Supporting Material

Atomistic Simulations of Phosphatidylcholines and Cholesteryl Esters in High Density Lipoprotein-Sized Lipid Droplet and Trilayer: Clues to Cholesteryl Ester Transport and Storage

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SUPPLEMENTARY MATERIAL

Force field

Force field parameters are described in detail in earlier simulation studies of bulk CO system and POPC bilayer (1, 2). It should be noted that the previous simulation of bulk COs was carried out using the ffgmx force field (GROMOS87). In order to simulate POPCs (described by Berger's lipid parameters) with COs, we changed the van der Waals interaction parameters of COs to the corresponding Berger's lipid parameters, since it is well known that the van der Waals interactions between the ffgmx and Berger lipid parameters are greatly overestimated (two different force fields are basically mixed) (3). The van der Waals parameters for the oleate chain of CO were taken from the oleate chain of POPC as described in the Berger's lipid parameters. Cholesterol body's van der Waals parameters where chosen so that similar carbon atoms, e. g. carbon atoms forming double bonds, are described by similar atom types in the oleate chain and cholesterol body as it was done in the previous simulation of bulk CO system. Atom types based on Berger lipid parameters (4) are found in the topology file of CO that is showed later in the SM. For water, we employed the SPC water model (5, 6).

Simulation details

The MD simulations were performed using GROMACS 4.0 Beta (7). In the trilayer system, initially the Berendsen thermostat and barostat (8) with 0.1 ps and 1.0 ps coupling constants, in respective order, were used in the simulation of the trilayer system. After the simulation time of 40 ns, the schemes were switched to the Nóse-Hoover thermostat (9, 10) and the Parrinello-Rahman barostat (11) to produce the more realistic NpT ensemble (see below).

In the droplet simulation, only the Nóse-Hoover and Parrinello-Rahman coupling schemes were used. The coupling constants used for the thermostat and the barostat were 0.1 ps and 1.0 ps, respectively, and these values for these two schemes were also used in the trilayer simulations. Temperature was set to 330 K in order to produce liquid state for COs, like in the previous simulation of isotropic CO carried out by Heikelä et al (1).

In both trilayer and droplet simulations semi-isotropic and isotropic pressure couplings were used, respectively, with reference pressure of 1.0 bar. The van der Waals interactions were chosen to have a cutoff at 1.0 nm. Electrostatic interactions were evaluated by using the reaction field technique (12) with a cut-off of 2.0 nm and a dielectric constant of 80. This combination has been shown to produce reliable results in lipid bilayer simulations (13). The bonds of lipid molecules were constrained by using LINCS (14) and water molecules by using SETTLE (15). Time step was set to 2 fs.

Additional data analysis information

To characterize intermolecular orientation order between CO molecules, we defined the director of CO as a vector from C_b to C_a. Then we defined the ring-ring correlation function as

$$S_{RR} = \frac{1}{2}\left\langle 3\cos^2\varphi - 1 \right\rangle, \tag{1}$$

where φ is the angle between the directors of two different CO molecules (see Fig. 1 in the article). The order parameter S_{RR} was computed as a function of the distance between the centers of the directors. In order to calculate the intramolecular angle distribution of CO, we defined an angle between the director and the oleate chain of CO (angle between vectors formed by atoms C_b-C_c and

C_b-C_a). The angle thus describes the average orientation of the oleate chain with respect to the ring structure, and its distribution P(angle) allowed us to gain insight into the structure and orientation properties of individual CO molecules. Using the same approach, we considered the average orientation of the short hydrocarbon chain by a vector from C_a to C_d at the other end of the cholesterol ring structure. Then, the average orientation of the fatty acyl chain segments with respect to the steroid structure of the same cholesteryl ester molecule was described by an order parameter

$$S_{CD,k} = \frac{1}{2}\left\langle 3\cos^2\beta_k - 1 \right\rangle, \tag{2}$$

where β_k is the angle between the director and a C–H bond at the kth carbon atom in the oleate chain. In the case of POPC molecules, we calculated S_{CD} order parameters (deuterium order parameters) of the acyl chains with respect to the normal of the trilayer or the local normal of the spherical droplet. For this purpose, as the apolar hydrogens are not explicitly present in united-atom simulations, we reconstructed the corresponding C–H vectors using backbone chain configuration.

In addition to these previously done analyses we monitored the angle formed by the director of CO (vector C_B-C_A, see Fig. 1 in the article) and the normal of the system as a function of distance from the center of mass (COM) of the droplet or from the x-y plane of the geometrical center (GC) of the trilayer.

In order to study the ordering of the director angle of CO respect to the normal of the system we also defined the order parameter

$$S_{RN} = \frac{1}{2}\left\langle 3\cos^2\alpha - 1 \right\rangle, \tag{3}$$

where α is the angle between the director and the normal of the system. S_{RN} order parameter was calculated as a function of distance from the COM or the x-y plane of GC to study the distance dependence of the ordering of CO director.

Simulation snapshots for the additional lipid droplet simulation.

Here, we initially placed six COs outside of the particle as seen in one of the three simulation snapshots (0 ns) in Figure S1 below. In five nanoseconds all six COs readily diffused and localized into the core of lipid droplet indicating that the mixing of the lipids is well conserved in our simulations.
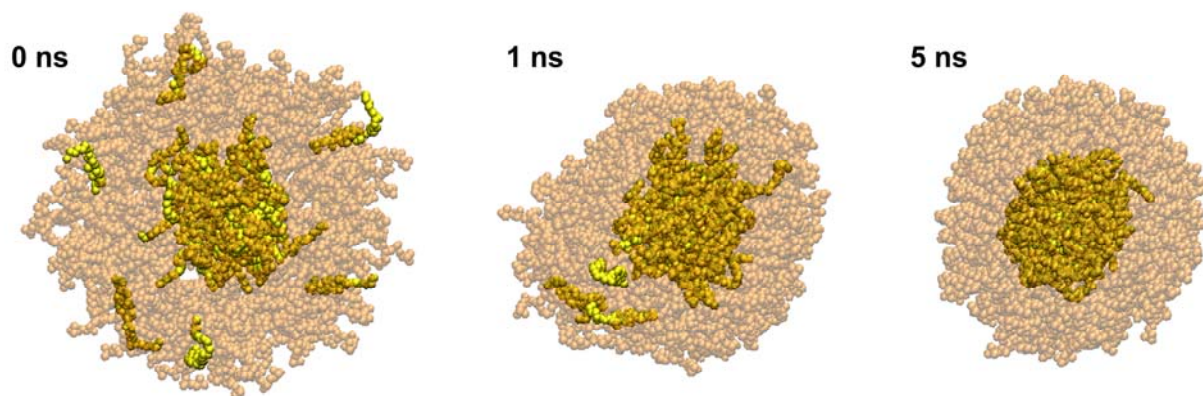
Figure S1. Molecules are visualized using van der Waals radii. The POPC molecules are shown in orange with transparency whereas CO molecules appear in yellow. For clarity water molecules are not shown.

Additional intermolecular properties

The intermolecular orientational order parameter S_{RR} between the directors of COs (defined as the C_B - C_A vector) was determined imilarly to the isotropic CO system (1) and is shown in Figure S2 as a function of distance between the center of masses of the CO directors. Apparently the profiles suggest that within the distance range of 0.4-1.5 nm the most prevailing intermolecular orientation is parallel or antiparallel, approaching a random orientation at longer intermolecular distances. Intermolecular correlation is very similar in the droplet and the trilayer systems and also in the isotropic bulk CO system studied earlier (1). This type of intermolecular arrangement is also supported by atomic distributions shown in Figure 3 (in the article), as the density peaks of carbonyl oxygens and the C_A atom are consistent with the short-range stacking of the sterol bodies revealed by the S_{RR} profiles.

The intermolecular orientation of COs at the liquid state at very short distances interestingly resembles the suggested structure of COs in the crystal-phase (16). In addition, the observed parallel and antiparallel orientations starting from the intermolecular distance of 0.4 nm accords with the earlier conclusions based on the X-ray studies of various CEs (17). Furthermore, the acyl chain-ring stacking was also observed, which could induce ordering to the acyl chain of COs. In Figure S4 snapshots are shown from the trilayer simulation representing the examples of the above mentioned intermolecular arrangements.
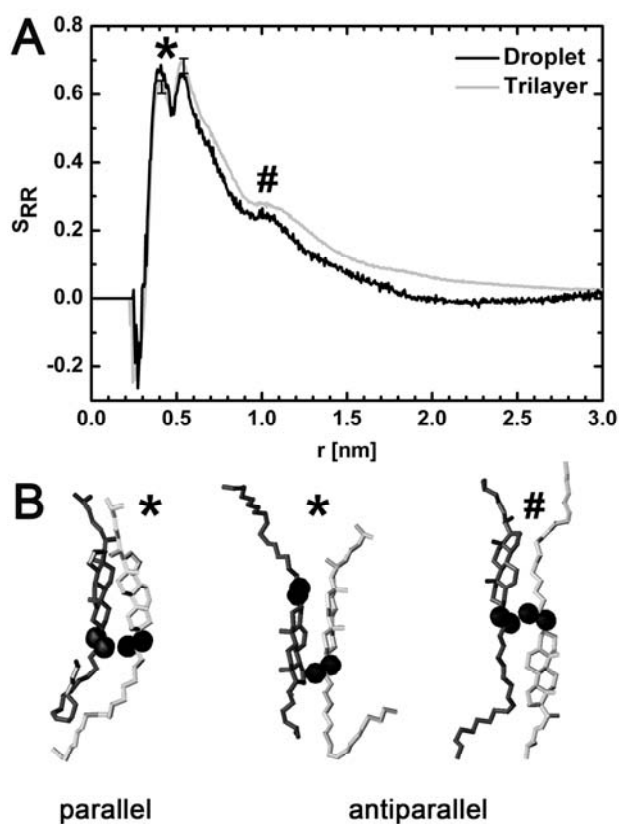
Figure S2. A) Orientational ordering of sterol rings (indicated by the director vector shown in Figure 1) as a function of distance between the centers of directors. **B)** Snapshot conformations from the

simulations presenting situations causing the two positive peaks in A). The first and the second peaks in A) arise from the antiparallel (oleate chains point to different directions) and parallel conformations of COs with the centers of cholesterol directors close by (marked with *). The weak third peak arises either from antiparallel conformations of COs with higher distance between the directors than in the first and second peak (marked with #) or possibly from slight second nearest-neighbor ordering. The oxygen atoms of COs are marked with black van der Waals spheres to clarify the orientations of COs.

Additional intramolecular properties

Phospholipid head group orientation

Figure S3 shows the probability distribution of the angle between the phosphorus-nitrogen (P-N) vector of the head group and the local normal of the system. The distributions show how the prevailing orientation of the head group is slightly more towards the water phase in the small lipid droplet. Comparison to our POPC bilayer simulation at the temperature of 330 K revealed that the P-N distribution profile in the trilayer simulation is identical to the bilayer simulation (data not shown). Possible biological implications of the difference in the orientation distribution between the planar and highly spherical surface could be related to the resulting difference in the electrostatic surface of the systems, which rises due to the difference in the prevailing orientation of the P-N dipole.
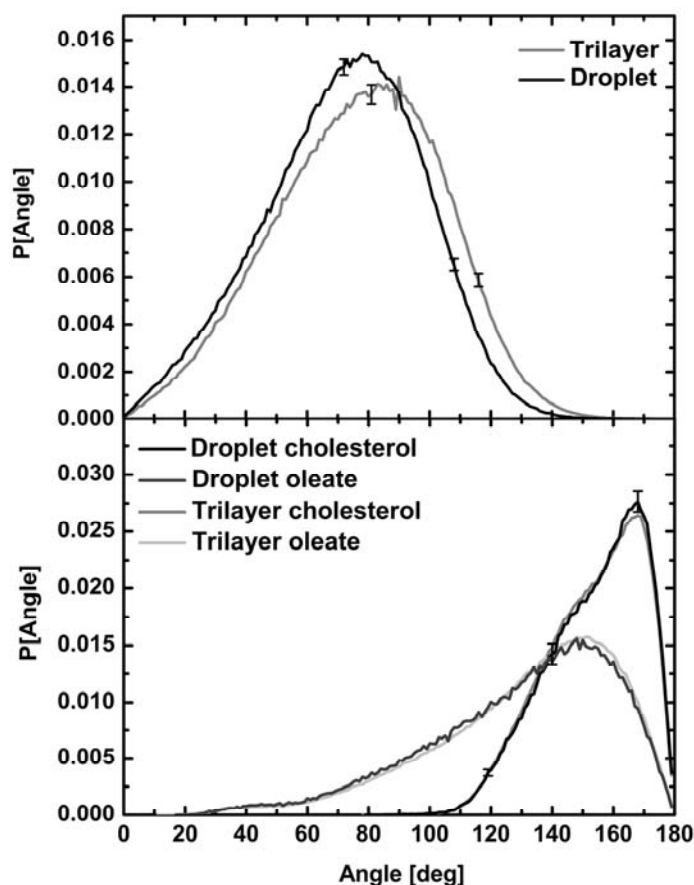
Figure S3. Distribution of the angle between the head group P-N vector and the local normal in the droplet and trilayer (upper panel). Intramolecular angle distribution of the oleate chain with respect to the CO director and the distribution of the short cholesterol chain with respect to the negative CO director (lower panel).

Intramolecular angle distribution of CO

Figure S3 shows also the probability distribution of the intramolecular angles between the oleate chain or the short acyl chain and the cholesterol director of CO. The distribution of the angle between the short chain and the ring structure of CO shows similar features like in the isotropic system, i.e. the chain is mostly aligned along the ring with a maximum bending angle of ~90°. The distribution of the angle between the oleate chain and the director ranges from ~25° to ~180° with a peak at ~150°. The angle distributions show that the most prevailing conformation of CO molecules is extended. However, also minor amounts of strongly bent "horseshoe" or U-shaped conformations with angles of ~ 25° - 50° are observed in both systems.

These findings are in accordance with X-ray diffraction data and neutron scattering experiments concerning the mesophases of CEs, which indicate that bulk CEs adopt nearly extended conformations in the isotropic phase (17, 18).

Topology for cholesteryl oleate

```
; Cholesteryl Oleate
;
; Based on Cholesterol of Hoeltje and Brandt and POPC from Tielemann and
ffgmx.rtp.
;
; Mikko Heikelä, 2002
; Fixed: Mikko Heikelä, January 2005
; Further improved: Mikko Heikelä, February 2005
;          incorporated sensible next-to-double-bond dihedrals from
;          ab initio work of Bahar et.al. (changes indicated by popc-fix).
;          J. Phys. Chem. B. 2004, 108, 7170-7179
;
; Bulk simulation of cholesteryl oleate by Heikela et al.
; Biophysical Journal, 2006, 90, 2247-2257
;
; Artturi Koivuniemi, 2008
; Van der Waals parameters modified to produce consistent interactions with
; Berger lipid parameters.
;
;
; Uses standard Gromacs united-atom force-field (ffgmx.* files)
;
;                                    21          26
;                                    |           |
;                          13 15          20  23      25
;                         /      \|  __  / \ / \ / \
;                          12      14  19 22  24      27
;                          |           |   |
;               3  1  11          16  18
;              /      \|/  \       / \  /
;             4        2    10   17
;             |        |    |
;             5        7    9
;            / \      / \\ /
;     ...-28  6      8
;
;                                        CH3     CH3
;                                        |           |
```

```
;                              CH2 CH3  CH1 CH2 CH1
;                             /     \|  __ / \ / \ / \
;                            CH2      C  CH CH2 CH2 CH3
;                             |           |   |
;                  CH2CH3CH        CH CH2
;                 /     \|/ \     / \  /
;             CH2      C   CH   CH2
;              |           |     |
;             CH        C   CH2
;            /  \      / \\ /
;          -O   CH2   CH
;
[ moleculetype ]
;name      nrexcl
CHOL            3

[ atoms ]
;  nr     type   resnr   residu    atom    cgnr     charge    ; total charge
; The following comes from Hoeltje & Brandts cholesterol
      1    LP3       1    CHOL      C1       1         0
      2     LC       1    CHOL      C2       2         0
      3    LP2       1    CHOL      C3       3         0
      4    LP2       1    CHOL      C4       4         0
; Charges at the ester bond adapted from DPPC in ffgmx.rtp.
      5    LH1       1    CHOL      C5       5        0.10
; Next two atoms get replaced by ester bridge to the oleic acid
;     6     OA       1    CHOL      O6       5       -0.54
;     7     HO       1    CHOL      H        5        0.40
      6    LP2       1    CHOL      C8       6         0
      7     LC       1    CHOL      C9       7         0
      8    LH1       1    CHOL      C10      8         0
      9    LP2       1    CHOL      C11      9         0
     10    LH1       1    CHOL      C12     10         0
     11    LH1       1    CHOL      C13     11         0
     12    LP2       1    CHOL      C14     12         0
     13    LP2       1    CHOL      C15     13         0
     14     LC       1    CHOL      C16     14         0
     15    LP3       1    CHOL      C17     15         0
     16    LH1       1    CHOL      C18     16         0
     17    LP2       1    CHOL      C19     17         0
     18    LP2       1    CHOL      C20     18         0
     19    LH1       1    CHOL      C21     19         0
     20    LH1       1    CHOL      C22     20         0
     21    LP3       1    CHOL      C23     21         0
     22    LP2       1    CHOL      C24     22         0
     23    LP2       1    CHOL      C25     23         0
     24    LP2       1    CHOL      C26     24         0
     25    LH1       1    CHOL      C27     25         0
     26    LP3       1    CHOL      C28     26         0
     27    LP3       1    CHOL      C29     27         0

; Adapted from DPPC in ffgmx.rtp
;
;[ DPPC ]
; [ atoms ]

     28    LOS       1    CHOL      O30      5       -0.18
     29     LC       1    CHOL      C31      5        0.27
     30     LO       1    CHOL      O32      5       -0.19
     31    LP2       1    CHOL      C33     28         0
     32    LP2       1    CHOL      C34     29         0
```

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    33      LP2       1    CHOL    C35     30      0
    34      LP2       1    CHOL    C36     31      0
    35      LP2       1    CHOL    C37     32      0
    36      LP2       1    CHOL    C38     33      0
    37      LP2       1    CHOL    C39     34      0
    38      LH1       1    CHOL    C40     35      0
    39      LH1       1    CHOL    C41     36      0
    40      LP2       1    CHOL    C42     37      0
    41      LP2       1    CHOL    C43     38      0
    42      LP2       1    CHOL    C44     39      0
    43      LP2       1    CHOL    C45     40      0
    44      LP2       1    CHOL    C46     41      0
    45      LP2       1    CHOL    C47     42      0
    46      LP2       1    CHOL    C48     43      0
    47      LP3       1    CHOL    C49     44      0
;
;
; cholesterol.itp:
;
; All values were taken from the most corresponding parameters in ffgmxnb.itp
; and ffgmxbon.itp
;
[ bonds ]
;  ai    aj funct          c0              c1
    1      2    1        0.153         334720.
    2      3    1        0.153         334720.
    3      4    1        0.153          334720
    4      5    1        0.153          334720
; Removed bonds that relate to the atoms that are replaced by the ester bond
    5      6    1        0.153          334720
    6      7    1      0.153            334720
    7      2    1        0.153         334720.
    7      8    1        0.139          418400
    8      9    1        0.153         334720.
    9     10    1        0.153          334720
   10     11    1        0.153          334720
    2     11    1        0.153         334720.
   11     12    1        0.153          334720
   12     13    1        0.153          334720
   13     14    1        0.153         334720.
   14     15    1        0.153         334720.
   16     14    1        0.153         334720.
   16     10    1        0.153          334720
   16     17    1        0.153          334720
   17     18    1        0.153          334720
   18     19    1      0.153          334720
   14     19    1        0.153         334720.
   19     20    1        0.153         334720.
   20     21    1      0.153          334720.
   20     22    1      0.153          334720.
   22     23    1      0.153          334720.
   23     24    1      0.153          334720.
   24     25    1      0.153          334720.
   25     26    1      0.153          334720.
   25     27    1      0.153          334720.
; The rest adapted from Tielemans POPC

    5     28    1      0.1435                251000.
   28     29    1      0.136                 376600.
   29     30         1            0.123             502100.
   29     31         1            0.153             334700.
```

```
    31    32            1        0.153          334700.
    32    33            1          0.153            334700.
    33    34            1        0.153          334700.
    34    35            1        0.153          334700.
    35    36            1        0.153          334700.
    36    37            1        0.153          334700.
    37    38            1        0.153          334700.
    38    39            1          0.139                418400.
    39    40            1          0.153          334700.
    40    41            1          0.153          334700.
    41    42            1        0.153          334700.
    42    43            1          0.153            334700.
    43    44            1          0.153            334700.
    44    45            1        0.153          334700.
    45    46            1        0.153          334700.
    46    47            1        0.153          334700.


[ pairs ]
;  ai    aj funct            c0              c1
    1     4    1
    1     6    1
    1     8    1
    1    10    1
    1    12    1
    2     9    1
    2    13    1
    2    16    1
    3    28    1
    3     8    1
    3    10    1
    3    12    1
    4    29    1
    4    11    1
    5     8    1
    5    30    1  ; fixed to be like in popc
    5    31    1  ; fixed to be like in popc
   28     7    1
   29     6    1
    6     9    1
    6    11    1
    7    10    1
    7    12    1
    8    16    1
    9    12    1
    9    14    1
    9    17    1
   10    13    1
   10    15    1
   10    18    1
   10    19    1
   11    14    1
   11    17    1
   12    15    1
   12    19    1
   13    17    1
   13    18    1
   13    20    1
   14    21    1
   14    22    1
   15    17    1
```

```
   15     18     1
   15     20     1
   16     20     1
   17     20     1
   18     21     1
   18     22     1
   19     23     1
   20     24     1
   21     23     1
   22     25     1
   23     26     1
   23     27     1
;Adapted from popc.itp
   28     32     1
   29     33     1
   30     32     1
   37     40     1     ; (popc-fix)
;  36     39     1     ; pair around double bond (popc-fix)
;  38     41     1     ; pair around double bond (popc-fix)


[ angles ]
;from cholesterol.itp
;  ai     aj     ak funct              c0              c1
    7      2     11     1                  111.          460.240
    7      2      1     1                  109.5         460.240 ;according to
crystal data
    7      2      3     1                  111.          460.240
   11      2      1     1      111.          460.240
   11      2      3     1      111.          460.240
    1      2      3     1      111.          460.240
    2      3      4     1      111.          460.240
    3      4      5     1      111.000       460.240
    4      5      6     1                  109.500       460.240
    4      5     28     1                  106.000       397.480
    6      5     28     1                  106.000       397.480
;  29     28      5     1      Took corresponding from POPC since it had params.
    7      6      5     1      111.000       460.240
    6      7      8     1                  120.000       418.400
    6      7      2     1                  120.          460.240
    8      7      2     1      120.000       418.400
    9      8      7     1                  126.000       418.400
   10      9      8     1      111.          460.240
   11     10     16     1                  111.000       460.240
   11     10      9     1                  111.000       460.240
   16     10      9     1      111.000       460.240
   12     11     10     1      111.000       460.240
   12     11      2     1      111.          460.240
   10     11      2     1                  111.          460.240
   13     12     11     1      111.000       460.240
   14     13     12     1                  111.000       460.240
   19     14     15     1      111.          460.240
   19     14     16     1      111.          460.240
   19     14     13     1      111.          460.240
   15     14     16     1      111.          460.240
   15     14     13     1      111.          460.240
   16     14     13     1      111.          460.240
   17     16     14     1      111.          460.240
   17     16     10     1      111.000       460.240
   14     16     10     1      111.          460.240
   16     17     18     1                  111.000       460.240
   17     18     19     1                  111.000       460.240
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```
    18      19      20     1           111.000        460.240
    18      19      14     1           111.          460.240
    20      19      14     1           111.          460.240
    21      20      22     1                    111.000        460.240
    21      20      19     1           111.000        460.240
    22      20      19     1           111.000        460.240
    23      22      20     1           111.000        460.240
    24      23      22     1           111.000        460.240
    25      24      23     1           111.000        460.240
    26      25      27     1           111.000        460.240
    26      25      24     1           111.000        460.240
    27      25      24     1           111.000        460.240
;from popc.itp
         5      28      29     1 0.12000E+03 0.41840E+03
        28      29      30     1 0.12400E+03 0.50210E+03
        28      29      31     1 0.11500E+03 0.50210E+03
        29      31      32     1 0.11100E+03 0.46020E+03
        30      29      31     1 0.12100E+03 0.50210E+03
        31      32      33     1 0.11100E+03 0.46020E+03
        32      33      34     1 0.11100E+03 0.46020E+03
        33      34      35     1 0.11100E+03 0.46020E+03
        34      35      36     1 0.11100E+03 0.46020E+03
        35      36      37     1 0.11100E+03 0.46020E+03
        36      37      38     1 0.11100E+03 0.46020E+03
        37      38      39     1    120.000     502.080   ; cis thingies
        38      39      40     1    120.000     502.080   ; cis thingies
        39      40      41     1 0.11100E+03 0.46020E+03
        40      41      42     1 0.11100E+03 0.46020E+03
        41      42      43     1 0.11100E+03 0.46020E+03
        42      43      44     1 0.11100E+03 0.46020E+03
        43      44      45     1 0.11100E+03 0.46020E+03
    44      45      46     1 0.11100E+03 0.46020E+03
    45      46      47     1 0.11100E+03 0.46020E+03

[ dihedrals ]
;  ai     aj     ak     al funct
     4      5      28     29     1      0.000        3.766        3
     4      5       6      7     1      0.000        5.858        3
     6      5       4      3     1      0.000        5.858        3
     5      4       3      2     1      0.000        5.858        3
     4      3       2      7     1      0.000        0.418        6
     7      2      11     12     1      0.000        0.418        6
    11      2       7      6     1    180.000       41.840        2
     2      7       8      9     1    180.000       41.840        2
     2      7       6      5     1    0.000        0.418          6
     7      8       9     10     1    180.000       41.840        2
     8      9      10     11     1      0.000        5.858        3
    11     10      16     17     1      0.000        5.858        3
    16     10      11     12     1      0.000        5.858        3
    10     11      12     13     1      0.000        5.858        3
    11     12      13     14     1      0.000        5.858        3
    12     13      14     19     1      0.000        0.418        6
    13     14      16     17     1      0.000        0.418        6
    13     14      19     20     1      0.000        0.418        6
    18     19      20     21     1      0.000        5.858        3
    17     18      19     20     1      0.000        5.858        3
    19     18      17     16     1      0.000        5.858        3
    18     17      16     10     1      0.000        5.858        3
    19     20      22     23     1      0.000        5.858        3
    20     22      23     24     1      0.000        5.858        3
    22     23      24     25     1      0.000        5.858        3
```

```
    23     24     25     26     1    0.000        5.858       3
; From popc.itp
;  ai    aj    ak     al funct    phi0     cp     mult
    28     5      6      7     1    0.000        5.858       3    ;These hold the
oxygen
    28     5      4      3     1    0.000        5.858       3    ;where it should be
;fix (added 2005)
     5     28     29     31     1    180.0   16.74   2  180.0  16.74   2
    28     29     31     32     1    0.0     0.42    6
    29     31     32     33     1    0.0     5.86    3
    31     32     33     34     3
    32     33     34     35     3
    33     34     35     36     3
    34     35     36     37     3
; popc-fix: neighborhood-of the double bond changed
;   35     36     37     38     3 ;(old)
; CH1-CH2-CH2-CH2   7  8  9  10  => C37-C38-C39-C40
;   Note that atom names and numbers differ by 2 because esterification
;   removes two atoms from cholesterol but atom names in cholesterol
;   have not been changed.
;
    38     37     36     35     1    0.000        3.34957  1 0.000       3.34957  1
    38     37     36     35     1    180.000  -1.66004  2 180.000  -1.66004  2
    38     37     36     35     1    0.000        7.33265  3

; 36     37     38     39     1 0.000        5.858       3 ;(old)
; CH1-CH1-CH2-CH2   1 2 3 4 =>  C38-C39-C40=C41
;
    39     38     37     36     1    0.000        7.47     1 0.000       7.47     1
    39     38     37     36     1    0.000        3.9      2 0.000       3.9      2
    39     38     37     36     1    180.000  1.1      3
    39     38     37     36     1    0.000       -2.8425   0 0.000      -2.8425   0

; Commented out already in popc.itp, why?
; Improper used instead, thats why.
;   37     38     39     40     1

;   38     39     40     41     1 0.000        5.858       3 ;(old)
; CH1-CH1-CH2-CH2   1 2 3 4 =>  C40=C41-C42-C43
;
    41     40     39     38     1    0.000        7.47     1 0.000       7.47     1
    41     40     39     38     1    0.000        3.9      2 0.000       3.9      2
    41     40     39     38     1    180.000  1.1      3
    41     40     39     38     1    0.000       -2.8425   0 0.000      -2.8425   0

;   39     40     41     42     3 ;(old)
;                   C41-C42-C43-C44
;
    39     40     41     42     1    0.000        3.34957  1 0.000       3.34957  1
    39     40     41     42     1    180.000  -1.66004  2 180.000  -1.66004  2
    39     40     41     42     1    0.000        7.33265  3
; popc-fix: changes to double-bond neighborhood end here
    40     41     42     43     3
    41     42     43     44     3
    42     43     44     45     3
    43     44     45     46     3
    44     45     46     47     3


[ dihedrals ]
;from cholesterol
;  ai    aj    ak     al funct
```

```
         2       11        3        1        2        0.000       167.360
         5        6        4       28        2       35.264       334.720
        10       11       16        9        2       35.264       334.720
        11       12        2       10        2       35.264       334.720
        14       13       19       16        2       35.264       334.720
        16       10       17       14        2       35.264       334.720
        19       20       14       18        2       35.264       334.720
        20       22       19       21        2       35.264       334.720
         2        7        8        9        2        0.000       167.360
         7        2        6        8        2        0.000       167.360
         7        8        2        6        2        0.000       167.360

;from popc

;         5       28        4        6        2 35.264       0.33470E+03
         29       28       31       30        2 0.00000E+00 0.16740E+03
         37       38       39       40        2 0.000       167.360
```

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