Twin Tailed Surfactant Induced Conformational Changes in Bovine Serum Albumin: A Detailed Spectroscopic and Physicochemical Study

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Supplementary Information

S1: Potentiometric Measurements

The neutral ion-pair complexes of ditetradecyldimethyl ammonium bromide-sodium dioctyl sulfosuccinate ($DTDA^+DSS^-$) used in the dioctyl sulfosuccinate (DSS^-) ion-selective membrane were prepared as follows: Equimolar aqueous solutions of ditetradecyldimethyl ammonium bromide and sodium dioctyl sulfosuccinate were mixed and after continuous stirring for a considerable time, the white precipitates of ion-pair $DTDA^+DSS^-$ were obtained. The precipitates were washed thoroughly and repeatedly with double distilled water and re-crystallized thrice from acetone.

The PVC (176 mg), ion-pair complex $DTDA^+DSS^-$ (5 mg) and plasticizer, DOA (550.0 mg) were mixed and dissolved in minimum quantity of THF. This ratio of proportions for all components of membrane represents the best system in terms of the slope values, correlation coefficient, linear range, detection limit etc. The resulting mixture was poured into 50-mm petri dish after removing the air bubbles and THF was allowed to evaporate at room temperature. The resulting membrane was cut to size, attached to PVC tubes with PVC glue, and equilibrated in 25 mM AOT solution (internal reference solution: 25 mM AOT in 1 mM NaCl).

S2: Turbidity Measurements

The turbidity measurements were carried out by using a digital Nephelo-Turbidity meter 132 from Systronics at 25 ˚C. The light beam source (Tungsten lamp) in combination with optical components produce a converging light beam which is then scattered by colloidal particles and scattered light is sensed by a photocell appeared in arbitrary nephelo turbidity units (N.T.U). The sample cell was filled 25 ml of BSA solution (10 or 20 μM concentration) and DTDAB solution was titrated into the sample cell with constant stirring and sufficient time equilibrations. All the measurements were repeated at least three times.

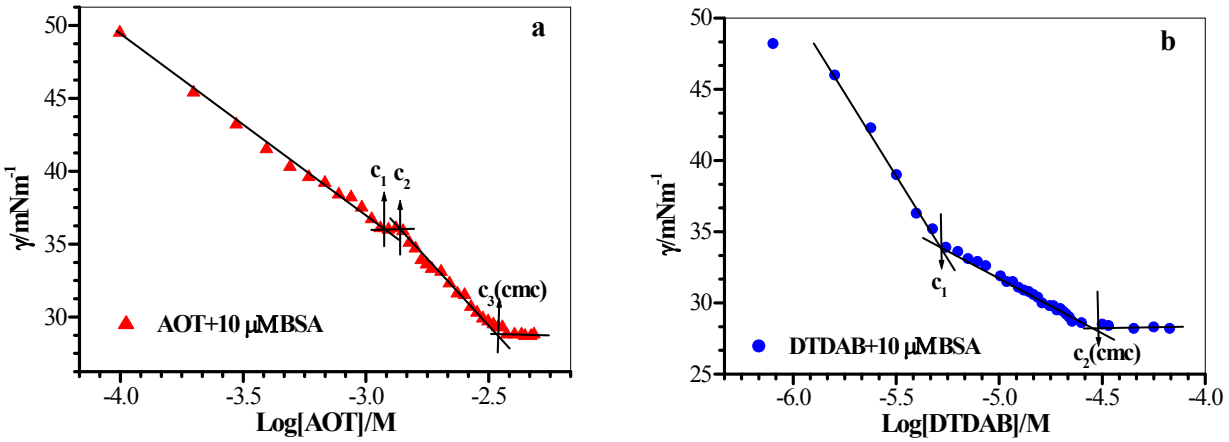

Fig. S1: Surface tension as a function of Log [surfactant] in the presence of BSA (**a**) AOT (**b**) DTDAB

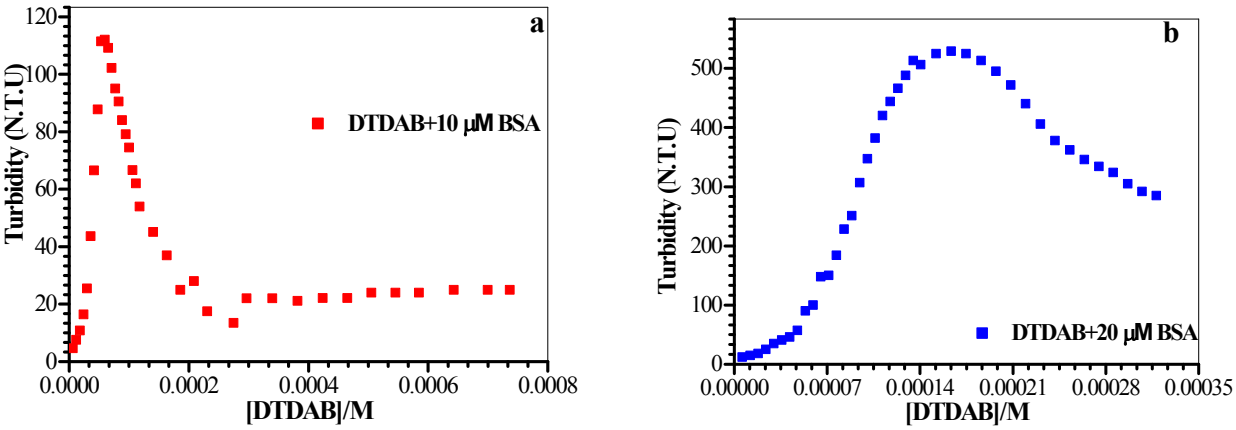

Fig. S2: Tubidity (N.T.U) as a function of [DTDAB] in the presence of BSA at (**a**) 10 μM (**b**) 20 μM

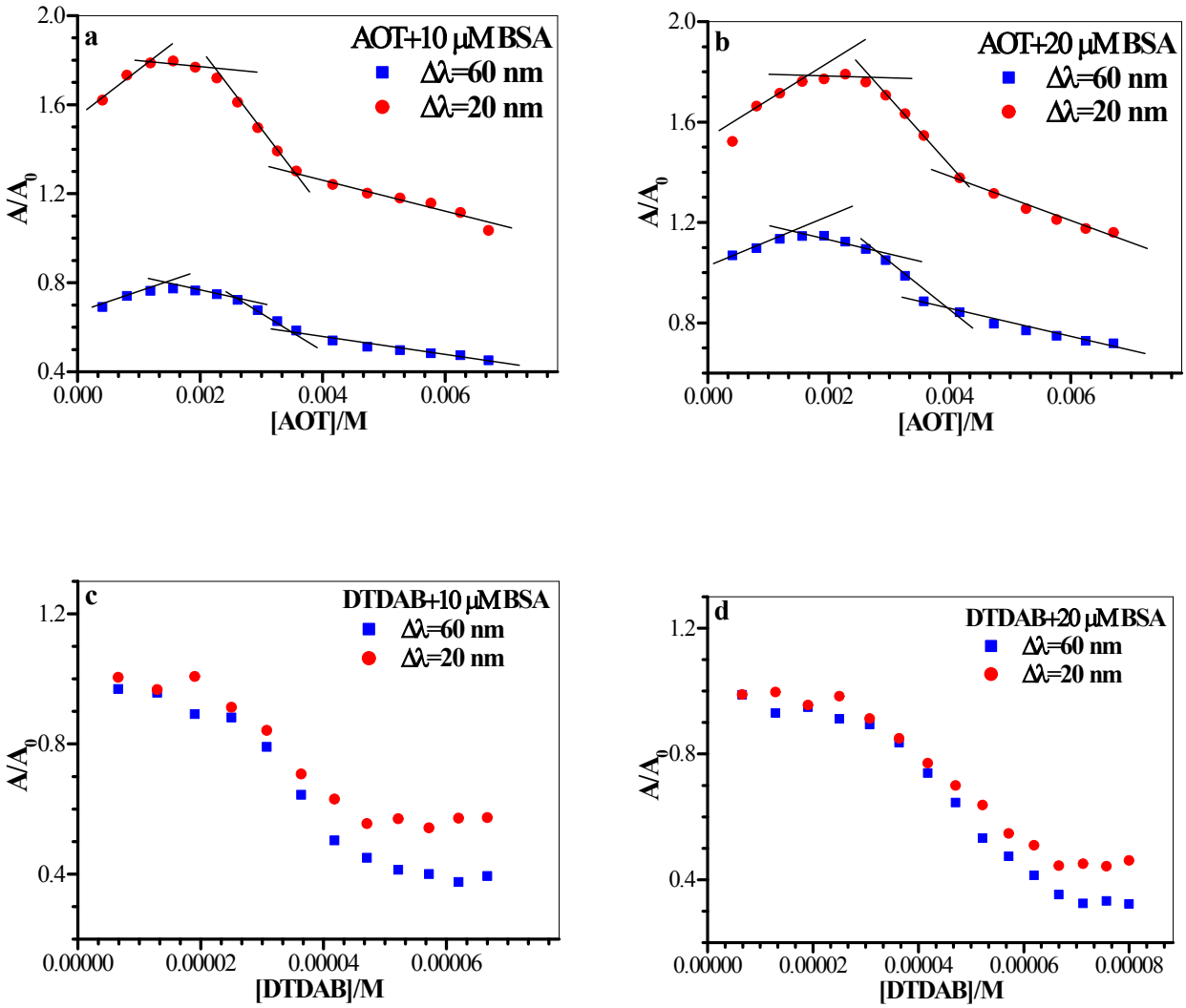

Fig. S3: Normalized area ratios (A_0/A) as a function of [surfactant] obtained from synchronous fluorescence spectra at $\Delta\lambda$ = 60 nm and at $\Delta\lambda$ = 20 nm for (a) AOT+BSA (10 μM) (b) AOT+BSA (20 μM) (c) DTDAB+BSA (10 μM) (d) DTDAB+BSA (20 μM)

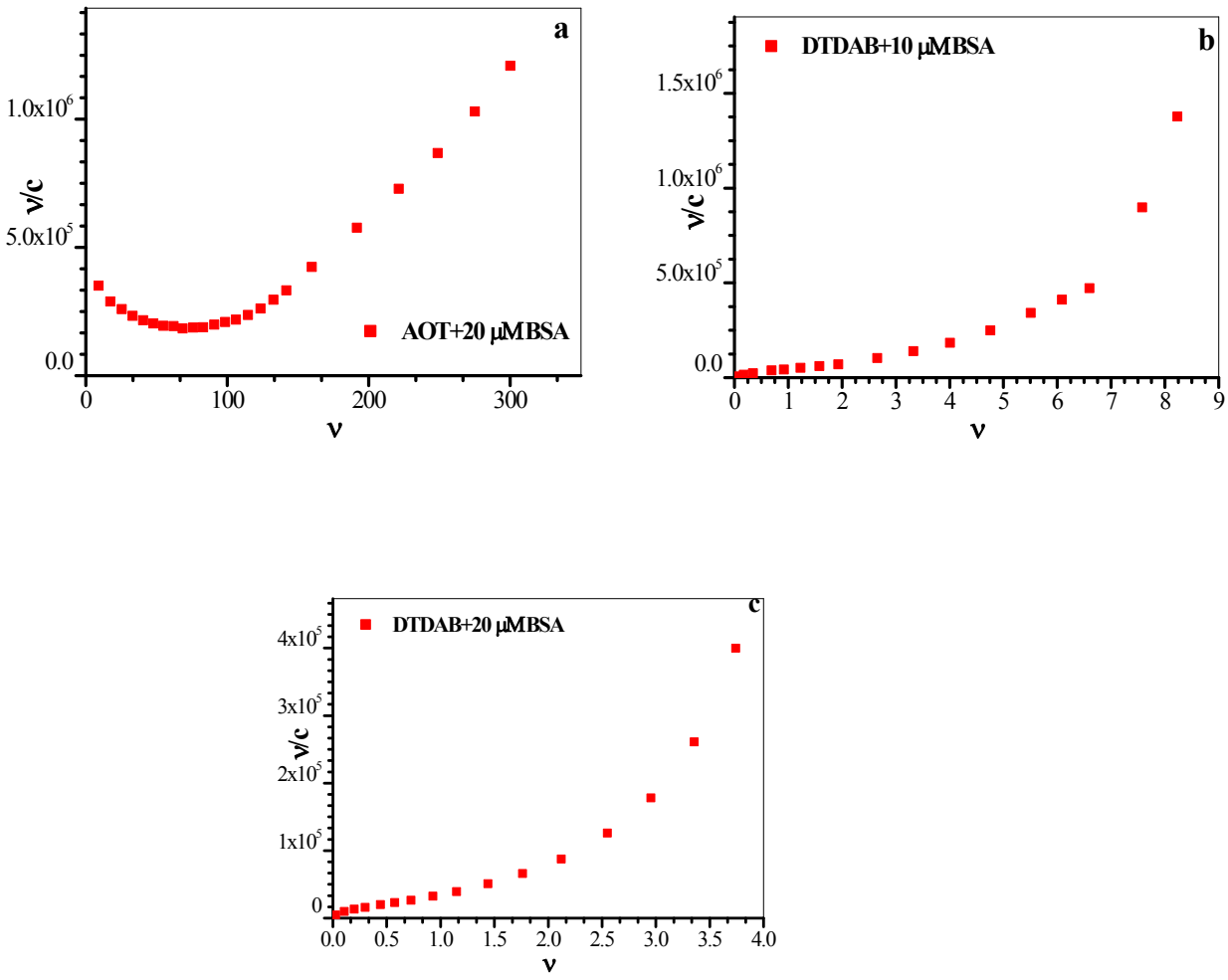

Fig. S4: Scatchard plots of (**a**) 20 μM BSA with AOT (**b**) 10 μM BSA with DTDAB (**c**) 20 μM BSA with DTDAB

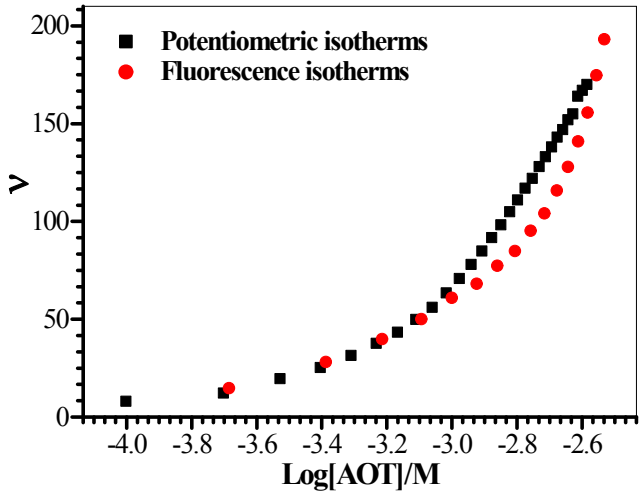

Fig.S5: Binding isotherms obtained from potentiometric and fluorescence measurements for AOT + 10 μM BSA

Table S1: The various transition concentrations: C_1, C_2 and Critical micelle concentration (C_3-cmc) obtained from synchronous fluorescence spectra at $\Delta\lambda = 60$ nm and at $\Delta\lambda = 20$ nm

System	C_1 (10^{-3} M)	C_2 (10^{-3} M)	C_3(*cmc*) (10^{-3} M)
Synchronous fluorescence at Δλ = 60 nm			
AOT+BSA (10 µM)	1.43	2.60	3.58
AOT+BSA (20 µM)	1.64	2.72	4.16
Synchronous fluorescence at Δλ = 20 nm			
AOT+BSA (10 µM)	1.18	2.24	3.55
AOT+BSA (20 µM)	1.56	2.64	4.16

Table S2: The various transition concentrations: C_1, and Critical micelle concentration (C_2-*cmc*) obtained from synchronous fluorescence spectra at $\Delta\lambda = 60$ nm and at $\Delta\lambda = 20$ nm

System	C_1 (10^{-5} M)	C_2(*cmc*) (10^{-5} M)
Synchronous fluorescence at Δλ = 60 nm		
DTDAB+BSA (10 µM)	2.69	4.63
DTDAB +BSA (20 µM)	2.49	6.63
Synchronous fluorescence at Δλ = 20 nm		
DTDAB +BSA (10 µM)	2.69	4.63
DTDAB +BSA (20 µM)	2.49	6.63

Table 6: *cmc* and thermodynamic parameters: Gibbs free energy, enthalpy and entropy of micellization (ΔG_{mic}, ΔH_{mic} and ΔS_{mic} respectively) at 25±1 °C obtained from ITC measurements.

System	*cmc* (10^{-3} M)	ΔG_{mic} (kJ/mol)	ΔH_{mic} (kJ/mol)	ΔS_{mic} (J/(mol.K))
AOT	2.28	-25.04	3.25	94.88
AOT+BSA (10 µM)	2.32	-25.01	3.22	94.70
AOT+BSA (20 µM)	2.67	-24.65	3.09	93.03
	cmc	**ΔG_{mic}**	**ΔH_{mic}**	**ΔS_{mic}**
	(10^{-5} M)	**(kJ/mol)**	**(kJ/mol)**	**(J/(mol.K))**
DTDAB	3.23	-35.59	-3.48	107.70
DTDAB+BSA (10 µM)	5.83	-34.13	-0.22	113.73
DTDAB+BSA (20 µM)	6.11	-34.01	-0.22	113.30