Electronic Supplementary Information

Exploring the structure and stability of pentameric amyloid β peptide aggregate in aqueous ammonium-based ionic liquid solutions

Subhadip Sahoo[a] and Sanjoy Bandyopadhyay*[b]

[a] *Centre for Computational and Data Sciences, Indian Institute of Technology Kharagpur, Kharagpur - 721302, India*
[b] *Molecular Modeling Laboratory, Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur - 721302, India; E-mail: sanjoy@chem.iitkgp.ac.in*

Table SI-1 Initial cell dimension, number of solvent and cosolvent molecules used during the center-of-mass (com) pulling simulation for Aβ pentameric system in pure aqueous and aqueous ammoinum-based IL solution

system	cell dimension(Å^3)	solvent molecules		
		N_{Water}	N_{Cation}	N_{Anion}
TMAC	60×50×120	8467	434	434
ChoC	60×50×120	7541	434	434
TBAC	60×50×120	4026	434	434
Pure	60×50×120	11251	0	0

Table SI-2 Average interaction energies (in kcal mol^{-1}) of water and ammonium-based IL components present at the exterior surface ($\langle E^{surf} \rangle$) of the Aβ pentamer in pure aqueous medium and in binary water-IL solutions

system	cation			anion			water		
	vdw	elec	tot	vdw	elec	tot	vdw	elec	tot
TMAC	-1.02	-60.10	-61.12	-0.82	51.18	50.36	-0.62	-9.93	-10.55
ChoC	-3.03	-59.77	-62.80	-0.80	50.12	49.32	-0.63	-11.25	-11.88
TBAC	-11.08	-56.61	-67.69	-0.71	48.45	47.77	-0.60	-10.97	-11.57
Pure	-	-	-	-	-	-	-0.52	-9.37	9.89

Table SI-3 Average interaction energies (in kcal mol^{-1}) of water and ammonium-based IL components present inside the core ($\langle E^{core} \rangle$) of the Aβ pentamers in pure aqueous medium and in binary water-IL solutions

system	cation			anion			water		
	vdw	elec	tot	vdw	elec	tot	vdw	elec	tot
TMAC	-1.82	-69.54	-71.36	-	-	-	-0.78	-15.46	-16.24
ChoC	-4.23	-74.02	-78.80	-0.90	49.32	48.42	-0.80	-17.44	-18.24
TBAC	-13.23	-70.79	-84.02	-0.92	53.3	52.38	-0.78	-18.23	-19.01
Pure	-	-	-	-	-	-	-0.72	-12.5	-13.22

Table SI-4 Average side-chain interaction energies (in kcal mol^{-1}) of positive, negative, polar and non-polar residues of the Aβ pentamer with water and the ammonium-based IL components ($\langle E^{res} \rangle$) in pure aqueous medium and in binary water-IL solutions

residue	TMAC			ChoC			TBAC			Pure
	cation	anion	water	cation	anion	water	cation	anion	water	water
positive	86.33	-78.40	-3.87	82.77	-84.27	-2.63	76.50	-92.40	-5.89	-3.23
negative	-187.08	150.34	-6.73	-151.73	157.02	-4.44	-157.72	163.53	-5.24	-4.28
polar	-1.62	-2.93	-3.84	-2.66	-7.95	-4.44	-2.24	-11.90	-5.58	-3.23
nonpolar	-3.72	0.64	-6.02	-6.68	-0.97	-5.98	-9.63	-5.56	-7.21	-2.23

Table SI-5 Average number of protein-water hydrogen bonds (N_{PW}) formed around different peptide segments (N-term, turn, and C-term) for the Aβ pentamer in presence of different ammonium-based IL solution. For comparison the data in pure aqueous solution are included

system	N_{PW}		
	N-term	turn	C-term
TMAC	65.93($\pm$6.27)	34.56($\pm$3.54)	38.84($\pm$3.29)
ChoC	64.33($\pm$4.19)	31.11 ($\pm$3.12)	33.43($\pm$3.12)
TBAC	60.17($\pm$5.30)	19.02($\pm$3.27)	26.58($\pm$3.16)
Pure	86.93($\pm$5.02)	39.98($\pm$3.13)	46.00($\pm$3.33)

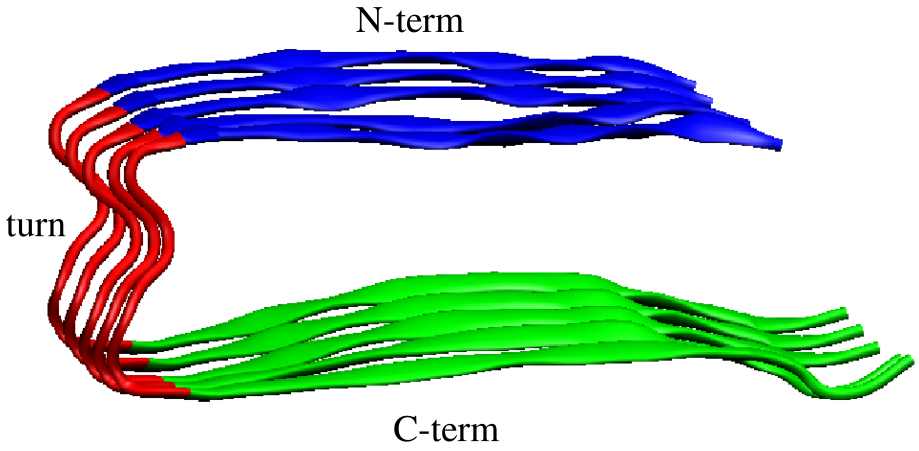

Fig. SI-1 A schematic representation of pentameric form of Aβ oligomer. For, visual clarity different segments of the monomers in the oligomer are color-coded differently, where Nterm, turn and Cterm are marked in blue, red and green colour respectively.

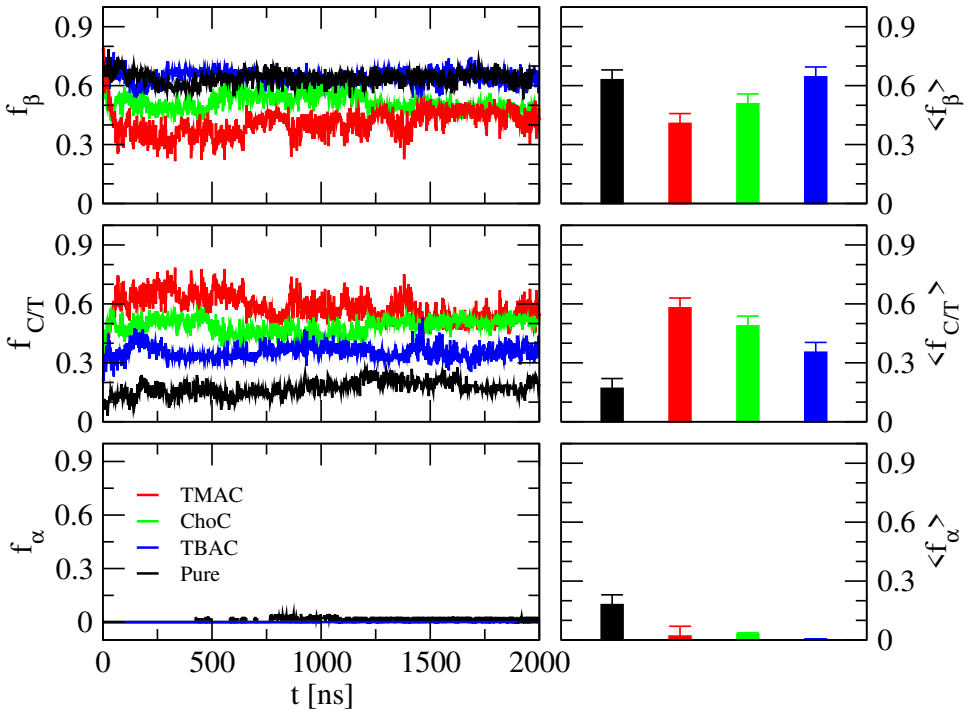

Fig. SI-2 Time evolutions of the fractions of β-strand, turn/coil and α-helical contents of the Aβ oligomer in pure aqueous medium and in binary water-IL solutions.

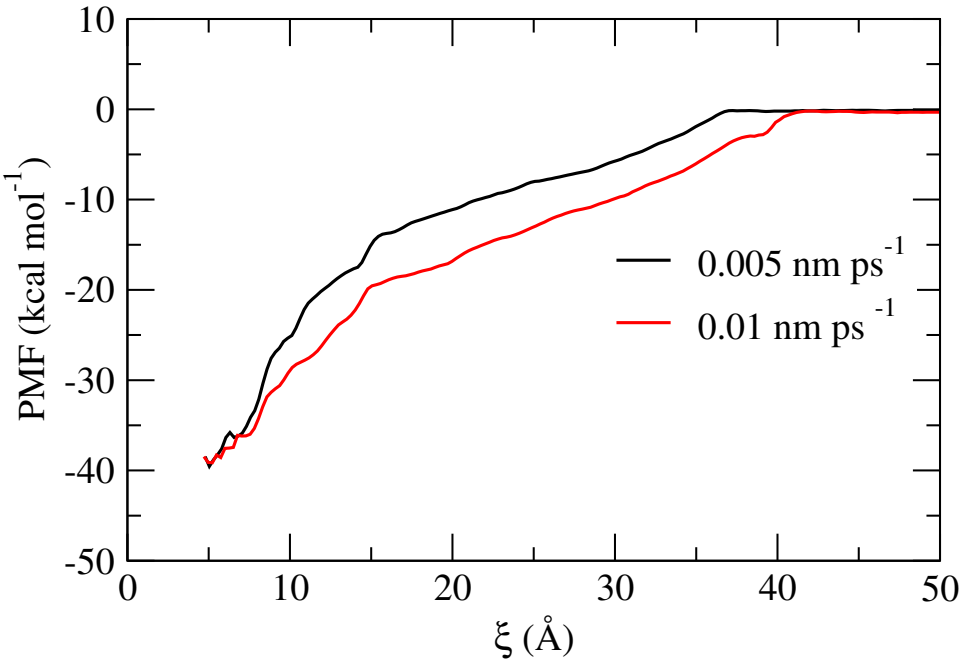

Fig. SI-3 Variation of the potential of mean force (PMF) along the reaction coordinate for Aβ Pentamer in pure aqueous solution by employing different pulling speeds.