Salt effect on mixed composition membranes containing an antioxidant lipophilic edaravone derivative: a computational-experimental study

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Parameter file for C18-EdV:

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[ moleculetype ]

; name   nrexcl

EDV          3


[ atoms ]

; nr       type      resnr     residu    atom     cgnr      charge    mass
   1    CG2R61     1     EDV     C1     1     0.176    12.0110   ; qtot  0.176
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   6    CG2R61     1     EDV     C6     6    -0.116    12.0110   ; qtot -0.405
   7    CG2R52     1     EDV     C7     7     0.675    12.0110   ; qtot  0.270
   8    CG3C51     1     EDV     C8     8    -0.399    12.0110   ; qtot -0.129
   9    NG2R53     1     EDV     N1     9     0.211    14.0070   ; qtot  0.082
  10    NG2R50     1     EDV     N2     10    -0.785    14.0070   ; qtot -0.703
  11     CG331     1     EDV     C9     11    -0.185    12.0110   ; qtot -0.888
  12    CG2R53     1     EDV     C10    12     0.334    12.0110   ; qtot -0.554
  13     OG2D1     1     EDV     O      13    -0.434    15.9994   ; qtot -0.988
  14     CG321     1     EDV     C11    14    -0.197    12.0110   ; qtot -1.185
  15     CG321     1     EDV     C12    15    -0.167    12.0110   ; qtot -1.352
  16     CG321     1     EDV     C13    16    -0.175    12.0110   ; qtot -1.527
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28	CG321	1	EDV	C25	28	-0.179	12.0110	; qtot -3.686
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30	CG321	1	EDV	C27	30	-0.177	12.0110	; qtot -4.044
31	CG331	1	EDV	C28	31	-0.273	12.0110	; qtot -4.317
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37	HGA1	1	EDV	H6	37	0.142	1.0080	; qtot -3.600
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43	HGA2	1	EDV	H12	43	0.090	1.0080	; qtot -3.060
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   76     HGA3    1    EDV   H45    76     0.090    1.0080  ; qtot -0.090
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List of atoms:

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 CG2R53    6   12.0110    0.334    A   3.91995435982e-01   8.368000e-02
 CG2R61    6   12.0110    0.176    A   3.55005321205e-01   2.928800e-01
 CG321     6   12.0110   -0.197    A   3.58141284692e-01   2.343040e-01 ;  3.38541512893e-01   4.184000e-02
  CG331    6   12.0110   -0.185    A   3.65268474438e-01   3.263520e-01 ;  3.38541512893e-01   4.184000e-02
 CG3C51    6   12.0110   -0.399    A   3.58141284692e-01   1.506240e-01 ;  3.38541512893e-01   4.184000e-02
   HGA1    1    1.0080    0.142    A   2.38760856462e-01   1.882800e-01
   HGA2    1    1.0080    0.090    A   2.38760856462e-01   1.464400e-01
   HGA3    1    1.0080    0.090    A   2.38760856462e-01   1.004160e-01
  HGR61    1    1.0080    0.115    A   2.42003727796e-01   1.255200e-01
 NG2R50    7   14.0070   -0.785    A   3.29632525712e-01   8.368000e-01
 NG2R53    7   14.0070    0.211    A   3.29632525712e-01   8.368000e-01
  OG2D1    8   15.9994   -0.434    A   3.02905564168e-01   5.020800e-01 ;  2.49451641079e-01   5.020800e-01

[ bondtypes ]
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 CG2R52   CG321    1  1.500000e-01  2.468560e+05
 CG2R52   CG331    1  1.500000e-01  1.921544e+05
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CG2R52 NG2R50 1 1.315000e-01 3.347200e+05

CG2R53 CG2R61 1 1.440000e-01 2.510400e+05

CG2R53 CG321 1 1.500000e-01 3.556400e+05

CG2R53 CG331 1 1.500000e-01 3.556400e+05

CG2R53 CG3C51 1 1.530000e-01 2.510400e+05

CG2R53 NG2R50 1 1.320000e-01 3.347200e+05

CG2R53 NG2R53 1 1.380000e-01 3.849280e+05

CG2R53 OG2D1 1 1.235000e-01 4.769760e+05

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CG2R61 CG321 1 1.490000e-01 1.924640e+05

CG2R61 CG331 1 1.490000e-01 1.924640e+05

CG2R61 HGR61 1 1.080000e-01 2.845120e+05

CG2R61 NG2R53 1 1.414000e-01 2.552240e+05

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CG321 CG331 1 1.528000e-01 1.861880e+05

CG321 CG3C51 1 1.528000e-01 1.861880e+05

CG321 HGA2 1 1.111000e-01 2.585712e+05

CG321 NG2R53 1 1.430000e-01 2.677760e+05

CG331 CG331 1 1.530000e-01 1.861880e+05

CG331 CG3C51 1 1.528000e-01 1.861880e+05

CG331 HGA3 1 1.111000e-01 2.694496e+05

CG331 NG2R53 1 1.430000e-01 2.677760e+05

CG3C51 CG3C51 1 1.518000e-01 1.631760e+05

CG3C51 HGA1 1 1.100000e-01 2.568976e+05

NG2R50 NG2R50 1 1.290000e-01 2.845120e+05

NG2R50 NG2R53 1 1.355000e-01 3.012480e+05

[pairtypes]

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CG2R52 CG3C51 1 3.65268474438e-01 5.91706954497e-02

CG2R52 OG2D1 1 3.20723538531e-01 2.04973301676e-01

CG2R53 CG321 1 3.65268474438e-01 5.91706954497e-02

CG2R53 CG331 1 3.65268474438e-01 5.91706954497e-02

CG2R53 CG3C51 1 3.65268474438e-01 5.91706954497e-02

CG2R53 OG2D1 1 3.20723538531e-01 2.04973301676e-01

CG2R61 CG321 1 3.46773417049e-01 1.10698234855e-01

CG2R61 CG331 1 3.46773417049e-01 1.10698234855e-01

CG2R61 CG3C51 1 3.46773417049e-01 1.10698234855e-01

CG2R61 OG2D1 1 3.02228481142e-01 3.83469934154e-01

CG321 CG321 1 3.38541512893e-01 4.18400000000e-02

CG321 CG331 1 3.38541512893e-01 4.18400000000e-02

CG321 CG3C51 1 3.38541512893e-01 4.18400000000e-02

CG321 HGA1 1 2.88651184677e-01 8.87560431745e-02

CG321 HGA2 1 2.88651184677e-01 7.82754725313e-02

CG321 HGA3 1 2.88651184677e-01 6.48182492821e-02

CG321 HGR61 1 2.90272620344e-01 7.24690057887e-02

CG321 NG2R50 1 3.34087019303e-01 1.87114168357e-01

CG321 NG2R53 1 3.34087019303e-01 1.87114168357e-01

CG321 OG2D1 1 2.93996576986e-01 1.44938011577e-01

CG331 CG331 1 3.38541512893e-01 4.18400000000e-02

CG331 CG3C51 1 3.38541512893e-01 4.18400000000e-02

CG331 HGA1 1 2.88651184677e-01 8.87560431745e-02

CG331 HGA2 1 2.88651184677e-01 7.82754725313e-02

CG331 HGA3 1 2.88651184677e-01 6.48182492821e-02

CG331 HGR61 1 2.90272620344e-01 7.24690057887e-02

CG331 NG2R50 1 3.34087019303e-01 1.87114168357e-01

CG331 NG2R53 1 3.34087019303e-01 1.87114168357e-01

CG331 OG2D1 1 2.93996576986e-01 1.44938011577e-01

CG3C51 CG3C51 1 3.38541512893e-01 4.18400000000e-02

CG3C51 HGA1 1 2.88651184677e-01 8.87560431745e-02

CG3C51 HGA2 1 2.88651184677e-01 7.82754725313e-02

CG3C51 HGA3 1 2.88651184677e-01 6.48182492821e-02

CG3C51 HGR61 1 2.90272620344e-01 7.24690057887e-02

CG3C51 NG2R50 1 3.34087019303e-01 1.87114168357e-01

CG3C51 NG2R53 1 3.34087019303e-01 1.87114168357e-01

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  HGA1   OG2D1    1  2.44106248770e-01  3.07459952514e-01
  HGA2   OG2D1    1  2.44106248770e-01  2.71154190821e-01
  HGA3   OG2D1    1  2.44106248770e-01  2.24537002029e-01
 HGR61   OG2D1    1  2.45727684437e-01  2.51040000000e-01
 NG2R50   OG2D1    1  2.89542083396e-01  6.48182492821e-01
 NG2R53   OG2D1    1  2.89542083396e-01  6.48182492821e-01
  OG2D1   OG2D1    1  2.49451641079e-01  5.02080000000e-01

[ angletypes ]
; i         j         k         func      th0       cth       S0        Kub
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 CG2R52   CG321   CG321    5  1.1100000e+02  4.8534400e+02  0.0000000e+00  0.0000000e+00
 CG2R52   CG321    HGA2    5  1.0950000e+02  4.1840000e+02  0.0000000e+00  0.0000000e+00
 CG2R52   CG331    HGA3    5  1.0950000e+02  4.6024000e+02  0.0000000e+00  0.0000000e+00
 CG2R52  CG3C51  CG2R53    5  1.0800000e+02  3.7656000e+02  0.0000000e+00  0.0000000e+00
 CG2R52  CG3C51   CG321    5  1.0300000e+02  3.7656000e+02  0.0000000e+00  0.0000000e+00
 CG2R52  CG3C51    HGA1    5  1.1100000e+02  4.8534400e+02  0.0000000e+00  0.0000000e+00
 CG2R52  NG2R50  NG2R53    5  1.0350000e+02  1.3388800e+03  0.0000000e+00  0.0000000e+00
 CG2R53  CG2R61  CG2R61    5  1.2000000e+02  2.6777600e+02  0.0000000e+00  0.0000000e+00
 CG2R53   CG321   CG321    5  1.1100000e+02  4.9371200e+02  0.0000000e+00  0.0000000e+00
 CG2R53   CG321   CG331    5  1.1100000e+02  4.9371200e+02  0.0000000e+00  0.0000000e+00
 CG2R53   CG321    HGA2    5  1.0950000e+02  4.6024000e+02  0.0000000e+00  0.0000000e+00
 CG2R53   CG331    HGA3    5  1.0950000e+02  4.6024000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  CG3C51   CG321    5  1.0300000e+02  3.7656000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  CG3C51    HGA1    5  1.1100000e+02  4.8534400e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R50  CG2R53    5  1.0100000e+02  8.3680000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R50  NG2R50    5  1.0590000e+02  9.2048000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R53  CG2R53    5  1.2050000e+02  4.6024000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R53  CG2R61    5  1.2700000e+02  3.3472000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R53   CG321    5  1.2000000e+02  4.1840000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R53   CG331    5  1.2400000e+02  2.5104000e+02  0.0000000e+00  0.0000000e+00
 CG2R53  NG2R53  NG2R50    5  1.1100000e+02  2.9288000e+02  0.0000000e+00  0.0000000e+00
 CG2R61  CG2R53  NG2R50    5  1.2450000e+02  2.0920000e+02  0.0000000e+00  0.0000000e+00
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CG2R61 CG2R61 CG321 5 1.2000000e+02 3.8325440e+02 0.0000000e+00 0.0000000e+00

CG2R61 CG2R61 CG331 5 1.2000000e+02 3.8325440e+02 0.0000000e+00 0.0000000e+00

CG2R61 CG2R61 HGR61 5 1.2000000e+02 2.5104000e+02 2.1525000e-01 1.8409600e+04

CG2R61 CG2R61 NG2R53 5 1.2000000e+02 3.3472000e+02 2.4162000e-01 2.9288000e+04

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CG2R61 CG321 CG331 5 1.0750000e+02 4.3346240e+02 0.0000000e+00 0.0000000e+00

CG2R61 CG321 HGA2 5 1.0750000e+02 4.1254240e+02 0.0000000e+00 0.0000000e+00

CG2R61 CG331 HGA3 5 1.0750000e+02 4.1254240e+02 0.0000000e+00 0.0000000e+00

CG2R61 NG2R53 NG2R50 5 1.1800000e+02 3.3472000e+02 0.0000000e+00 0.0000000e+00

CG321 CG2R52 NG2R50 5 1.2000000e+02 3.7656000e+02 0.0000000e+00 0.0000000e+00

CG321 CG2R53 NG2R50 5 1.2300000e+02 3.8325440e+02 0.0000000e+00 0.0000000e+00

CG321 CG321 CG321 5 1.1360000e+02 4.8827280e+02 2.5610000e-01 9.3386880e+03

CG321 CG321 CG331 5 1.1500000e+02 4.8534400e+02 2.5610000e-01 6.6944000e+03

CG321 CG321 CG3C51 5 1.1200000e+02 4.4350400e+02 2.5610000e-01 6.6944000e+03

CG321 CG321 HGA2 5 1.1010000e+02 2.2175200e+02 2.1790000e-01 1.8853104e+04

CG321 CG321 NG2R53 5 1.1350000e+02 5.8576000e+02 0.0000000e+00 0.0000000e+00

CG321 CG331 HGA3 5 1.1010000e+02 2.8953280e+02 2.1790000e-01 1.8853104e+04

CG321 CG3C51 CG3C51 5 1.1500000e+02 4.8534400e+02 2.5610000e-01 6.6944000e+03

CG321 CG3C51 HGA1 5 1.1010000e+02 2.8953280e+02 2.1790000e-01 1.8853104e+04

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CG331 CG2R53 NG2R50 5 1.2300000e+02 3.8325440e+02 0.0000000e+00 0.0000000e+00

CG331 CG321 CG331 5 1.1400000e+02 4.4643280e+02 2.5610000e-01 6.6944000e+03

CG331 CG321 HGA2 5 1.1010000e+02 2.8953280e+02 2.1790000e-01 1.8853104e+04

CG331 CG321 NG2R53 5 1.2000000e+02 5.8576000e+02 0.0000000e+00 0.0000000e+00

CG331 CG331 HGA3 5 1.1010000e+02 3.1380000e+02 2.1790000e-01 1.8853104e+04

CG331 CG3C51 CG3C51 5 1.1500000e+02 4.8534400e+02 2.5610000e-01 6.6944000e+03

CG331 CG3C51 HGA1 5 1.1010000e+02 2.8953280e+02 2.1790000e-01 1.8853104e+04

CG3C51 CG2R52 NG2R50 5 1.1200000e+02 1.4225600e+03 0.0000000e+00 0.0000000e+00

CG3C51 CG2R53 NG2R53 5 1.0550000e+02 1.0041600e+03 0.0000000e+00 0.0000000e+00

CG3C51 CG2R53 OG2D1 5 1.2670000e+02 5.4392000e+02 0.0000000e+00 0.0000000e+00

CG3C51 CG321 HGA2 5 1.1010000e+02 2.8953280e+02 2.1790000e-01 1.8853104e+04

CG3C51 CG331 HGA3 5 1.1010000e+02 2.8953280e+02 2.1790000e-01 1.8853104e+04

CG3C51 CG3C51 CG3C51 5 1.0950000e+02 4.8534400e+02 2.5610000e-01 9.3386880e+03

CG3C51 CG3C51 HGA1 5 1.1140000e+02 2.9288000e+02 2.1790000e-01 1.8853104e+04

HGA2 CG321 HGA2 5 1.0900000e+02 2.9706400e+02 1.8020000e-01 4.5187200e+03

HGA3 CG331 HGA3 5 1.0840000e+02 2.9706400e+02 1.8020000e-01 4.5187200e+03

NG2R50 CG2R53 NG2R50 5 1.1100000e+02 8.3680000e+02 0.0000000e+00 0.0000000e+00

NG2R50 NG2R50 NG2R50 5 1.0820000e+02 1.3388800e+03 0.0000000e+00 0.0000000e+00

NG2R53 CG2R53 NG2R53 5 1.0440000e+02 6.2760000e+02 0.0000000e+00 0.0000000e+00

NG2R53 CG2R53 OG2D1 5 1.2780000e+02 5.4392000e+02 0.0000000e+00 0.0000000e+00

NG2R53 CG321 HGA2 5 1.0950000e+02 4.3095200e+02 0.0000000e+00 0.0000000e+00

NG2R53 CG331 HGA3 5 1.0900000e+02 3.2635200e+02 0.0000000e+00 0.0000000e+00

[dihedraltypes]

; i j k l func phi0 cp mult

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CG2R52 CG321 CG321 HGA2 9 0.000000e+00 8.368000e-01 3

CG2R52 NG2R50 NG2R53 CG2R53 9 1.800000e+02 4.184000e+01 2

CG2R52 NG2R50 NG2R53 CG2R61 9 1.800000e+02 5.857600e+00 2

CG2R53 CG2R61 CG2R61 CG2R61 9 1.800000e+02 1.255200e+01 2

CG2R53 CG2R61 CG2R61 HGR61 9 1.800000e+02 8.368000e+00 2

CG2R53 CG321 CG321 HGA2 9 0.000000e+00 8.368000e-01 3

CG2R53 CG321 CG331 HGA3 9 0.000000e+00 6.694400e-01 3

CG2R53 NG2R50 NG2R50 NG2R50 9 1.800000e+02 6.485200e+01 2

CG2R61 CG2R61 CG2R61 CG2R61 9 1.800000e+02 1.297040e+01 2

CG2R61 CG2R61 CG2R61 CG321 9 1.800000e+02 1.297040e+01 2

CG2R61 CG2R61 CG2R61 CG331 9 1.800000e+02 1.297040e+01 2

CG2R61 CG2R61 CG2R61 HGR61 9 1.800000e+02 1.757280e+01 2

CG2R61 CG2R61 CG2R61 NG2R53 9 1.800000e+02 1.297040e+01 2

CG2R61 CG2R61 CG321 CG2R61 9 1.800000e+02 9.623200e-01 2

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CG2R61 CG2R61 CG321 CG331 9 1.800000e+02 9.623200e-01 2

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CG2R61 CG2R61 CG331 HGA3 9 0.000000e+00 8.368000e-03 6

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CG2R61 CG2R61 NG2R53 CG2R53 9 1.800000e+02 4.602400e+00 2

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CG2R61 CG321 CG321 CG321 9 0.000000e+00 1.673600e-01 3

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CG2R61 CG321 CG321 HGA2 9 0.000000e+00 1.673600e-01 3

CG2R61 CG321 CG331 HGA3 9 0.000000e+00 1.673600e-01 3

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CG321 CG2R61 CG2R61 HGR61 9 1.800000e+02 1.004160e+01 2

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CG321 CG3C51 CG3C51 HGA1 9 0.000000e+00 7.949600e-01 3

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CG3C51 CG2R52 CG331 HGA3 9 0.000000e+00 1.471931e+00 3

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CG3C51 CG2R53 NG2R53 CG2R53 9 1.800000e+02 8.368000e-01 2

CG3C51 CG2R53 NG2R53 CG2R61 9 1.800000e+02 8.368000e-01 2

CG3C51 CG2R53 NG2R53 CG321 9 1.800000e+02 8.368000e-01 2

CG3C51 CG2R53 NG2R53 CG331 9 1.800000e+02 8.368000e-01 2

CG3C51 CG2R53 NG2R53 NG2R50 9 1.800000e+02 8.368000e-01 2

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HGA1 CG3C51 CG3C51 HGA1 9 0.000000e+00 7.949600e-01 3

HGA2 CG321 CG321 HGA2 9 0.000000e+00 9.204800e-01 3

HGA2 CG321 CG331 HGA3 9 0.000000e+00 6.694400e-01 3

HGA2 CG321 CG3C51 CG2R52 9 0.000000e+00 0.000000e+00 3

HGA2 CG321 CG3C51 CG2R53 9 0.000000e+00 0.000000e+00 3

HGA2 CG321 CG3C51 CG3C51 9 0.000000e+00 6.694400e-01 3

HGA2 CG321 CG3C51 HGA1 9 0.000000e+00 6.694400e-01 3

HGA2 CG321 NG2R53 CG2R53 9 0.000000e+00 0.000000e+00 1

HGA3 CG331 CG331 HGA3 9 0.000000e+00 6.485200e-01 3

HGA3 CG331 CG3C51 CG3C51 9 0.000000e+00 6.694400e-01 3

HGA3 CG331 CG3C51 HGA1 9 0.000000e+00 6.694400e-01 3

HGA3 CG331 NG2R53 CG2R53 9 0.000000e+00 4.184000e-01 3

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NG2R50 CG2R52 CG321 CG321 9 0.000000e+00 7.949600e-01 3

NG2R50 CG2R52 CG321 HGA2 9 0.000000e+00 7.949600e-01 3

NG2R50 CG2R52 CG331 HGA3 9 0.000000e+00 7.949600e-01 3

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NG2R50 CG2R52 CG3C51 CG321 9 1.800000e+02 1.171520e+01 3

NG2R50 CG2R52 CG3C51 HGA1 9 0.000000e+00 5.857600e+00 3

NG2R50 CG2R53 CG2R61 CG2R61 9 0.000000e+00 4.184000e-01 4

NG2R50 CG2R53 CG2R61 CG2R61 9 1.800000e+02 3.723760e+00 2

NG2R50 CG2R53 CG321 CG321 9 0.000000e+00 6.234160e-02 2

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NG2R50 CG2R53 CG321 CG321 9 1.800000e+02 1.522139e+00 1

NG2R50 CG2R53 CG321 CG331 9 0.000000e+00 6.234160e-02 2

NG2R50 CG2R53 CG321 CG331 9 0.000000e+00 1.234280e-01 6

NG2R50 CG2R53 CG321 CG331 9 1.800000e+02 1.188674e+00 3

NG2R50 CG2R53 CG321 CG331 9 1.800000e+02 1.522139e+00 1

NG2R50 CG2R53 CG321 HGA2 9 0.000000e+00 7.949600e-01 3

NG2R50 CG2R53 CG331 HGA3 9 0.000000e+00 7.949600e-01 3

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NG2R50 CG2R53 NG2R50 NG2R50 9 1.800000e+02 5.251422e+01 2

NG2R53 CG2R53 CG3C51 CG2R52 9 1.800000e+02 4.184000e+00 3

NG2R53 CG2R53 CG3C51 CG321 9 1.800000e+02 4.184000e+00 3

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NG2R53 CG2R61 CG2R61 HGR61 9 1.800000e+02 1.004160e+01 2

NG2R53 CG321 CG321 HGA2 9 0.000000e+00 8.158800e-01 3

NG2R53 CG321 CG331 HGA3 9 0.000000e+00 8.158800e-01 3

OG2D1 CG2R53 CG3C51 CG2R52 9 0.000000e+00 3.347200e-01 3

OG2D1 CG2R53 CG3C51 CG321 9 0.000000e+00 3.347200e-01 3

OG2D1 CG2R53 CG3C51 HGA1 9 0.000000e+00 0.000000e+00 3

OG2D1 CG2R53 NG2R53 CG2R53 9 1.800000e+02 4.602400e+00 2

OG2D1 CG2R53 NG2R53 CG2R61 9 1.800000e+02 8.368000e-01 2

OG2D1 CG2R53 NG2R53 CG321 9 1.800000e+02 1.046000e+01 2

```
 OG2D1  CG2R53  NG2R53   CG331    9  1.800000e+02  8.368000e-01     2
 OG2D1  CG2R53  NG2R53  NG2R50    9  1.800000e+02  8.368000e-01     2

[ dihedraltypes ]
; i          j          k          l          func      q0         cq
 CG2R53  CG3C51  NG2R53   OG2D1    2  0.000000e+00  7.531200e+02
 CG2R53  NG2R53  NG2R53   OG2D1    2  0.000000e+00  7.531200e+02
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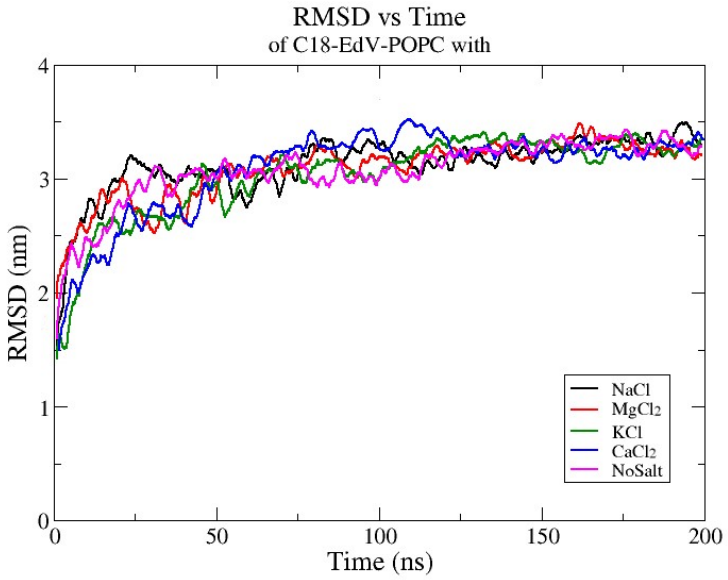

Fig. S1: root-mean-square deviation (RMSD) of POPC and C18-EdV in function of time

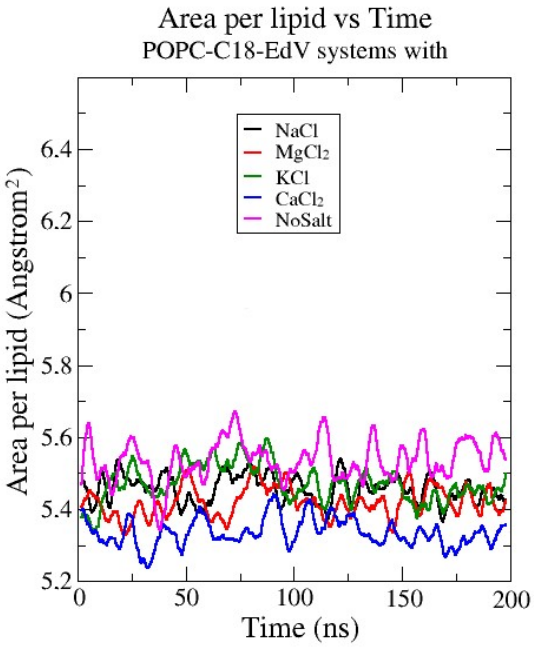

Fig. S2: *Area per lipid* of POPC-C18-EdV systems in function of time