Supporting information for:

Limited Perturbation of a DPPC Bilayer by Fluorescent Lipid Probes: A Molecular Dynamics Study

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S1 DiI Topology Files

The topology files for DiI-C18:0, DiI-C18:2 and DiI-C12:0 are listed below:

S1.1 DiI-C18:0

```
[ moleculetype ]
; Name nrexcl
DII      3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr    charge      mass
     1        LP3      1  DII      C1     1     0.000  15.0350
     2        LP2      1  DII      C2     2     0.000  14.0270
     3        LP2      1  DII      C3     3     0.000  14.0270
     4        LP2      1  DII      C4     4     0.000  14.0270
     5        LP2      1  DII      C5     5     0.000  14.0270
     6        LP2      1  DII      C6     6     0.000  14.0270
     7        LP2      1  DII      C7     7     0.000  14.0270
     8        LP2      1  DII      C8     8     0.000  14.0270
     9        LP2      1  DII      C9     9     0.000  14.0270
    10        LP2      1  DII     C10    10     0.000  14.0270
    11        LP2      1  DII     C11    11     0.000  14.0270
    12        LP2      1  DII     C12    12     0.000  14.0270
    13        LP2      1  DII     C13    13     0.000  14.0270
    14        LP2      1  DII     C14    14     0.000  14.0270
    15        LP2      1  DII     C15    15     0.000  14.0270
    16        LP2      1  DII     C16    16     0.000  14.0270
    17        LP2      1  DII     C17    17     0.000  14.0270
    18        LP2      1  DII     C18    18     0.150  14.0270
    19         NR      1  DII     N19    19    -0.010  14.0067
    20          C      1  DII     C20    20     0.100  12.0110
    21        CR1      1  DII     C21    21    -0.040  13.0190
    22        CR1      1  DII     C22    22     0.040  13.0190
    23        CR1      1  DII     C23    23     0.010  13.0190
    24        CR1      1  DII     C24    24     0.010  13.0190
    25          C      1  DII     C25    25    -0.100  12.0110
    26        CH1      1  DII     C26    26     0.400  12.0110
    27        CH3      1  DII     C27    27    -0.060  15.0350
    28        CH3      1  DII     C28    28    -0.070  15.0350
    29          C      1  DII     C29    29     0.300  12.0110
    30        CR1      1  DII     C30    30    -0.430  13.0190
    31        CR1      1  DII     C31    31     0.370  13.0190
    32        CR1      1  DII     C32    32    -0.340  13.0190
    33          C      1  DII     C33    33     0.410  12.0110
    34        CH1      1  DII     C34    34     0.140  12.0110
    35        CH3      1  DII     C35    35    -0.030  15.0350
    36        CH3      1  DII     C36    36    -0.040  15.0350
    37          C      1  DII     C37    37     0.030  12.0110
    38        CR1      1  DII     C38    38    -0.020  13.0190
    39        CR1      1  DII     C39    39     0.010  13.0190
    40        CR1      1  DII     C40    40     0.040  13.0190
    41        CR1      1  DII     C41    41    -0.060  13.0190
    42          C      1  DII     C42    42     0.140  12.0110
    43          N      1  DII     N43    43    -0.100  14.0067
    44        LP2      1  DII     C44    44     0.150  14.0270
    45        LP2      1  DII     C45    45     0.000  14.0270
    46        LP2      1  DII     C46    46     0.000  14.0270
    47        LP2      1  DII     C47    47     0.000  14.0270
    48        LP2      1  DII     C48    48     0.000  14.0270
    49        LP2      1  DII     C49    49     0.000  14.0270
    50        LP2      1  DII     C50    50     0.000  14.0270
    51        LP2      1  DII     C51    51     0.000  14.0270
    52        LP2      1  DII     C52    52     0.000  14.0270
    53        LP2      1  DII     C53    53     0.000  14.0270
    54        LP2      1  DII     C54    54     0.000  14.0270
    55        LP2      1  DII     C55    55     0.000  14.0270
    56        LP2      1  DII     C56    56     0.000  14.0270
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    57       LP2     1  DII     C57    57    0.000  14.0270
    58       LP2     1  DII     C58    58    0.000  14.0270
    59       LP2     1  DII     C59    59    0.000  14.0270
    60       LP2     1  DII     C60    60    0.000  14.0270
    61       LP3     1  DII     C61    61    0.000  15.0350

[ bonds ]
; ai   aj   fu    c0, c1, ...
   1    2    1    0.153    334720.0    0.153    334720.0 ;   CAA  CAR
   2    3    1    0.153    334720.0    0.153    334720.0 ;   CAR  CAT
   3    4    1    0.153    334720.0    0.153    334720.0 ;   CAT  CAV
   4    5    1    0.153    334720.0    0.153    334720.0 ;   CAV  CAX
   5    6    1    0.153    334720.0    0.153    334720.0 ;   CAX  CAZ
   6    7    1    0.153    334720.0    0.153    334720.0 ;   CAZ  CBB
   7    8    1    0.153    334720.0    0.153    334720.0 ;   CBB  CBD
   8    9    1    0.153    334720.0    0.153    334720.0 ;   CBD  CBF
   9   10    1    0.153    334720.0    0.153    334720.0 ;   CBF  CBH
  10   11    1    0.153    334720.0    0.153    334720.0 ;   CBH  CBJ
  11   12    1    0.153    334720.0    0.153    334720.0 ;   CBJ  CBL
  12   13    1    0.153    334720.0    0.153    334720.0 ;   CBL  CBN
  13   14    1    0.153    334720.0    0.153    334720.0 ;   CBN  CBP
  14   15    1    0.153    334720.0    0.153    334720.0 ;   CBP  CBR
  15   16    1    0.153    334720.0    0.153    334720.0 ;   CBR  CBT
  16   17    1    0.153    334720.0    0.153    334720.0 ;   CBT  CBV
  17   18    1    0.153    334720.0    0.153    334720.0 ;   CBV  CBX
  18   19    1    0.147    376560.0    0.147    376560.0 ;   CBX  NCF
  19   20    1    0.141    418400.0    0.133    418400.0 ;   NCF  CCB
  19   29    1    0.133    418400.0    0.133    418400.0 ;   NCF  CBZ
  20   21    1    0.139    418400.0    0.139    418400.0 ;   CCB  CAN
  20   25    1    0.139    418400.0    0.139    418400.0 ;   CCB  CCD
  21   22    1    0.139    418400.0    0.139    418400.0 ;   CAN  CAJ
  22   23    1    0.139    418400.0    0.139    418400.0 ;   CAJ  CAL
  23   24    1    0.139    418400.0    0.139    418400.0 ;   CAL  CAP
  24   25    1    0.139    418400.0    0.139    418400.0 ;   CAP  CCD
  25   26    1    0.153    334720.0    0.153    334720.0 ;   CCD  CCH
  26   27    1    0.153    334720.0    0.153    334720.0 ;   CCH  CAC
  26   28    1    0.153    334720.0    0.153    334720.0 ;   CCH  CAD
  26   29    1    0.153    334720.0    0.153    334720.0 ;   CCH  CBZ
  29   30    1    0.139    418400.0    0.139    418400.0 ;   CBZ  CAH
  30   31    1    0.139    418400.0    0.139    418400.0 ;   CAH  CAG
  31   32    1    0.139    418400.0    0.139    418400.0 ;   CAG  CAI
  32   33    1    0.139    418400.0    0.139    418400.0 ;   CAI  CCA
  33   34    1    0.153    334720.0    0.153    334720.0 ;   CCA  CCI
  33   43    1    0.133    418400.0    0.133    418400.0 ;   CCA  NCG
  34   35    1    0.153    334720.0    0.153    334720.0 ;   CCI  CAE
  34   36    1    0.153    334720.0    0.153    334720.0 ;   CCI  CAF
  34   37    1    0.153    334720.0    0.153    334720.0 ;   CCI  CCE
  37   38    1    0.139    418400.0    0.139    418400.0 ;   CCE  CAQ
  37   42    1    0.139    418400.0    0.139    418400.0 ;   CCE  CCC
  38   39    1    0.139    418400.0    0.139    418400.0 ;   CAQ  CAM
  39   40    1    0.139    418400.0    0.139    418400.0 ;   CAM  CAK
  40   41    1    0.139    418400.0    0.139    418400.0 ;   CAK  CAO
  41   42    1    0.139    418400.0    0.139    418400.0 ;   CAO  CCC
  42   43    1    0.141    418400.0    0.133    418400.0 ;   CCC  NCG
  43   44    1    0.147    376560.0    0.147    376560.0 ;   NCG  CBY
  44   45    1    0.153    334720.0    0.153    334720.0 ;   CBY  CBW
  45   46    1    0.153    334720.0    0.153    334720.0 ;   CBW  CBU
  46   47    1    0.153    334720.0    0.153    334720.0 ;   CBU  CBS
  47   48    1    0.153    334720.0    0.153    334720.0 ;   CBS  CBQ
  48   49    1    0.153    334720.0    0.153    334720.0 ;   CBQ  CBO
  49   50    1    0.153    334720.0    0.153    334720.0 ;   CBO  CBM
  50   51    1    0.153    334720.0    0.153    334720.0 ;   CBM  CBK
  51   52    1    0.153    334720.0    0.153    334720.0 ;   CBK  CBI
  52   53    1    0.153    334720.0    0.153    334720.0 ;   CBI  CBG
  53   54    1    0.153    334720.0    0.153    334720.0 ;   CBG  CBE
  54   55    1    0.153    334720.0    0.153    334720.0 ;   CBE  CBC
  55   56    1    0.153    334720.0    0.153    334720.0 ;   CBC  CBA
  56   57    1    0.153    334720.0    0.153    334720.0 ;   CBA  CAY
  57   58    1    0.153    334720.0    0.153    334720.0 ;   CAY  CAW
  58   59    1    0.153    334720.0    0.153    334720.0 ;   CAW  CAU
  59   60    1    0.153    334720.0    0.153    334720.0 ;   CAU  CAS
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  60  61   1    0.153    334720.0    0.153    334720.0 ;   CAS  CAB

[ pairs ]
; ai  aj  fu    c0, c1, ...
  19  22   1                                          ;   NCF  CAJ
  19  24   1                                          ;   NCF  CAP
  19  27   1                                          ;   NCF  CAC
  19  28   1                                          ;   NCF  CAD
  19  31   1                                          ;   NCF  CAG
  20  23   1                                          ;   CCB  CAL
  20  27   1                                          ;   CCB  CAC
  20  28   1                                          ;   CCB  CAD
  20  30   1                                          ;   CCB  CAH
  21  24   1                                          ;   CAN  CAP
  21  26   1                                          ;   CAN  CCH
  21  29   1                                          ;   CAN  CBZ
  22  25   1                                          ;   CAJ  CCD
  23  26   1                                          ;   CAL  CCH
  24  27   1                                          ;   CAP  CAC
  24  28   1                                          ;   CAP  CAD
  24  29   1                                          ;   CAP  CBZ
  25  30   1                                          ;   CCD  CAH
  26  31   1                                          ;   CCH  CAG
  27  30   1                                          ;   CAC  CAH
  28  30   1                                          ;   CAD  CAH
  29  32   1                                          ;   CBZ  CAI
  30  33   1                                          ;   CAH  CCA
  31  34   1                                          ;   CAG  CCI
  31  43   1                                          ;   CAG  NCG
  32  35   1                                          ;   CAI  CAE
  32  36   1                                          ;   CAI  CAF
  32  37   1                                          ;   CAI  CCE
  32  42   1                                          ;   CAI  CCC
  33  38   1                                          ;   CCA  CAQ
  33  41   1                                          ;   CCA  CAO
  34  39   1                                          ;   CCI  CAM
  34  41   1                                          ;   CCI  CAO
  35  38   1                                          ;   CAE  CAQ
  35  42   1                                          ;   CAE  CCC
  35  43   1                                          ;   CAE  NCG
  36  38   1                                          ;   CAF  CAQ
  36  42   1                                          ;   CAF  CCC
  36  43   1                                          ;   CAF  NCG
  37  40   1                                          ;   CCE  CAK
  38  41   1                                          ;   CAQ  CAO
  38  43   1                                          ;   CAQ  NCG
  39  42   1                                          ;   CAM  CCC
  40  43   1                                          ;   CAK  NCG


[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   1   2   3   1    111.0       460.2    111.0       460.2 ;   CAA  CAR  CAT
   2   3   4   1    111.0       460.2    111.0       460.2 ;   CAR  CAT  CAV
   3   4   5   1    111.0       460.2    111.0       460.2 ;   CAT  CAV  CAX
   4   5   6   1    111.0       460.2    111.0       460.2 ;   CAV  CAX  CAZ
   5   6   7   1    111.0       460.2    111.0       460.2 ;   CAX  CAZ  CBB
   6   7   8   1    111.0       460.2    111.0       460.2 ;   CAZ  CBB  CBD
   7   8   9   1    111.0       460.2    111.0       460.2 ;   CBB  CBD  CBF
   8   9  10   1    111.0       460.2    111.0       460.2 ;   CBD  CBF  CBH
   9  10  11   1    111.0       460.2    111.0       460.2 ;   CBF  CBH  CBJ
  10  11  12   1    111.0       460.2    111.0       460.2 ;   CBH  CBJ  CBL
  11  12  13   1    111.0       460.2    111.0       460.2 ;   CBJ  CBL  CBN
  12  13  14   1    111.0       460.2    111.0       460.2 ;   CBL  CBN  CBP
  13  14  15   1    111.0       460.2    111.0       460.2 ;   CBN  CBP  CBR
  14  15  16   1    111.0       460.2    111.0       460.2 ;   CBP  CBR  CBT
  15  16  17   1    111.0       460.2    111.0       460.2 ;   CBR  CBT  CBV
  16  17  18   1    111.0       460.2    111.0       460.2 ;   CBT  CBV  CBX
  17  18  19   1    109.5       460.2    109.5       460.2 ;   CBV  CBX  NCF
  18  19  20   1    120.0       418.4    120.0       418.4 ;   CBX  NCF  CCB
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  18  19  29   1    120.0       418.4    120.0       418.4 ;   CBX  NCF  CBZ
  20  19  29   1    108.0       418.4    108.0       418.4 ;   CCB  NCF  CBZ
  19  20  21   1    120.0       418.4    120.0       418.4 ;   NCF  CCB  CAN
  19  20  25   1    108.0       418.4    108.0       418.4 ;   NCF  CCB  CCD
  21  20  25   1    120.0       418.4    120.0       418.4 ;   CAN  CCB  CCD
  20  21  22   1    120.0       418.4    120.0       418.4 ;   CCB  CAN  CAJ
  21  22  23   1    120.0       418.4    120.0       418.4 ;   CAN  CAJ  CAL
  22  23  24   1    120.0       418.4    120.0       418.4 ;   CAJ  CAL  CAP
  23  24  25   1    120.0       418.4    120.0       418.4 ;   CAL  CAP  CCD
  20  25  24   1    120.0       418.4    120.0       418.4 ;   CCB  CCD  CAP
  20  25  26   1    108.0       418.4    108.0       418.4 ;   CCB  CCD  CCH
  24  25  26   1    132.0       418.4    132.0       418.4 ;   CAP  CCD  CCH
  25  26  27   1    109.5       397.5    109.5       397.5 ;   CCD  CCH  CAC
  25  26  28   1    109.5       397.5    109.5       397.5 ;   CCD  CCH  CAD
  25  26  29   1    104.0       460.2    104.0       460.2 ;   CCD  CCH  CBZ
  27  26  28   1    111.0       460.2    111.0       460.2 ;   CAC  CCH  CAD
  27  26  29   1    109.5       397.5    109.5       397.5 ;   CAC  CCH  CBZ
  28  26  29   1    109.5       397.5    109.5       397.5 ;   CAD  CCH  CBZ
  19  29  26   1    108.0       418.4    108.0       418.4 ;   NCF  CBZ  CCH
  19  29  30   1    132.0       418.4    132.0       418.4 ;   NCF  CBZ  CAH
  26  29  30   1    132.0       418.4    132.0       418.4 ;   CCH  CBZ  CAH
  29  30  31   1    120.0       418.4    120.0       418.4 ;   CBZ  CAH  CAG
  30  31  32   1    135.0       418.4    135.0       418.4 ;   CAH  CAG  CAI
  31  32  33   1    125.0       418.4    125.0       418.4 ;   CAG  CAI  CCA
  32  33  34   1    120.0       418.4    120.0       418.4 ;   CAI  CCA  CCI
  32  33  43   1    132.0       418.4    132.0       418.4 ;   CAI  CCA  NCG
  34  33  43   1    108.0       418.4    108.0       418.4 ;   CCI  CCA  NCG
  33  34  35   1    109.5       397.5    109.5       397.5 ;   CCA  CCI  CAE
  33  34  36   1    109.5       397.5    109.5       397.5 ;   CCA  CCI  CAF
  33  34  37   1    104.0       460.2    104.0       460.2 ;   CCA  CCI  CCE
  35  34  36   1    111.0       460.2    111.0       460.2 ;   CAE  CCI  CAF
  35  34  37   1    109.5       397.5    109.5       397.5 ;   CAE  CCI  CCE
  36  34  37   1    109.5       397.5    109.5       397.5 ;   CAF  CCI  CCE
  34  37  38   1    132.0       418.4    132.0       418.4 ;   CCI  CCE  CAQ
  34  37  42   1    108.0       418.4    108.0       418.4 ;   CCI  CCE  CCC
  38  37  42   1    120.0       418.4    120.0       418.4 ;   CAQ  CCE  CCC
  37  38  39   1    120.0       418.4    120.0       418.4 ;   CCE  CAQ  CAM
  38  39  40   1    120.0       418.4    120.0       418.4 ;   CAQ  CAM  CAK
  39  40  41   1    120.0       418.4    120.0       418.4 ;   CAM  CAK  CAO
  40  41  42   1    120.0       418.4    120.0       418.4 ;   CAK  CAO  CCC
  37  42  41   1    120.0       418.4    120.0       418.4 ;   CCE  CCC  CAO
  37  42  43   1    108.0       418.4    108.0       418.4 ;   CCE  CCC  NCG
  41  42  43   1    132.0       418.4    132.0       418.4 ;   CAO  CCC  NCG
  33  43  42   1    108.0       418.4    108.0       418.4 ;   CCA  NCG  CCC
  33  43  44   1    120.0       418.4    120.0       418.4 ;   CCA  NCG  CBY
  42  43  44   1    120.0       418.4    120.0       418.4 ;   CCC  NCG  CBY
  43  44  45   1    109.5       460.2    109.5       460.2 ;   NCG  CBY  CBW
  44  45  46   1    111.0       460.2    111.0       460.2 ;   CBY  CBW  CBU
  45  46  47   1    111.0       460.2    111.0       460.2 ;   CBW  CBU  CBS
  46  47  48   1    111.0       460.2    111.0       460.2 ;   CBU  CBS  CBQ
  47  48  49   1    111.0       460.2    111.0       460.2 ;   CBS  CBQ  CBO
  48  49  50   1    111.0       460.2    111.0       460.2 ;   CBQ  CBO  CBM
  49  50  51   1    111.0       460.2    111.0       460.2 ;   CBO  CBM  CBK
  50  51  52   1    111.0       460.2    111.0       460.2 ;   CBM  CBK  CBI
  51  52  53   1    111.0       460.2    111.0       460.2 ;   CBK  CBI  CBG
  52  53  54   1    111.0       460.2    111.0       460.2 ;   CBI  CBG  CBE
  53  54  55   1    111.0       460.2    111.0       460.2 ;   CBG  CBE  CBC
  54  55  56   1    111.0       460.2    111.0       460.2 ;   CBE  CBC  CBA
  55  56  57   1    111.0       460.2    111.0       460.2 ;   CBC  CBA  CAY
  56  57  58   1    111.0       460.2    111.0       460.2 ;   CBA  CAY  CAW
  57  58  59   1    111.0       460.2    111.0       460.2 ;   CAY  CAW  CAU
  58  59  60   1    111.0       460.2    111.0       460.2 ;   CAW  CAU  CAS
  59  60  61   1    111.0       460.2    111.0       460.2 ;   CAU  CAS  CAB

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
  19  18  20  29   2      0.0 1673.6       0.0 1673.6  ; imp   NCF  CBX  CCB  CBZ
  20  25  21  19   2      0.0 1673.6       0.0 1673.6  ; imp   CCB  CCD  CAN  NCF
  25  20  26  24   2      0.0 1673.6       0.0 1673.6  ; imp   CCD  CCB  CCH  CAP
  29  30  26  19   2      0.0 1673.6       0.0 1673.6  ; imp   CBZ  CAH  CCH  NCF
  33  32  34  43   2      0.0 1673.6       0.0 1673.6  ; imp   CCA  CAI  CCI  NCG
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  37  34  42  38   2      0.0 1673.6       0.0 1673.6  ; imp   CCE  CCI  CCC  CAQ
  42  37  41  43   2      0.0 1673.6       0.0 1673.6  ; imp   CCC  CCE  CAO  NCG
  43  33  42  44   2      0.0 1673.6       0.0 1673.6  ; imp   NCG  CCA  CCC  CBY
  26  25  28  27   2     35.3  836.8      35.3  836.8  ; imp   CCH  CCD  CAD  CAC
  34  33  35  36   2     35.3  836.8      35.3  836.8  ; imp   CCI  CCA  CAE  CAF
  37  38  39  40   2      0.0 1673.6       0.0 1673.6  ; imp   CCE  CAQ  CAM  CAK
  38  39  40  41   2      0.0 1673.6       0.0 1673.6  ; imp   CAQ  CAM  CAK  CAO
  39  40  41  42   2      0.0 1673.6       0.0 1673.6  ; imp   CAM  CAK  CAO  CCC
  40  41  42  37   2      0.0 1673.6       0.0 1673.6  ; imp   CAK  CAO  CCC  CCE
  41  42  37  38   2      0.0 1673.6       0.0 1673.6  ; imp   CAO  CCC  CCE  CAQ
  42  37  38  39   2      0.0 1673.6       0.0 1673.6  ; imp   CCC  CCE  CAQ  CAM
  20  21  22  23   2      0.0 1673.6       0.0 1673.6  ; imp   CCB  CAN  CAJ  CAL
  21  22  23  24   2      0.0 1673.6       0.0 1673.6  ; imp   CAN  CAJ  CAL  CAP
  22  23  24  25   2      0.0 1673.6       0.0 1673.6  ; imp   CAJ  CAL  CAP  CCD
  23  24  25  20   2      0.0 1673.6       0.0 1673.6  ; imp   CAL  CAP  CCD  CCB
  24  25  20  21   2      0.0 1673.6       0.0 1673.6  ; imp   CAP  CCD  CCB  CAN
  25  20  21  22   2      0.0 1673.6       0.0 1673.6  ; imp   CCD  CCB  CAN  CAJ
   4   3   2   1   3
   5   4   3   2   3
   6   5   4   3   3
   7   6   5   4   3
   8   7   6   5   3
   9   8   7   6   3
  10   9   8   7   3
  11  10   9   8   3
  12  11  10   9   3
  13  12  11  10   3
  14  13  12  11   3
  15  14  13  12   3
  16  15  14  13   3
  17  16  15  14   3
  18  17  16  15   3
  19  18  17  16   1      0.0    5.9 3      0.0    5.9 3 ; dih   NCF  CBX  CBV  CBT
  17  18  19  29   1      0.0    3.8 6      0.0    3.8 6 ; dih   CBV  CBX  NCF  CBZ
  18  19  20  25   1    180.0   33.5 2    180.0   33.5 2 ; dih   CBX  NCF  CCB  CCD
  18  19  29  30   1    180.0   33.5 2    180.0   33.5 2 ; dih   CBX  NCF  CBZ  CAH
  20  25  26  29   1      0.0    0.4 6      0.0    0.4 6 ; dih   CCB  CCD  CCH  CBZ
  25  26  29  30   1      0.0    0.4 6      0.0    0.4 6 ; dih   CCD  CCH  CBZ  CAH
  19  29  30  31   1    180.0   41.8 2    180.0   41.8 2 ; dih   NCF  CBZ  CAH  CAG
  29  30  31  32   1    180.0   41.8 2    180.0   41.8 2 ; dih   CBZ  CAH  CAG  CAI
  30  31  32  33   1    180.0   41.8 2    180.0   41.8 2 ; dih   CAH  CAG  CAI  CCA
  43  33  32  31   1    180.0   41.8 2    180.0   41.8 2 ; dih   NCG  CCA  CAI  CAG
  32  33  34  37   1      0.0    0.4 6      0.0    0.4 6 ; dih   CAI  CCA  CCI  CCE
  32  33  43  44   1    180.0   33.5 2    180.0   33.5 2 ; dih   CAI  CCA  NCG  CBY
  33  34  37  42   1      0.0    0.4 6      0.0    0.4 6 ; dih   CCA  CCI  CCE  CCC
  37  42  43  44   1    180.0   33.5 2    180.0   33.5 2 ; dih   CCE  CCC  NCG  CBY
  33  43  44  45   1      0.0    3.8 6      0.0    3.8 6 ; dih   CCA  NCG  CBY  CBW
  46  45  44  43   1      0.0    5.9 3      0.0    5.9 3 ; dih   CBU  CBW  CBY  NCG
  47  46  45  44   3
  48  47  46  45   3
  49  48  47  46   3
  50  49  48  47   3
  51  50  49  48   3
  52  51  50  49   3
  53  52  51  50   3
  54  53  52  51   3
  55  54  53  52   3
  56  55  54  53   3
  57  56  55  54   3
  58  57  56  55   3
  59  58  57  56   3
  60  59  58  57   3
  61  60  59  58   3

; Strong position restraints for InflateGRO
;#ifdef STRONG_POSRES
;#include "strong_posre.itp"
;#endif
```

S1.2 DiI-C18:2

```
[ moleculetype ]
; Name nrexcl
DII      3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr   charge     mass
     1        LP3      1  DII      C1     1    0.000  15.0350
     2        LP2      1  DII      C2     2    0.000  14.0270
     3        LP2      1  DII      C3     3    0.000  14.0270
     4        LP2      1  DII      C4     4    0.000  14.0270
     5        LP2      1  DII      C5     5    0.000  14.0270
     6        LH1      1  DII      C6     6    0.000  13.0190
     7        LH1      1  DII      C7     7    0.000  13.0190
     8        LP2      1  DII      C8     8    0.000  14.0270
     9        LH1      1  DII      C9     9    0.000  13.0190
    10        LH1      1  DII     C10    10    0.000  13.0190
    11        LP2      1  DII     C11    11    0.000  14.0270
    12        LP2      1  DII     C12    12    0.000  14.0270
    13        LP2      1  DII     C13    13    0.000  14.0270
    14        LP2      1  DII     C14    14    0.000  14.0270
    15        LP2      1  DII     C15    15    0.000  14.0270
    16        LP2      1  DII     C16    16    0.000  14.0270
    17        LP2      1  DII     C17    17    0.000  14.0270
    18        LP2      1  DII     C18    18    0.150  14.0270
    19         NR      1  DII     N19    19   -0.010  14.0067
    20          C      1  DII     C20    20    0.100  12.0110
    21        CR1      1  DII     C21    21   -0.040  13.0190
    22        CR1      1  DII     C22    22    0.040  13.0190
    23        CR1      1  DII     C23    23    0.010  13.0190
    24        CR1      1  DII     C24    24    0.010  13.0190
    25          C      1  DII     C25    25   -0.100  12.0110
    26        CH1      1  DII     C26    26    0.400  12.0110
    27        CH3      1  DII     C27    27   -0.060  15.0350
    28        CH3      1  DII     C28    28   -0.070  15.0350
    29          C      1  DII     C29    29    0.300  12.0110
    30        CR1      1  DII     C30    30   -0.430  13.0190
    31        CR1      1  DII     C31    31    0.370  13.0190
    32        CR1      1  DII     C32    32   -0.340  13.0190
    33          C      1  DII     C33    33    0.410  12.0110
    34        CH1      1  DII     C34    34    0.140  12.0110
    35        CH3      1  DII     C35    35   -0.030  15.0350
    36        CH3      1  DII     C36    36   -0.040  15.0350
    37          C      1  DII     C37    37    0.030  12.0110
    38        CR1      1  DII     C38    38   -0.020  13.0190
    39        CR1      1  DII     C39    39    0.010  13.0190
    40        CR1      1  DII     C40    40    0.040  13.0190
    41        CR1      1  DII     C41    41   -0.060  13.0190
    42          C      1  DII     C42    42    0.140  12.0110
    43          N      1  DII     N43    43   -0.100  14.0067
    44        LP2      1  DII     C44    44    0.150  14.0270
    45        LP2      1  DII     C45    45    0.000  14.0270
    46        LP2      1  DII     C46    46    0.000  14.0270
    47        LP2      1  DII     C47    47    0.000  14.0270
    48        LP2      1  DII     C48    48    0.000  14.0270
    49        LP2      1  DII     C49    49    0.000  14.0270
    50        LP2      1  DII     C50    50    0.000  14.0270
    51        LP2      1  DII     C51    51    0.000  14.0270
    52        LH1      1  DII     C52    52    0.000  13.0190
    53        LH1      1  DII     C53    53    0.000  13.0190
    54        LP2      1  DII     C54    54    0.000  14.0270
    55        LH1      1  DII     C55    55    0.000  13.0190
    56        LH1      1  DII     C56    56    0.000  13.0190
    57        LP2      1  DII     C57    57    0.000  14.0270
    58        LP2      1  DII     C58    58    0.000  14.0270
    59        LP2      1  DII     C59    59    0.000  14.0270
    60        LP2      1  DII     C60    60    0.000  14.0270
    61        LP3      1  DII     C61    61    0.000  15.0350
```

```
[ bonds ]
; ai   aj   fu    c0, c1, ...
    1    2    1    0.153    334720.0    0.153    334720.0 ;   CAA  CAR
    2    3    1    0.153    334720.0    0.153    334720.0 ;   CAR  CAT
    3    4    1    0.153    334720.0    0.153    334720.0 ;   CAT  CAV
    4    5    1    0.153    334720.0    0.153    334720.0 ;   CAV  CAX
    5    6    1    0.153    334720.0    0.153    334720.0 ;   CAX  CAZ

    6    7    1    0.139    418400.0    0.139    418400.0 ;   CAZ  CBB

    7    8    1    0.153    334720.0    0.153    334720.0 ;   CBB  CBD
    8    9    1    0.153    334720.0    0.153    334720.0 ;   CBD  CBF

    9   10    1    0.139    418400.0    0.139    418400.0 ;   CBF  CBH

   10   11    1    0.153    334720.0    0.153    334720.0 ;   CBH  CBJ
   11   12    1    0.153    334720.0    0.153    334720.0 ;   CBJ  CBL
   12   13    1    0.153    334720.0    0.153    334720.0 ;   CBL  CBN
   13   14    1    0.153    334720.0    0.153    334720.0 ;   CBN  CBP
   14   15    1    0.153    334720.0    0.153    334720.0 ;   CBP  CBR
   15   16    1    0.153    334720.0    0.153    334720.0 ;   CBR  CBT
   16   17    1    0.153    334720.0    0.153    334720.0 ;   CBT  CBV
   17   18    1    0.153    334720.0    0.153    334720.0 ;   CBV  CBX
   18   19    1    0.147    376560.0    0.147    376560.0 ;   CBX  NCF
   19   20    1    0.141    418400.0    0.133    418400.0 ;   NCF  CCB
   19   29    1    0.133    418400.0    0.133    418400.0 ;   NCF  CBZ
   20   21    1    0.139    418400.0    0.139    418400.0 ;   CCB  CAN
   20   25    1    0.139    418400.0    0.139    418400.0 ;   CCB  CCD
   21   22    1    0.139    418400.0    0.139    418400.0 ;   CAN  CAJ
   22   23    1    0.139    418400.0    0.139    418400.0 ;   CAJ  CAL
   23   24    1    0.139    418400.0    0.139    418400.0 ;   CAL  CAP
   24   25    1    0.139    418400.0    0.139    418400.0 ;   CAP  CCD
   25   26    1    0.153    334720.0    0.153    334720.0 ;   CCD  CCH
   26   27    1    0.153    334720.0    0.153    334720.0 ;   CCH  CAC
   26   28    1    0.153    334720.0    0.153    334720.0 ;   CCH  CAD
   26   29    1    0.153    334720.0    0.153    334720.0 ;   CCH  CBZ
   29   30    1    0.139    418400.0    0.139    418400.0 ;   CBZ  CAH
   30   31    1    0.139    418400.0    0.139    418400.0 ;   CAH  CAG
   31   32    1    0.139    418400.0    0.139    418400.0 ;   CAG  CAI
   32   33    1    0.139    418400.0    0.139    418400.0 ;   CAI  CCA
   33   34    1    0.153    334720.0    0.153    334720.0 ;   CCA  CCI
   33   43    1    0.133    418400.0    0.133    418400.0 ;   CCA  NCG
   34   35    1    0.153    334720.0    0.153    334720.0 ;   CCI  CAE
   34   36    1    0.153    334720.0    0.153    334720.0 ;   CCI  CAF
   34   37    1    0.153    334720.0    0.153    334720.0 ;   CCI  CCE
   37   38    1    0.139    418400.0    0.139    418400.0 ;   CCE  CAQ
   37   42    1    0.139    418400.0    0.139    418400.0 ;   CCE  CCC
   38   39    1    0.139    418400.0    0.139    418400.0 ;   CAQ  CAM
   39   40    1    0.139    418400.0    0.139    418400.0 ;   CAM  CAK
   40   41    1    0.139    418400.0    0.139    418400.0 ;   CAK  CAO
   41   42    1    0.139    418400.0    0.139    418400.0 ;   CAO  CCC
   42   43    1    0.141    418400.0    0.133    418400.0 ;   CCC  NCG
   43   44    1    0.147    376560.0    0.147    376560.0 ;   NCG  CBY
   44   45    1    0.153    334720.0    0.153    334720.0 ;   CBY  CBW
   45   46    1    0.153    334720.0    0.153    334720.0 ;   CBW  CBU
   46   47    1    0.153    334720.0    0.153    334720.0 ;   CBU  CBS
   47   48    1    0.153    334720.0    0.153    334720.0 ;   CBS  CBQ
   48   49    1    0.153    334720.0    0.153    334720.0 ;   CBQ  CBO
   49   50    1    0.153    334720.0    0.153    334720.0 ;   CBO  CBM
   50   51    1    0.153    334720.0    0.153    334720.0 ;   CBM  CBK
   51   52    1    0.153    334720.0    0.153    334720.0 ;   CBK  CBI

   52   53    1    0.139    418400.0    0.139    418400.0 ;   CBI  CBG

   53   54    1    0.153    334720.0    0.153    334720.0 ;   CBG  CBE
   54   55    1    0.153    334720.0    0.153    334720.0 ;   CBE  CBC

   55   56    1    0.139    418400.0    0.139    418400.0 ;   CBC  CBA

   56   57    1    0.153    334720.0    0.153    334720.0 ;   CBA  CAY
   57   58    1    0.153    334720.0    0.153    334720.0 ;   CAY  CAW
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  58  59   1    0.153    334720.0    0.153    334720.0 ;   CAW  CAU
  59  60   1    0.153    334720.0    0.153    334720.0 ;   CAU  CAS
  60  61   1    0.153    334720.0    0.153    334720.0 ;   CAS  CAB

[ pairs ]
; ai  aj  fu    c0, c1, ...
  19  22   1                                          ;   NCF  CAJ
  19  24   1                                          ;   NCF  CAP
  19  27   1                                          ;   NCF  CAC
  19  28   1                                          ;   NCF  CAD
  19  31   1                                          ;   NCF  CAG
  20  23   1                                          ;   CCB  CAL
  20  27   1                                          ;   CCB  CAC
  20  28   1                                          ;   CCB  CAD
  20  30   1                                          ;   CCB  CAH
  21  24   1                                          ;   CAN  CAP
  21  26   1                                          ;   CAN  CCH
  21  29   1                                          ;   CAN  CBZ
  22  25   1                                          ;   CAJ  CCD
  23  26   1                                          ;   CAL  CCH
  24  27   1                                          ;   CAP  CAC
  24  28   1                                          ;   CAP  CAD
  24  29   1                                          ;   CAP  CBZ
  25  30   1                                          ;   CCD  CAH
  26  31   1                                          ;   CCH  CAG
  27  30   1                                          ;   CAC  CAH
  28  30   1                                          ;   CAD  CAH
  29  32   1                                          ;   CBZ  CAI
  30  33   1                                          ;   CAH  CCA
  31  34   1                                          ;   CAG  CCI
  31  43   1                                          ;   CAG  NCG
  32  35   1                                          ;   CAI  CAE
  32  36   1                                          ;   CAI  CAF
  32  37   1                                          ;   CAI  CCE
  32  42   1                                          ;   CAI  CCC
  33  38   1                                          ;   CCA  CAQ
  33  41   1                                          ;   CCA  CAO
  34  39   1                                          ;   CCI  CAM
  34  41   1                                          ;   CCI  CAO
  35  38   1                                          ;   CAE  CAQ
  35  42   1                                          ;   CAE  CCC
  35  43   1                                          ;   CAE  NCG
  36  38   1                                          ;   CAF  CAQ
  36  42   1                                          ;   CAF  CCC
  36  43   1                                          ;   CAF  NCG
  37  40   1                                          ;   CCE  CAK
  38  41   1                                          ;   CAQ  CAO
  38  43   1                                          ;   CAQ  NCG
  39  42   1                                          ;   CAM  CCC
  40  43   1                                          ;   CAK  NCG


[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   1   2   3   1    111.0       460.2    111.0       460.2 ;   CAA  CAR  CAT
   2   3   4   1    111.0       460.2    111.0       460.2 ;   CAR  CAT  CAV
   3   4   5   1    111.0       460.2    111.0       460.2 ;   CAT  CAV  CAX
   4   5   6   1    111.0       460.2    111.0       460.2 ;   CAV  CAX  CAZ

   5   6   7   1    120.0       502.08    120.0       502.08 ;   CAX  CAZ  CBB
   6   7   8   1    120.0       502.08    120.0       502.08 ;   CAZ  CBB  CBD

   7   8   9   1    111.0       460.2    111.0       460.2 ;   CBB  CBD  CBF

   8   9  10   1    120.0       502.08    120.0       502.08 ;   CBD  CBF  CBH
   9  10  11   1    120.0       502.08    120.0       502.08 ;   CBF  CBH  CBJ

  10  11  12   1    111.0       460.2    111.0       460.2 ;   CBH  CBJ  CBL
  11  12  13   1    111.0       460.2    111.0       460.2 ;   CBJ  CBL  CBN
  12  13  14   1    111.0       460.2    111.0       460.2 ;   CBL  CBN  CBP
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13  14  15   1    111.0       460.2    111.0       460.2 ;   CBN  CBP  CBR
14  15  16   1    111.0       460.2    111.0       460.2 ;   CBP  CBR  CBT
15  16  17   1    111.0       460.2    111.0       460.2 ;   CBR  CBT  CBV
16  17  18   1    111.0       460.2    111.0       460.2 ;   CBT  CBV  CBX
17  18  19   1    109.5       460.2    109.5       460.2 ;   CBV  CBX  NCF
18  19  20   1    120.0       418.4    120.0       418.4 ;   CBX  NCF  CCB
18  19  29   1    120.0       418.4    120.0       418.4 ;   CBX  NCF  CBZ
20  19  29   1    108.0       418.4    108.0       418.4 ;   CCB  NCF  CBZ
19  20  21   1    120.0       418.4    120.0       418.4 ;   NCF  CCB  CAN
19  20  25   1    108.0       418.4    108.0       418.4 ;   NCF  CCB  CCD
21  20  25   1    120.0       418.4    120.0       418.4 ;   CAN  CCB  CCD
20  21  22   1    120.0       418.4    120.0       418.4 ;   CCB  CAN  CAJ
21  22  23   1    120.0       418.4    120.0       418.4 ;   CAN  CAJ  CAL
22  23  24   1    120.0       418.4    120.0       418.4 ;   CAJ  CAL  CAP
23  24  25   1    120.0       418.4    120.0       418.4 ;   CAL  CAP  CCD
20  25  24   1    120.0       418.4    120.0       418.4 ;   CCB  CCD  CAP
20  25  26   1    108.0       418.4    108.0       418.4 ;   CCB  CCD  CCH
24  25  26   1    132.0       418.4    132.0       418.4 ;   CAP  CCD  CCH
25  26  27   1    109.5       397.5    109.5       397.5 ;   CCD  CCH  CAC
25  26  28   1    109.5       397.5    109.5       397.5 ;   CCD  CCH  CAD
25  26  29   1    104.0       460.2    104.0       460.2 ;   CCD  CCH  CBZ
27  26  28   1    111.0       460.2    111.0       460.2 ;   CAC  CCH  CAD
27  26  29   1    109.5       397.5    109.5       397.5 ;   CAC  CCH  CBZ
28  26  29   1    109.5       397.5    109.5       397.5 ;   CAD  CCH  CBZ
19  29  26   1    108.0       418.4    108.0       418.4 ;   NCF  CBZ  CCH
19  29  30   1    132.0       418.4    132.0       418.4 ;   NCF  CBZ  CAH
26  29  30   1    132.0       418.4    132.0       418.4 ;   CCH  CBZ  CAH
29  30  31   1    120.0       418.4    120.0       418.4 ;   CBZ  CAH  CAG
30  31  32   1    135.0       418.4    135.0       418.4 ;   CAH  CAG  CAI
31  32  33   1    125.0       418.4    125.0       418.4 ;   CAG  CAI  CCA
32  33  34   1    120.0       418.4    120.0       418.4 ;   CAI  CCA  CCI
32  33  43   1    132.0       418.4    132.0       418.4 ;   CAI  CCA  NCG
34  33  43   1    108.0       418.4    108.0       418.4 ;   CCI  CCA  NCG
33  34  35   1    109.5       397.5    109.5       397.5 ;   CCA  CCI  CAE
33  34  36   1    109.5       397.5    109.5       397.5 ;   CCA  CCI  CAF
33  34  37   1    104.0       460.2    104.0       460.2 ;   CCA  CCI  CCE
35  34  36   1    111.0       460.2    111.0       460.2 ;   CAE  CCI  CAF
35  34  37   1    109.5       397.5    109.5       397.5 ;   CAE  CCI  CCE
36  34  37   1    109.5       397.5    109.5       397.5 ;   CAF  CCI  CCE
34  37  38   1    132.0       418.4    132.0       418.4 ;   CCI  CCE  CAQ
34  37  42   1    108.0       418.4    108.0       418.4 ;   CCI  CCE  CCC
38  37  42   1    120.0       418.4    120.0       418.4 ;   CAQ  CCE  CCC
37  38  39   1    120.0       418.4    120.0       418.4 ;   CCE  CAQ  CAM
38  39  40   1    120.0       418.4    120.0       418.4 ;   CAQ  CAM  CAK
39  40  41   1    120.0       418.4    120.0       418.4 ;   CAM  CAK  CAO
40  41  42   1    120.0       418.4    120.0       418.4 ;   CAK  CAO  CCC
37  42  41   1    120.0       418.4    120.0       418.4 ;   CCE  CCC  CAO
37  42  43   1    108.0       418.4    108.0       418.4 ;   CCE  CCC  NCG
41  42  43   1    132.0       418.4    132.0       418.4 ;   CAO  CCC  NCG
33  43  42   1    108.0       418.4    108.0       418.4 ;   CCA  NCG  CCC
33  43  44   1    120.0       418.4    120.0       418.4 ;   CCA  NCG  CBY
42  43  44   1    120.0       418.4    120.0       418.4 ;   CCC  NCG  CBY
43  44  45   1    109.5       460.2    109.5       460.2 ;   NCG  CBY  CBW
44  45  46   1    111.0       460.2    111.0       460.2 ;   CBY  CBW  CBU
45  46  47   1    111.0       460.2    111.0       460.2 ;   CBW  CBU  CBS
46  47  48   1    111.0       460.2    111.0       460.2 ;   CBU  CBS  CBQ
47  48  49   1    111.0       460.2    111.0       460.2 ;   CBS  CBQ  CBO
48  49  50   1    111.0       460.2    111.0       460.2 ;   CBQ  CBO  CBM
49  50  51   1    111.0       460.2    111.0       460.2 ;   CBO  CBM  CBK
50  51  52   1    111.0       460.2    111.0       460.2 ;   CBM  CBK  CBI

51  52  53   1    111.0       460.2    111.0       460.2 ;   CBK  CBI  CBG
52  53  54   1    111.0       460.2    111.0       460.2 ;   CBI  CBG  CBE

53  54  55   1    111.0       460.2    111.0       460.2 ;   CBG  CBE  CBC

54  55  56   1    120.0       502.08    120.0       502.08 ;   CBE  CBC  CBA
55  56  57   1    120.0       502.08    120.0       502.08 ;   CBC  CBA  CAY
56  57  58   1    111.0       460.2    111.0       460.2 ;   CBA  CAY  CAW
57  58  59   1    111.0       460.2    111.0       460.2 ;   CAY  CAW  CAU
58  59  60   1    111.0       460.2    111.0       460.2 ;   CAW  CAU  CAS
```

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  59  60  61   1    111.0       460.2    111.0       460.2 ;   CAU  CAS  CAB

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
  19  18  20  29   2      0.0 1673.6       0.0 1673.6  ; imp   NCF  CBX  CCB  CBZ
  20  25  21  19   2      0.0 1673.6       0.0 1673.6  ; imp   CCB  CCD  CAN  NCF
  25  20  26  24   2      0.0 1673.6       0.0 1673.6  ; imp   CCD  CCB  CCH  CAP
  29  30  26  19   2      0.0 1673.6       0.0 1673.6  ; imp   CBZ  CAH  CCH  NCF
  33  32  34  43   2      0.0 1673.6       0.0 1673.6  ; imp   CCA  CAI  CCI  NCG
  37  34  42  38   2      0.0 1673.6       0.0 1673.6  ; imp   CCE  CCI  CCC  CAQ
  42  37  41  43   2      0.0 1673.6       0.0 1673.6  ; imp   CCC  CCE  CAO  NCG
  43  33  42  44   2      0.0 1673.6       0.0 1673.6  ; imp   NCG  CCA  CCC  CBY
  26  25  28  27   2     35.3  836.8      35.3  836.8  ; imp   CCH  CCD  CAD  CAC
  34  33  35  36   2     35.3  836.8      35.3  836.8  ; imp   CCI  CCA  CAE  CAF
  37  38  39  40   2      0.0 1673.6       0.0 1673.6  ; imp   CCE  CAQ  CAM  CAK
  38  39  40  41   2      0.0 1673.6       0.0 1673.6  ; imp   CAQ  CAM  CAK  CAO
  39  40  41  42   2      0.0 1673.6       0.0 1673.6  ; imp   CAM  CAK  CAO  CCC
  40  41  42  37   2      0.0 1673.6       0.0 1673.6  ; imp   CAK  CAO  CCC  CCE
  41  42  37  38   2      0.0 1673.6       0.0 1673.6  ; imp   CAO  CCC  CCE  CAQ
  42  37  38  39   2      0.0 1673.6       0.0 1673.6  ; imp   CCC  CCE  CAQ  CAM
  20  21  22  23   2      0.0 1673.6       0.0 1673.6  ; imp   CCB  CAN  CAJ  CAL
  21  22  23  24   2      0.0 1673.6       0.0 1673.6  ; imp   CAN  CAJ  CAL  CAP
  22  23  24  25   2      0.0 1673.6       0.0 1673.6  ; imp   CAJ  CAL  CAP  CCD
  23  24  25  20   2      0.0 1673.6       0.0 1673.6  ; imp   CAL  CAP  CCD  CCB
  24  25  20  21   2      0.0 1673.6       0.0 1673.6  ; imp   CAP  CCD  CCB  CAN
  25  20  21  22   2      0.0 1673.6       0.0 1673.6  ; imp   CCD  CCB  CAN  CAJ
   4   3   2   1   3
   5   4   3   2   3
   6   5   4   3   3
   7   6   5   4   1      0.0    5.858 3      0.0    5.858 3
;   8   7   6   5   3
   9   8   7   6   1      0.0    5.858 3      0.0    5.858 3
  10   9   8   7   1      0.0    5.858 3      0.0    5.858 3
;  11  10   9   8   3
  12  11  10   9   1      0.0    5.858 3      0.0    5.858 3
  13  12  11  10   3
  14  13  12  11   3
  15  14  13  12   3
  16  15  14  13   3
  17  16  15  14   3
  18  17  16  15   3
  19  18  17  16   1      0.0    5.9 3        0.0    5.9 3 ; dih   NCF  CBX  CBV  CBT
  17  18  19  29   1      0.0    3.8 6        0.0    3.8 6 ; dih   CBV  CBX  NCF  CBZ
  18  19  20  25   1    180.0   33.5 2     180.0   33.5 2 ; dih   CBX  NCF  CCB  CCD
  18  19  29  30   1    180.0   33.5 2     180.0   33.5 2 ; dih   CBX  NCF  CBZ  CAH
  20  25  26  29   1      0.0    0.4 6        0.0    0.4 6 ; dih   CCB  CCD  CCH  CBZ
  25  26  29  30   1      0.0    0.4 6        0.0    0.4 6 ; dih   CCD  CCH  CBZ  CAH
  19  29  30  31   1    180.0   41.8 2     180.0   41.8 2 ; dih   NCF  CBZ  CAH  CAG
  29  30  31  32   1    180.0   41.8 2     180.0   41.8 2 ; dih   CBZ  CAH  CAG  CAI
  30  31  32  33   1    180.0   41.8 2     180.0   41.8 2 ; dih   CAH  CAG  CAI  CCA
  43  33  32  31   1    180.0   41.8 2     180.0   41.8 2 ; dih   NCG  CCA  CAI  CAG
  32  33  34  37   1      0.0    0.4 6        0.0    0.4 6 ; dih   CAI  CCA  CCI  CCE
  32  33  43  44   1    180.0   33.5 2     180.0   33.5 2 ; dih   CAI  CCA  NCG  CBY
  33  34  37  42   1      0.0    0.4 6        0.0    0.4 6 ; dih   CCA  CCI  CCE  CCC
  37  42  43  44   1    180.0   33.5 2     180.0   33.5 2 ; dih   CCE  CCC  NCG  CBY
  33  43  44  45   1      0.0    3.8 6        0.0    3.8 6 ; dih   CCA  NCG  CBY  CBW
  46  45  44  43   1      0.0    5.9 3        0.0    5.9 3 ; dih   CBU  CBW  CBY  NCG
  47  46  45  44   3
  48  47  46  45   3
  49  48  47  46   3
  50  49  48  47   3
  51  50  49  48   3
  52  51  50  49   3
  53  52  51  50   1      0.0    5.858 3      0.0    5.858 3
 ; 54  53  52  51   3
  55  54  53  52   1      0.0    5.858 3      0.0    5.858 3
  56  55  54  53   1      0.0    5.858 3      0.0    5.858 3
;  57  56  55  54   3
  58  57  56  55   1      0.0    5.858 3      0.0    5.858 3
  59  58  57  56   3
  60  59  58  57   3
```

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  61   60   59   58    3

[ dihedrals ]
;  ai    aj    ak    al funct
       11       10        9        8        2 0.000       167.360
        8        7        6        5        2 0.000       167.360
       54       53       52       51        2 0.000       167.360
       57       56       55       54        2 0.000       167.360

; Strong position restraints for InflateGRO
#ifdef STRONG_POSRES
#include "strong_posre.itp"
#endif
```

S1.3 DiI-C12:0

```
[ moleculetype ]
; Name nrexcl
DII      3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr   charge     mass
     1        LP3      1  DII      C1     1    0.000  15.0350
     2        LP2      1  DII      C2     2    0.000  14.0270
     3        LP2      1  DII      C3     3    0.000  14.0270
     4        LP2      1  DII      C4     4    0.000  14.0270
     5        LP2      1  DII      C5     5    0.000  14.0270
     6        LP2      1  DII      C6     6    0.000  14.0270
     7        LP2      1  DII      C7     7    0.000  14.0270
     8        LP2      1  DII      C8     8    0.000  14.0270
     9        LP2      1  DII      C9     9    0.000  14.0270
    10        LP2      1  DII     C10    10    0.000  14.0270
    11        LP2      1  DII     C11    11    0.000  14.0270
    12        LP2      1  DII     C12    12    0.150  14.0270
    13         NR      1  DII     N13    13   -0.010  14.0067
    14          C      1  DII     C14    14    0.100  12.0110
    15        CR1      1  DII     C15    15   -0.040  13.0190
    16        CR1      1  DII     C16    16    0.040  13.0190
    17        CR1      1  DII     C17    17    0.010  13.0190
    18        CR1      1  DII     C18    18    0.010  13.0190
    19          C      1  DII     C19    19   -0.100  12.0110
    20        CH1      1  DII     C20    20    0.400  12.0110
    21        CH3      1  DII     C21    21   -0.060  15.0350
    22        CH3      1  DII     C22    22   -0.070  15.0350
    23          C      1  DII     C23    23    0.300  12.0110
    24        CR1      1  DII     C24    24   -0.430  13.0190
    25        CR1      1  DII     C25    25    0.370  13.0190
    26        CR1      1  DII     C26    26   -0.340  13.0190
    27          C      1  DII     C27    27    0.410  12.0110
    28        CH1      1  DII     C28    28    0.140  12.0110
    29        CH3      1  DII     C29    29   -0.030  15.0350
    30        CH3      1  DII     C30    30   -0.040  15.0350
    31          C      1  DII     C31    31    0.030  12.0110
    32        CR1      1  DII     C32    32   -0.020  13.0190
    33        CR1      1  DII     C33    33    0.010  13.0190
    34        CR1      1  DII     C34    34    0.040  13.0190
    35        CR1      1  DII     C35    35   -0.060  13.0190
    36          C      1  DII     C36    36    0.140  12.0110
    37          N      1  DII     N37    37   -0.100  14.0067
    38        LP2      1  DII     C38    38    0.150  14.0270
    39        LP2      1  DII     C39    39    0.000  14.0270
    40        LP2      1  DII     C40    40    0.000  14.0270
    41        LP2      1  DII     C41    41    0.000  14.0270
    42        LP2      1  DII     C42    42    0.000  14.0270
    43        LP2      1  DII     C43    43    0.000  14.0270
    44        LP2      1  DII     C44    44    0.000  14.0270
    45        LP2      1  DII     C45    45    0.000  14.0270
    46        LP2      1  DII     C46    46    0.000  14.0270
    47        LP2      1  DII     C47    47    0.000  14.0270
    48        LP2      1  DII     C48    48    0.000  14.0270
    49        LP3      1  DII     C49    49    0.000  15.0350

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   1    0.153    334720.0    0.153    334720.0 ;   CBB  CBD
   2   3   1    0.153    334720.0    0.153    334720.0 ;   CBD  CBF
   3   4   1    0.153    334720.0    0.153    334720.0 ;   CBF  CBH
   4   5   1    0.153    334720.0    0.153    334720.0 ;   CBH  CBJ
   5   6   1    0.153    334720.0    0.153    334720.0 ;   CBJ  CBL
   6   7   1    0.153    334720.0    0.153    334720.0 ;   CBL  CBN
   7   8   1    0.153    334720.0    0.153    334720.0 ;   CBN  CBP
   8   9   1    0.153    334720.0    0.153    334720.0 ;   CBP  CBR
   9  10   1    0.153    334720.0    0.153    334720.0 ;   CBR  CBT
  10  11   1    0.153    334720.0    0.153    334720.0 ;   CBT  CBV
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  11  12   1    0.153    334720.0    0.153    334720.0 ;   CBV  CBX
  12  13   1    0.147    376560.0    0.147    376560.0 ;   CBX  NCF
  13  14   1    0.141    418400.0    0.133    418400.0 ;   NCF  CCB
  13  23   1    0.133    418400.0    0.133    418400.0 ;   NCF  CBZ
  14  15   1    0.139    418400.0    0.139    418400.0 ;   CCB  CAN
  14  19   1    0.139    418400.0    0.139    418400.0 ;   CCB  CCD
  15  16   1    0.139    418400.0    0.139    418400.0 ;   CAN  CAJ
  16  17   1    0.139    418400.0    0.139    418400.0 ;   CAJ  CAL
  17  18   1    0.139    418400.0    0.139    418400.0 ;   CAL  CAP
  18  19   1    0.139    418400.0    0.139    418400.0 ;   CAP  CCD
  19  20   1    0.153    334720.0    0.153    334720.0 ;   CCD  CCH
  20  21   1    0.153    334720.0    0.153    334720.0 ;   CCH  CAC
  20  22   1    0.153    334720.0    0.153    334720.0 ;   CCH  CAD
  20  23   1    0.153    334720.0    0.153    334720.0 ;   CCH  CBZ
  23  24   1    0.139    418400.0    0.139    418400.0 ;   CBZ  CAH
  24  25   1    0.139    418400.0    0.139    418400.0 ;   CAH  CAG
  25  26   1    0.139    418400.0    0.139    418400.0 ;   CAG  CAI
  26  27   1    0.139    418400.0    0.139    418400.0 ;   CAI  CCA
  27  28   1    0.153    334720.0    0.153    334720.0 ;   CCA  CCI
  27  37   1    0.133    418400.0    0.133    418400.0 ;   CCA  NCG
  28  29   1    0.153    334720.0    0.153    334720.0 ;   CCI  CAE
  28  30   1    0.153    334720.0    0.153    334720.0 ;   CCI  CAF
  28  31   1    0.153    334720.0    0.153    334720.0 ;   CCI  CCE
  31  32   1    0.139    418400.0    0.139    418400.0 ;   CCE  CAQ
  31  36   1    0.139    418400.0    0.139    418400.0 ;   CCE  CCC
  32  33   1    0.139    418400.0    0.139    418400.0 ;   CAQ  CAM
  33  34   1    0.139    418400.0    0.139    418400.0 ;   CAM  CAK
  34  35   1    0.139    418400.0    0.139    418400.0 ;   CAK  CAO
  35  36   1    0.139    418400.0    0.139    418400.0 ;   CAO  CCC
  36  37   1    0.141    418400.0    0.133    418400.0 ;   CCC  NCG
  37  38   1    0.147    376560.0    0.147    376560.0 ;   NCG  CBY
  38  39   1    0.153    334720.0    0.153    334720.0 ;   CBY  CBW
  39  40   1    0.153    334720.0    0.153    334720.0 ;   CBW  CBU
  40  41   1    0.153    334720.0    0.153    334720.0 ;   CBU  CBS
  41  42   1    0.153    334720.0    0.153    334720.0 ;   CBS  CBQ
  42  43   1    0.153    334720.0    0.153    334720.0 ;   CBQ  CBO
  43  44   1    0.153    334720.0    0.153    334720.0 ;   CBO  CBM
  44  45   1    0.153    334720.0    0.153    334720.0 ;   CBM  CBK
  45  46   1    0.153    334720.0    0.153    334720.0 ;   CBK  CBI
  46  47   1    0.153    334720.0    0.153    334720.0 ;   CBI  CBG
  47  48   1    0.153    334720.0    0.153    334720.0 ;   CBG  CBE
  48  49   1    0.153    334720.0    0.153    334720.0 ;   CBE  CBC

[ pairs ]
; ai  aj  fu    c0, c1, ...
  13  16   1                                          ;   NCF  CAJ
  13  18   1                                          ;   NCF  CAP
  13  21   1                                          ;   NCF  CAC
  13  22   1                                          ;   NCF  CAD
  13  25   1                                          ;   NCF  CAG
  14  17   1                                          ;   CCB  CAL
  14  21   1                                          ;   CCB  CAC
  14  22   1                                          ;   CCB  CAD
  14  24   1                                          ;   CCB  CAH
  15  18   1                                          ;   CAN  CAP
  15  20   1                                          ;   CAN  CCH
  15  23   1                                          ;   CAN  CBZ
  16  19   1                                          ;   CAJ  CCD
  17  20   1                                          ;   CAL  CCH
  18  21   1                                          ;   CAP  CAC
  18  22   1                                          ;   CAP  CAD
  18  23   1                                          ;   CAP  CBZ
  19  24   1                                          ;   CCD  CAH
  20  25   1                                          ;   CCH  CAG
  21  24   1                                          ;   CAC  CAH
  22  24   1                                          ;   CAD  CAH
  23  26   1                                          ;   CBZ  CAI
  24  27   1                                          ;   CAH  CCA
  25  28   1                                          ;   CAG  CCI
  25  37   1                                          ;   CAG  NCG
  26  29   1                                          ;   CAI  CAE
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  26  30   1                                          ;   CAI  CAF
  26  31   1                                          ;   CAI  CCE
  26  36   1                                          ;   CAI  CCC
  27  32   1                                          ;   CCA  CAQ
  27  35   1                                          ;   CCA  CAO
  28  33   1                                          ;   CCI  CAM
  28  35   1                                          ;   CCI  CAO
  29  32   1                                          ;   CAE  CAQ
  29  36   1                                          ;   CAE  CCC
  29  37   1                                          ;   CAE  NCG
  30  32   1                                          ;   CAF  CAQ
  30  36   1                                          ;   CAF  CCC
  30  37   1                                          ;   CAF  NCG
  31  34   1                                          ;   CCE  CAK
  32  35   1                                          ;   CAQ  CAO
  32  37   1                                          ;   CAQ  NCG
  33  36   1                                          ;   CAM  CCC
  34  37   1                                          ;   CAK  NCG


[ angles ]
; ai   aj   ak   fu    c0, c1, ...
    1    2    3    1    111.0       460.2    111.0       460.2 ;   CBB  CBD  CBF
    2    3    4    1    111.0       460.2    111.0       460.2 ;   CBD  CBF  CBH
    3    4    5    1    111.0       460.2    111.0       460.2 ;   CBF  CBH  CBJ
    4    5    6    1    111.0       460.2    111.0       460.2 ;   CBH  CBJ  CBL
    5    6    7    1    111.0       460.2    111.0       460.2 ;   CBJ  CBL  CBN
    6    7    8    1    111.0       460.2    111.0       460.2 ;   CBL  CBN  CBP
    7    8    9    1    111.0       460.2    111.0       460.2 ;   CBN  CBP  CBR
    8    9   10    1    111.0       460.2    111.0       460.2 ;   CBP  CBR  CBT
    9   10   11    1    111.0       460.2    111.0       460.2 ;   CBR  CBT  CBV
   10   11   12    1    111.0       460.2    111.0       460.2 ;   CBT  CBV  CBX
   11   12   13    1    109.5       460.2    109.5       460.2 ;   CBV  CBX  NCF
   12   13   14    1    120.0       418.4    120.0       418.4 ;   CBX  NCF  CCB
   12   13   23    1    120.0       418.4    120.0       418.4 ;   CBX  NCF  CBZ
   14   13   23    1    108.0       418.4    108.0       418.4 ;   CCB  NCF  CBZ
   13   14   15    1    120.0       418.4    120.0       418.4 ;   NCF  CCB  CAN
   13   14   19    1    108.0       418.4    108.0       418.4 ;   NCF  CCB  CCD
   15   14   19    1    120.0       418.4    120.0       418.4 ;   CAN  CCB  CCD
   14   15   16    1    120.0       418.4    120.0       418.4 ;   CCB  CAN  CAJ
   15   16   17    1    120.0       418.4    120.0       418.4 ;   CAN  CAJ  CAL
   16   17   18    1    120.0       418.4    120.0       418.4 ;   CAJ  CAL  CAP
   17   18   19    1    120.0       418.4    120.0       418.4 ;   CAL  CAP  CCD
   14   19   18    1    120.0       418.4    120.0       418.4 ;   CCB  CCD  CAP
   14   19   20    1    108.0       418.4    108.0       418.4 ;   CCB  CCD  CCH
   18   19   20    1    132.0       418.4    132.0       418.4 ;   CAP  CCD  CCH
   19   20   21    1    109.5       397.5    109.5       397.5 ;   CCD  CCH  CAC
   19   20   22    1    109.5       397.5    109.5       397.5 ;   CCD  CCH  CAD
   19   20   23    1    104.0       460.2    104.0       460.2 ;   CCD  CCH  CBZ
   21   20   22    1    111.0       460.2    111.0       460.2 ;   CAC  CCH  CAD
   21   20   23    1    109.5       397.5    109.5       397.5 ;   CAC  CCH  CBZ
   22   20   23    1    109.5       397.5    109.5       397.5 ;   CAD  CCH  CBZ
   13   23   20    1    108.0       418.4    108.0       418.4 ;   NCF  CBZ  CCH
   13   23   24    1    132.0       418.4    132.0       418.4 ;   NCF  CBZ  CAH
   20   23   24    1    132.0       418.4    132.0       418.4 ;   CCH  CBZ  CAH
   23   24   25    1    120.0       418.4    120.0       418.4 ;   CBZ  CAH  CAG
   24   25   26    1    135.0       418.4    135.0       418.4 ;   CAH  CAG  CAI
   25   26   27    1    125.0       418.4    125.0       418.4 ;   CAG  CAI  CCA
   26   27   28    1    120.0       418.4    120.0       418.4 ;   CAI  CCA  CCI
   26   27   37    1    132.0       418.4    132.0       418.4 ;   CAI  CCA  NCG
   28   27   37    1    108.0       418.4    108.0       418.4 ;   CCI  CCA  NCG
   27   28   29    1    109.5       397.5    109.5       397.5 ;   CCA  CCI  CAE
   27   28   30    1    109.5       397.5    109.5       397.5 ;   CCA  CCI  CAF
   27   28   31    1    104.0       460.2    104.0       460.2 ;   CCA  CCI  CCE
   29   28   30    1    111.0       460.2    111.0       460.2 ;   CAE  CCI  CAF
   29   28   31    1    109.5       397.5    109.5       397.5 ;   CAE  CCI  CCE
   30   28   31    1    109.5       397.5    109.5       397.5 ;   CAF  CCI  CCE
   28   31   32    1    132.0       418.4    132.0       418.4 ;   CCI  CCE  CAQ
   28   31   36    1    108.0       418.4    108.0       418.4 ;   CCI  CCE  CCC
   32   31   36    1    120.0       418.4    120.0       418.4 ;   CAQ  CCE  CCC
```

```
  31  32  33   1    120.0       418.4    120.0       418.4 ;   CCE  CAQ  CAM
  32  33  34   1    120.0       418.4    120.0       418.4 ;   CAQ  CAM  CAK
  33  34  35   1    120.0       418.4    120.0       418.4 ;   CAM  CAK  CAO
  34  35  36   1    120.0       418.4    120.0       418.4 ;   CAK  CAO  CCC
  31  36  35   1    120.0       418.4    120.0       418.4 ;   CCE  CCC  CAO
  31  36  37   1    108.0       418.4    108.0       418.4 ;   CCE  CCC  NCG
  35  36  37   1    132.0       418.4    132.0       418.4 ;   CAO  CCC  NCG
  27  37  36   1    108.0       418.4    108.0       418.4 ;   CCA  NCG  CCC
  27  37  38   1    120.0       418.4    120.0       418.4 ;   CCA  NCG  CBY
  36  37  38   1    120.0       418.4    120.0       418.4 ;   CCC  NCG  CBY
  37  38  39   1    109.5       460.2    109.5       460.2 ;   NCG  CBY  CBW
  38  39  40   1    111.0       460.2    111.0       460.2 ;   CBY  CBW  CBU
  39  40  41   1    111.0       460.2    111.0       460.2 ;   CBW  CBU  CBS
  40  41  42   1    111.0       460.2    111.0       460.2 ;   CBU  CBS  CBQ
  41  42  43   1    111.0       460.2    111.0       460.2 ;   CBS  CBQ  CBO
  42  43  44   1    111.0       460.2    111.0       460.2 ;   CBQ  CBO  CBM
  43  44  45   1    111.0       460.2    111.0       460.2 ;   CBO  CBM  CBK
  44  45  46   1    111.0       460.2    111.0       460.2 ;   CBM  CBK  CBI
  45  46  47   1    111.0       460.2    111.0       460.2 ;   CBK  CBI  CBG
  46  47  48   1    111.0       460.2    111.0       460.2 ;   CBI  CBG  CBE
  47  48  49   1    111.0       460.2    111.0       460.2 ;   CBG  CBE  CBC

[ dihedrals ]
; ai   aj   ak   al   fu    c0, c1, m, ... FIXED
  13   12   14   23    2      0.0 1673.6       0.0 1673.6  ; imp   NCF  CBX  CCB  CBZ
  14   19   15   13    2      0.0 1673.6       0.0 1673.6  ; imp   CCB  CCD  CAN  NCF
  19   14   20   18    2      0.0 1673.6       0.0 1673.6  ; imp   CCD  CCB  CCH  CAP
  23   24   20   13    2      0.0 1673.6       0.0 1673.6  ; imp   CBZ  CAH  CCH  NCF
  27   26   28   37    2      0.0 1673.6       0.0 1673.6  ; imp   CCA  CAI  CCI  NCG
  31   28   36   32    2      0.0 1673.6       0.0 1673.6  ; imp   CCE  CCI  CCC  CAQ
  36   31   35   37    2      0.0 1673.6       0.0 1673.6  ; imp   CCC  CCE  CAO  NCG
  37   27   36   38    2      0.0 1673.6       0.0 1673.6  ; imp   NCG  CCA  CCC  CBY
  20   19   22   21    2     35.3  836.8      35.3  836.8  ; imp   CCH  CCD  CAD  CAC
  28   27   29   30    2     35.3  836.8      35.3  836.8  ; imp   CCI  CCA  CAE  CAF
  31   32   33   34    2      0.0 1673.6       0.0 1673.6  ; imp   CCE  CAQ  CAM  CAK
  32   33   34   35    2      0.0 1673.6       0.0 1673.6  ; imp   CAQ  CAM  CAK  CAO
  33   34   35   36    2      0.0 1673.6       0.0 1673.6  ; imp   CAM  CAK  CAO  CCC
  34   35   36   31    2      0.0 1673.6       0.0 1673.6  ; imp   CAK  CAO  CCC  CCE
  35   36   31   32    2      0.0 1673.6       0.0 1673.6  ; imp   CAO  CCC  CCE  CAQ
  36   31   32   33    2      0.0 1673.6       0.0 1673.6  ; imp   CCC  CCE  CAQ  CAM
  14   15   16   17    2      0.0 1673.6       0.0 1673.6  ; imp   CCB  CAN  CAJ  CAL
  15   16   17   18    2      0.0 1673.6       0.0 1673.6  ; imp   CAN  CAJ  CAL  CAP
  16   17   18   19    2      0.0 1673.6       0.0 1673.6  ; imp   CAJ  CAL  CAP  CCD
  17   18   19   14    2      0.0 1673.6       0.0 1673.6  ; imp   CAL  CAP  CCD  CCB
  18   19   14   15    2      0.0 1673.6       0.0 1673.6  ; imp   CAP  CCD  CCB  CAN
  19   14   15   16    2      0.0 1673.6       0.0 1673.6  ; imp   CCD  CCB  CAN  CAJ
   4    3    2    1    3
   5    4    3    2    3
   6    5    4    3    3
   7    6    5    4    3
   8    7    6    5    3
   9    8    7    6    3
  10    9    8    7    3
  11   10    9    8    3
  12   11   10    9    3
  13   12   11   10    1      0.0    5.9 3      0.0    5.9 3 ; dih   NCF  CBX  CBV  CBT
  11   12   13   23    1      0.0    3.8 6      0.0    3.8 6 ; dih   CBV  CBX  NCF  CBZ
  12   13   14   19    1    180.0   33.5 2    180.0   33.5 2 ; dih   CBX  NCF  CCB  CCD
  12   13   23   24    1    180.0   33.5 2    180.0   33.5 2 ; dih   CBX  NCF  CBZ  CAH
  14   19   20   23    1      0.0    0.4 6      0.0    0.4 6 ; dih   CCB  CCD  CCH  CBZ
  19   20   23   24    1      0.0    0.4 6      0.0    0.4 6 ; dih   CCD  CCH  CBZ  CAH
  13   23   24   25    1    180.0   41.8 2    180.0   41.8 2 ; dih   NCF  CBZ  CAH  CAG
  23   24   25   26    1    180.0   41.8 2    180.0   41.8 2 ; dih   CBZ  CAH  CAG  CAI
  24   25   26   27    1    180.0   41.8 2    180.0   41.8 2 ; dih   CAH  CAG  CAI  CCA
  37   27   26   25    1    180.0   41.8 2    180.0   41.8 2 ; dih   NCG  CCA  CAI  CAG
  26   27   28   31    1      0.0    0.4 6      0.0    0.4 6 ; dih   CAI  CCA  CCI  CCE
  26   27   37   38    1    180.0   33.5 2    180.0   33.5 2 ; dih   CAI  CCA  NCG  CBY
  27   28   31   36    1      0.0    0.4 6      0.0    0.4 6 ; dih   CCA  CCI  CCE  CCC
  31   36   37   38    1    180.0   33.5 2    180.0   33.5 2 ; dih   CCE  CCC  NCG  CBY
  26   37   38   39    1      0.0    3.8 6      0.0    3.8 6 ; dih   CCA  NCG  CBY  CBW
  40   39   38   37    1      0.0    5.9 3      0.0    5.9 3 ; dih   CBU  CBW  CBY  NCG
```

```
  41   40   39   38    3
  42   41   40   39    3
  43   42   41   40    3
  44   43   42   41    3
  45   44   43   42    3
  46   45   44   43    3
  47   46   45   44    3
  48   47   46   45    3
  49   48   47   46    3

; Strong position restraints for InflateGRO
#ifdef STRONG_POSRES
#include "strong_posre.itp"
#endif
```

S2 Simulation Setup

Construction of the desired bilayers was a multi-step process. First, the PDB file of a template bilayer consisting of 128 DPPC molecules and water was obtained from the Tieleman website [http://people.ucalgary.ca/~tieleman/download.html]. Water was then removed and the system was tiled 2 times in both the *x* and *y* dimensions to create a bilayer with 512 DPPC molecules, with the *z*-axis being normal to the bilayer. One DPPC per leaflet was chosen so that their separation distance, including periodic copies, was maximized. These two DPPC molecules were then removed from the template bilayer and replaced with either two identical probe molecules (DiI-C18:0, DiI-C18:2, DiI-C12:0) or two DPPC (as a control). These inserted molecules were randomly rotated about their z-axis, and placed at the (*x,y*) position of the removed DPPC molecule. To minimize the possibility of atomic overlap, the inserted molecules were initially placed so that they were protruding from the bilayer, with only the ends of their hydrocarbon chains within the bilayer, and energy minimization was performed to reduce unfavorable interactions or overlaps. The inserted molecules were then moved 1 nm into the bilayer in 0.05 nm increments along the bilayer normal, with energy minimization performed at each step.

We tested a variety of simulation parameters, choosing particular values based on their ability to reproduce experimentally measured parameters. Importantly, we found that our results are robust even under different conditions including a lower hydration level or lower pressure (results not shown). We also saw that for the pure DPPC control simulations, insertion of the DPPC molecule did not cause bilayer perturbations.

Table S1. Number of lipids per shell after partitioning. The shell assignments described in Equation 3 partition the leaflets such that there are ~ 6*n* lipids in shell *n*, for all systems studied. For shell $n > 7$ the shell diameters exceed the (*x,y*) box dimensions, leading to a decrease in the number of lipids per shell for the remaining shells.

inserted molecule	leaf	shell 0	shell 1	shell 2	shell 3	shell 4	shell 5	shell 6	shell 7	shell 8	shell 9	shell 10	shell 11
DPPC	same		6.01±0.02	12.00±0.03	18.04±0.03	23.99±0.03	30.00±0.04	35.99±0.04	42.00±0.04	44.23±0.05	24.86±0.04	13.32±0.03	4.56±0.01
DPPC	opp.	1.000±0.007	6.00±0.02	12.00±0.03	18.00±0.04	23.99±0.05	30.01±0.03	35.99±0.03	42.01±0.05	44.23±0.04	24.88±0.04	13.32±0.03	4.56±0.01
DiI-C18:0	same		6.0±0.1	12.1±0.3	18.1±0.4	24.0±0.4	30.1±0.6	36.0±0.5	41.8±0.5	44.3±0.6	24.8±0.5	13.3±0.4	4.5±0.1
DiI-C18:0	opp.	0.97±0.09	5.8±0.2	12.0±0.3	18.2±0.3	24.2±0.3	30.0±0.4	36.1±0.5	41.9±0.5	44.0±0.6	24.6±0.3	12.9±0.3	4.4±0.2
DiI-C18:2	same		5.9±0.2	12.0±0.3	18.1±0.3	24.1±0.4	30.1±0.4	36.2±0.4	41.7±0.4	44.3±0.4	24.7±0.3	13.3±0.2	4.6±0.2
DiI-C18:2	opp.	0.97±0.09	5.8±0.1	12.0±0.3	18.2±0.3	24.0±0.4	30.1±0.6	36.1±0.5	41.8±0.4	44.1±0.4	24.6±0.3	12.9±0.2	4.4±0.2
DiI-C12:0	same		5.9±0.2	12.2±0.4	17.9±0.4	24.0±0.5	29.9±0.4	36.4±0.5	41.8±0.5	44.3±0.4	24.7±0.5	13.2±0.3	4.5±0.1
DiI-C12:0	opp.	0.98±0.09	5.9±0.2	12.0±0.2	17.9±0.4	24.2±0.4	30.1±0.4	35.9±0.5	42.0±0.6	44.2±0.6	24.5±0.4	12.9±0.3	4.4±0.2

Table S2. DPPC chain order by shell. The average acyl chain order parameter S_{CD} (Eq. 4) for DPPC partitioned into shells, for each leaflet. Overall average for each system is shown in the last column.

inserted molecule	leaf	shell 0	shell 1	shell 2	shell 3	shell 4	shell 5	shell 6	shell 7	shell 8	shell 9	shell 10	shell 11	Avg.
DPPC	same		0.169 ±0.001	0.166 ±0.001	0.165 ±0.001	0.165 ±0.001	0.165 ±0.001	0.165 ±0.001	0.165± 0.001	0.165± 0.001	0.165± 0.001	0.166± 0.001	0.166± 0.001	**0.165±0.001**
DPPC	opp.	0.165 ±0.002	0.166 ±0.002	0.166 ±0.002	0.166 ±0.001	0.165 ±0.001	0.165 ±0.001	0.165 ±0.001	0.165 ±0.001	0.165 ±0.001	0.166 ±0.001	0.165 ±0.001	0.166 ±0.001	
DiI-C18:0	same		0.15±0.01	0.172 ±0.009	0.171 ±0.006	0.169 ±0.004	0.167 ±0.004	0.166 ±0.003	0.165 ±0.004	0.165 ±0.004	0.167 ±0.004	0.166 ±0.006	0.16 ±0.01	**0.166±0.001**
DiI-C18:0	opp.	0.15±0.01	0.158 ±0.008	0.166 ±0.006	0.170 ±0.005	0.170 ±0.004	0.168 ±0.004	0.166 ±0.002	0.165 ±0.002	0.165 ±0.003	0.166 ±0.004	0.165 ±0.007	0.16±0.01	
DiI-C18:2	same		0.148 ±0.009	0.169 ±0.005	0.170 ±0.005	0.170 ±0.005	0.169 ±0.003	0.167 ±0.004	0.165 ±0.002	0.165 ±0.003	0.165 ±0.003	0.165 ±0.005	0.16±0.01	**0.166±0.001**
DiI-C18:2	opp.	0.15±0.01	0.16±0.01	0.164 ±0.007	0.170 ±0.004	0.170 ±0.004	0.168 ±0.003	0.167 ±0.004	0.166 ±0.003	0.165 ±0.003	0.166 ±0.005	0.166 ±0.006	0.17±0.01	
DiI-C12:0	same		0.152 ±0.009	0.171 ±0.006	0.169 ±0.005	0.168 ±0.004	0.167 ±0.004	0.167 ±0.003	0.166 ±0.002	0.166 ±0.003	0.166 ±0.004	0.164 ±0.006	0.16±0.01	**0.1664±0.0008**
DiI-C12:0	opp.	0.16±0.01	0.16±0.01	0.164 ±0.008	0.168 ±0.004	0.168 ±0.004	0.167 ±0.004	0.167 ±0.003	0.166 ±0.003	0.166 ±0.003	0.166 ±0.004	0.164 ±0.007	0.16±0.01	

Table S3. P-N vector angle by shell with respect to the bilayer normal. The average P-N vector angle of all shells in each leaflet for each system is shown. Overall average for each system is shown in the last column.

inserted molecule	leaf	shell 0	shell 1	shell 2	shell 3	shell 4	shell 5	shell 6	shell 7	shell 8	shell 9	shell 10	shell 11	Avg
DPPC	same		79.6±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.6±0.2	79.5±0.2	**79.5±0.2**
DPPC	opp.	79.6±0.4	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	79.5±0.2	
DiI-C18:0	same		71±2	77±2	79±1	79±1	80±1	79.3±0.7	79.4±0.7	79.5±0.6	78.9±0.9	79±1	79±2	**79.1±0.2**
DiI-C18:0	opp.	79±4	79±2	79±1	79±1	79.4±0.9	79.4±0.7	79.3±0.8	79.2±0.6	79±1	78.4±0.8	77±1	77±3	
DiI-C18:2	same		71±3	78±2	79±1	79±1	79.2±0.9	79.5±0.7	79.4±0.8	79.5±0.8	79.3±0.9	79±1	79±2	**79.0±0.2**
DiI-C18:2	opp.	80±4	79±2	79±1	79±1	79.0±0.9	79.5±0.7	79.2±0.6	79.4±0.7	79.0±0.7	78.6±0.8	78±2	77±3	
DiI-C12:0	same		71±2	78±1	79±1	79±1	79.4±0.9	79.4±0.9	79.3±0.6	79.4±0.7	79.2±0.6	80±1	79±2	**79.0±0.1**
DiI-C12:0	opp.	80±5	79±1	79±2	79±1	79±1	79.5±0.7	79.4±0.6	79.3±0.7	79.0±0.8	79.5±0.9	78±1	77±4	

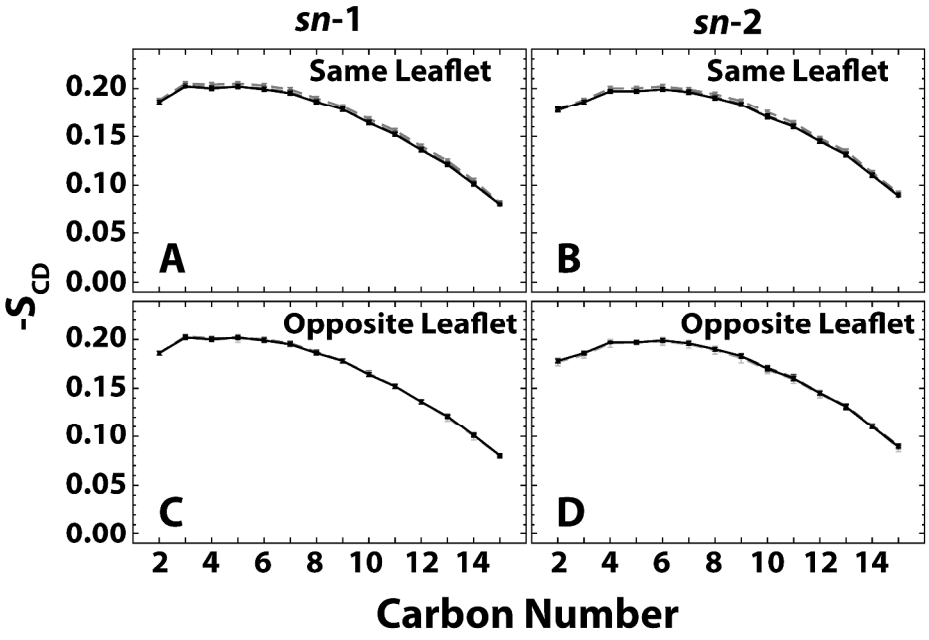

Figure S1. Order parameter by shell for a pure DPPC bilayer reveals a partitioning artifact. Order parameter of DPPC carbons shown for same leaflet lipids (*A,B*) and opposite leaflet lipids (*C,D*) for a pure DPPC bilayer. Shells $n \leq 3$ are shown (gray dashed) with darker grays indicating increasing shell number. Overall average order for the pure DPPC bilayers (black solid) is shown for comparison. For same leaflet lipids, first shell order is marginally increased due to the partitioning scheme, while opposite leaflet lipids are unaffected.

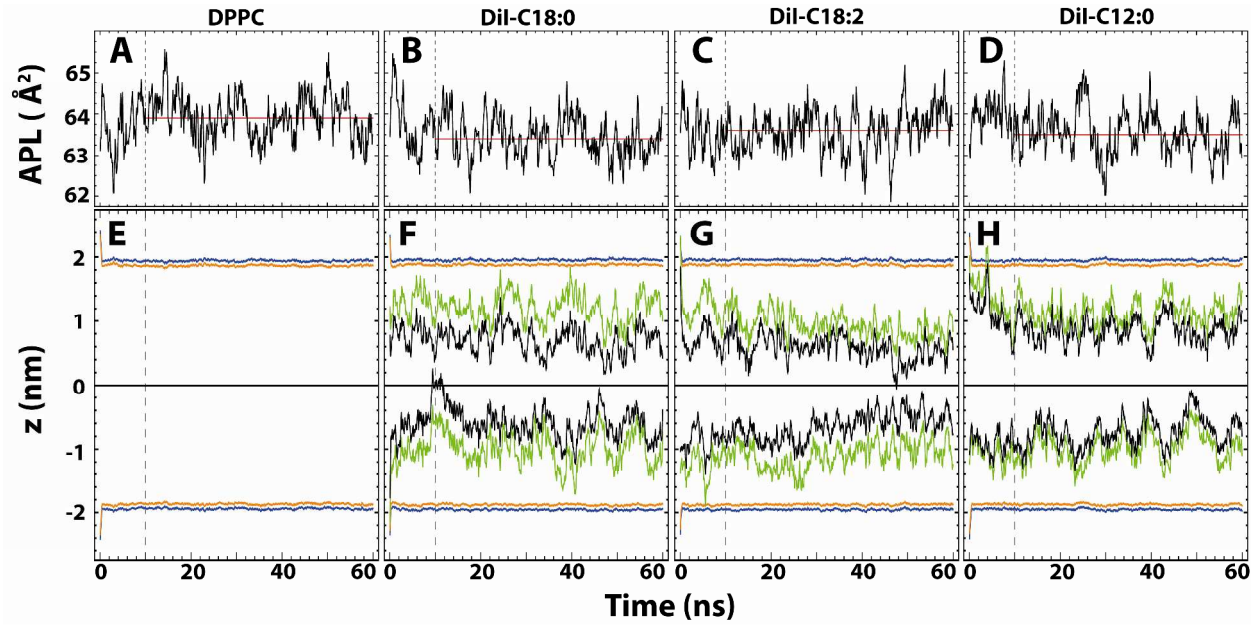

Figure S2. Representative data showing equilibration of pure DPPC and DiI-containing, simulations. *A-D*, APL during a representative 60 ns simulation of the systems studied. The average value over the final 50 ns is shown (red line). *E-H*, transverse bilayer position with respect to the bilayer midplane (z = 0 nm) of DPPC nitrogen (blue) and phosphate (yellow), and center-of-mass of the DiI chromophore (green) and entire DiI molecule (black).

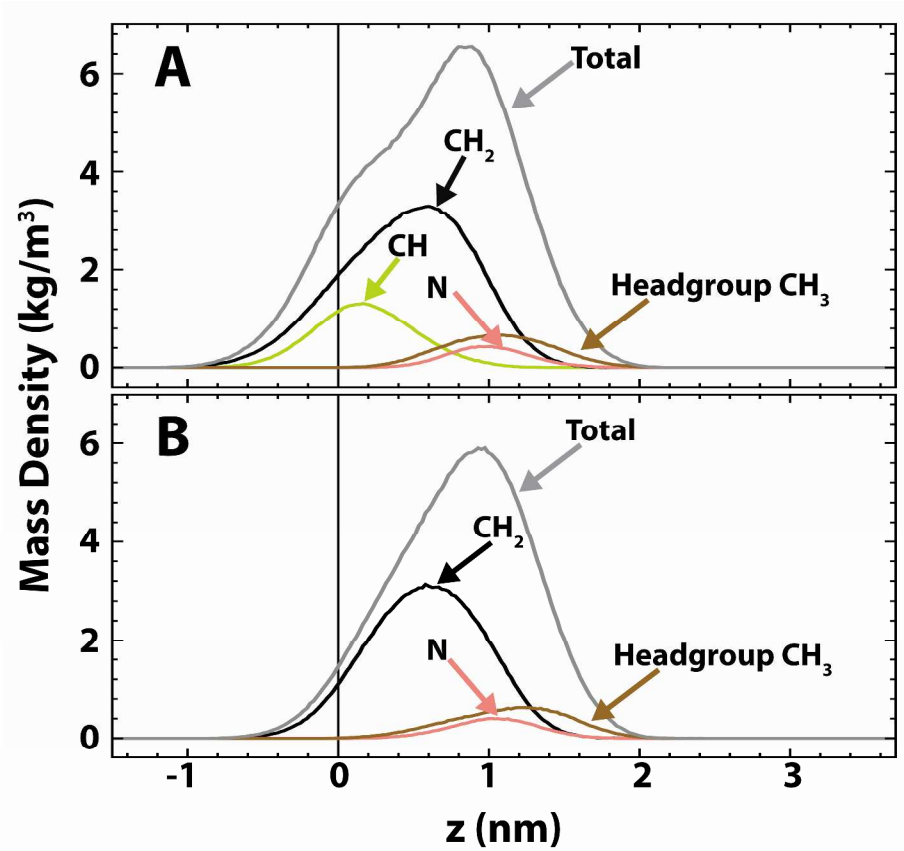

Figure S3. Average single-leaflet mass density profiles for simulations. *A*, average densities of DiI-C18:2 components. *B*, average densities for DiI-C12:0 components. Bilayer midplane at z = 0 nm.

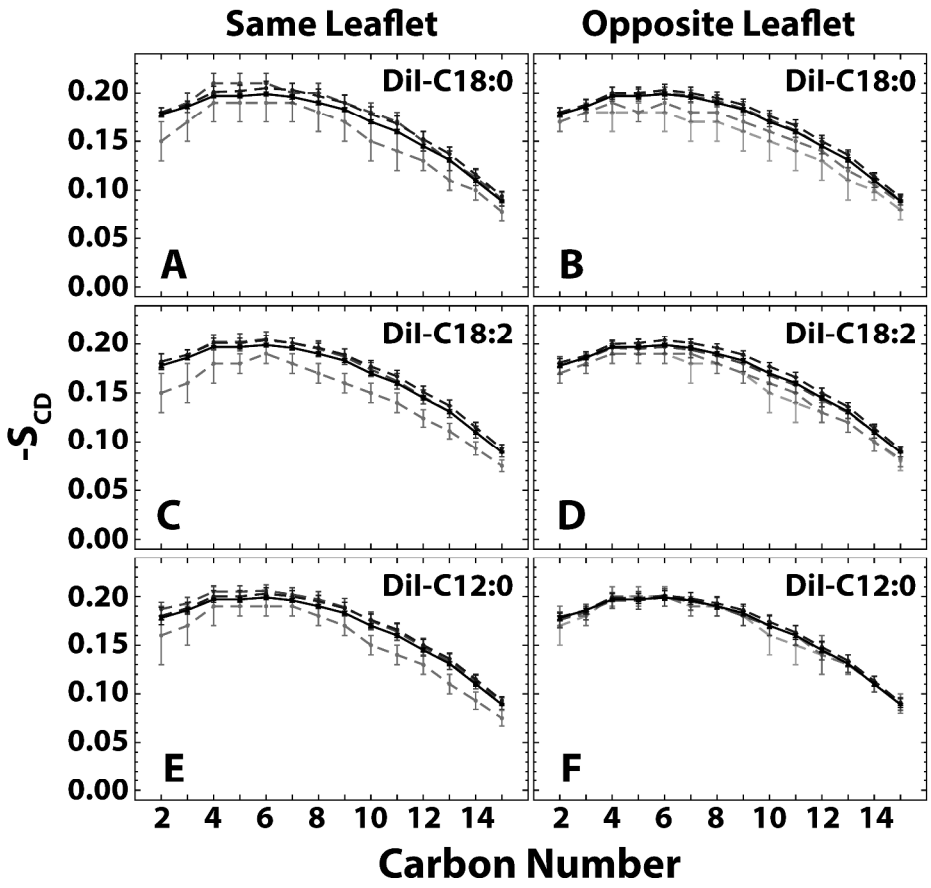

Figure S4. DPPC *sn*-2 carbon order perturbation depends on shell, not carbon number. Order parameter of DPPC *sn*-2 carbons shown for same leaflet lipids (*left*) and opposite leaflet lipids (*right*) for bilayers containing DiI-C18:0 (*A,B*), DiI-C18:2 (*C,D*) and DiI-C12:0 (*E,F*). Shells $n \leq 3$ are shown (gray dashed), with darker grays indicating increased shell number. Overall average *sn*-2 order for pure DPPC bilayers (black solid) is shown for comparison. Error bars indicate the standard deviation.

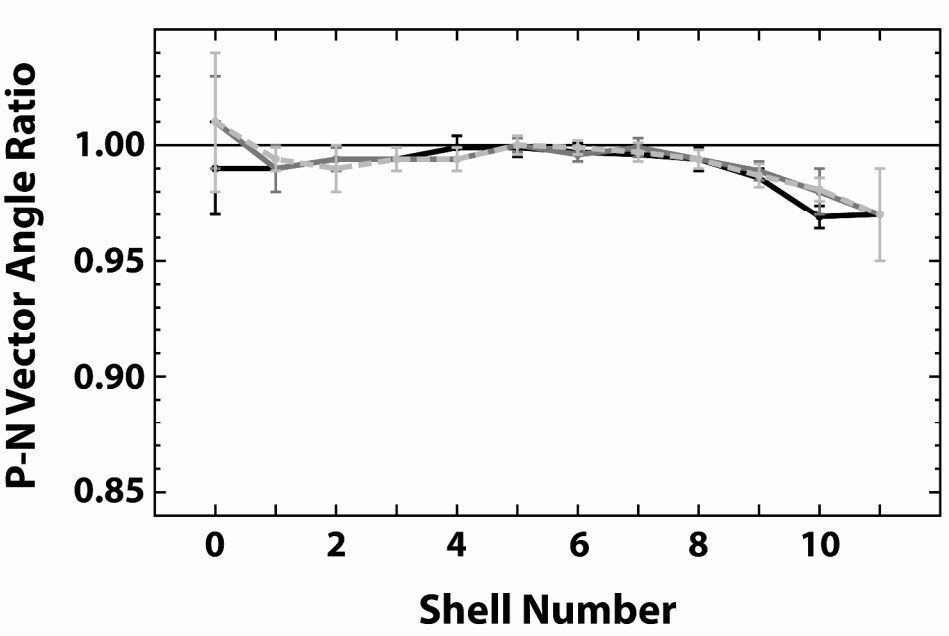

Figure S5. DPPC headgroups show no preferential orientation in the leaflet opposite the probe. P-N vector angle ratio by shell for opposite leaflet lipids in bilayers containing DiI-C18:0 (black), DiI-C18:2 (dark gray) and DiI-C12:0 (light gray dashed) compared to the pure DPPC simulations. Error bars indicate 95% confidence intervals.