Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Conformational dynamics of amyloid-β(16-22) peptide in aqueous ionic liquids

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Table S1. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in water.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β -sheet	β -bridge
180	0.76						0.15	0.02
170	0.77						0.14	0.02
160	0.60						0.33	0.01
150	0.52						0.41	0.01
140	0.46						0.47	
130	0.81						0.04	0.08
120	0.72						0.16	0.06
110	0.74						0.15	0.04
100	0.88	0.05						
90	0.81	0.01					0.05	0.07
80	0.50						0.41	0.02
70	0.93							0.01
60	0.93							
50	0.93		0.01					
40	0.81	0.01	0.11					
30	0.75	0.01	0.18					
20	0.60	0.07	0.24		0.03			
10	0.56	0.04	0.31		0.03			
0	0.50	0.11	0.31		0.01			
-10	0.40	0.11	0.39		0.03			
-20	0.39	0.12	0.36	0.01	0.06			
-30	0.35	0.05	0.24	0.25	0.04			
-40	0.28	0.01	0.06	0.58	0.01			
-50	0.27		0.03	0.64				
-60	0.27		0.01	0.65				
-70	0.30		0.08	0.40		0.15		
-80	0.38	0.05	0.29	0.10		0.10		
-90	0.54	0.20	0.13			0.06		
-100	0.57	0.33	0.03					

Table S2. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in 10% (w/w) EAM.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β -sheet	β -bridge
180	0.77						0.11	0.06
170	0.72						0.16	0.05
160	0.76						0.16	0.02
150	0.65						0.26	0.03
140	0.30						0.63	
130	0.43						0.50	
120	0.50						0.43	
110	0.27						0.66	
100	0.31						0.62	
90	0.43						0.50	
80	0.51						0.40	0.02
70	0.80						0.08	0.05
60	0.89						0.01	0.03
50	0.90						0.01	0.02
40	0.89	0.01	0.04					
30	0.73	0.02	0.19					
20	0.60	0.07	0.25		0.01			
10	0.45	0.03	0.44		0.04			
0	0.40	0.09	0.33	0.01	0.11			
-10	0.38	0.01	0.16	0.04	0.35			
-20	0.31	0.01	0.20	0.27	0.16			
-30	0.29		0.11	0.52	0..02			
-40	0.30		0.05	0.58				
-50	0.30		0.05	0.56		0.03		
-60	0.31	0.02	0.15	0.28		0.17		
-70	0.31	0.01	0.05	0.29		0.26		
-80	0.32	0.02	0.19	0.02		0.38		
-90	0.46	0.11	0.28			0.08		
-100	0.63	0.27	0.03					

Table S3. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in 70% (w/w) EAM.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β -sheet	β -bridge
180	0.64						0.28	0.01
170	0.48						0.44	0.02
160	0.30						0.63	0.01
150	0.30						0.63	
140	0.30						0.62	
130	0.30						0.62	0.01
120	0.27						0.66	
110	0.38						0.55	
100	0.40						0.53	
90	0.60						0.33	
80	0.67						0.25	0.02
70	0.83						0.06	0.04
60	0.93							
50	0.93							
40	0.93							
30	0.93							
20	0.90		0.03					
10	0.62	0.04	0.26		0.02			
0	0.48	0.02	0.28		0.16			
-10	0.39	0.03	0.29	0.01	0.20			
-20	0.39	0.08	0.19	0.22	0.05			
-30	0.31		0.23	0.30	0.08			
-40	0.28		0.03	0.62				
-50	0.28		0.01	0.64				
-60	0.27			0.66				
-70	0.32		0.13	0.40		0.08		
-80	0.34		0.28	0.30		0.01		
-90	0.41	0.08	0.13	0.27		0.03		
-100	0.49	0.15	0.13			0.16		

Table S4. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in 10% (w/w) EAN.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β –sheet	β -bridge
180	0.75						0.15	0.03
170	0.59						0.33	0.01
160	0.57						0.36	0.01
150	0.56						0.37	
140	0.39						0.54	
130	0.52						0.41	
120	0.63						0.30	
110	0.53						0.40	
100	0.61						0.32	
90	0.70						0.24	
80	0.53						0.37	0.03
70	0.75						0.12	0.07
60	0.89						0.01	0.03
50	0.92							0.01
40	0.93		0.01					
30	0.73	0.10	0.10					
20	0.61	0.04	0.29					
10	0.52	0.08	0.33					
0	0.50	0.14	0.30					
-10	0.42	0.16	0.22	0.02	0.11			
-20	0.45	0.19	0.29					
-30	0.40	0.20	0.20	0.12	0.01			
-40	0.36	0.11	0.13	0.32		0.01		
-50	0.29		0.01	0.63				
-60	0.28		0.01	0.61		0.05		
-70	0.42	0.13	0.19	0.13		0.06		
-80	0.50	0.24	0.11	0.01		0.07		
-90	0.60	0.24	0.09					
-100	0.63	0.29	0.01					

Table S5. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in 70% (w/w) EAN.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β –sheet	β -bridge
180	0.54						0.39	0.01
170	0.40						0.53	0.01
160	0.43						0.48	0.02
150	0.39						0.54	
140	0.28						0.65	
130	0.27						0.67	
120	0.28						0.66	
110	0.28						0.66	
100	0.34						0.59	
90	0.45						0.48	
80	0.58						0.33	0.03
70	0.78						0.12	0.03
60	0.93							
50	0.93							
40	0.91	0.03						
30	0.88	0.05	0.01					
20	0.61	0.09	0.22		0.01			
10	0.48	0.08	0.30		0.07			
0	0.48	0.05	0.32		0.09			
-10	0.48	0.02	0.28		0.15			
-20	0.48	0.03	0.41		0.02			
-30	0.48		0.35	0.10				
-40	0.44		0.26	0.23				
-50	0.40		0.21	0.33				
-60	0.40		0.20	0.33				
-70	0.44		0.20	0.29				
-80	0.55	0.09	0.20	0.09				
-90	0.58	0.12	0.23					
-100	0.56	0.16	0.21					

Table S6. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in 10% (w/w) TEAM.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β –sheet	β -bridge
180	0.86						0.02	0.06
170	0.68						0.24	0.01
160	0.41						0.52	
150	0.37						0.56	0.01
140	0.31						0.62	
130	0.69						0.21	0.03
120	0.81						0.01	0.12
110	0.82	0.06						0.05
100	0.84	0.08	0.01					0.01
90	0.81	0.04	0.03					0.06
80	0.73	0.04	0.08					0.08
70	0.88	0.05						
60	0.82	0.08	0.03					
50	0.80	0.08	0.05					
40	0.80	0.07	0.06					
30	0.67	0.17	0.09					
20	0.60	0.17	0.16					
10	0.59	0.13	0.20		0.01			
0	0.54	0.10	0.27		0.02			
-10	0.47	0.12	0.15	0.01	0.18			
-20	0.44	0.16	0.14	0.08	0.11			
-30	0.42	0.13	0.12	0.23	0.03			
-40	0.47	0.06	0.10	0.30				
-50	0.50	0.08	0.06	0.29				
-60	0.55	0.08	0.14	0.06		0.11		
-70	0.46	0.12	0.06	0.01		0.29		
-80	0.37	0.09	0.24			0.23		
-90	0.60	0.28	0.06					
-100	0.62	0.30	0.01					

Table S7. Secondary structure elements with average Ψ angle for peptide dimer (16-22) in 70% (w/w) TEAM.

Average Ψ	Coil	Bend	Turn	α -helix	3_{10}-helix	5-helix	β -sheet	β -bridge
180	0.50						0.42	0.02
170	0.42						0.51	0.01
160	0.44						0.49	
150	0.30						0.63	
140	0.27						0.66	
130	0.29						0.64	
120	0.27						0.67	
110	0.27						0.66	
100	0.27						0.66	
90	0.32						0.61	
80	0.49						0.42	0.02
70	0.79						0.10	0.04
60	0.93							
50	0.93							
40	0.93							
30	0.91		0.02					
20	0.92		0.02					
10	0.61	0.04	0.21		0.07			
0	0.53		0.21		0.19			
-10	0.48	0.05	0.10		0.31			
-20	0.45	0.07	0.10		0.32			
-30	0.40	0.01	0.24		0.29			
-40	0.40		0.25	0.17	0.11			
-50	0.40		0.21	0.33				
-60	0.41	0.01	0.18	0.33				
-70	0.40		0.20	0.33				
-80	0.42	0.04	0.14	0.33				
-90	0.47	0.13	0.04	0.29				
-100	0.53	0.14	0.24		0.03			

Table S8. Coordination numbers of water oxygen atoms, anion oxygen atoms around each amide hydrogen and water hydrogens, cation hydrogens around each amide oxygen of peptide dimer (16-22) in water, 10% and 70% (w/w) EAM, EAN and TEAM IL.

System	RDF	10% (w/w) IL		70% (w/w) IL	
		α–helix	β–sheet	α–helix	β–sheet
Water	Amide_H – Water_O	0.39	0.85 (Coil)	–	–
	Amide_O – Water_H	1.12	1.57 (Coil)	–	–
EAM	Amide_H – Water_O	0.03	0.42	0.153	0.16
	Amide_H – Anion_O	0.54	0.13	0.39	0.56
	Amide_O – Cation_H	0.05	0.03	0.16	0.43
	Amide_O – Water_H	1.19	1.13	0.80	0.40
EAN	Amide_H – Water_O	0.21	0.40	0.12	0.15
	Amide_H – Anion_O	0.52	0.19	0.73	0.54
	Amide_O – Cation_H	0. 09	0.04	0.35	0.42
	Amide_O – Water_H	1.11	1.18	0.67	0.48
TEAM	Amide_H – Water_O	0.34	0.45	0.11	0.27
	Amide_H – Anion_O	0.34	0.12	0.25	0.23
	Amide_O – Cation_H	0.01	0.001	0.08	0.04
	Amide_O – Water_H	1.35	1.16	0.60	0.67

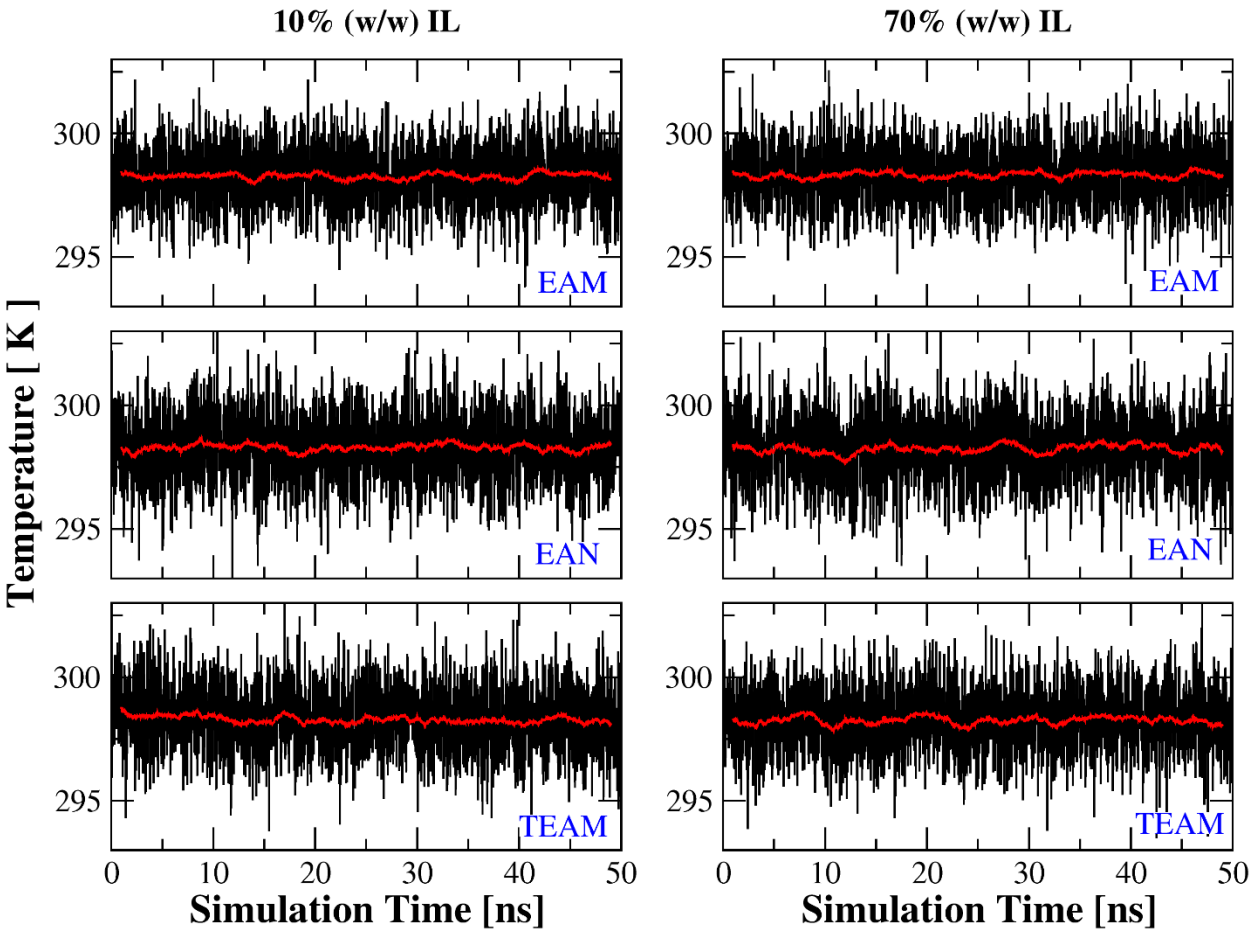

Figure S1. Temperature of the system along the equilibrium simulation of 50 ns with running average for 10 and 70% (w/w) EAM, EAN and TEAM ILs.

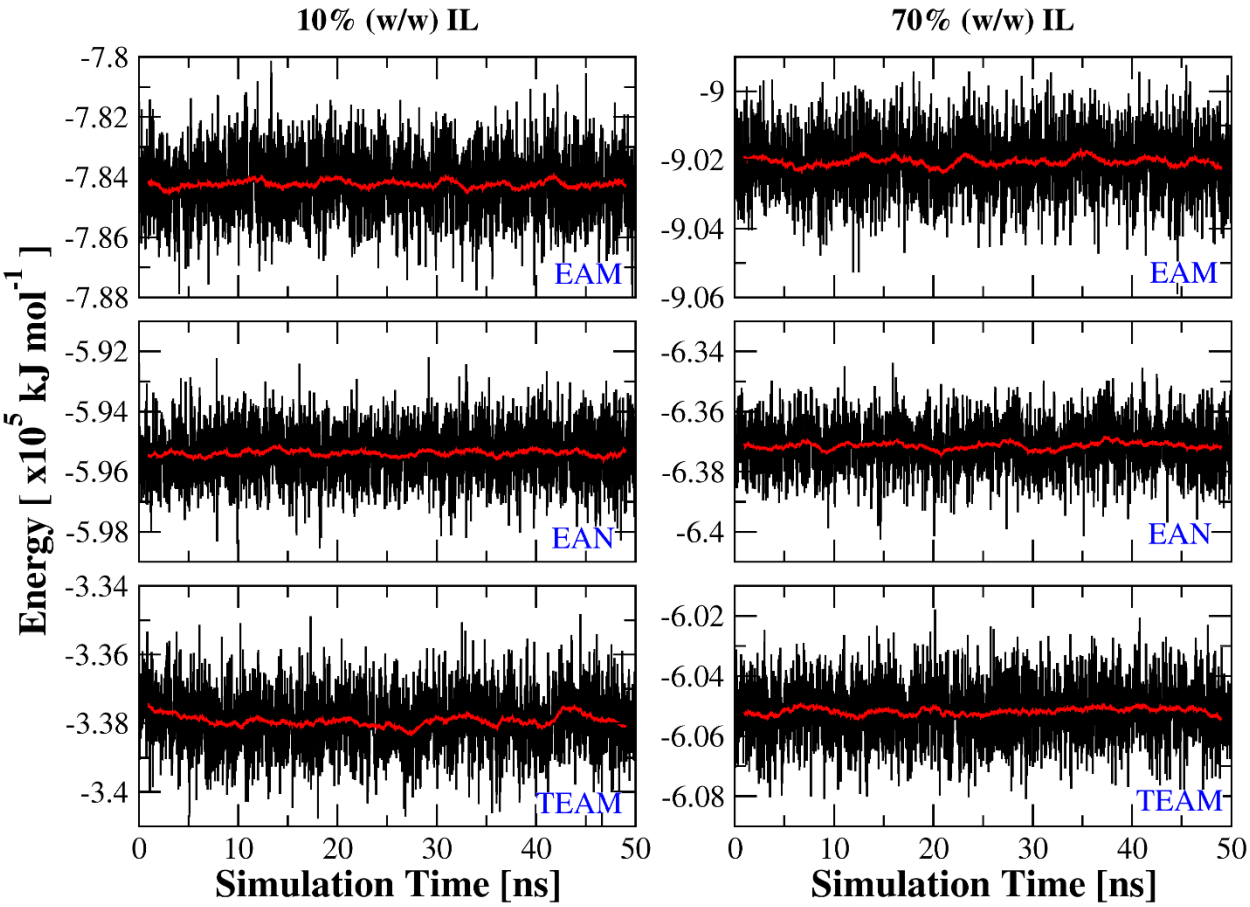

Figure S2. Total energy of the system along the equilibrium simulation of 50 ns with running average for 10 and 70% (w/w) EAM, EAN and TEAM ILs.

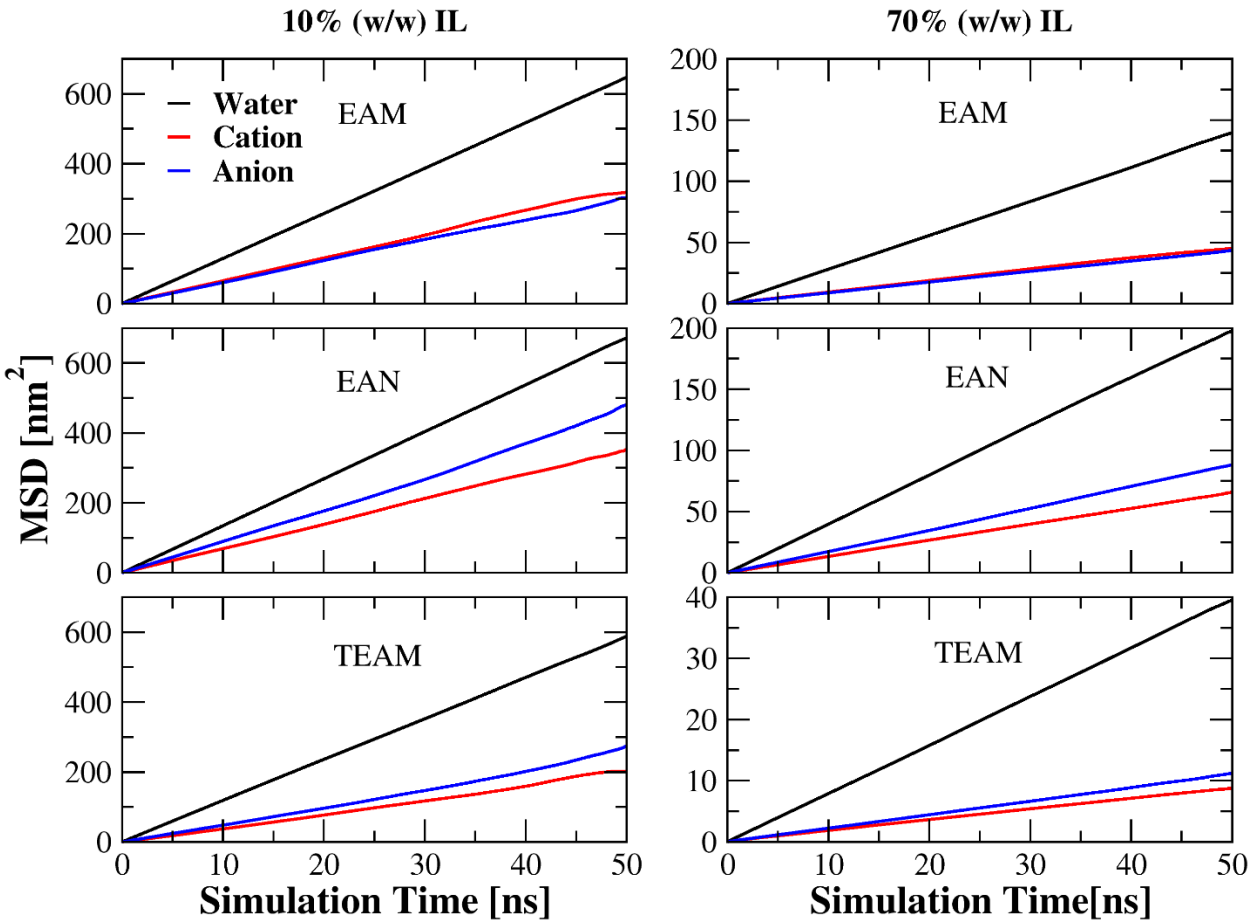

Figure S3. Mean squared displacement of water, cation and anion along the equilibration of 50 ns in 10 and 70% (w/w) EAM, EAN and TEAM ILs.

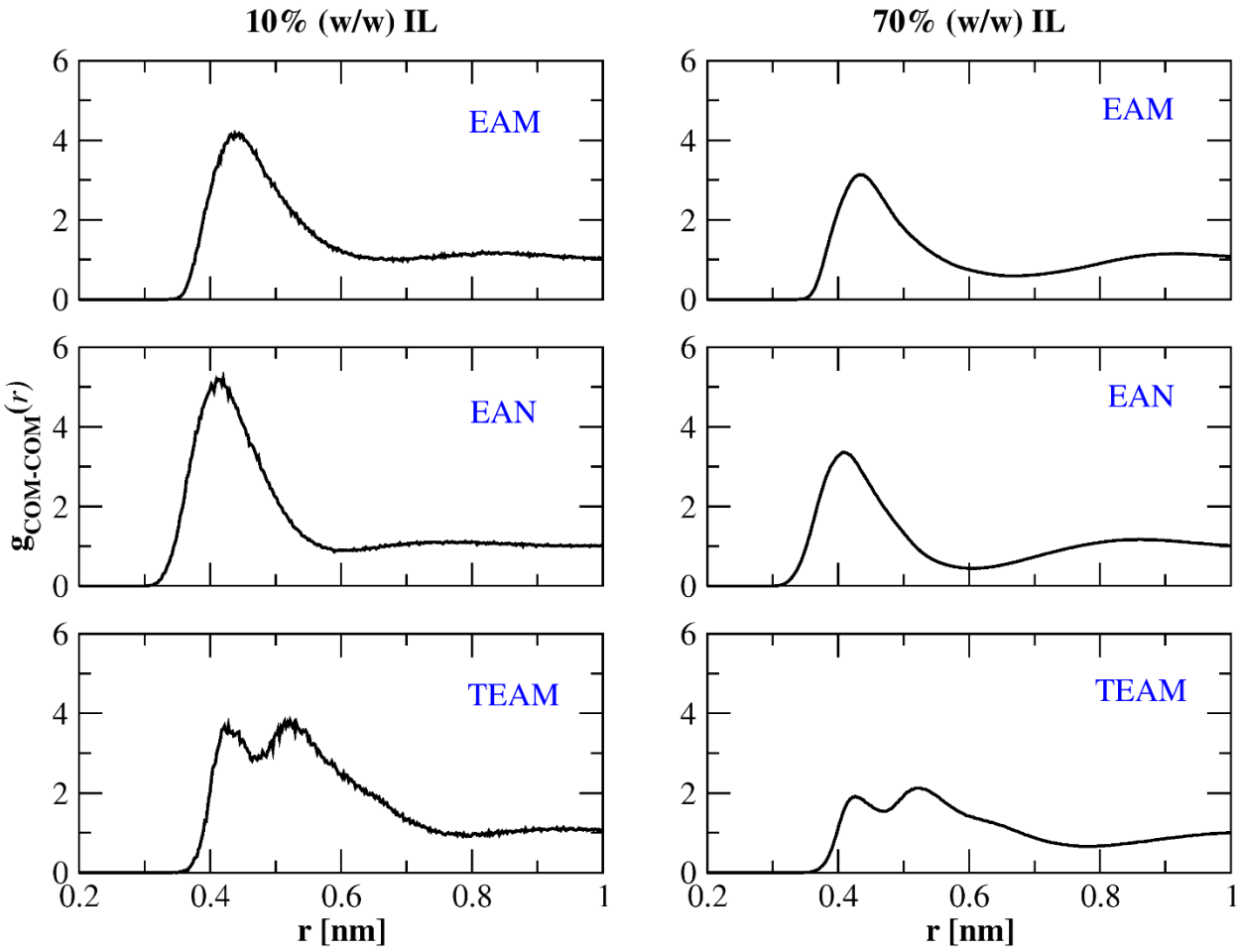

Figure S4. COM-COM radial distribution functions of anion around cation in 10 and 70% (w/w) EAM, EAN and TEAM IL.

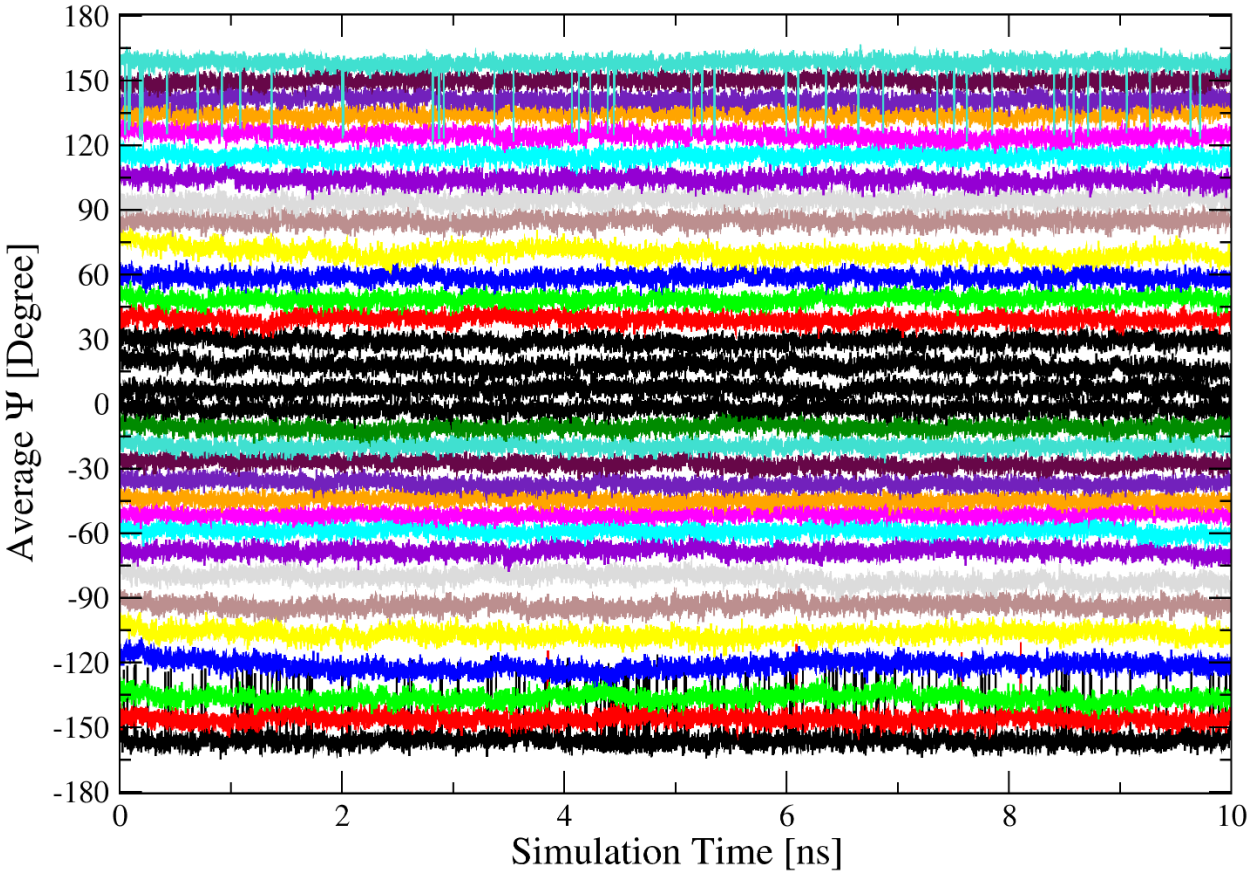

Figure S5. Average Ψ angle along with the simulation time for peptide dimer in water.

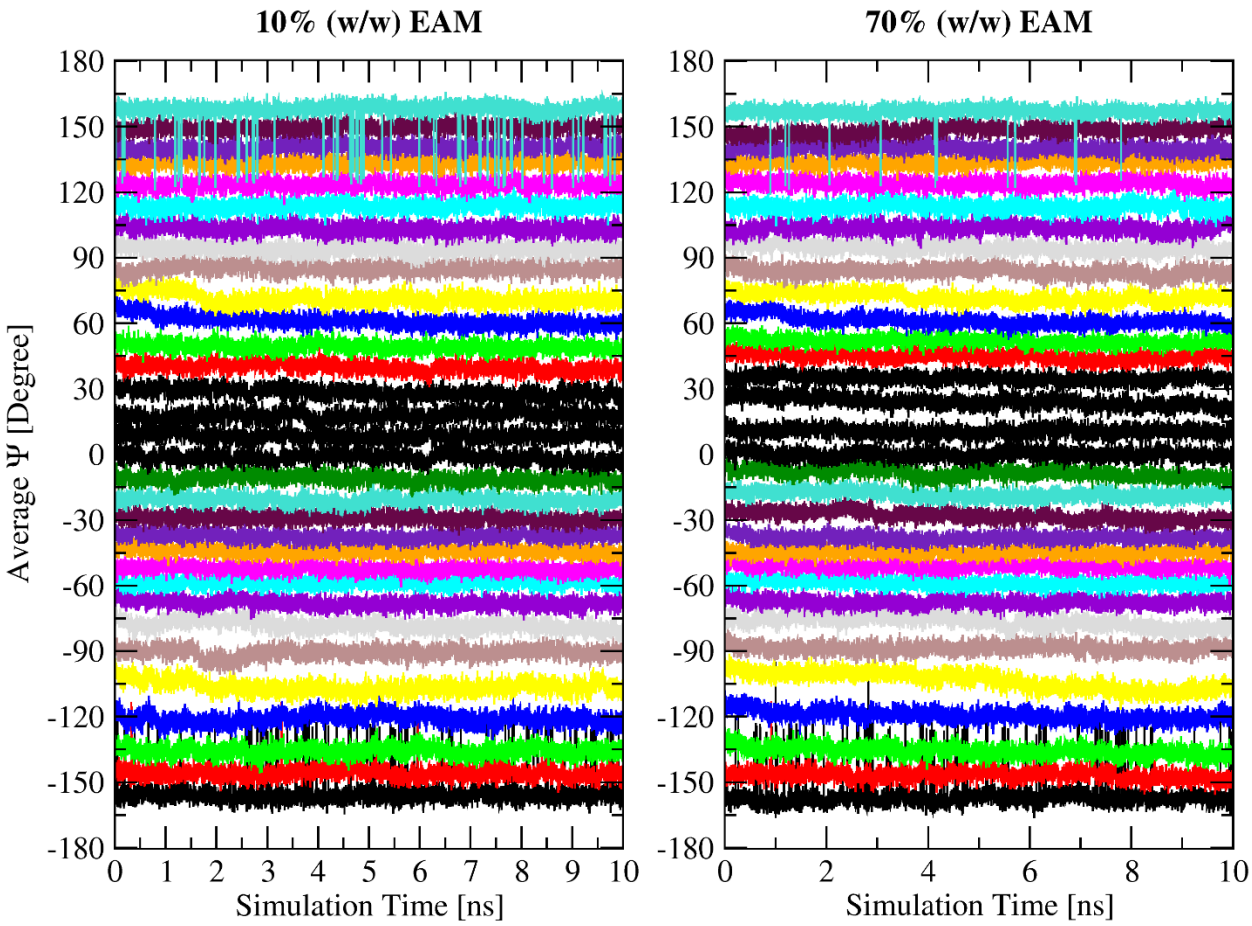

Figure S6. Average Ψ angle along with the simulation time for peptide dimer in 10% and 70% (w/w) EAM IL.

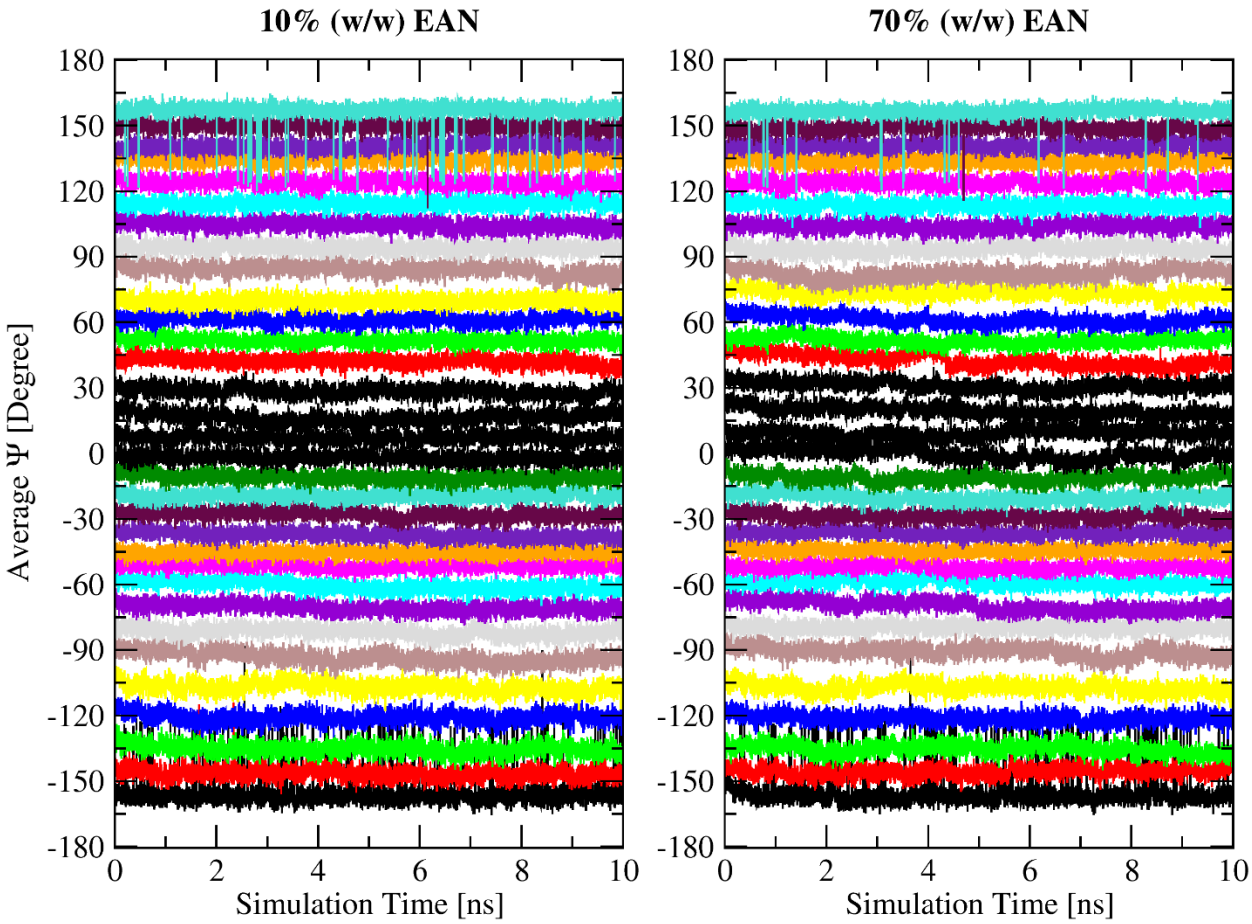

Figure S7. Average Ψ angle along with the simulation time for peptide dimer in 10% and 70% (w/w) EAN IL.

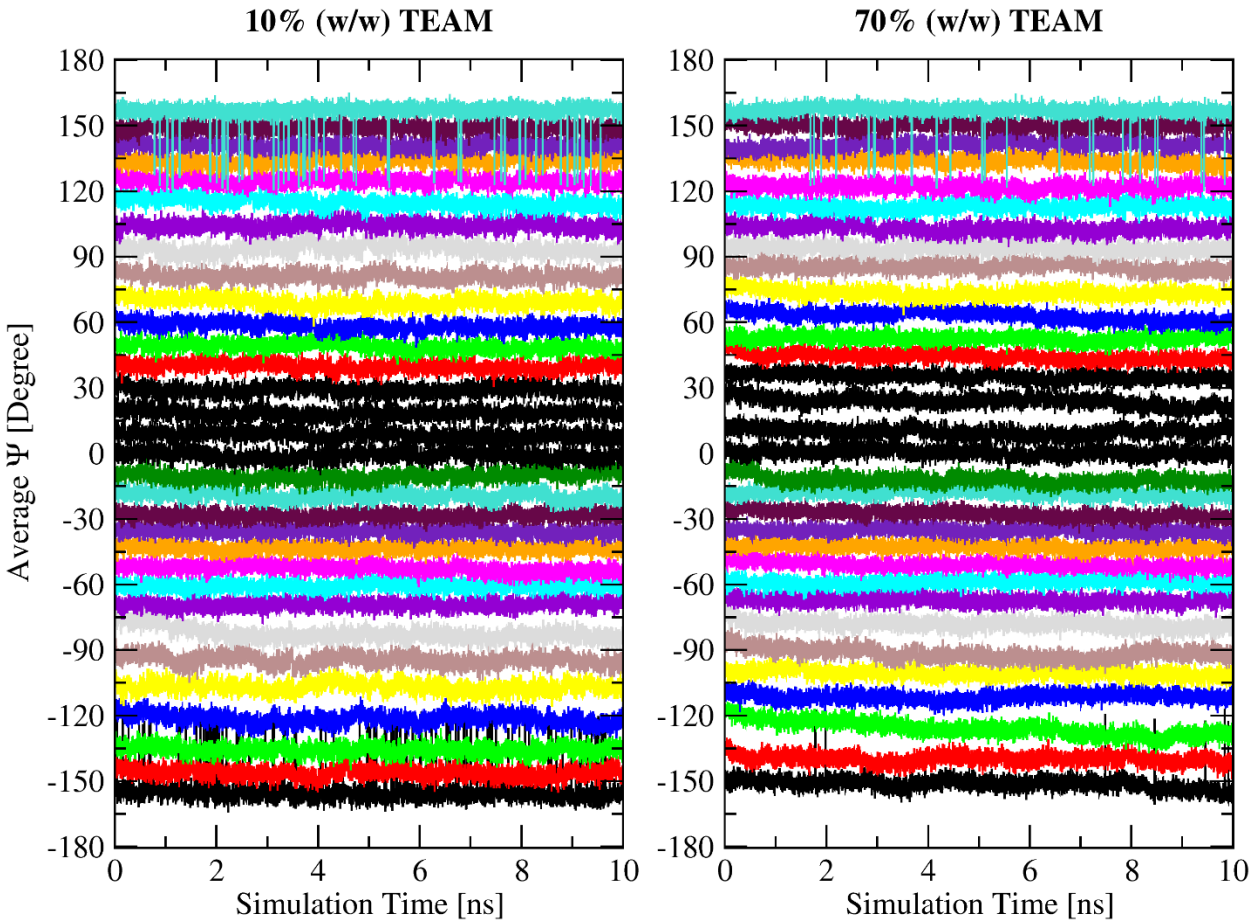

Figure S8. Average Ψ angle along with the simulation time for peptide dimer in 10% and 70% (w/w) TEAM IL.

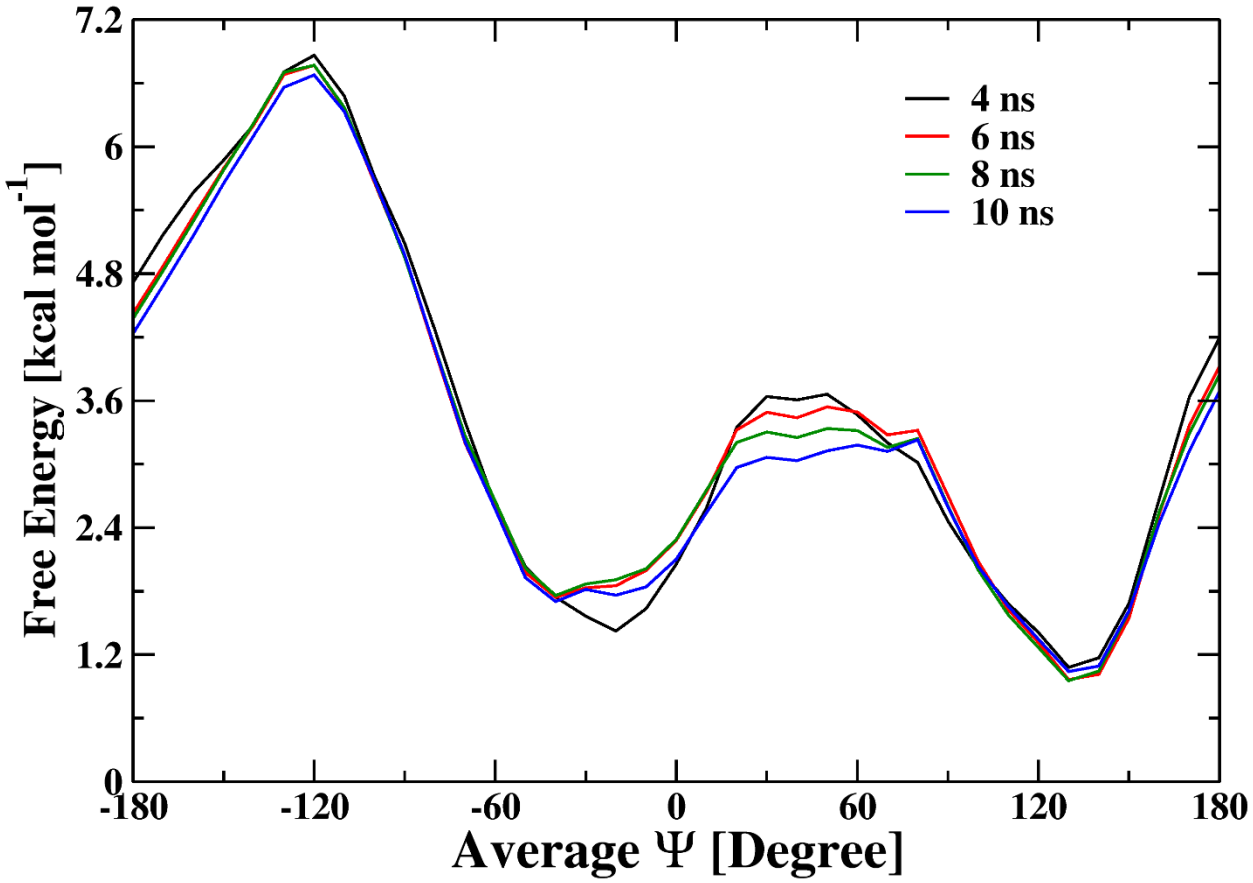

Figure S9. Convergence of the free energy profile with simulation time for peptide dimer in water.

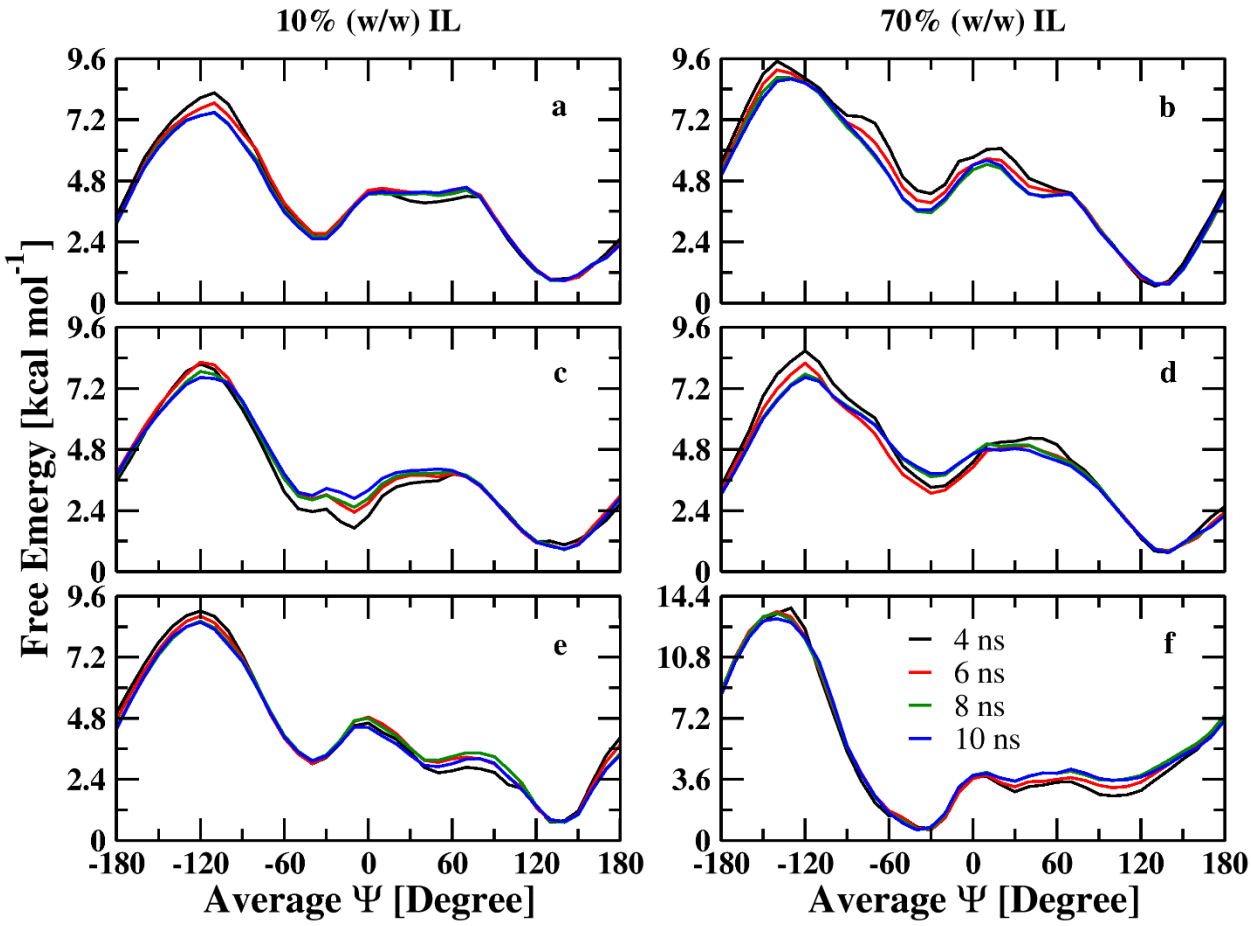

Figure S10. Convergence of the free energy profile with simulation time for peptide dimer in 10 and 70% (w/w) EAM (a, b), EAN (c, d) and TEAM (e, f) ILs.

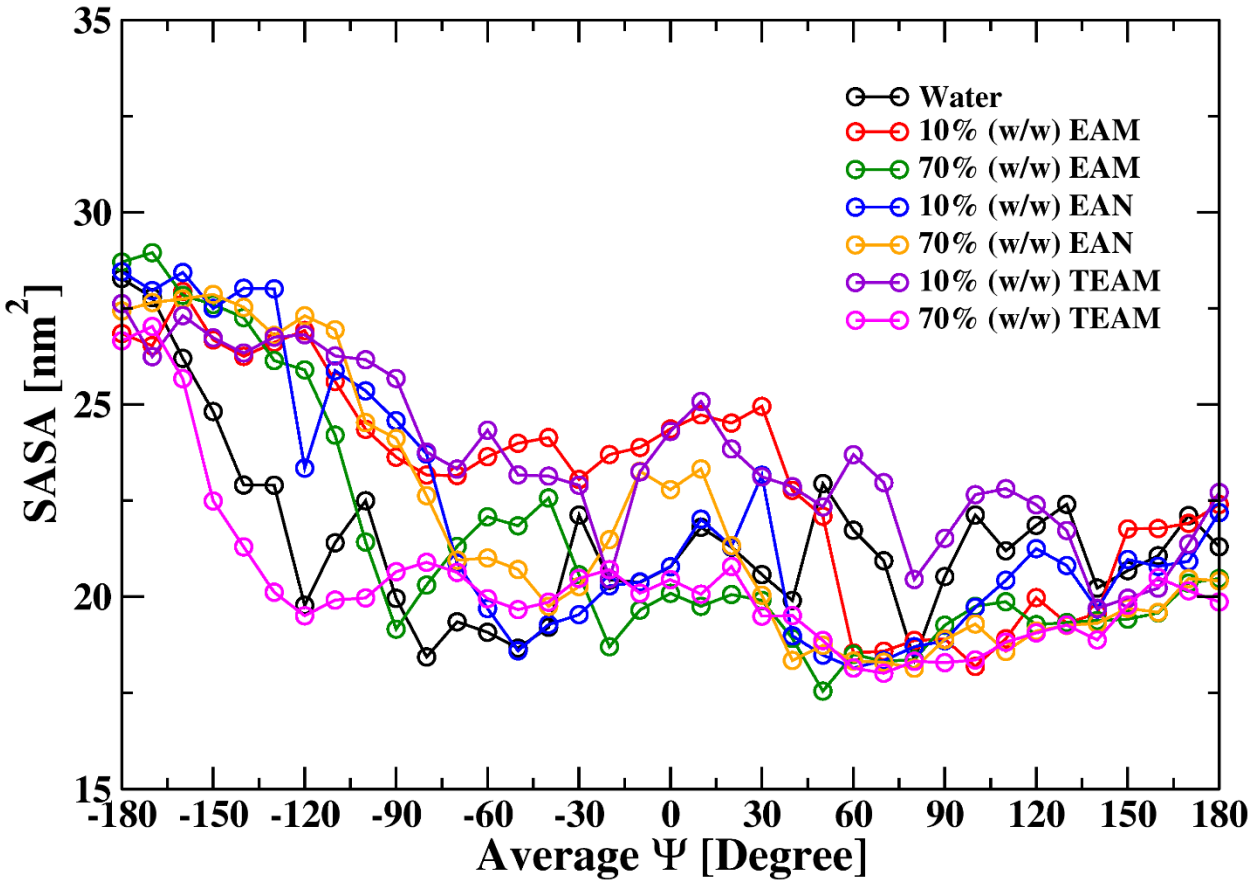

Figure S11. The solvent-accessible surface area of the peptide dimer with changing average Ψ angle in water, 10% and 70% (w/w) EAM, EAN and TEAM IL.

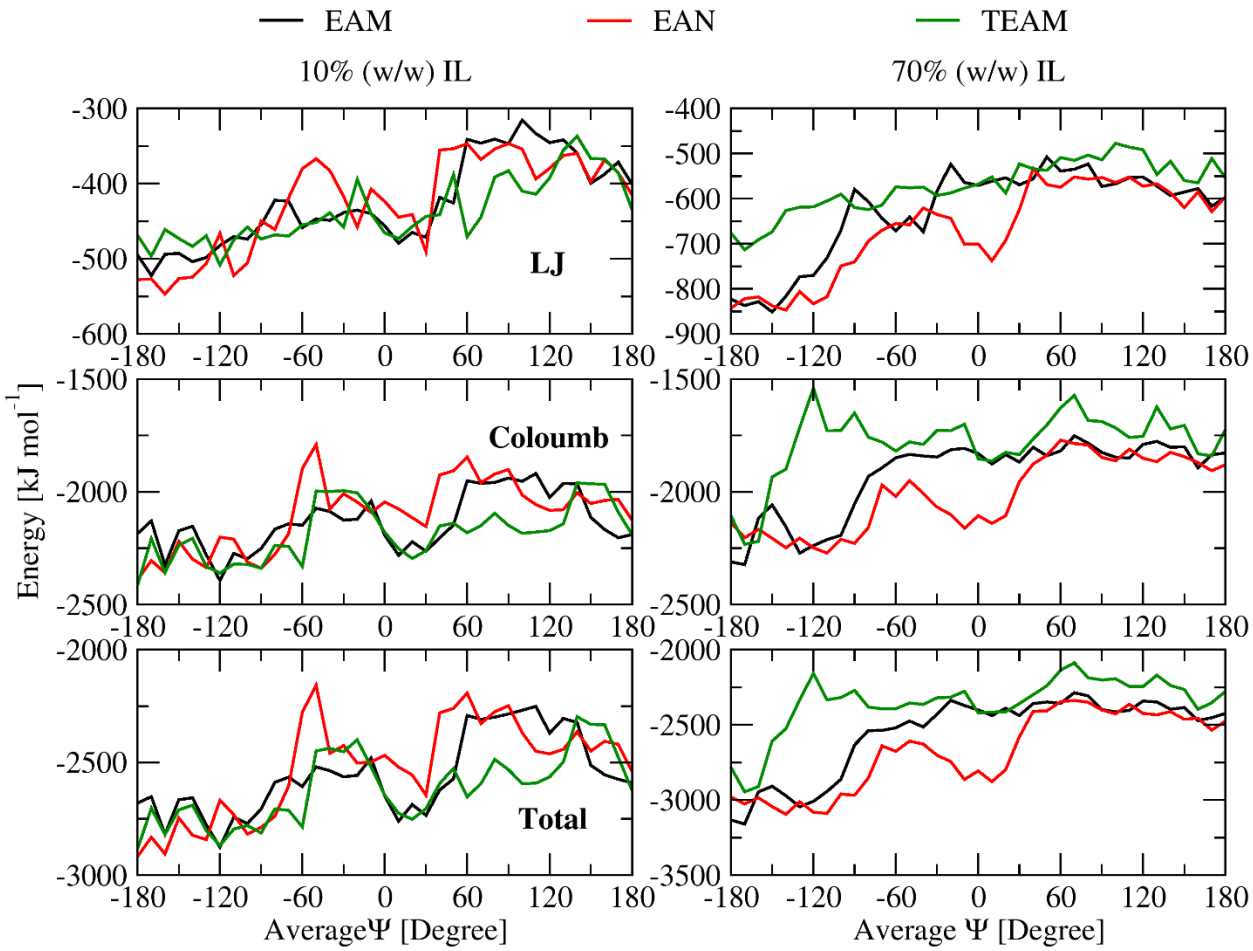

Figure S12. vdWs, Coulomb and total interaction energies between peptide and solvent with average Ψ angle in 10% and 70% (w/w) EAM, EAN and TEAM IL.

Optimized coordinates of Ethylammonium (EA), Triethylammonium (TEA), Mesylate and Nitrate ions.

Ethylammonium

Atom	x	y	z
C1	0.425	0.199	0.189
H1	0.430	0.136	0.278
H2	0.514	0.262	0.189
H3	0.430	0.136	0.100
C2	0.302	0.287	0.189
H4	0.296	0.350	0.101
H5	0.296	0.350	0.278
N1	0.173	0.202	0.189
H6	0.115	0.220	0.272
H7	0.115	0.221	0.107
H8	0.195	0.102	0.189

Triethylammonium

Atom	x	y	z
C2	0.243	0.190	0.202
H4	0.170	0.118	0.241
H5	0.191	0.253	0.130
H6	0.320	0.132	0.150
C1	0.298	0.268	0.319
H2	0.344	0.202	0.393
H3	0.220	0.325	0.370
N1	0.407	0.369	0.283
H1	0.434	0.413	0.371
C5	0.359	0.481	0.193
H12	0.448	0.539	0.167
H13	0.322	0.435	0.102
C6	0.255	0.570	0.258
H14	0.234	0.654	0.192
H15	0.160	0.519	0.276
H16	0.290	0.612	0.353
C3	0.532	0.302	0.228
H7	0.539	0.205	0.278
H8	0.514	0.283	0.122
C4	0.657	0.384	0.252
H9	0.743	0.328	0.215
H10	0.656	0.480	0.200
H11	0.674	0.402	0.358

Mesylate

Atom	x	y	z
C1	0.135	0.221	0.220
H1	0.100	0.297	0.150
H2	0.100	0.243	0.321
H3	0.100	0.122	0.189
S1	0.317	0.221	0.220
O2	0.354	0.357	0.264
O3	0.354	0.190	0.081
O1	0.354	0.115	0.317

Nitrate

Atom	x	y	z
O1	0.100	0.132	0.318
N1	0.100	0.195	0.209
O3	0.100	0.321	0.209
O2	0.100	0.132	0.100

Force-field parameters of the ionic liquid ions are given in the form of .itp files.

ea.itp

```
[ moleculetype ]
; Name            nrexcl
eam               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
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     2         HC      1    EAM     H1      2    0.10212   1.000000
     3         HC      1    EAM     H2      3    0.10212   1.000000
     4         HC      1    EAM     H3      4    0.10212   1.000000
     5         CT      1    EAM     C2      5    0.094624 12.000000
     6         H1      1    EAM     H4      6    0.083008  1.000000
     7         H1      1    EAM     H5      7    0.083008  1.000000
     8          N      1    EAM     N1      8   -0.379448 14.000000
     9          H      1    EAM     H6      9    0.283504  1.000000
    10          H      1    EAM     H7     10    0.283504  1.000000
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[ bonds ]
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    8    11     1  1.0330e-01  3.0878e+05
    5     6     1  1.0910e-01  2.8342e+05
    5     7     1  1.0910e-01  2.8342e+05
    1     2     1  1.0920e-01  2.8225e+05
    1     3     1  1.0920e-01  2.8225e+05
    1     4     1  1.0920e-01  2.8225e+05
    5     8     1  1.4990e-01  2.4568e+05
    1     5     1  1.5350e-01  2.5363e+05

[ pairs ]
;  ai    aj funct
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     7    10      1
     7    11      1
     6     9      1
     6    10      1
     6    11      1
     4     6      1
     4     7      1
     4     8      1
     3     6      1
```

```
    3     7     1
    3     8     1
    2     6     1
    2     7     1
    2     8     1
    1     9     1
    1    10     1
    1    11     1

[ angles ]
;  ai    aj    ak funct  theta   cth
   10     8    11     1  1.0811e+02  3.3907e+02
    9     8    10     1  1.0811e+02  3.3907e+02
    9     8    11     1  1.0811e+02  3.3907e+02
    7     5     8     1  1.0791e+02  4.1020e+02
    6     5     7     1  1.1074e+02  3.2669e+02
    6     5     8     1  1.0791e+02  4.1020e+02
    5     8     9     1  1.1011e+02  3.8652e+02
    5     8    10     1  1.1011e+02  3.8652e+02
    5     8    11     1  1.1011e+02  3.8652e+02
    4     1     5     1  1.1005e+02  3.8802e+02
    3     1     4     1  1.0835e+02  3.2995e+02
    3     1     5     1  1.1005e+02  3.8802e+02
    2     1     3     1  1.0835e+02  3.2995e+02
    2     1     4     1  1.0835e+02  3.2995e+02
    2     1     5     1  1.1005e+02  3.8802e+02
    1     5     6     1  1.1174e+02  3.8510e+02
    1     5     7     1  1.1174e+02  3.8510e+02
    1     5     8     1  1.1432e+02  5.3932e+02

[ dihedrals ]
;i  j   k  l    func   C0  ...  C5
    7    5    8    9     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    7    5    8   10     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    7    5    8   11     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    6    5    8    9     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    6    5    8   10     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    6    5    8   11     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    4    1    5    6     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    4    1    5    7     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    4    1    5    8     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    3    1    5    6     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    3    1    5    7     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    3    1    5    8     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    2    1    5    6     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
    2    1    5    7     3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
```

```
   2    1    5    8     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000     ;
   1    5    8    9     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000     ;
   1    5    8    10    3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000     ;
   1    5    8    11    3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000     ;
```

nitrate.itp

```
[ moleculetype ]
; Name            nrexcl
nitrate           3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
    1         O2      1    NIT     O1      1   -0.539408 16.000000
    2          N      1    NIT     N1      2    0.818224 14.000000
    3         O2      1    NIT     O2      3   -0.539408 16.000000
    4         O2      1    NIT     O3      4   -0.539408 16.000000

[ bonds ]
;  ai    aj funct  r  k
   2     3     1  1.2190e-01  6.3697e+05
   2     4     1  1.2190e-01  6.3697e+05
   1     2     1  1.2190e-01  6.3697e+05

[ pairs ]
;  ai    aj funct

[ angles ]
;  ai    aj    ak funct  theta   cth
   3     2     4     1  1.2513e+02  6.4559e+02
   1     2     3     1  1.2513e+02  6.4559e+02
   1     2     4     1  1.2513e+02  6.4559e+02
```

tea.itp

```
[ moleculetype ]
; Name            nrexcl
tea               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
    1         CT      1    TEA     C2      1   -0.190376 12.000000
```

```
   2       HC     1    TEA     H4      2    0.09144   1.000000
   3       HC     1    TEA     H5      3    0.09144   1.000000
   4       HC     1    TEA     H6      4    0.09144   1.000000
   5       CT     1    TEA     C1      5   -0.066968 12.000000
   6       H1     1    TEA     H2      6    0.111376  1.000000
   7       H1     1    TEA     H3      7    0.111376  1.000000
   8        N     1    TEA     N1      8   -0.17632  14.000000
   9        H     1    TEA     H1      9    0.257136  1.000000
  10       CT     1    TEA     C5     10   -0.066968 12.000000
  11       H1     1    TEA    H12     11    0.111376  1.000000
  12       H1     1    TEA    H13     12    0.111376  1.000000
  13       CT     1    TEA     C6     13   -0.190376 12.000000
  14       HC     1    TEA    H14     14    0.09144   1.000000
  15       HC     1    TEA    H15     15    0.09144   1.000000
  16       HC     1    TEA    H16     16    0.09144   1.000000
  17       CT     1    TEA     C3     17   -0.066968 12.000000
  18       H1     1    TEA     H7     18    0.111376  1.000000
  19       H1     1    TEA     H8     19    0.111376  1.000000
  20       CT     1    TEA     C4     20   -0.190376 12.000000
  21       HC     1    TEA     H9     21    0.09144   1.000000
  22       HC     1    TEA    H10     22    0.09144   1.000000
  23       HC     1    TEA    H11     23    0.09144   1.000000

[ bonds ]
;  ai    aj funct  r  k
   20    21     1  1.0920e-01  2.8225e+05
   20    22     1  1.0920e-01  2.8225e+05
   20    23     1  1.0920e-01  2.8225e+05
   17    18     1  1.0910e-01  2.8342e+05
   17    19     1  1.0910e-01  2.8342e+05
   13    14     1  1.0920e-01  2.8225e+05
   13    15     1  1.0920e-01  2.8225e+05
   13    16     1  1.0920e-01  2.8225e+05
   10    11     1  1.0910e-01  2.8342e+05
   10    12     1  1.0910e-01  2.8342e+05
    8     9     1  1.0330e-01  3.0878e+05
    5     6     1  1.0910e-01  2.8342e+05
    5     7     1  1.0910e-01  2.8342e+05
    1     2     1  1.0920e-01  2.8225e+05
    1     3     1  1.0920e-01  2.8225e+05
    1     4     1  1.0920e-01  2.8225e+05
   17    20     1  1.5350e-01  2.5363e+05
   10    13     1  1.5350e-01  2.5363e+05
    8    10     1  1.4990e-01  2.4568e+05
    8    17     1  1.4990e-01  2.4568e+05
    5     8     1  1.4990e-01  2.4568e+05
```

```
    1     5     1  1.5350e-01  2.5363e+05

[ pairs ]
;  ai    aj funct
    19     21      1
    19     22      1
    19     23      1
    18     21      1
    18     22      1
    18     23      1
    12     17      1
    12     14      1
    12     15      1
    12     16      1
    11     17      1
    11     14      1
    11     15      1
    11     16      1
    10     18      1
    10     19      1
     9     11      1
     9     12      1
     9     13      1
     9     18      1
     9     19      1
     9     20      1
     8     14      1
     8     15      1
     8     16      1
     8     21      1
     8     22      1
     8     23      1
     7      9      1
     7     10      1
     7     17      1
     6      9      1
     6     10      1
     6     17      1
     5     11      1
     5     12      1
     5     18      1
     5     19      1
     4      6      1
     4      7      1
     4      8      1
     3      6      1
```

```
   3     7     1
   3     8     1
   2     6     1
   2     7     1
   2     8     1
   1     9     1
  13    17     1
  10    20     1
   5    13     1
   5    20     1
   1    10     1
   1    17     1

[ angles ]
;  ai    aj    ak funct  theta   cth
  22    20    23     1  1.0835e+02  3.2995e+02
  21    20    22     1  1.0835e+02  3.2995e+02
  21    20    23     1  1.0835e+02  3.2995e+02
  19    17    20     1  1.1174e+02  3.8510e+02
  18    17    19     1  1.1074e+02  3.2669e+02
  18    17    20     1  1.1174e+02  3.8510e+02
  17    20    21     1  1.1005e+02  3.8802e+02
  17    20    22     1  1.1005e+02  3.8802e+02
  17    20    23     1  1.1005e+02  3.8802e+02
  15    13    16     1  1.0835e+02  3.2995e+02
  14    13    15     1  1.0835e+02  3.2995e+02
  14    13    16     1  1.0835e+02  3.2995e+02
  12    10    13     1  1.1174e+02  3.8510e+02
  11    10    12     1  1.1074e+02  3.2669e+02
  11    10    13     1  1.1174e+02  3.8510e+02
  10    13    14     1  1.1005e+02  3.8802e+02
  10    13    15     1  1.1005e+02  3.8802e+02
  10    13    16     1  1.1005e+02  3.8802e+02
   9     8    10     1  1.1011e+02  3.8652e+02
   9     8    17     1  1.1011e+02  3.8652e+02
   8    10    11     1  1.0791e+02  4.1020e+02
   8    10    12     1  1.0791e+02  4.1020e+02
   8    17    18     1  1.0791e+02  4.1020e+02
   8    17    19     1  1.0791e+02  4.1020e+02
   7     5     8     1  1.0791e+02  4.1020e+02
   6     5     7     1  1.1074e+02  3.2669e+02
   6     5     8     1  1.0791e+02  4.1020e+02
   5     8     9     1  1.1011e+02  3.8652e+02
   4     1     5     1  1.1005e+02  3.8802e+02
   3     1     4     1  1.0835e+02  3.2995e+02
   3     1     5     1  1.1005e+02  3.8802e+02
```

```
   2    1    3    1  1.0835e+02  3.2995e+02
   2    1    4    1  1.0835e+02  3.2995e+02
   2    1    5    1  1.1005e+02  3.8802e+02
   1    5    6    1  1.1174e+02  3.8510e+02
   1    5    7    1  1.1174e+02  3.8510e+02
  10    8   17    1  1.1064e+02  5.2585e+02
   8   10   13    1  1.1432e+02  5.3932e+02
   8   17   20    1  1.1432e+02  5.3932e+02
   5    8   10    1  1.1064e+02  5.2585e+02
   5    8   17    1  1.1064e+02  5.2585e+02
   1    5    8    1  1.1432e+02  5.3932e+02

[ dihedrals ]
;i  j   k  l    func   C0  ...  C5
   19   17   20   21    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   19   17   20   22    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   19   17   20   23    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   18   17   20   21    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   18   17   20   22    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   18   17   20   23    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   12   10   8   17    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   12   10   13   14    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   12   10   13   15    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   12   10   13   16    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   11   10   8   17    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   11   10   13   14    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   11   10   13   15    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   11   10   13   16    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   10   8   17   18    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   10   8   17   19    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   9   8   10   11    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   9   8   10   12    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   9   8   10   13    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   9   8   17   18    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   9   8   17   19    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   9   8   17   20    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   8   10   13   14    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   8   10   13   15    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   8   10   13   16    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   8   17   20   21    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   8   17   20   22    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   8   17   20   23    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   7   5   8   9    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   7   5   8   10    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   7   5   8   17    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
   6   5   8   9    3    0.65270    1.95811    0.00000   -2.61082    0.00000    0.00000    ;
```

```
   6    5    8    10    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   6    5    8    17    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   5    8    10   11    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   5    8    10   12    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   5    8    17   18    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   5    8    17   19    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   4    1    5    6     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   4    1    5    7     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   4    1    5    8     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   3    1    5    6     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   3    1    5    7     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   3    1    5    8     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   2    1    5    6     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   2    1    5    7     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   2    1    5    8     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   1    5    8    9     3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   13   10   8    17    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   10   8    17   20    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   5    8    10   13    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   5    8    17   20    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   1    5    8    10    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
   1    5    8    17    3    0.65270    1.95811    0.00000    -2.61082    0.00000    0.00000    ;
```

mesylate.itp

```
[ moleculetype ]
; Name            nrexcl
mesylate            3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         CT      1    MES     C1      1   -0.314216 12.000000
     2         H1      1    MES     H1      2    0.071328  1.000000
     3         H1      1    MES     H2      3    0.071328  1.000000
     4         H1      1    MES     H3      4    0.071328  1.000000
     5          S      1    MES     S1      5    0.985656 32.100000
     6         O2      1    MES     O2      6   -0.561808 16.000000
     7         O2      1    MES     O3      7   -0.561808 16.000000
     8         O2      1    MES     O1      8   -0.561808  16.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0930e-01  2.8108e+05
    1     3     1  1.0930e-01  2.8108e+05
    1     4     1  1.0930e-01  2.8108e+05
    5     6     1  1.4360e-01  4.5279e+05
```

```
   5     7     1  1.4360e-01  4.5279e+05
   5     8     1  1.4360e-01  4.5279e+05
   1     5     1  1.7740e-01  2.1255e+05

[ pairs ]
;  ai    aj funct
    4     6     1
    4     7     1
    4     8     1
    3     6     1
    3     7     1
    3     8     1
    2     6     1
    2     7     1
    2     8     1

[ angles ]
;  ai    aj    ak funct  theta   cth
    4     1     5     1  1.0811e+02  3.6702e+02
    3     1     4     1  1.0955e+02  3.2786e+02
    3     1     5     1  1.0811e+02  3.6702e+02
    2     1     3     1  1.0955e+02  3.2786e+02
    2     1     4     1  1.0955e+02  3.2786e+02
    2     1     5     1  1.0811e+02  3.6702e+02
    7     5     8     1  1.1973e+02  6.2409e+02
    6     5     7     1  1.1973e+02  6.2409e+02
    6     5     8     1  1.1973e+02  6.2409e+02
    1     5     6     1  1.0832e+02  5.5723e+02
    1     5     7     1  1.0832e+02  5.5723e+02
    1     5     8     1  1.0832e+02  5.5723e+02

[ dihedrals ]
;i  j   k  l    func   C0  ...  C5
    4    1    5    6     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    4    1    5    7     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    4    1    5    8     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    3    1    5    6     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    3    1    5    7     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    3    1    5    8     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    2    1    5    6     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    2    1    5    7     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
    2    1    5    8     3     0.60250     1.80749     0.00000    -2.40998     0.00000     0.00000    ;
```