in the portions 0-5 ns, 0-7.5 ns and 0-10 ns are very similar indicating that the free energy surfaces in the last 5ns of the PMF profiles have converged.

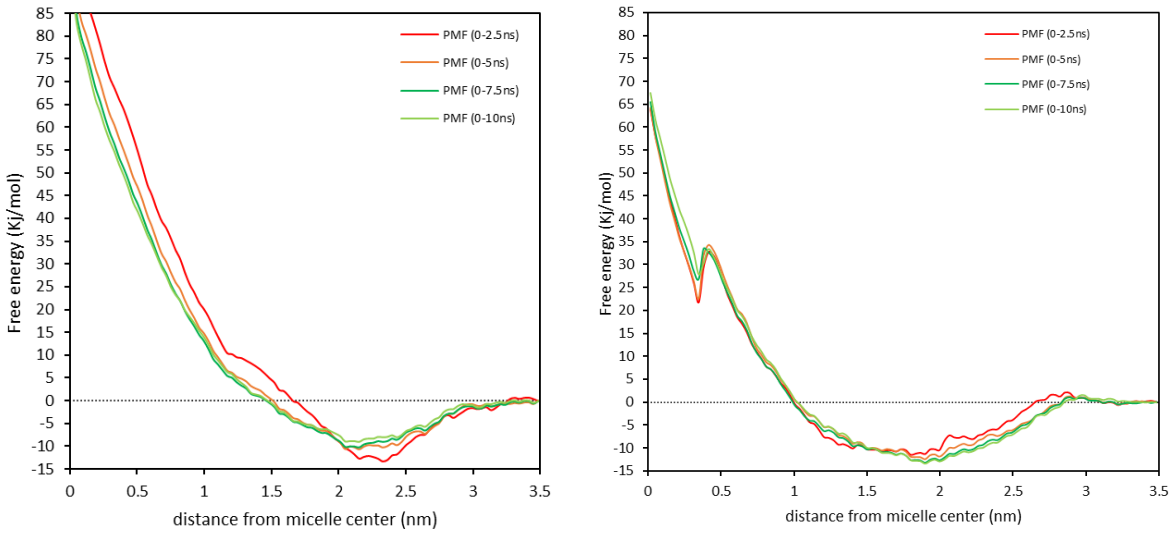

Figure S1: Convergence of PMF for caprate at different time portions of the 36 windows for the **a)** non-polarizable force field and **b)** polarizable force field.

Parametrization of SLES, capric acid and caprate ion with the CHARMM Drude FF

Initial residue topologies and parameters for SLES, capric acid and caprate were assigned based on analogy with those already available in the Drude force field. In the case of SLES, a new atom-type was introduced for the sulfur atom in sulfate wherein the Lennard-Jones parameters were taken from Drude force field parameter of phosphorus atom of phosphate[2]. Since the missing parameters were mainly associated with the head-group of SLES, a prototype structure was prepared by attaching the head-group of SLES to a neutral methyl moiety. This procedure allows patching of the head-group parameters with the rest of the aliphatic chain of the concerned molecule. The head-group parameters were refined to improve the agreement with QM water-interactions, molecular polarizability and the intramolecular stretching, bending and twisting patterns along with the dihedral potential energy scan. The QM target data were generated by using

the Gaussian03 software[3]. The structure of methylsulfate was initially optimized at MP2/6-31G*[4] level of theory. The optimized structure was then subjected to single point calculation at MP2/cc-pVQZ[5] level of theory to obtain the molecular polarizability. Target data for partial charges were based on water-methylsulfate dimer interaction (Figure S2) optimized at the MP2/aug-cc-pVDZ[6] model chemistry. The interaction energies between water and methylsulfate were calculated by subtracting their monomer energies obtained from single-point calculation at MP2/aug-cc-pVDZ level of theory from the total energy of water-methylsulfate complexes. A scan of the potential energy surface (PES) along the C-O-S-O dihedral was performed at MP2/aug-cc-pVDZ model chemistry.

The Drude-force field parameters of the head-group were parametrized using CHARMM-c42b1[7] targeting the above QM data. The bond and angle parameters were adjusted such that molecular mechanics (MM) optimized geometry matches the QM geometry. Values for QM and MM bonds, angles and dihedrals and their differences for the optimized geometries are reported in Table S1. The dihedral parameter of the C-O-S-O dihedral was modified to reproduce the QM PES. The plot of MM and QM PES against the C-O-S-O dihedral is given in Figure S3. The alpha and Thole parameters were adjusted to match QM molecular polarizability values and are reported in Table S2. The MM interaction energies of methylsulfate with water are reported in Table S3 in comparison to the corresponding QM values. The MM values are systematically less favourable than the QM values. However, this difference was not corrected based on a calculation of the free energy of aqueous solvation of methylsulfate, yielding a value of -84.05 kcal/mol, which is in good agreement with -80.12 kcal/mol as predicted by COSMOtherm program. Details of the free energy of aqueous solvation calculation are shown along with final residue topologies and parameters for not currently available in the Drude force fields are presented in Tables S4, S5 and S6.

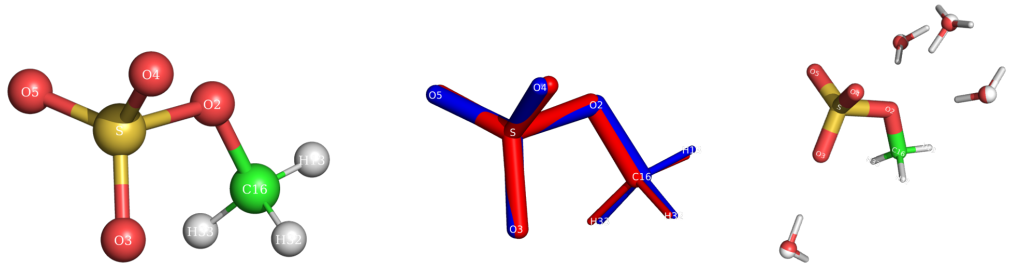

Figure S2: a) Molecular structure of minimized methylsulfate, **b)** comparison of 3D coordinates obtained from QM and MM after parametrization, and **c)** four different orientations of water interacting with methylsulfate used for fitting the MM charges combined in a single image.

Table S1: Internal coordinates of methylsulfate (C(H1)(H2)(H3)-O1-S(O2)(O3)(O4)$^-$) obtained from optimized QM (MP2/6-31G*) and the Drude polarizable MM calculations.

#IC_LIST	QM_V	MM_V	ΔV(MM-QM)
C-O1	1.408	1.474	0.067
C-H1	1.107	1.111	0.004
C-H2	1.107	1.113	0.006
C-H3	1.107	1.113	0.006
S-O1	1.751	1.774	0.023
S-O2	1.493	1.499	0.006
S-O3	1.485	1.493	0.007
S-O4	1.485	1.493	0.007
H1-C-O1	106.498	109.631	3.132
H1-C-H2	108.620	108.396	-0.224
H1-C-H3	108.620	108.396	-0.224
O1-C-H2	112.990	110.591	-2.399
O1-C-H3	112.990	110.591	-2.399
H2-C-H3	106.995	109.178	2.183
C-O1-S	114.386	114.935	0.549
O1-S-O2	103.445	107.775	4.329
O1-S-O3	102.122	99.099	-3.023
O1-S-O4	102.122	99.099	-3.023
O2-S-O3	115.357	115.718	0.361
O2-S-O4	115.357	115.718	0.361
O3-S-O4	115.503	115.920	0.417
H1-C-O1-S	180.000	-180.000	0.000
H2-C-O1-S	-60.831	-60.533	-0.299
H3-C-O1-S	60.831	60.533	-0.298
C-O1-S-O2	0.003	0.000	-0.003
C-O1-S-O3	120.117	120.854	0.737
C-O1-S-O4	-120.111	-120.854	0.743

QM_V and MM_V are distances, angles and dihedral values obtained from QM and MM calculations, respectively. ΔV(MM-QM) is the difference between MM and QM values. Distance values are in Å, and angles and dihedral values are in degrees.

Table S2: Values of components of molecular polarizability (Pxx, Pyy and Pzz) and total molecular polarizability (P_{tot}) of methylsulfate obtained from QM (MP2/cc-pVQZ) and Drude polarizable MM calculations.

Polarizability	QM_Pol	MM_Pol	ΔPol(MM-QM)
$\mathbf{P}_{xx}$	5.931	5.671	-0.260
$\mathbf{P}_{yy}$	4.552	5.672	1.120
$\mathbf{P}_{zz}$	4.615	5.703	1.088
$\mathbf{P}_{tot}$	5.033	5.682	0.649

QM_Pol and MM_Pol are polarizability values (xx, yy and zz components) obtained from QM and MM calculations, respectively. ΔPol(MM-QM) is the difference between MM and QM values. Polarizability values are represented in $Å^3$.

Table S3: Interaction energies and corresponding distances between water and methylsulfate obtained from QM (MP2/aug-cc-pvDZ) and the Drude polarizable MM calculations. Various entries correspond to different orientation of water molecules placed to represent maximum interaction with different oxygen atoms in methylsulfate.

Complex	QM_IE	MM_IE	ΔIE(MM-QM)	QM_D	MM_D	ΔD(MM-QM)
SULF_O2_WAT	-10.980	-4.539	6.441	1.96	2.14	0.18
SULF_O3_WAT	-12.568	-10.108	2.460	1.83	1.98	0.15
SULF_O4_WAT	-12.805	-9.959	2.846	1.83	1.98	0.15
SULF_O5_WAT	-12.465	-10.051	2.414	1.83	1.98	0.15

QM_IE and MM_IE are interaction energies obtained from QM and MM calculations, respectively; QM_D and MM_D are distances between concerned oxygen atom with closest hydrogen atom of the water molecule in water in QM and MM calculations, respectively. Energy values are in kcal/mol. Distance values are in Å.

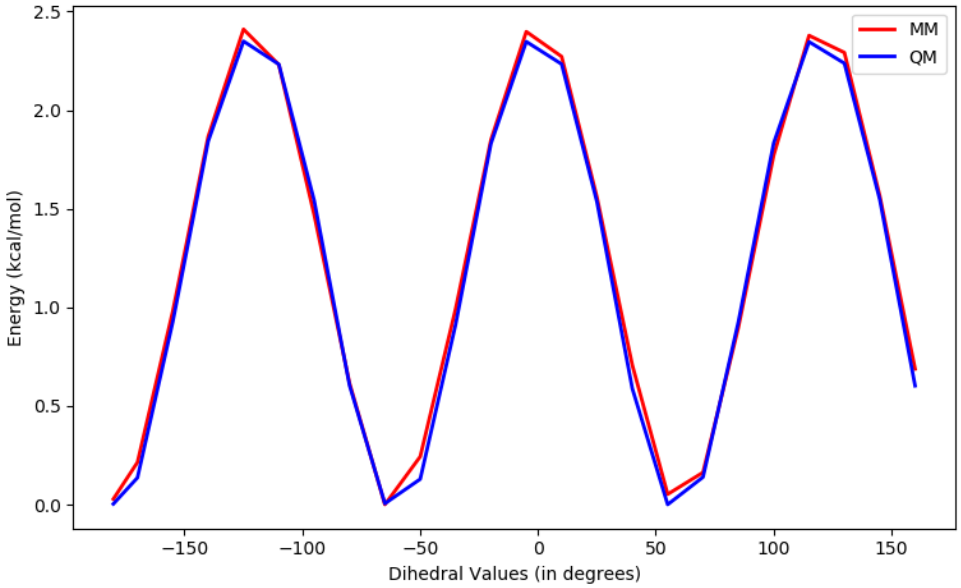

Figure S3: Relaxed potential energy scan of C-O1-S-O2 dihedral of methylsulfate obtained from QM (MP2/aug-cc-pvDZ) and the Drude polarizable MM calculations.

Free energy of hydration

Free energy of hydration was calculated via free energy perturbation method using the staged protocol developed by Deng and Roux.[2] In this procedure, free energy is divided into nonpolar (LJ potential) and electrostatic contributions. The nonpolar contribution is further divided into repulsive and dispersive (attractive) part using Weeks, Chandler and Andersen (WCA) scheme. Following equations show the calculation of free energy of hydration and the obtained energies for methylsulfate. We note that there is no experimental estimate of the free energy of hydration of methylsulfate available such that the results are included only for informational purposes.

$$\Delta G^{hyd} = \Delta G^{aq} - \Delta G^{vac} + zF\Phi + corr + lrc = -84.05\ kcal/mol \quad \text{Eq. 2}$$

$$\Delta G^{aq} = \Delta G^{aq}_{nonp} + \Delta G^{aq}_{elec} = 14.23 + (-24.08) = -9.86 \quad \text{Eq. 2a}$$

$$\Delta G^{aq}_{nonp} = \Delta G^{aq}_{rep} + \Delta G^{aq}_{dis} = 31.19 + (-16.97) = 14.23;\ \Delta G^{aq}_{elec} = -24.08 \quad \text{Eq. 2b}$$

$$\Delta G^{vac} = \Delta G^{vac}_{nonp} + \Delta G^{vac}_{elec} = 14.05 + 74.62 = 88.67 \quad \text{Eq. 2c}$$

$$\Delta G^{vac}_{nonp} = \Delta G^{vac}_{rep} + \Delta G^{vac}_{dis} = 15.04 + (-0.990943) = 14.0512;\ \Delta G^{vac}_{elec} = 74.62 \quad \text{Eq. 2d}$$

$$\mathrm{z} = -1;\ \mathrm{F} = 23.06\ ;\ \Phi = -0.540\ ;\ \mathrm{corr} = 0.0\ ;\ lrc = -0.12 \quad \text{Eq. 2e}$$

In Eq. 1, ΔG^{hyd} , ΔG^{aq} , $\Delta G^{vac}, z, F, \Phi, corr, lrc$ are free energy of hydration of methylsulfate, free energy of methylsulfate in water, free energy of methylsulfate in gas, total charge, Faraday constant, electrostatic Galvani potential at the liquid vacuum interface, entropy related contributions and long range correction computed using particle mesh Ewald summation, respectively. The terms ΔG^{aq}_{nonp} and ΔG^{aq}_{elec}, are nonpolar (LJ potential) and electrostatic contributions to aqueous free energy. LJ potential is further divided into ΔG^{aq}_{rep} and ΔG^{aq}_{dis} terms representing repulsive and dispersive terms. Similar notation are used for free energy in vacuum as $\Delta G^{vac}_{nonp}, \Delta G^{vac}_{rep}, \Delta G^{vac}_{dis}$ and ΔG^{vac}_{elec}.

Table S4. Drude toppar stream file with topology and parameters for SLES molecule.

```
* DRUDE topology and parameter stream file for ! sulfate
*

!requires toppar_drude_master*.str

read rtf card append
* Topology for Drude nucleic acids
*
38

DEFA FIRS NONE LAST NONE
AUTOGENERATE ANGLES DIHEDRALS DRUDE

RESI LES     -1.000
GROUP           ! CHARGE   CH_PENALTY
ATOM C16    CD32C   -0.371 ALPHA -1.678   THOLE 0.862
ATOM O2     OD30B   -0.279 ALPHA -0.670   THOLE 0.181
ATOM S      SD1A     1.930 ALPHA -0.930   THOLE 1.098
ATOM O3     OD2C2B  -0.850 ALPHA -0.990   THOLE 1.083
ATOM O4     OD2C2B  -0.850 ALPHA -0.990   THOLE 1.083
ATOM O5     OD2C2B  -0.850 ALPHA -0.990   THOLE 1.083
ATOM H32    HDA2A    0.135
ATOM H33    HDA2A    0.135
GROUP
ATOM C13    CD32A   -0.120  ALPHA -1.887  THOLE 0.456
ATOM H26    HDA2A    0.060
ATOM H27    HDA2A    0.060
ATOM C14    CD32A   -0.004  ALPHA -1.696  THOLE 0.918
ATOM H28    HDA2A    0.060
ATOM H29    HDA2A    0.060
ATOM O1     OD30A    0.000  ALPHA -0.705  THOLE 1.312
ATOM LP1A   LPD     -0.116
ATOM LP1B   LPD     -0.116
ATOM C15    CD32A   -0.004  ALPHA -1.798  THOLE 1.074
ATOM H30    HDA2A    0.060
ATOM H31    HDA2A    0.060
GROUP
ATOM C1     CD33A   -0.177  ALPHA -2.051  THOLE 1.3
ATOM H1     HDA3A    0.059
ATOM H2     HDA3A    0.059
ATOM H3     HDA3A    0.059
GROUP
ATOM C2     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H4     HDA2A    0.078
ATOM H5     HDA2A    0.078
GROUP
ATOM C3     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H6     HDA2A    0.078
ATOM H7     HDA2A    0.078
GROUP
ATOM C4     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H8     HDA2A    0.078
ATOM H9     HDA2A    0.078
GROUP
```

```
ATOM C5     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H10    HDA2A    0.078
ATOM H11    HDA2A    0.078
GROUP
ATOM C6     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H12    HDA2A    0.078
ATOM H13    HDA2A    0.078
GROUP
ATOM C7     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H14    HDA2A    0.078
ATOM H15    HDA2A    0.078
GROUP
ATOM C8     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H16    HDA2A    0.078
ATOM H17    HDA2A    0.078
GROUP
ATOM C9     CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H18    HDA2A    0.078
ATOM H19    HDA2A    0.078
GROUP
ATOM C10    CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H20    HDA2A    0.078
ATOM H21    HDA2A    0.078
GROUP
ATOM C11    CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H22    HDA2A    0.078
ATOM H23    HDA2A    0.078
GROUP
ATOM C12    CD32A   -0.156  ALPHA -1.660  THOLE 1.3
ATOM H24    HDA2A    0.078
ATOM H25    HDA2A    0.078

BOND  C1   C2     C2   C3     C3   C4     C4   C5
BOND  C5   C6     C6   C7     C7   C8     C8   C9   C9   C10
BOND  C10  C11    C11  C12    C12  C13
BOND  C1   H1     C1   H2     C1   H3     C2   H4   C2   H5
BOND  C3   H6     C3   H7     C4   H8     C4   H9
BOND  C5   H10    C5   H11    C6   H12    C6   H13
BOND  C7   H14    C7   H15    C8   H16    C8   H17
BOND  C9   H18    C9   H19    C10  H20   C10   H21  C11  H22
BOND  C11  H23    C12  H24    C12  H25
BOND C13   C14    C14  O1     O1   C15   C13   H27  C13  H26
BOND C14   H29    C14  H28    C15  H31   C15   H30  C16  C15
BOND O1    LP1A   O1   LP1B   O4    S    O3    S    H32   C16
BOND S     O2     S     O5    H33   C16  C16   O2

LONEPAIR bisector LP1A O1 C15 C14 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP1B O1 C15 C14 distance 0.35 angle 110.0 dihe 270.0
END

read param card append
* Parameters generated by analogy by
* CHARMM Drude Force Field program version 2.2.0
*

! Penalties lower than 10 indicate the analogy is fair; penalties between 10
! and 50 mean some basic validation is recommended; penalties higher than
! 50 indicate poor analogy and mandate extensive validation/optimization.

BONDS
OD2C2B   SD1A      525.00      1.493  ! DMP, cmb, 06/09
OD30B    SD1A      240.00      1.701  ! DMP, cmb, 06/09
SD1A     LPD         0.00      0.000  ! DMP
CD32A    OD30A     360.00      1.415
CD32C    OD30B     335.00      1.420

ANGLES
SD1A     OD30B    CD32C     75.00     98.38     ! DMP, cmb, 06/09
OD2C2B   SD1A     OD2C2B    60.00     115.35    ! DMP, csd, EH/IV 2007
OD2C2B   SD1A     OD30B     90.00     98.44     ! DMP, csd, EH/IV 2007**better molvib fit
OD30B    CD32C    HDA2A     60.00    109.50
OD30B    CD32C    CD32A     75.70    110.10
CD32C    CD32A    OD30A     75.70    110.10

DIHEDRALS
CD32C    OD30B    SD1A     OD2C2B      5.056    2   180.00
SD1A     OD30B    CD32C    HDA2A       0.000    3     0.00 ! DMP, cmb, 06/09
OD30B    CD32C    CD32A    OD30A       0.3681   1     0.00
OD30B    CD32C    CD32A    OD30A       1.2036   2     0.00
OD30B    CD32C    CD32A    OD30A       0.1171   3     0.00
OD30B    CD32C    CD32A    OD30A       0.1612   4     0.00
```

```
OD30B     CD32C     CD32A     OD30A        0.0340   5      0.00
OD30B     CD32C     CD32A     OD30A        0.0225   6      0.00
OD30B     CD32C     CD32A     HDA2A        0.190    3      0.00
HDA2A     CD32C     CD32A     OD30A        0.190    3      0.00
CD32C     CD32A     OD30A     CD32A        0.570    1      0.00
CD32C     CD32A     OD30A     CD32A        0.290    2      0.00
CD32C     CD32A     OD30A     CD32A        0.430    3      0.00
CD32A     CD32C     OD30B     SD1A         0.203    1    180.00
CD32A     CD32C     OD30B     SD1A         0.182    2      0.00
CD32A     CD32C     OD30B     SD1A         0.123    3    180.00
CD32A     CD32C     OD30B     SD1A         0.089    4      0.00
CD32A     CD32C     OD30B     SD1A         0.143    5    180.00
CD32A     CD32C     OD30B     SD1A         0.093    6    180.00

IMPROPERS

NONBONDED nbxmod  5 atom vatom cdiel vdistance switch vswitch -
cutnb 16.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

SD1A      0.0   -0.2700     1.9000 ! DMP, lipids

END
RETURN
```

Table S5. Drude toppar stream file with topology and parameters for CA molecule.

```
* DRUDE topology and parameter stream file
*

!requires toppar_drude_master*.str

!ioformat extended


read rtf card append
* Topology for Drude lipids
*
38

DEFA FIRS NONE LAST NONE
AUTOGENERATE ANGLES DIHEDRALS DRUDE  !note use of DRUD

RESI CAC            0.000 ! param penalty=   0.600 ; charge penalty=   1.952
GROUP            ! CHARGE   CH_PENALTY
ATOM C8     CD32C  -0.208  ALPHA -2.114 THOLE 0.750 ! -0.208
ATOM H15    HDA2A   0.092
ATOM H16    HDA2A   0.092
ATOM C10    CD2O3A  0.858  ALPHA -1.207 THOLE 0.708
ATOM O1     OD2C3A  0.000  ALPHA -0.922 THOLE 1.539
ATOM LPP1   LPD    -0.319
ATOM LPP2   LPD    -0.319
ATOM O2     OD30D   0.000  ALPHA -1.280 THOLE 1.124
ATOM LPP3   LPD    -0.285
ATOM LPP4   LPD    -0.285
ATOM H20    HDP1A   0.374
GROUP
ATOM C9     CD33A  -0.177  ALPHA -2.051  THOLE 1.3
ATOM H17    HDA3A   0.059
ATOM H18    HDA3A   0.059
ATOM H19    HDA3A   0.059
GROUP
ATOM C2     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H3     HDA2A   0.078
ATOM H4     HDA2A   0.078
GROUP
ATOM C3     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H5     HDA2A   0.078
ATOM H6     HDA2A   0.078
GROUP
ATOM C4     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H7     HDA2A   0.078
ATOM H8     HDA2A   0.078
GROUP
ATOM C5     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H9     HDA2A   0.078
ATOM H10    HDA2A   0.078
GROUP
ATOM C6     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H11    HDA2A   0.078
```

```
ATOM H12    HDA2A   0.078
GROUP
ATOM C7     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H13    HDA2A   0.078
ATOM H14    HDA2A   0.078
GROUP
ATOM C1     CD32A  -0.156  ALPHA -1.660  THOLE 1.3
ATOM H1     HDA2A   0.078
ATOM H2     HDA2A   0.078

BOND C1   C2   C2   C4  C3   C5  C4   C6  C5   C7  C6   C8  C7   C9
BOND C8   C10  C1   C3  C10  O1  C10  O2  C1   H1  C1   H2  C2   H3
BOND C2   H4   C3   H5  C3   H6  C4   H7  C4   H8  C5   H9  C5   H10
BOND C6   H11  C6   H12 C7   H13 C7   H14 C8   H15 C8   H16 C9   H17
BOND C9   H18  C9   H19 O2   H20 O1  LPP1 O1  LPP2 O2  LPP3 O2  LPP4
IMPR C10    C8     O1     O2

!standard carbonyl
LONEPAIR relative LPP1 O1 C10 O2 distance 0.30 angle 91.0 dihe   0.0
LONEPAIR relative LPP2 O1 C10 O2 distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY O1 C10 LPP1 LPP2  A11 0.6968  A22 1.2194

!from MeOH
LONEPAIR relative LPP3 O2 C10 H20 distance 0.35 angle 110.9 dihe  91.0
LONEPAIR relative LPP4 O2 C10 H20 distance 0.35 angle 110.9 dihe 269.0
ANISOTROPY O2 C10 LPP3 LPP4  A11 0.8108  A22 1.2162

END
```

Table S6. Drude toppar stream file with topology and parameters for Caprate ion molecule.

```
* DRUDE topology and parameter stream file
*

!requires toppar_drude_master*.str

!ioformat extended

read rtf card append
* Topology for Drude lipids
*
38

DEFA FIRS NONE LAST NONE
AUTOGENERATE ANGLES DIHEDRALS DRUDE  !note use of DRUD

RESI CAP           -1.000 !
GROUP
ATOM C8     CD32C  -0.190  ALPHA -2.528  THOLE 1.414
ATOM H15    HDA2A   0.004
ATOM H16    HDA2A   0.004
ATOM C10    CD2O2A  0.708  ALPHA -1.016  THOLE 0.899
ATOM O1     OD2C2A  0.003  ALPHA -0.699  THOLE 2.399
ATOM LP1A   LPD    -0.383
ATOM LP1B   LPD    -0.383
ATOM O2     OD2C2A  0.003  ALPHA -0.699  THOLE 2.399
ATOM LP2A   LPD    -0.383
ATOM LP2B   LPD    -0.383
GROUP
ATOM C9     CD33A  -0.177  ALPHA -2.051  THOLE 1.300
ATOM H17    HDA3A   0.059
ATOM H18    HDA3A   0.059
ATOM H19    HDA3A   0.059
GROUP
ATOM C2     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H4     HDA2A   0.078
ATOM H3     HDA2A   0.078
GROUP
ATOM C3     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H6     HDA2A   0.078
ATOM H5     HDA2A   0.078
GROUP
ATOM C4     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H8     HDA2A   0.078
ATOM H7     HDA2A   0.078
GROUP
ATOM C5     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H10    HDA2A   0.078
ATOM H9     HDA2A   0.078
GROUP
```

```
ATOM C6     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H12    HDA2A   0.078
ATOM H11    HDA2A   0.078
GROUP
ATOM C7     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H14    HDA2A   0.078
ATOM H13    HDA2A   0.078
GROUP
ATOM C1     CD32A  -0.156  ALPHA -1.660  THOLE 1.300
ATOM H1     HDA2A   0.078
ATOM H2     HDA2A   0.078

BOND C1   C2   C2   C4   C3   C5   C4   C6   C5   C7
BOND C6   C8   C7   C9   C8   C10  C1   C3
BOND C10  O1   C10  O2
BOND C1   H1   C1   H2   C2   H3   C2   H4   C3   H5
BOND C3   H6   C4   H7   C4   H8   C5   H9   C5   H10
BOND C6   H11  C6   H12  C7   H13  C7   H14  C8   H15
BOND C8   H16  C9   H17  C9   H18  C9   H19
BOND O1  LP1A    O1  LP1B    O2  LP2A    O2  LP2B
IMPR C10    C8     O1     O2

LONEPAIR relative LP1A O1 C10 C8  distance 0.35 angle 110.0 dihe   0.0
LONEPAIR relative LP1B O1 C10 C8  distance 0.35 angle 110.0 dihe 180.0
LONEPAIR relative LP2A O2 C10 C8  distance 0.35 angle 110.0 dihe   0.0
LONEPAIR relative LP2B O2 C10 C8  distance 0.35 angle 110.0 dihe 180.0
ANISOTROPY O1 C10 LP1A LP1B A11 0.7229 A22 1.265
ANISOTROPY O2 C10 LP2A LP2B A11 0.7229 A22 1.265

END

read param card append
* Parameters generated by analogy by
* CHARMM Drude Force Field program version 2.2.0
*
ANGLES

CD2O2A   CD32C    CD32A     30.60    120.70                 ! CTER, PEML, Glu


DIHEDRALS
CD2O2A   CD32C    CD32A    CD32A       0.200    3     0.00 !
CD2O2A   CD32C    CD32A    HDA2A       0.200    3     0.00 !
OD2C2A   CD2O2A   CD32C    CD32A       0.200    3     0.00 !

IMPROPERS

CD2O2A   CD32C    OD2C2A   OD2C2A      71.000   0     0.00 ! CTER, Gly


END
RETURN
```

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