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SUPPORTING INFORMATION

for

Ammonium Based stabilizers Effectively Counteract the Urea – Conferred Denaturation in a Small Protein: Insights from Molecular Dynamics Simulations

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Serial number	Ionic species	Atom name	Partial charge
1	TEA	N	-0.1658
2	TEA	C	-0.4425
3	TEA	C	-0.6560
4	TEA	H	0.2520
5	TEA	H	0.2760
6	TEA	H	0.2543
7	TEA	H	0.2670
8	TEA	H	0.2277
9	TEA	C	-0.1595
10	TEA	C	-0.8210
11	TEA	H	0.2303
12	TEA	H	0.2450
13	TEA	H	0.2622
14	TEA	H	0.2650
15	TEA	H	0.2112
16	TEA	C	-0.4373
17	TEA	C	-0.5282
18	TEA	H	0.2379
19	TEA	H	0.2731
20	TEA	H	0.2594
21	TEA	H	0.2481
22	TEA	H	0.2324
23	TEA	H	0.4684

Table S1. Partial charges on different atoms of triethylammonium (TEA) ions constituting the TEAA molecule.

Serial number	Ionic species	Atom name	Partial charge
1	ACE	C	-0.7072
2	ACE	H	0.1873
3	ACE	H	0.1893
4	ACE	H	0.2014
5	ACE	C	0.4021
6	ACE	O	-0.5632
7	ACE	O	-0.7098

Table S2. Partial charges on different atoms of acetate (ACE) ions constituting the TEAA molecule.

Serial number	Ionic species	Atom name	Partial charge
1	Choline	N	-0.8625
2	Choline	C	-0.2838
3	Choline	C	-0.0605
4	Choline	H	0.2869
5	Choline	H	0.2870
6	Choline	H	0.2011
7	Choline	H	0.2012
8	Choline	C	-0.3634
9	Choline	H	0.2806
10	Choline	H	0.2792
11	Choline	H	0.2806
12	Choline	C	-0.3639
13	Choline	H	0.2861
14	Choline	H	0.2627
15	Choline	H	0.2793
16	Choline	C	-0.3641
17	Choline	H	0.2861
18	Choline	H	0.2793
19	Choline	H	0.2627
20	Choline	O	-0.6798
21	Choline	H	0.5053

Table S3. Partial charges on different atoms of Choline ions constituting the ChCl molecule.

Bond parameters			
Bond type	**Ionic species**	**Force constant (kJ mol^{-1} nm^{-2})**	**Equilibrium bond length (nm)**
N-H	TEA	363171	0.100
N-C	TEA	307105	0.147
C-H	TEA	284512	0.107
C-C	TEA	224262	0.154
C-O	ACE	548960	0.125
C-H	ACE	284512	0.109
C-C	ACE	265265	0.152
Angle parameters			
Angle type	**Ionic species**	**Force constant (kJ mol^{-1} rad^{-2}**	**Equilibrium angle (degree)**
N-C-H (alkyl hydrogen)	TEA	292.880	109.515
N-C-C	TEA	669.440	109.457
C-C-H	TEA	313.800	109.432
C-N-H (N-terminal hydrogen)	TEA	292.880	109.437
H-C-C	ACE	292.900	109.500
H-C-H	ACE	276.100	107.800
O-C-C	ACE	585.800	117.000
O-C-O	ACE	669.400	126.000
Dihedral parameters			
Dihedral type	**Ionic species**	**Phase (degree)**	**Multiplicity**
H-N-C-C	TEA	0	3
O-C-C-H	ACE	0	3

Table S4. Bonded interaction parameters for the molecule TEAA compatible with the OPLS-AA force field.

Bond parameters			
Bond type	**Ionic species**	**Force constant (kJ mol^{-1} nm^{-2})**	**Equilibrium bond length (nm)**
O-H	Choline	463000	0.095
C-O	Choline	268000	0.141
C-H	Choline	285000	0.109
C-C	Choline	224000	0.153
C-N	Choline	307000	0.147
Angle parameters			
Angle type	**Ionic species**	**Force constant (kJ mol^{-1} rad^{-2}**	**Equilibrium angle (degree)**
C-N-C	Choline	418.4	113.0
C-C-H (alkane Hydrogen)	Choline	313.8	110.7
H-C-H	Choline	276.1	107.8
N-C-H	Choline	292.9	109.5
N-C-C	Choline	669.4	111.2
H-C-O	Choline	292.9	109.5
C-C-O	Choline	418.4	109.5
C-O-H (alcohol hydrogen)	Choline	460.2	108.5
Dihedral parameters			
Dihedral type	**Ionic species**	**Phase (degree)**	**Multiplicity**
H-O-C-H	Choline	0	3
H-O-C-C	Choline	0	3
O-C-C-H	Choline	0	3
O-C-C-N	Choline	0	3
H-C-C-H	Choline	0	3
H-C-C-N	Choline	0	3
H-C-N-C	Choline	0	3
C-C-N-C	Choline	0	3

Table S5. Bonded interaction parameters for the REL ion compatible with the OPLS-AA force field.

System	N_p	N_u	N_{IL} (TEA and ACE)	N_{ChCl} (REL and Cl)	N_W	V (nm^3)	d (kg/m^3)	T (K)	P (bar)
PW	1	0	0	0	4485	145.651 ± 0.0016	969.862 ± 0.011	329.998 ± 0.0013	1.1105 ± 0.0003
PUW	1	680	0	0	2300	125.214 ± 0.0014	1148.17 ± 0.0130	329.965 ± 0.0009	1.134 ± 0.0004
PUILW (5:1)	1	680	136	0	1179	123.126 ± 0.0052	1186.67 ± 0.05	329.94 ± 0.0012	1.132 ± 0.0008
PUILW (2:1)	1	680	340	0	2522	124.604 ± 0.0068	1126.46 ± 0.035	329.948 ± 0.0008	1.0746 ± 0.0001
PUChClW (5:1)	1	680	0	136	1418	126.182 ± 0.0035	1181.98 ± 0.033	329.947 ± 0.0009	1.1287 ± 0.0003
PUChClW (2:1)	1	680	0	340	1000	157.051 ± 0.009	1169.72 ± 0.067	329.937 ± 0.0007	1.10456 ± 0.0003

Table S6. Brief overview of all the six simulated systems. N_P, N_U, N_{IL}, N_{ChCl}, and N_W refer to the number of small protein HP-36, urea, ions from TEAA, ions from the ChCl and water molecules respectively. Systems PW, PUW, PUILW (5:1), PUILW (2:1), PUChClW (5:1) and PUChClW (2:1) denote the small protein in pure water, in aqueous urea, in mixed urea-TEAA (lower concentration), in mixed urea-TEAA (higher concentration), in mixed urea-ChCl (lower concentration) and in mixed urea-TEAA (higher concentration). V, d, T, P represent the cubic box volume, density, temperature and pressure of each of the simulated systems respectively. Standard errors provided are calculated from two independent simulations for each system.