Supplementary Material

Aggregation Behavior of Cetyldimethylethylammonium Bromide under the Influence of Bovine Serum Albumin in Aqueous/ Electrolyte Solutions at Various Temperatures and Compositions: Conductivity and Molecular Dynamics Study

FaridAhmed[a,b], Mohammad Robel Molla[a,b], MousumiSaha[c], ImrulShahriar[c], Mohammad Saidur Rahman[a,d], Mohammad A. Halim[c], Malik Abdul Rub[e,f], Md. Anamul Hoque[a,*], Abdullah M. Asiri[e,f]

[a]*Department of Chemistry, Jahangirnagar University, Savar, Dhaka- 1342, Bangladesh*
[b]*Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka, Bangladesh*
[c]*Division of Quantum Chemistry, The Red-Green Research Centre, BICCB, Dhaka, Bangladesh*
[d]*Department of Chemical Engineering, Faculty of Engineering, University of Malaya, 50603, Kuala Lumpur, Malaysia*
[e]*Chemistry Department, Faculty of Science, King Abdulaziz University, Jeddah-21589, Saudi Arabia*
[f]*Center of Excellence for Advanced Materials Research, King Abdulaziz University, Jeddah 21589, Saudi Arabia*

[*]*Correspondence address:*

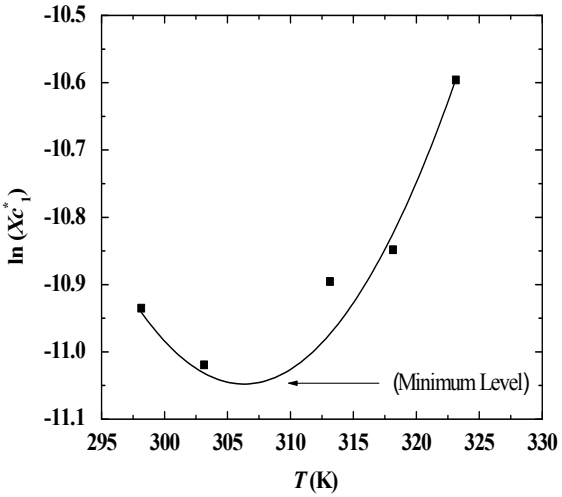
Professor Dr. Md. AnamulHoque
Department of Chemistry
Jahangirnagar University
Savar, Dhaka-1342, Bangladesh
Tel: PABX: 880-2-7791045-51, extension: 1437
Fax: 880-2-7791052
Email: ahoque_ju@yahoo.com, ahoque_ju@juniv.edu

SM Table 1

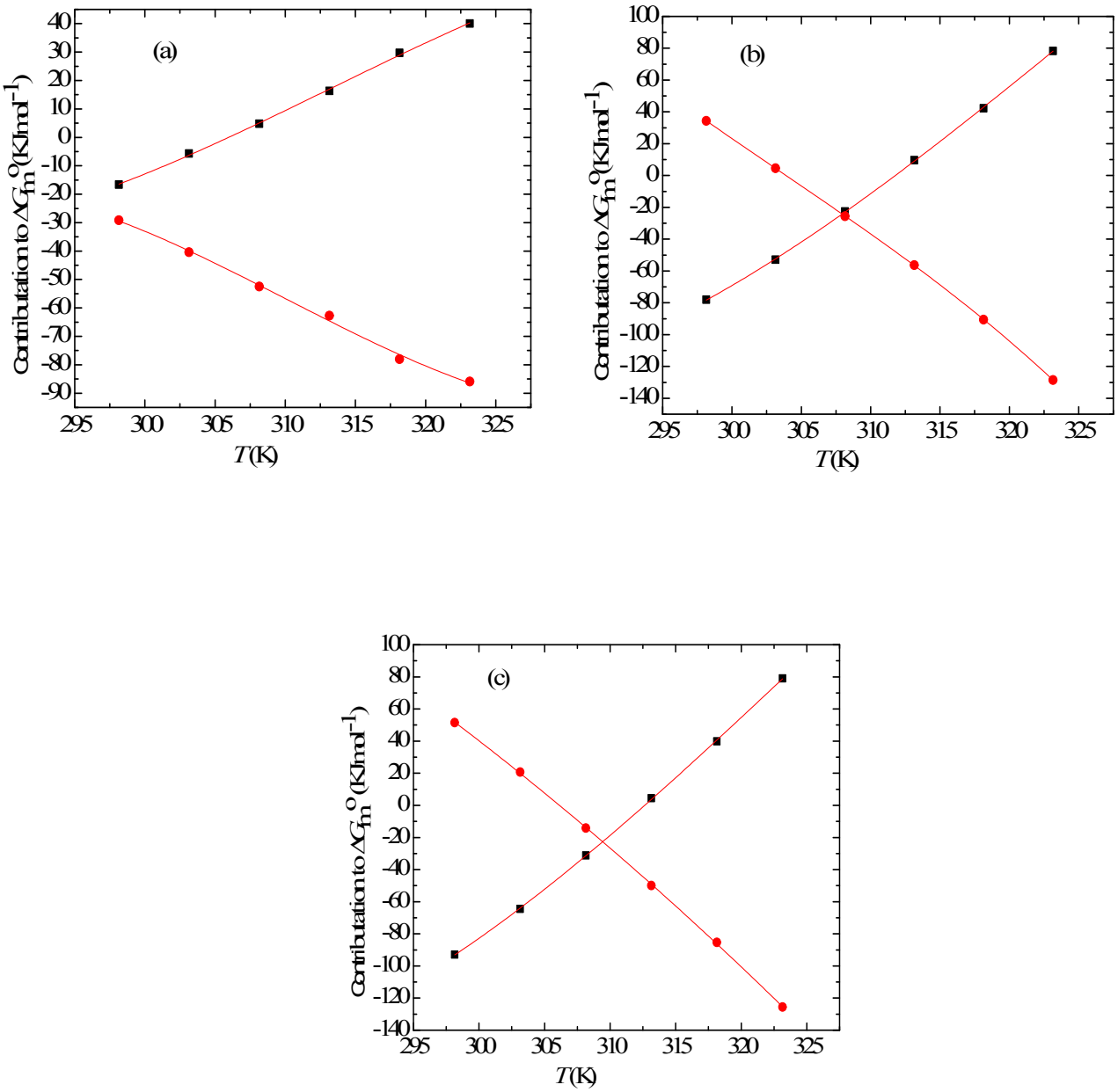
Thermodynamic parameters of transfer for the micellization of BSA mediated CDMEAB solution (with/ without salt of different ionic strength)[a]

System	Medium	$I_{Salt/}$ mmol.kg^{-1}	T/K	$\Delta G^0_{1,m,tr}$	$\Delta G^0_{2,m,tr}$	$\Delta G^0_{3,m,tr}$	$\Delta H^0_{1,m,tr}$	$\Delta H^0_{2,m,tr}$	$\Delta H^0_{3,m,tr}$	$\Delta C^0_{1,m,tr}$	$\Delta C^0_{2,m,tr}$	$\Delta C^0_{3,m,tr}$
				kJ mol^{-1}			kJ mol^{-1}			kJ K^{-1} mol^{-1}		
BSA+CDMEAB	H_2O	0.00	298.15	0.92	-2.11	0.55	25.02	-13.04	-8.59	-1.60	-0.16	-0.38
			303.15	3.48	3.46	2.20	17.48	-14.02	-10.13	-1.87	-0.13	-0.43
			308.15	2.10	1.02	2.69	5.70	-13.94	-12.53	-2.13	-0.08	-0.49
			313.15	3.54	2.40	2.07	-5.16	-14.49	-15.35	-2.40	-0.04	-0.53
			318.15	1.95	4.17	0.73	-16.05	-15.20	-18.20	-2.66	0.00	-0.58
			323.15	5.30	1.81	0.66	-31.65	-14.38	-20.82	-2.90	0.04	-0.63
BSA+CDMEAB	H_2O+NaCl	1.50	298.15	3.06	5.43	4.94	-36.42	-85.60	-16.27	1.41	3.07	0.40
			303.15	1.20	2.98	1.65	-29.74	-72.31	-15.41	1.52	3.60	0.55
			308.15	1.55	0.92	2.69	-21.73	-51.49	-11.20	1.66	4.16	0.70
			313.15	3.20	1.00	2.11	-11.92	-27.09	-6.80	1.80	4.71	0.88
			318.15	2.00	0.84	1.72	-3.46	-2.98	-2.43	1.94	5.27	1.03
			323.15	1.05	1.07	1.74	6.69	23.30	2.78	2.07	5.81	1.19
BSA+CDMEAB	H_2O+Na_2SO_4	1.50	298.15	5.35	5.13	4.70	-51.25	-4.92	-1.52	2.06	0.08	0.02
			303.15	5.80	6.28	3.19	-41.27	-4.34	-1.60	2.18	0.10	0.05
			308.15	4.42	4.63	2.77	-30.34	-3.44	-1.14	2.29	0.13	0.07
			313.15	4.49	6.23	4.01	-17.08	-3.28	-0.42	2.42	0.16	0.14
			318.15	4.85	6.30	4.02	-5.84	-2.51	0.06	2.54	0.19	0.15
			323.15	4.65	5.75	3.77	7.39	-1.07	0.88	2.66	0.21	0.18

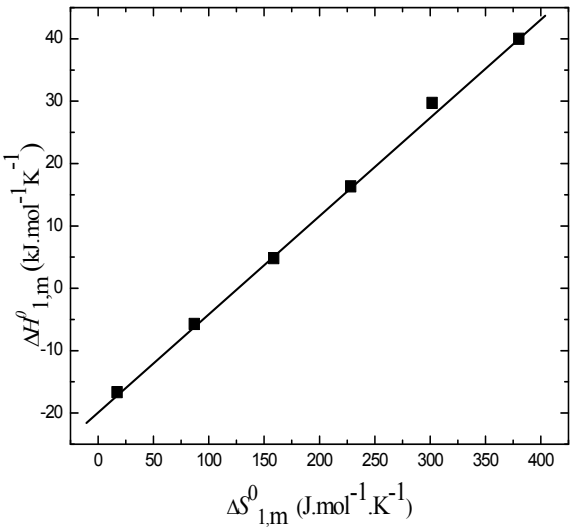
[a]Relative standard uncertainties (u_r) limits are $u_r(\Delta G^0_{m.tr.})$, $u_r(\Delta H^0_{m.tr.})$ and $u_r(\Delta C^0_{p.m.tr.})$ are 0.03, 0.04, and 0.04 respectively



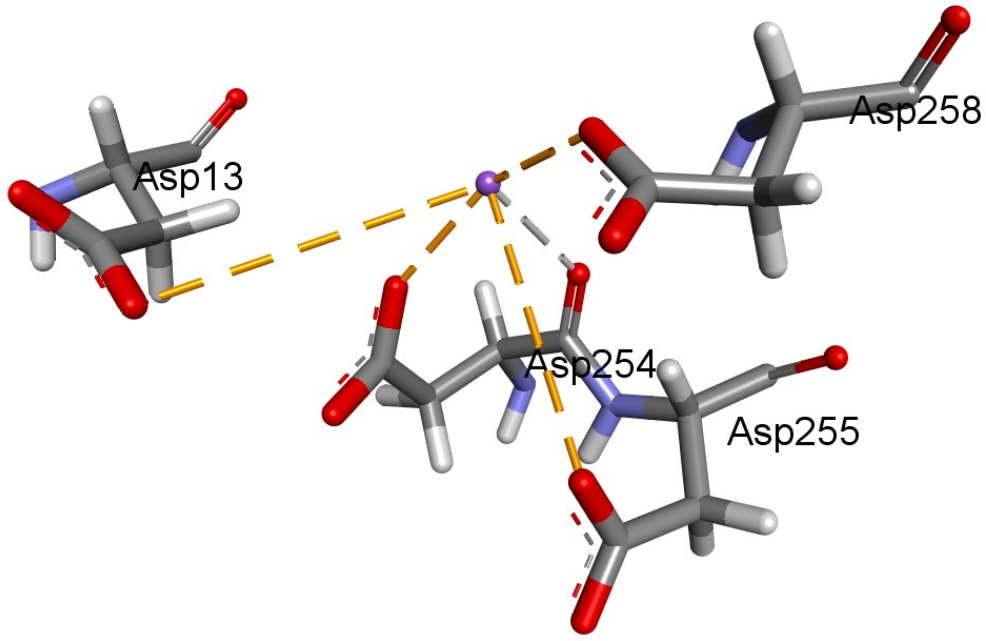
SM Fig. 1. Plot of ln (Xc^*_1) versus T for (BSA+CDMEAB) system containing 0.03 mmol.kg^{-1} BSA in aqueous solution



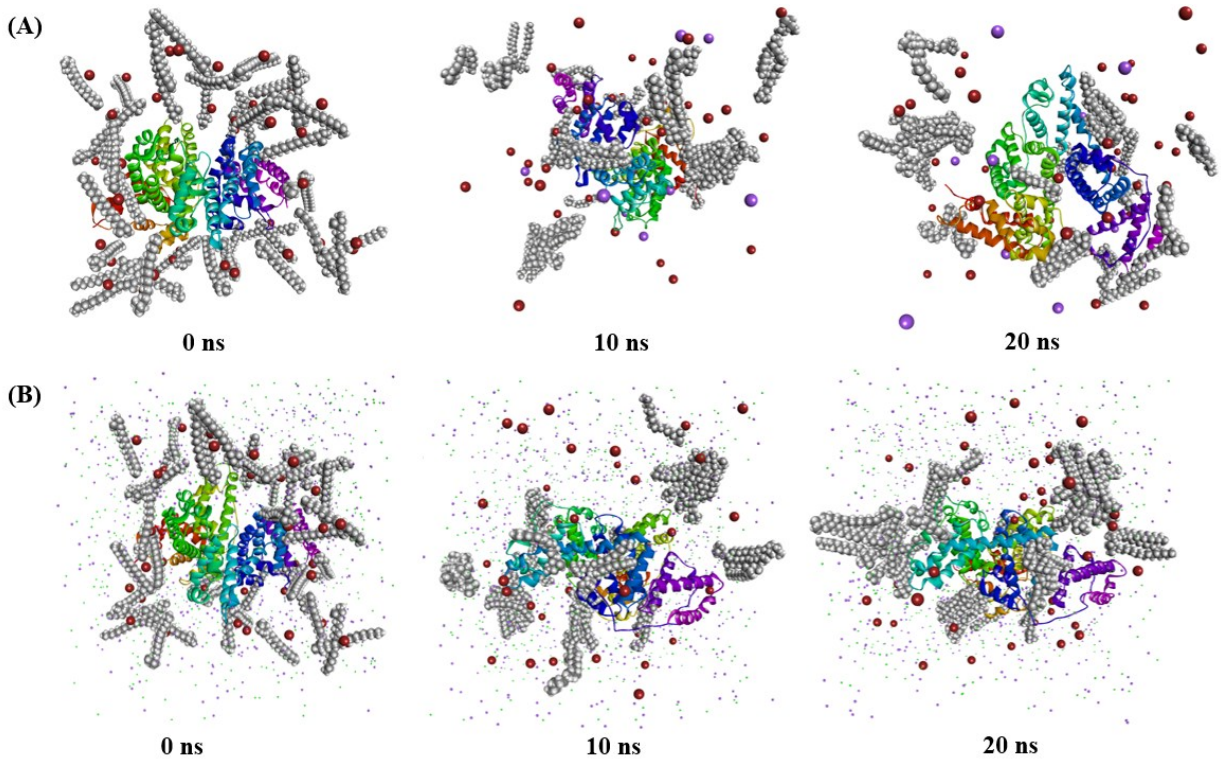
SM Fig. 2. Representative plots of contribution of enthalpy, $\Delta H^0_{1,m}$ (■) and entropy, $-T\Delta S^0_{1,m}$ (●) to $\Delta G^0_{1,m}$ for (CDMEAB+BSA) mixed system containing 0.03 mmol.kg^{-1} BSA in (a) water, (b) aqueous solution of NaCl (ionic strength, I = 1.50 mmol.kg^{-1}) and (c) aqueous solution of Na_2SO_4 (ionic strength, I = 1.50 mmol.kg^{-1})



SM Fig. 3. Plot of enthalpy-entropy compensation event for (BSA+CDMEAB) systems having 0.03 mmol.kg^{-1} BSA solution in an aqueous medium for c_1^*



SM Fig. 4. Interaction of sodium ion (in purple) with four negatively charged amino acid residues of BSA (obtained from a simulation snapshot at 20 ns)



SM Fig. 5. Simulation snapshots of BSA+CDMEAB in (A) H_2O and (B) H_2O+NaCl