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******* FILE DS_OPLS.itp *******

[ moleculetype ]
; Name   nrexcl
DS      3

[ atoms ]
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    3    O_DS        1    DS      O2    1   -0.654
    4    O_DS        1    DS      O3    1   -0.654
    5    OS_DS       1    DS      OS    2   -0.459
    6    opls_443    1    DS      C1    2    0.017
    7    opls_444    1    DS     H11    2    0.06
    8    opls_444    1    DS     H12    2    0.06
    9    opls_136    1    DS      C2    3   -0.12
   10    opls_140    1    DS     H21    3    0.06
   11    opls_140    1    DS     H22    3    0.06
   12    opls_136    1    DS      C3    3   -0.12
   13    opls_140    1    DS     H31    3    0.06
   14    opls_140    1    DS     H32    3    0.06
   15    opls_136    1    DS      C4    4   -0.12
   16    opls_140    1    DS     H41    4    0.06
   17    opls_140    1    DS     H42    4    0.06
   18    opls_136    1    DS      C5    4   -0.12
   19    opls_140    1    DS     H51    4    0.06
   20    opls_140    1    DS     H52    4    0.06
   21    opls_136    1    DS      C6    5   -0.12
   22    opls_140    1    DS     H61    5    0.06
   23    opls_140    1    DS     H62    5    0.06
   24    opls_136    1    DS      C7    6   -0.12
   25    opls_140    1    DS     H71    6    0.06
   26    opls_140    1    DS     H72    6    0.06
   27    opls_136    1    DS      C8    6   -0.12
   28    opls_140    1    DS     H81    6    0.06
   29    opls_140    1    DS     H82    6    0.06
   30    opls_136    1    DS      C9    7   -0.12
   31    opls_140    1    DS     H91    7    0.06
   32    opls_140    1    DS     H92    7    0.06
   33    opls_136    1    DS     C10    7   -0.12
   34    opls_140    1    DS     HA1    7    0.06
   35    opls_140    1    DS     HA2    7    0.06
   36    opls_136    1    DS     C11    8   -0.12
   37    opls_140    1    DS     HB1    8    0.06
   38    opls_140    1    DS     HB2    8    0.06
   39    opls_135    1    DS     C12    8   -0.18
   40    opls_140    1    DS     HC1    8    0.06
   41    opls_140    1    DS     HC2    8    0.06
   42    opls_140    1    DS     HC3    8    0.06

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   6     8     1
   6     9     1
```

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    39    41    1
    39    42    1

[ angles ]
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    13    12    15    1
    14    12    15    1
```

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   36    39    41    1
   36    39    42    1
   40    39    41    1
   40    39    42    1
   41    39    42    1

[ dihedrals ]
;  ai   aj   ak   al
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   3     1     5     6     3
   4     1     5     6     3
   1     5     6     7     3
```

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1	5	6	9	3
5	6	9	10	3
5	6	9	11	3
5	6	9	12	3
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7	6	9	11	HC_CT_CT_HC_long
7	6	9	12	3
8	6	9	10	HC_CT_CT_HC_long
8	6	9	11	HC_CT_CT_HC_long
8	6	9	12	3
6	9	12	13	3
6	9	12	14	3
6	9	12	15	CT_CT_CT_CT_long
10	9	12	13	HC_CT_CT_HC_long
10	9	12	14	HC_CT_CT_HC_long
10	9	12	15	3
11	9	12	13	HC_CT_CT_HC_long
11	9	12	14	HC_CT_CT_HC_long
11	9	12	15	3
9	12	15	16	3
9	12	15	17	3
9	12	15	18	CT_CT_CT_CT_long
13	12	15	16	HC_CT_CT_HC_long
13	12	15	17	HC_CT_CT_HC_long
13	12	15	18	3
14	12	15	16	HC_CT_CT_HC_long
14	12	15	17	HC_CT_CT_HC_long
14	12	15	18	3
12	15	18	19	3
12	15	18	20	3
12	15	18	21	CT_CT_CT_CT_long
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16	15	18	20	HC_CT_CT_HC_long
16	15	18	21	3
17	15	18	19	HC_CT_CT_HC_long
17	15	18	20	HC_CT_CT_HC_long
17	15	18	21	3
15	18	21	22	3
15	18	21	23	3
15	18	21	24	CT_CT_CT_CT_long
19	18	21	22	HC_CT_CT_HC_long
19	18	21	23	HC_CT_CT_HC_long
19	18	21	24	3
20	18	21	22	HC_CT_CT_HC_long
20	18	21	23	HC_CT_CT_HC_long
20	18	21	24	3
18	21	24	25	3
18	21	24	26	3
18	21	24	27	CT_CT_CT_CT_long
22	21	24	25	HC_CT_CT_HC_long
22	21	24	26	HC_CT_CT_HC_long
22	21	24	27	3
23	21	24	25	HC_CT_CT_HC_long
23	21	24	26	HC_CT_CT_HC_long
23	21	24	27	3
21	24	27	28	3
21	24	27	29	3
21	24	27	30	CT_CT_CT_CT_long
25	24	27	28	HC_CT_CT_HC_long
25	24	27	29	HC_CT_CT_HC_long

```
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   26    24    27    28    HC_CT_CT_HC_long
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   24    27    30    31    3
   24    27    30    32    3
   24    27    30    33    CT_CT_CT_CT_long
   28    27    30    31    HC_CT_CT_HC_long
   28    27    30    32    HC_CT_CT_HC_long
   28    27    30    33    3
   29    27    30    31    HC_CT_CT_HC_long
   29    27    30    32    HC_CT_CT_HC_long
   29    27    30    33    3
   27    30    33    34    3
   27    30    33    35    3
   27    30    33    36    CT_CT_CT_CT_long
   31    30    33    34    HC_CT_CT_HC_long
   31    30    33    35    HC_CT_CT_HC_long
   31    30    33    36    3
   32    30    33    34    HC_CT_CT_HC_long
   32    30    33    35    HC_CT_CT_HC_long
   32    30    33    36    3
   30    33    36    37    3
   30    33    36    38    3
   30    33    36    39    CT_CT_CT_CT_long
   34    33    36    37    HC_CT_CT_HC_long
   34    33    36    38    HC_CT_CT_HC_long
   34    33    36    39    3
   35    33    36    37    HC_CT_CT_HC_long
   35    33    36    38    HC_CT_CT_HC_long
   35    33    36    39    3
   33    36    39    40    3
   33    36    39    41    3
   33    36    39    42    3
   37    36    39    40    HC_CT_CT_HC_long
   37    36    39    41    HC_CT_CT_HC_long
   37    36    39    42    HC_CT_CT_HC_long
   38    36    39    40    HC_CT_CT_HC_long
   38    36    39    41    HC_CT_CT_HC_long
   38    36    39    42    HC_CT_CT_HC_long


******* FILE DS_params_OPLS.itp *******

; Karl J. Schweighofer, Ulrich Essmann, and Max Berkowitz
; Simulation of Sodium Dodecyl Sulfate at the Water-Vapor and Water-Carbon
; Tetrachloride Interfaces at Low Surface Coverage
; J. Phys. Chem. B 1997, 101, 3793-3799


[ atomtypes ]
OS_DS  OS    8      15.9994 -0.459   A     0.3        0.71128
O_DS   O2    8      15.9994 -0.654   A     0.315      0.8368
S_DS   SE   16      32.06    1.284   A     0.355      1.046

[ bondtypes ]
SE   OS     1    0.158     251040
SE   O2     1    0.146     376560

[ angletypes ]
CT   OS   SE      1    112.7      418.400
```

```
OS   SE   O2      1    102.6      426.768
O2   SE   O2      1    115.4      426.768

[ dihedraltypes ]
; OPLS for R2PO42-
SE   OS   CT   CT     3   12.51016   0.00000 -12.51016   0.00000   0.00000   0.00000
SE   OS   CT   HC     3    0.74684   2.24053   0.00000  -2.98738   0.00000   0.00000
CT   OS   SE   O2     3    1.17570   3.52711   0.00000  -4.70281   0.00000   0.00000


****** FILE C-C_long_dihs.itp *******

; Krzysztof Murzyn, Maciej Bratek, and Marta Pasenkiewicz-Gierula
; Refined OPLS All-Atom Force Field Parameters for n-Pentadecane,
; Methyl Acetate, and Dimethyl Phosphate
; J. Phys. Chem. B 2013, 117, 16388-16396


#define HC_CT_CT_HC_long      3    0.3138     0.9414     0.0000   -1.2552  0.0000  0.0000
#define CT_CT_CT_CT_long      3    2.209155   4.543825   0.77822  -7.5312  0.0000  0.0000


******* FILE topol_OPLS.top *******


#include "oplsaa.ff/forcefield.itp"
#include "C-C_long_dihs.itp"
#include "DS_params_OPLS.itp"

#include "DS_OPLS.itp"
#include "oplsaa.ff/ions.itp"
#include "oplsaa.ff/spc.itp"


[ system ]
; Name
SDS micelle

[ molecules ]
; Compound     #mols
DS               382
Na               873
Cl               491
SOL            71974


******* FILE DS_GAFF.itp *******

[ moleculetype ]
; Name   nrexcl
DS      3

[ atoms ]
;  nr  type  resnr  resid  atom  cgnr  charge
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    3    oP    1    DS      O2    1   -0.6383
    4    oP    1    DS      O3    1   -0.6383
    5    oT    1    DS      OS    2   -0.4483
    6    cA    1    DS      C1    2    0.2387
    7    hE    1    DS     H11    2   -0.012
```

```
     8    hE    1    DS     H12    2   -0.012
     9    cD    1    DS      C2    3    0.07293
    10    hL    1    DS     H21    3   -0.02823
    11    hL    1    DS     H22    3   -0.02823
    12    cD    1    DS      C3    3    0.0484
    13    hL    1    DS     H31    3   -0.0246
    14    hL    1    DS     H32    3   -0.0246
    15    cD    1    DS      C4    4    0.0343
    16    hL    1    DS     H41    4   -0.01713
    17    hL    1    DS     H42    4   -0.01713
    18    cD    1    DS      C5    4    0.02213
    19    hL    1    DS     H51    4   -0.01783
    20    hL    1    DS     H52    4   -0.01783
    21    cD    1    DS      C6    5    0.0286
    22    hL    1    DS     H61    5   -0.0151
    23    hL    1    DS     H62    5   -0.0151
    24    cD    1    DS      C7    6    0.02863
    25    hL    1    DS     H71    6   -0.0129
    26    hL    1    DS     H72    6   -0.0129
    27    cD    1    DS      C8    6    0.01827
    28    hL    1    DS     H81    6   -0.0134
    29    hL    1    DS     H82    6   -0.0134
    30    cD    1    DS      C9    7    0.02267
    31    hL    1    DS     H91    7   -0.01247
    32    hL    1    DS     H92    7   -0.01247
    33    cD    1    DS     C10    7    0.0222
    34    hL    1    DS     HA1    7   -0.01173
    35    hL    1    DS     HA2    7   -0.01173
    36    cD    1    DS     C11    8    0.05857
    37    hL    1    DS     HB1    8   -0.01573
    38    hL    1    DS     HB2    8   -0.01573
    39    cD    1    DS     C12    8   -0.05007
    40    hL    1    DS     HC1    8    0.00417
    41    hL    1    DS     HC2    8    0.00417
    42    hL    1    DS     HC3    8    0.00417

[ bonds ]
;  ai   aj
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    18    21    1
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    21    23    1
    21    24    1
```

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   36    38    1
   36    39    1
   39    40    1
   39    41    1
   39    42    1

[ angles ]
;  ai   aj   ak
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   2     1     5     1
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```

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   40    39    42    1
   41    39    42    1

[ dihedrals ]
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   1     5     6     8      9
   1     5     6     9      9
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   5     6     9     11     9
   5     6     9     12     9
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   8     6     9     11     9
   8     6     9     12     9
   6     9     12    13     9
   6     9     12    14     9
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29	27	30	31	9
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29	27	30	33	9
27	30	33	34	9
27	30	33	35	9

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   38    36    39    41     9
   38    36    39    42     9


******* FILE DS_params_GAFF.itp *******

; Karl J. Schweighofer, Ulrich Essmann, and Max Berkowitz
; Simulation of Sodium Dodecyl Sulfate at the Water-Vapor and
; Water-Carbon Tetrachloride Interfaces at Low Surface Coverage
; J. Phys. Chem. B 1997, 101, 3793-3799

; Hui Yan, Shi-Ling Yuan, Gui-Ying Xu, and Cheng-Bu Liu
; Effect of Ca2+ and Mg2+ Ions on Surfactant Solutions
; Investigated by Molecular Dynamics Simulation
; Langmuir 2010, 26, 10448-10459


[ atomtypes ]

s6          16      32.06    0.0000  A     3.56359e-01  1.04600e+00  ; s6 in GAFF

[ bondtypes ]

s6    oT     1    0.158    251040    ;  from Yan = from Schweighofer
s6    oP     1    0.146    376560    ;  from Schweighofer ~ from Yan

[ angletypes ]

cA   oT   s6     1    112.6     520.100    ;  from Yan = from Schweighofer
oT   s6   oP     1    102.6     426.768    ;  from Yan = from Schweighofer
oP   s6   oP     1    115.3     484.5      ;  from Yan

cA   cD   cD     1    110.63    528.94     ;  = cD-cD-cD
cA   cD   hL     1    110.05    388.02     ;  = cD-cD-hL
cD   cA   hE     1    110.07    387.94     ;  = cA-cA-hE
cD   cA   oT     1    108.42    567.18     ;  = cA-cA-oT

[ dihedraltypes ]
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cD   cD   cD   cA      9   180.0    1.302       1   ;  = cD-cD-cD-cD
cD   cD   cD   cA      9   180.0    0.5159      2   ;
cD   cD   cD   cA      9     0.0    0.4807      3   ;
cD   cD   cD   cA      9     0.0    0.9201      4   ;
cD   cD   cD   cA      9     0.0    0.9079      5   ;

cA   oT   s6   oP      9     0.0    3.347       2   ;  = cA-oT-p5-oP
cA   oT   s6   oP      9     0.0    3.347       2   ;
hE   cA   oT   s6      9     0.0    1.604       3   ;  = hE-cA-oT-pA
cD   cA   oT   s6      9     0.0    1.604       3   ;  = cA-cA-oT-pA
hL   cD   cA   oT      9     0.0    0           3   ;  = hE-cA-cA-oT
hL   cD   cA   oT      9     0.0    1.046       1   ;

hL   cD   cA   oT      9     0.0    0           3   ;  = hE-cA-cA-oT
hL   cD   cA   oT      9     0.0    1.046       1   ;
cD   cD   cA   oT      9     0.0    0.6510      3   ;  = cA-cA-cA-oT
hL   cD   cA   hE      9     0.0    0.6510      3   ;  = hA-cA-cA-hE
cD   cD   cA   hE      9     0.0    0.6510      3   ;  = cA-cA-cA-hE
cA   cD   cD   hL      9     0.0    0.6694      3   ;  = cD-cD-cD-hL


******* FILE topol_GAFF.top *******

#include "amber99.ff/forcefield.itp"
#include "AMBERLipid14.itp"
#include "DS_params_GAFF.itp"

#include "DS_GAFF.itp"
#include "amber99.ff/ions.itp"
#include "amber99.ff/spc.itp"

[ system ]
; Name
SDS micelle

[ molecules ]
; Compound     #mols
DS               382
Na               873
Cl               491
SOL            71974
```

```
******* FILE AMBERLipid14.itp *******

; AMBER Lipid 1.4 force field
;
; Callum J. Dickson, Benjamin D. Madej, Age A. Skjevik,
; Robin M. Betz, Knut Teigen, Ian R. Gould, Ross C. Walker
; LIPID14: The Amber Lipid Force Field
; J. Chem. Theory Comput. 2014, 10, 865-879


[ atomtypes ]
; name      at.num  mass     charge ptype  sigma     epsilon          ; in GAFF
cA           6      12.01    0.0000  A     3.39967e-01  4.57730e-01   ; c3
hA           1       1.008   0.0000  A     2.64953e-01  6.56888e-02   ; hc

cD           6      12.01    0.0000  A     3.39967e-01  4.57730e-01   ; c3  new in 14, = cA
hL           1       1.008   0.0000  A     0.260142     0.04184       ; hc  new in 14

hE           1       1.008   0.0000  A     2.47135e-01  6.56888e-02   ; h1
oS           8      16.00    0.0000  A     2.93997e-01  5.02080e-01   ; os  mod in 14
oT           8      16.00    0.0000  A     3.00001e-01  7.11280e-01   ; os
oC           8      16.00    0.0000  A     2.93997e-01  5.85760e-01   ; o   mod in 14
oO           8      16.00    0.0000  A     2.95992e-01  8.78640e-01   ; o
oP           8      16.00    0.0000  A     2.95992e-01  8.78640e-01   ; o

cB           6      12.01    0.0000  A     3.39967e-01  3.59824e-01   ; c2
cC           6      12.01    0.0000  A     3.39967e-01  2.92880e-01   ; c   mod in 14
hB           1       1.008   0.0000  A     2.59964e-01  6.27600e-02   ; ha
oH           8      16.00    0.0000  A     3.06647e-01  8.80314e-01   ; oh
hO           1       1.008   0.0000  A     0.00000e+00  0.00000e+00   ; ho
hX           1       1.008   0.0000  A     1.95998e-01  6.56888e-02   ; hx
hN           1       1.008   0.0000  A     1.06908e-01  6.56888e-02   ; hn
nA           7      14.01    0.0000  A     3.25000e-01  7.11280e-01   ; n4
pA          15      30.97    0.0000  A     3.74177e-01  8.36800e-01   ; p5

; name      at.num  mass     charge ptype  sigma     epsilon          ; in GLYCAM
oR           8      16.00    0.0000  A     0.306647     0.8803136     ; OH
hR           1       1.008   0.0000  A     0.0000       0.0000        ; HO
hS           1       1.008   0.0000  A     0.247135     0.0656888     ; H1
cR           6      12.01    0.0000  A     0.339967     0.4577296     ; CG
cP           6      12.01    0.0000  A     0.339967     0.4577296     ; CP

[ bondtypes ]

cA   cA     1    0.1535    253634.08    ;  Lipid11 v1.0 (GAFF c3-c3)
cA   cB     1    0.1508    274721.44    ;  Lipid11 v1.0 (GAFF c3-c2)
cA   cC     1    0.1508    274721.44    ;  Lipid11 v1.0 (GAFF c3-c )
cA   cD     1    0.1508    274721.44    ;  Lipid14 v2.0 (GAFF c3-c )
cA   hA     1    0.1092    282252.64    ;  Lipid11 v1.0 (GAFF c3-hc)
cA   hE     1    0.1093    281081.12    ;  Lipid11 v1.0 (GAFF c3-h1)
cA   hX     1    0.1091    283424.16    ;  Lipid11 v1.0 (GAFF c3-hx)
cA   nA     1    0.1499    245684.48    ;  Lipid11 v1.0 (GAFF c3-n4)
cA   oH     1    0.1426    262838.88    ;  Lipid11 v1.0 (GAFF c3-oh)
cA   oS     1    0.1439    252295.2     ;  Lipid11 v1.0 (GAFF c3-os)
cA   oT     1    0.1439    252295.2     ;  Lipid11 v1.0 (GAFF c3-os)
cB   cB     1    0.1324    493460.96    ;  Lipid11 v1.0 (GAFF c2-c2)
cB   hB     1    0.1087    288110.24    ;  Lipid11 v1.0 (GAFF c2-ha)
cC   oC     1    0.1214    542246.4     ;  Lipid11 v1.0 (GAFF c -o )
cC   oO     1    0.1214    542246.4     ;  Lipid11 v1.0 (GAFF c -o )
cC   oS     1    0.1343    344175.84    ;  Lipid11 v1.0 (GAFF c -os)
cD   cB     1    0.1508    274721.44    ;  Lipid14 v2.0 (GAFF c3-c2)
cD   cC     1    0.1508    274721.44    ;  Lipid14 v2.0 (GAFF c3-c )
cD   cD     1    0.1535    253634.08    ;  Lipid14 v2.0 (GAFF c3-c3)
cD   hL     1    0.1092    282252.64    ;  Lipid14 v2.0 (GAFF c3-hc)
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cP   cR     1    0.152     259408       ;  Lipid11 v1.0 (GLYCAM06g CP-CG)
cP   hS     1    0.109     284512       ;  Lipid11 v1.0 (GLYCAM06g CP-H1)
cP   oS     1    0.146     238488       ;  Lipid11 v1.0 (GLYCAM06g CP-OS)
cP   oT     1    0.146     238488       ;  Lipid11 v1.0 (GLYCAM06g CP-OS)
cR   cR     1    0.152     259408       ;  Lipid11 v1.0 (GLYCAM06g CG-CG)
cR   hS     1    0.109     284512       ;  Lipid11 v1.0 (GLYCAM06g CG-H1)
cR   oR     1    0.143     267776       ;  Lipid11 v1.0 (GLYCAM06g CG-OH)
hN   nA     1    0.1033    308779.2     ;  Lipid11 v1.0 (GAFF hn-n4)
hO   oH     1    0.0974    309281.28    ;  Lipid11 v1.0 (GAFF ho-oh)
hR   oR     1    0.096     462750.4     ;  Lipid11 v1.0 (GLYCAM06g HO-OH)
oC   pA     1    0.1481    408107.36    ;  Lipid11 v1.0 (GAFF o -p5)
oP   pA     1    0.1481    408107.36    ;  Lipid11 v1.0 (GAFF o -p5)
oH   pA     1    0.1625    268780.16    ;  Lipid11 v1.0 (GAFF oh-p5)
oS   pA     1    0.1602    286604       ;  Lipid11 v1.0 (GAFF os-p5)
oT   pA     1    0.1602    286604       ;  Lipid11 v1.0 (GAFF os-p5)

[ angletypes ]

cA   cA   cA     1    110.63    528.94     ;  Lipid11 v1.0 (GAFFc3-c3-c3)
cA   cA   cB     1    111.44    531.62     ;  Lipid11 v1.0 (GAFFc3-c3-c2)
cA   cA   cC     1    110.53    533.79     ;  Lipid11 v1.0 (GAFFc3-c3-c )
cA   cA   hA     1    110.05    388.02     ;  Lipid11 v1.0 (GAFFc3-c3-hc)
cA   cA   hE     1    110.07    387.94     ;  Lipid11 v1.0 (GAFFc3-c3-h1)
cA   cA   hL     1    110.05    388.02     ;  Lipid14 v2.0 (GAFFc3-c3-hc)
cA   cA   hX     1    111.74    385.10     ;  Lipid11 v1.0 (GAFFc3-c3-hx)
cA   cA   nA     1    114.32    539.32     ;  Lipid11 v1.0 (GAFFc3-c3-n4)
cA   cA   oH     1    109.43    566.68     ;  Lipid11 v1.0 (GAFFc3-c3-oh)
cA   cA   oS     1    108.42    567.18     ;  Lipid11 v1.0 (GAFFc3-c3-os)
cA   cA   oT     1    108.42    567.18     ;  Lipid11 v1.0 (GAFFc3-c3-os)
cA   cB   cA     1    116.52    524.67     ;  Lipid11 v1.0 (GAFFc3-c2-c3)
cA   cB   cB     1    123.42    538.31     ;  Lipid11 v1.0 (GAFFc3-c2-c2)
cA   cB   hB     1    117.30    382.08     ;  Lipid11 v1.0 (GAFFc3-c2-ha)
cA   cC   oC     1    123.11    569.28     ;  Lipid11 v1.0 (GAFFc3-c -o )
cA   cC   oO     1    123.11    569.28     ;  Lipid11 v1.0 (GAFFc3-c -o )
cA   cC   oS     1    111.96    579.57     ;  Lipid11 v1.0 (GAFFc3-c -os)
cA   nA   cA     1    110.64    525.85     ;  Lipid11 v1.0 (GAFFc3-n4-c3)
cA   nA   hN     1    110.11    386.51     ;  Lipid11 v1.0 (GAFFc3-n4-hn)
cA   oH   hO     1    108.16    394.05     ;  Lipid11 v1.0 (GAFFc3-oh-ho)
cA   oS   pA     1    118.00    518.82     ;  Lipid11 v1.0 (GAFFc3-os-p5)
cA   oS   cC     1    115.14    532.46     ;  Lipid11 v1.0 (GAFFc3-os-c )
cA   oT   pA     1    118.00    518.82     ;  Lipid11 v1.0 (GAFFc3-os-p5)
cB   cA   cB     1    112.08    534.97     ;  Lipid11 v1.0 (GAFFc2-c3-c2)
cB   cA   hA     1    110.49    393.55     ;  Lipid11 v1.0 (GAFFc2-c3-hc)
cB   cB   hB     1    120.94    418.73     ;  Lipid11 v1.0 (GAFFc2-c2-ha)
cB   cD   cB     1    112.08    534.97     ;  Lipid14 v2.0 (GAFFc2-c3-c2)
cB   cD   hL     1    110.49    393.55     ;  Lipid14 v2.0 (GAFFc2-c3-hc)
cC   cA   hA     1    109.68    394.97     ;  Lipid11 v1.0 (GAFFc -c3-hc)
cC   cA   hX     1    109.54    395.22     ;  Lipid11 v1.0 (GAFFc -c3-hx)
cC   cA   nA     1    114.21    544.51     ;  Lipid11 v1.0 (GAFFc -c3-n4)
cC   cD   hL     1    109.68    394.97     ;  Lipid14 v2.0 (GAFFc -c3-hc)
cD   cB   cB     1    123.42    538.31     ;  Lipid14 v2.0 (GAFFc3-c2-c2)
cD   cB   hB     1    117.30    382.08     ;  Lipid14 v2.0 (GAFFc3-c2-ha)
cD   cC   oC     1    123.11    569.28     ;  Lipid14 v2.0 (GAFFc3-c -o )
cD   cC   oS     1    111.96    579.57     ;  Lipid14 v2.0 (GAFFc3-c -os)
cD   cD   cB     1    111.44    531.62     ;  Lipid14 v2.0 (GAFFc3-c3-c2)
cD   cD   cC     1    110.53    533.79     ;  Lipid14 v2.0 (GAFFc3-c3-c )
cD   cD   cD     1    110.63    528.94     ;  Lipid14 v2.0 (GAFFc3-c3-c3)
cD   cD   hL     1    110.05    388.02     ;  Lipid14 v2.0 (GAFFc3-c3-hc)
cP   cR   cR     1    113.50    376.56     ;  Lipid11 v1.0 (GLYCAM06g CP-CG-CG)
cP   cR   hS     1    111.00    376.56     ;  Lipid11 v1.0 (GLYCAM06g CP-CG-H1)
cP   cR   oR     1    108.50    585.76     ;  Lipid11 v1.0 (GLYCAM06g CP-CG-OH == CP-CG-OS)
cP   oS   pA     1    119.00    418.4      ;  Lipid11 v1.0 (GLYCAM06g CP-OS-P )
cP   oT   pA     1    119.00    418.4      ;  Lipid11 v1.0 (GLYCAM06g CP-OS-P )
cR   cP   cR     1    113.50    376.56     ;  Lipid11 v1.0 (GLYCAM06g CG-CP-CG)
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cR   cP   hS     1    111.00    376.56     ;  Lipid11 v1.0 (GLYCAM06g CG-CP-H1)
cR   cP   oS     1    108.50    585.76     ;  Lipid11 v1.0 (GLYCAM06g CG-CP-OS)
cR   cP   oT     1    108.50    585.76     ;  Lipid11 v1.0 (GLYCAM06g CG-CP-OS)
cR   cR   cR     1    113.50    376.56     ;  Lipid11 v1.0 (GLYCAM06g CG-CG-CG)
cR   cR   hS     1    111.00    376.56     ;  Lipid11 v1.0 (GLYCAM06g CG-CG-H1)
cR   cR   oR     1    107.50    585.76     ;  Lipid11 v1.0 (GLYCAM06g CG-CG-OH)
cR   oR   hR     1    109.50    460.24     ;  Lipid11 v1.0 (GLYCAM06g CG-OH-HO)
hA   cA   hA     1    108.35    329.95     ;  Lipid11 v1.0 (GAFFhc-c3-hc)
hE   cA   hE     1    109.55    327.86     ;  Lipid11 v1.0 (GAFFh1-c3-h1)
hE   cA   oH     1    109.88    426.51     ;  Lipid11 v1.0 (GAFFha-c3-oh)
hE   cA   oS     1    108.82    425.43     ;  Lipid11 v1.0 (GAFFh1-c3-os)
hE   cA   oT     1    108.82    425.43     ;  Lipid11 v1.0 (GAFFh1-c3-os)
hL   cD   hL     1    108.35    329.95     ;  Lipid14 v2.0 (GAFFhc-c3-hc)
hN   nA   hN     1    108.11    339.07     ;  Lipid11 v1.0 (GAFFhn-n4-hn)
hO   oH   pA     1    110.14    369.45     ;  Lipid11 v1.0 (GAFFho-oh-p5)
hS   cP   oS     1    110.00    502.08     ;  Lipid11 v1.0 (GLYCAM06g H1-CP-OS)
hS   cP   oT     1    110.00    502.08     ;  Lipid11 v1.0 (GLYCAM06g H1-CP-OS)
hS   cR   oR     1    110.00    502.08     ;  Lipid11 v1.0 (GLYCAM06g H1-CG-OH)
hX   cA   hX     1    110.74    326.69     ;  Lipid11 v1.0 (GAFFhx-c3-hx)
hX   cA   nA     1    107.91    410.2      ;  Lipid11 v1.0 (GAFFhx-c3-n4)
oC   cC   oC     1    130.38    654.13     ;  Lipid11 v1.0 (GAFFo -c -o )
oO   cC   oO     1    130.38    654.13     ;  Lipid11 v1.0 (GAFFo -c -o )
oC   cC   oS     1    123.33    635.38     ;  Lipid11 v1.0 (GAFFo -c -os)
oC   pA   oC     1    115.80    615.3      ;  Lipid11 v1.0 (GAFFo -p5-o )
oC   pA   oH     1    115.26    585.59     ;  Lipid11 v1.0 (GAFFo -p5-oh)
oC   pA   oS     1    116.09    588.61     ;  Lipid11 v1.0 (GAFFo -p5-os)
oH   pA   oS     1    102.37    600.57     ;  Lipid11 v1.0 (GAFFoh-p5-os)
oH   pA   oT     1    102.37    600.57     ;  Lipid11 v1.0 (GAFFoh-p5-os)
oP   pA   oP     1    115.80    615.3      ;  Lipid11 v1.0 (GAFFo -p5-o )
oP   pA   oH     1    115.26    585.59     ;  Lipid11 v1.0 (GAFFo -p5-oh)
oP   pA   oT     1    116.09    588.61     ;  Lipid11 v1.0 (GAFFo -p5-os)
oS   pA   oS     1    101.77    606.76     ;  Lipid11 v1.0 (GAFFos-p5-os)
oT   pA   oT     1    101.77    606.76     ;  Lipid11 v1.0 (GAFFos-p5-os)

[ dihedraltypes ]

cA   cA   cA   cA      9     0.0    0.7531      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-c3-c3)
cA   cA   cA   cA      9   180.0    1.046       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-c3-c3)
cA   cA   cA   cA      9   180.0    0.8368      1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-c3-c3)
cA   cA   cA   cC      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cA   cA   cA   hA      9     0.0    0.6694      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-c3-hc)
cA   cA   cA   hE      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cA   cA   cA   oH      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cA   cA   cA   oS      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cA   cA   cA   oT      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cA   cA   cB   cA      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cA   cA   cB   cB      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cA   cA   cB   hB      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cA   cA   cC   oC      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -c3-X )
cA   cA   cC   oO      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -c3-X )
cA   cA   cC   oS      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -c3-X )
cA   cA   nA   cA      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-n4-X )
cA   cA   nA   hN      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-n4-X )
cA   cA   oH   hO      9     0.0    0.6694      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-oh-ho)
cA   cA   oH   hO      9     0.0    1.046       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-oh-ho)
cA   cA   oS   pA      9     0.0    1.604       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-os-X )
cA   cA   oT   pA      9     0.0    1.604       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-os-X )
cA   cB   cA   hA      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cA   cB   cB   hB      9   180.0   27.82        2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c2-c2-X )
cA   cB   cB   cA      9   180.0   27.82        2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c2-c2-c3)
cA   cB   cB   cA      9   180.0    7.950       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c2-c2-c3)
cA   cC   oS   cA      9   180.0   11.30        2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -os-X )
cA   nA   cA   hX      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-n4-X )
cA   oS   cC   oS      9   180.0   11.30        2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -os-X )
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cA   oS   pA   oC      9     0.0    3.347      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -os-p5-X )
cA   oS   pA   oH      9     0.0    1.046      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF oh-p5-os-c3)
cA   oS   pA   oH      9     0.0    5.021      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF oh-p5-os-c3)
cA   oS   pA   oS      9     0.0    1.046      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-os-p5-os)
cA   oS   pA   oS      9     0.0    5.021      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-os-p5-os)
cA   oT   pA   oP      9     0.0    3.347      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -os-p5-X )
cA   oT   pA   oP      9     0.0    3.347      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -os-p5-X )
cA   oT   pA   oH      9     0.0    1.046      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF oh-p5-os-c3)
cA   oT   pA   oH      9     0.0    5.021      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF oh-p5-os-c3)
cA   oT   pA   oT      9     0.0    1.046      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-os-p5-os)
cA   oT   pA   oT      9     0.0    5.021      2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-os-p5-os)
cB   cA   cA   cA      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cB   cA   cA   hA      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cB   cA   cA   hE      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cB   cA   cA   oH      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cB   cA   cB   cB      9     0.0    0          2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cB   cA   cB   hB      9     0.0    0          2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cB   cB   cD   cD      9     0.0    1.449      1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cB   cD   cD      9     0.0    2.333      2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cB   cD   cD      9     0.0    1.222      3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cB   cD   cD      9     0.0    0.3946     4   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cB   cD   cD      9     0.0    0.09456    5   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cD   cB   cB      9     0.0    0          2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
cB   cD   cB   hB      9     0.0    0          2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c3-c2-X )
cB   cD   cD   cC      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cB   cD   cD   cD      9   180.0    0.1050     1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cD   cD   cD      9   180.0    0.02259    2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cD   cD   cD      9     0.0    0.8397     3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cD   cD   cD      9     0.0    0.8799     4   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cD   cD   cD      9     0.0    0.3393     5   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cB   cD   cD   hL      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c3-c3-X )
cC   cA   cA   cB      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cC   cA   cA   hA      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cC   cA   cA   hE      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cC   cA   cA   oS      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cC   cA   cA   oT      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
cC   cA   nA   hN      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-n4-X )
cC   cD   cD   hL      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c3-c3-X )
cC   oS   cA   cA      9     0.0    1.602      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-os-c )
cC   oS   cA   cA      9   180.0    3.347      1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-c3-os-c )
cC   oS   cA   hE      9     0.0    1.604      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-os-X )
cD   cB   cB   cD      9   180.0    1.286      1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cB   cB   cD      9   180.0   16.76       2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cB   cB   cD      9     0.0    0.8326     3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cB   cB   cD      9     0.0    1.356      4   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cB   cB   cD      9     0.0    0.1736     5   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cB   cB   hB      9   180.0   27.82       2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c2-c2-X )
cD   cC   oS   cA      9   180.0   11.30       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -os-X )
cD   cC   oS   cD      9   180.0   11.30       2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c -os-X )
cD   cD   cC   oC      9   180.0    3.812      1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oC      9   180.0    3.089      2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oC      9     0.0    1.377      3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oC      9     0.0    2.453      4   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oC      9     0.0    0.5577     5   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oS      9   180.0    0.5130     1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oS      9   180.0    0.8594     2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oS      9     0.0    0.7540     3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oS      9     0.0    2.137      4   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cC   oS      9     0.0    0.5669     5   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cD   cC      9     0.0    0.6510     3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF )
cD   cD   cD   cD      9   180.0    1.302      1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cD   cD      9   180.0    0.5159     2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cD   cD      9     0.0    0.4807     3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cD   cD      9     0.0    0.9201     4   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
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cD   cD   cD   cD      9     0.0    0.9079      5   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.10 (paramfit)
cD   cD   cD   hL      9     0.0    0.6694      3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF c3-c3-c3-hc)
cP   cR   cR   cR      9     0.0    1.883       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-CG-CG-CG)
cP   cR   cR   hS      9     0.0    0.6276      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-CG-CG-H1)
cP   cR   cR   oR      9     0.0    0.4184      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-CG-CG-OH)
cP   cR   oR   hR      9     0.0    0.7531      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g Copied from CG-CG-OH-HO)
cP   oS   pA   oC      9     0.0    0.4184      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -O2)
cP   oS   pA   oC      9     0.0    2.092       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -O2)
cP   oS   pA   oC      9     0.0    0.4184      1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -O2)
cP   oS   pA   oS      9     0.0    2.092       3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -OS)
cP   oS   pA   oS      9     0.0    2.929       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -OS)
cP   oT   pA   oP      9     0.0    0.4184      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -O2)
cP   oT   pA   oP      9     0.0    2.092       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -O2)
cP   oT   pA   oP      9     0.0    0.4184      1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -O2)
cP   oT   pA   oT      9     0.0    2.092       3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -OS)
cP   oT   pA   oT      9     0.0    2.929       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CP-OS-P -OS)
cR   cP   cR   oR      9     0.0    1.130       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g Copied from CG-CP-CG-OS)
cR   cP   oS   pA      9     0.0    0.4184      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CP-OS-P )
cR   cP   oS   pA      9     0.0    0.2092      2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CP-OS-P )
cR   cP   oS   pA      9     0.0    5.021       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CP-OS-P )
cR   cP   oT   pA      9     0.0    0.4184      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CP-OS-P )
cR   cP   oT   pA      9     0.0    0.2092      2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CP-OS-P )
cR   cP   oT   pA      9     0.0    5.021       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CP-OS-P )
cR   cR   cR   cR      9     0.0    1.883       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-CG-CG)
cR   cR   cR   oR      9     0.0    0.4184      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-CG-OR)
cR   cR   cP   cR      9     0.0    1.883       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-CP-CG)
cR   cR   cP   hS      9     0.0    0.6276      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-CP-H1)
cR   cR   cP   oS      9     0.0    1.130       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-CP-OS)
cR   cR   cP   oT      9     0.0    1.130       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-CP-OS)
cR   cR   oR   hR      9     0.0    0.7531      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g CG-CG-OH-HO)
hA   cA   cA   hA      9     0.0    0.6276      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c3-hc)
hA   cA   cA   hE      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
hA   cA   cA   oH      9     0.0    0           3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c3-oh)
hA   cA   cA   oH      9     0.0    1.046       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c3-oh)
hA   cA   cB   cB      9   180.0    1.590       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c2-c2)
hA   cA   cB   cB      9     0.0    4.812       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c2-c2)
hA   cA   cB   hB      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c2-X )
hA   cA   cC   oC      9     0.0    3.347       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c -o )
hA   cA   cC   oC      9   180.0    0.3347      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF hc-c3-c -o )
hA   cA   cC   oS      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c -c3-X )
hB   cB   cB   hB      9   180.0   27.82        2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c2-c2-X )
hE   cA   cA   hE      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
hE   cA   cA   nA      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
hE   cA   cA   hX      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
hE   cA   cA   oH      9     0.0    0           3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF h1-c3-c3-oh)
hE   cA   cA   oH      9     0.0    1.046       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF h1-c3-c3-oh)
hE   cA   cA   oS      9     0.0    0           3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF h1-c3-c3-os)
hE   cA   cA   oS      9     0.0    1.046       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF h1-c3-c3-os)
hE   cA   cA   oT      9     0.0    0           3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF h1-c3-c3-os)
hE   cA   cA   oT      9     0.0    1.046       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF h1-c3-c3-os)
hE   cA   oH   hO      9     0.0    2.092       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-oh-X )
hE   cA   oS   pA      9     0.0    1.604       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-os-X )
hE   cA   oT   pA      9     0.0    1.604       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-os-X )
hB   cB   cD   cD      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c3-c2-X )
hB   cB   cD   hL      9     0.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c3-c2-X )
hL   cD   cB   cB      9   180.0    1.590       3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF hc-c3-c2-c2)
hL   cD   cB   cB      9     0.0    4.812       1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF hc-c3-c2-c2)
hL   cD   cC   oC      9     0.0    3.347       1   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF hc-c3-c -o )
hL   cD   cC   oC      9   180.0    0.3347      3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF hc-c3-c -o )
hL   cD   cC   oS      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF X -c -c3-X )
hL   cD   cD   hL      9     0.0    0.6276      3   ;  SCEE=1.2 SCNB=2.0 Lipid14 v2.0 (GAFF hc-c3-c3-hc)
hN   nA   cA   hX      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-n4-X )
hO   oH   pA   oC      9     0.0    2.231       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -p5-oh-X )
hO   oH   pA   oP      9     0.0    2.231       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -p5-oh-X )
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hO   oH   pA   oS      9     0.0    2.231       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -p5-oh-X )
hO   oH   pA   oT      9     0.0    2.231       3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -p5-oh-X )
hR   oR   cR   hS      9     0.0    0.7531      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g HO-OH-CG-H1)
hS   cP   cR   hS      9     0.0    0.7113      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CP-CG-H1)
hS   cR   cR   cR      9     0.0    0.6276      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CG-CG-CG)
hS   cR   cR   hS      9     0.0    0.7113      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CG-CG-H1)
hS   cR   cR   oR      9     0.0    0.2092      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g OH-CG-CG-H1)
hS   cR   cP   cR      9     0.0    0.6276      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CG-CP-CG)
hS   cR   cP   oS      9     0.0    0.2092      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CG-CP-OS)
hS   cR   cP   oT      9     0.0    0.2092      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CG-CP-OS)
hS   cR   cP   oT      9     0.0    0.2092      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CG-CP-OS)
hS   cP   oS   pA      9     0.0    0.2929      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CP-OS-P )
hS   cP   oT   pA      9     0.0    0.2929      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g H1-CP-OS-P )
hX   cA   cA   oS      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
hX   cA   cA   oT      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
hX   cA   cC   oC      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c -X )
hX   cA   cC   oO      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c -X )
nA   cA   cA   oS      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
nA   cA   cA   oT      9     0.0    0.6510      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c3-X )
nA   cA   cC   oC      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c -X )
nA   cA   cC   oO      9   180.0    0           2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF X -c3-c -X )
cA   oS   cC   oC      9   180.0   11.30        2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-os-c -o )
cA   oS   cC   oC      9   180.0    5.858       1   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF c3-os-c -o )
oH   cA   cA   oH      9     0.0    0.6025      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF oh-c3-c3-oh)
oH   cA   cA   oH      9     0.0    4.916       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF oh-c3-c3-oh)
oH   cA   cA   oS      9     0.0    0.6025      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-oh)
oH   cA   cA   oS      9     0.0    4.916       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-oh)
oH   cA   cA   oT      9     0.0    0.6025      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-oh)
oH   cA   cA   oT      9     0.0    4.916       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-oh)
oR   cR   cR   oR      9     0.0    0.4184      1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g OH-CG-CG-OH)
oR   cR   cR   oR      9     0.0    3.975       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g OH-CG-CG-OH)
oR   cR   cR   oR      9     0.0    2.301       3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g OH-CG-CG-OH)
oR   cR   cP   hS      9     0.0    0.2092      3   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g Copied from OH-CG-CG-H1)
oR   cR   cP   oS      9     0.0    4.602       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g copied from OH-CG-CG-OS)
oR   cR   cP   oS      9     0.0    1.046       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g copied from OH-CG-CG-OS)
oR   cR   cP   oT      9     0.0    4.602       1   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g copied from OH-CG-CG-OS)
oR   cR   cP   oT      9     0.0    1.046       2   ;  SCEE=1.0 SCNB=1.0 Lipid11 v1.0 (GLYCAM06g copied from OH-CG-CG-OS)
oS   cA   cA   oS      9     0.0    0.6025      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-os)
oS   cA   cA   oS      9     0.0    4.916       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-os)
oT   cA   cA   oS      9     0.0    0.6025      3   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-os)
oT   cA   cA   oS      9     0.0    4.916       2   ;  SCEE=1.2 SCNB=2.0 Lipid11 v1.0 (GAFF os-c3-c3-os)

; impropers
cD   oC   cC   oS      4   180.0   43.93        2   ;  Lipid14 v2.0 ester improper (GAFF X -X -c -o )
cB   cD   cB   hB      4   180.0    4.602       2   ;  Lipid14 v2.0 aliphatic improper (GAFF c2-c3-c2-ha - default)
cA   oC   cC   oC      4   180.0    4.602       2   ;  Lipid11 v1.0 carboxyl improper (GAFF c3-o -c -0 - default)
cB   cA   cB   cA      4   180.0    4.602       2   ;  Lipid11 v1.0 cholesterol aliphatic in ring (GAFF c2-c3-c2-c3- default)
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