Supporting Information

Influence of Salt and Temperature on the Self-assembly of Cyclic Peptides in Water: A Molecular Dynamics Study

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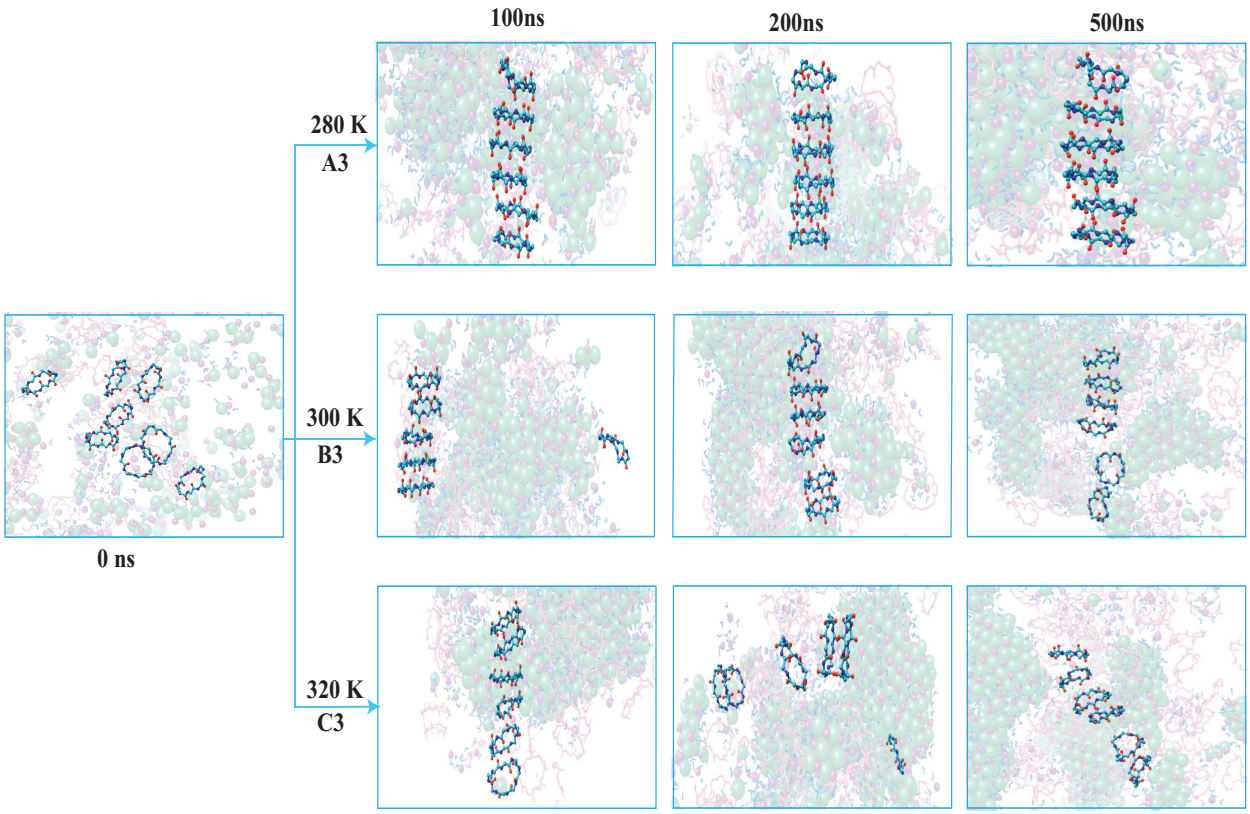

FIG. S1: Snapshots of cyclic peptide nanotube (CPNT) like structures formed in the systems (A3, B3, C3) at 280 K, 300 K, and 320 K at 0ns, 100ns, 200ns, and 500ns respectively

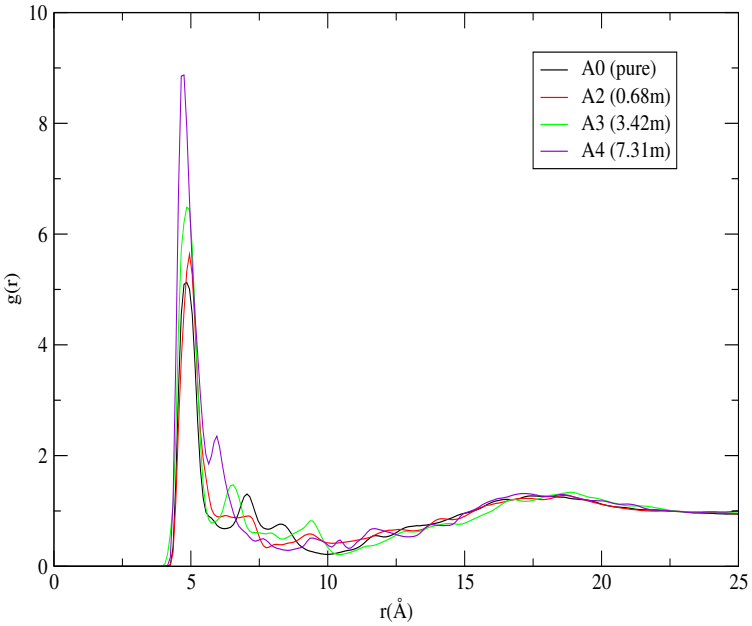

FIG. S2: Radial distribution functions of CP around a reference CP molecule calculated using center of mass of CP at 280 K

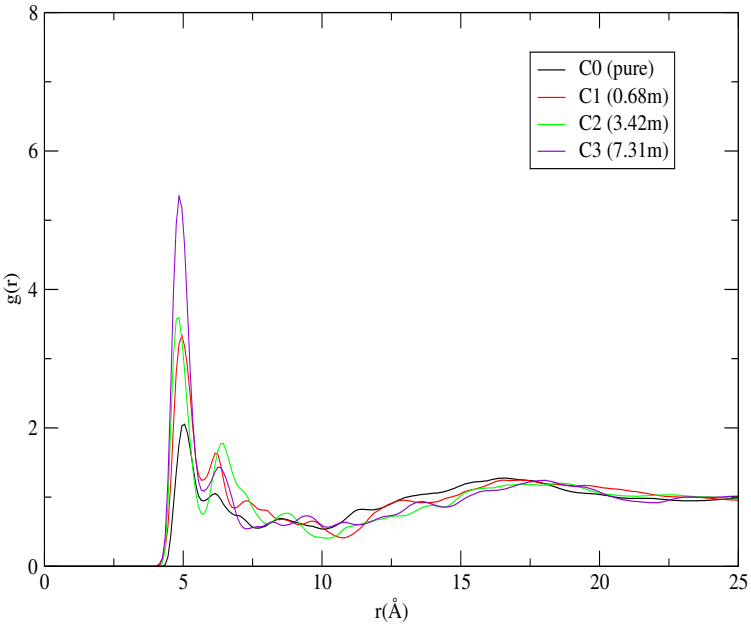

FIG. S3: Radial distribution functions of CP around a reference CP molecule calculated using center of mass of CP at 320 K

TABLE S1: Co-ordination (hydration) number around different hydrophilic and hydrophobic atomic sites of CP molecule in the considered systems at 280 K. The normalized values of hydration numbers are presented in parenthesis for each site

System	OD1	NZ	CG	CD2
A0	2.85	3.92	5.73	5.63
A1	2.61 (3.01)	3.79 (4.29)	5.60 (6.14)	5.56 (6.17)
A2	2.29 (2.56)	3.42 (3.82)	5.41 (5.97)	5.29 (5.84)
A3	2.12 (2.33)	3.29 (3.61)	5.14 (5.62)	5.02 (5.60)

TABLE S2: Co-ordination (hydration) number around different hydrophilic and hydrophobic atomic sites of CP molecule in the considered systems at 320 K. The normalized values of hydration numbers are presented in parenthesis for each site.

System	OD1	NZ	CG	CD2
C0	2.71	3.51	4.89	4.81
C1	2.30 (2.56)	3.49 (3.82)	4.87 (5.37)	4.82 (5.31)
C2	2.17 (2.34)	3.31 (3.66)	5.10 (5.63)	5.05 (5.58)
C3	2.32 (2.59)	3.43 (3.80)	5.33 (5.88)	5.31 (5.87)

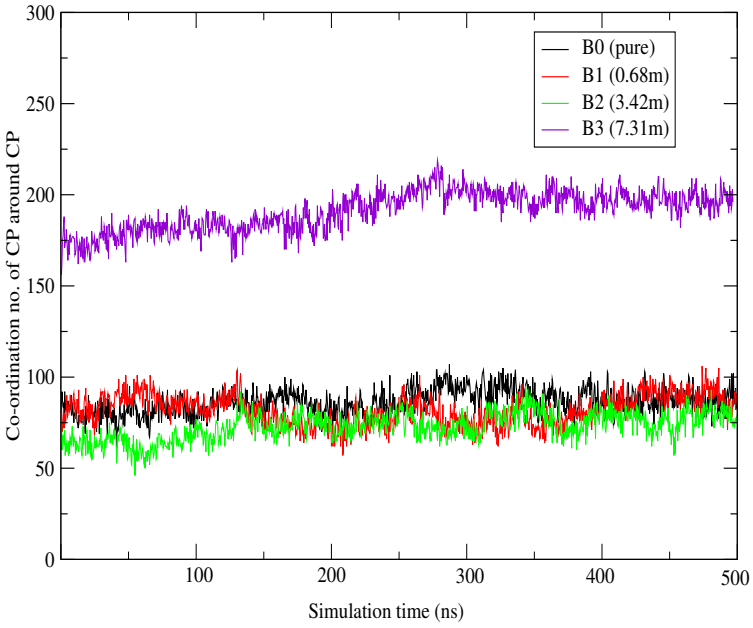

FIG. S4: The co-ordination number of CP around CP molecules versus simulation time for the systems B0, B1, B2, and B3 at 300 K.

TABLE S3: The average number of hydrogen bonds formed between water-water (per water) and site-water (per atom of CP) in all the systems considered at 280 K. Here, O and N are the backbone atoms of the CP while OD1 and NZ are the side chain atoms of aspartic acid and lysine respectively.

System	HB_{W-W}	HB_{O-W}	HB_{N-W}	HB_{OD1-W}	HB_{NZ-W}
A0	3.01	0.82	0.36	1.83	1.49
A1	2.92	0.77	0.35	1.65	1.47
A2	2.67	0.72	0.33	1.42	1.16
A3	2.48	0.69	0.28	1.26	1.06

TABLE S4: The average number of hydrogen bonds formed between water-water (per water) and site-water (per atom of CP) in all the systems considered at 320 K. Here, O and N are the backbone atoms of the CP while OD1 and NZ are the side chain atoms of aspartic acid and lysine respectively.

System	HB_{W-W}	HB_{O-W}	HB_{N-W}	HB_{OD1-W}	HB_{NZ-W}
C0	2.94	0.72	0.34	1.63	1.30
C1	2.87	0.69	0.33	1.47	1.32
C2	2.67	0.67	0.32	1.26	1.19
C3	2.50	0.68	0.32	1.25	1.12

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