Supporting information

Binding Interaction of an Anionic Amino Acid Surfactant with Bovine Serum Albumin: Physicochemical and Spectroscopic Investigations combined with Molecular Docking Study

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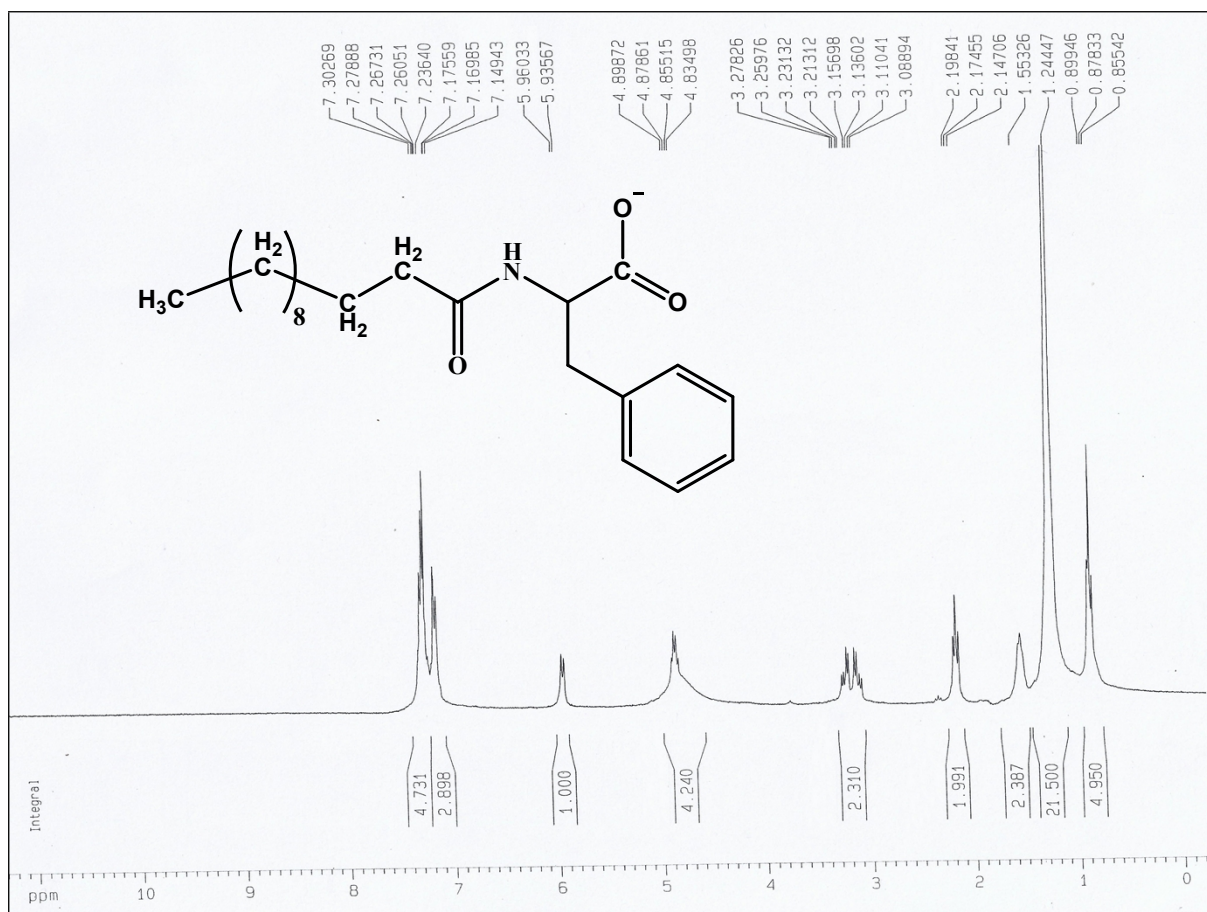E-mail addresses amahapatra@chemistry.jdvu.ac.in, ambikeshju@gmail.com

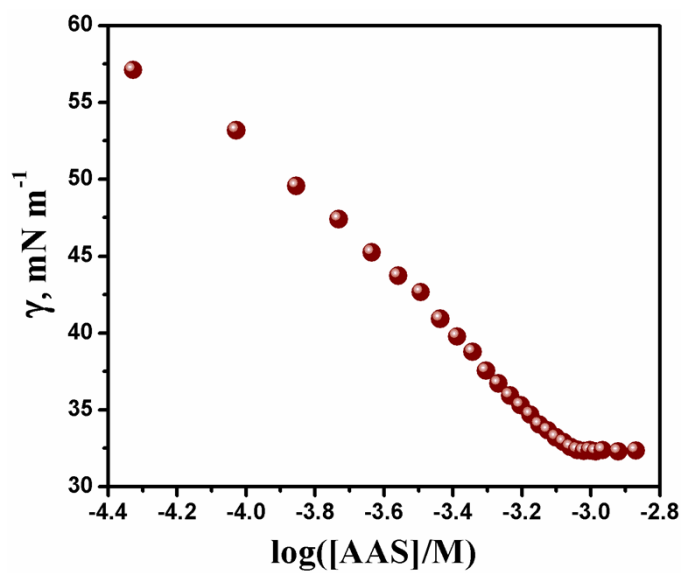Fig. S1: ^{1}H NMR spectra of *N*-dodecanoyl-L-phenylalanine.

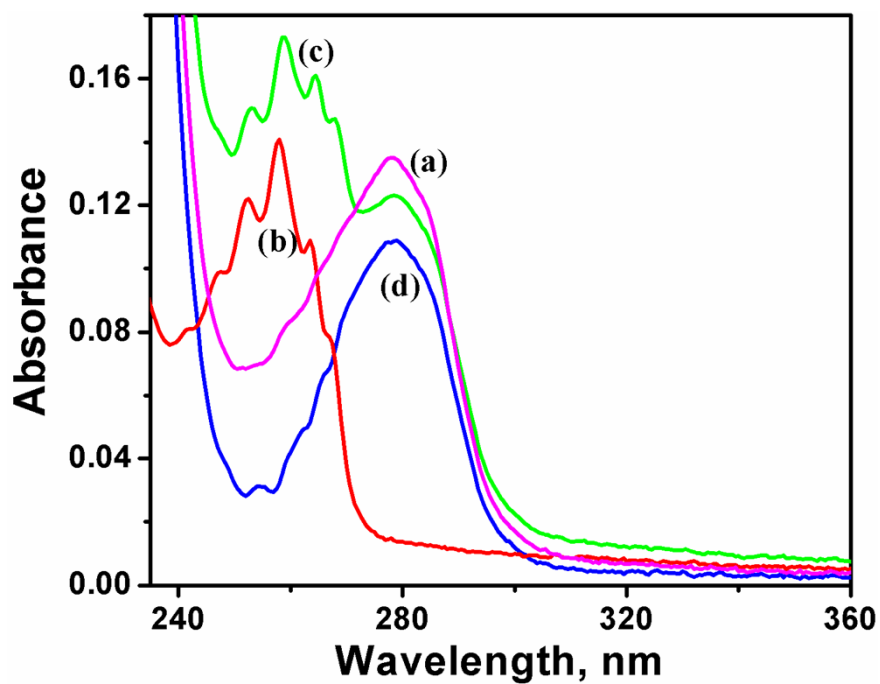Fig. S2: Variation of surface tension of AAS in pure water at 298 K.

Fig. S3: (a) absorption spectrum of BSA only, (b) absorption spectrum of AAS only, (c) absorption spectrum of BSA-AAS system at the same concentration of AAS and (d) difference of absorption spectrum between BSA-AAS system and AAS at 298 K; [BSA] = 3.0 μM, [AAS] = 2.0 mM.
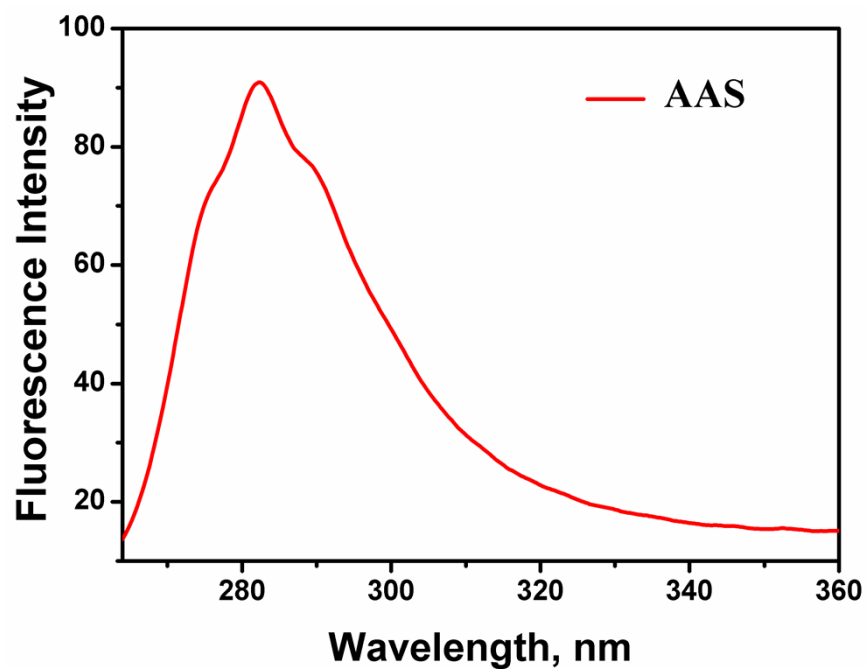

Fig. S4: Emission spectrum of AAS, λ_{ex} = 258 and λ_{em} = 282 nm, [AAS] = 2.0 mM, at 298 K.
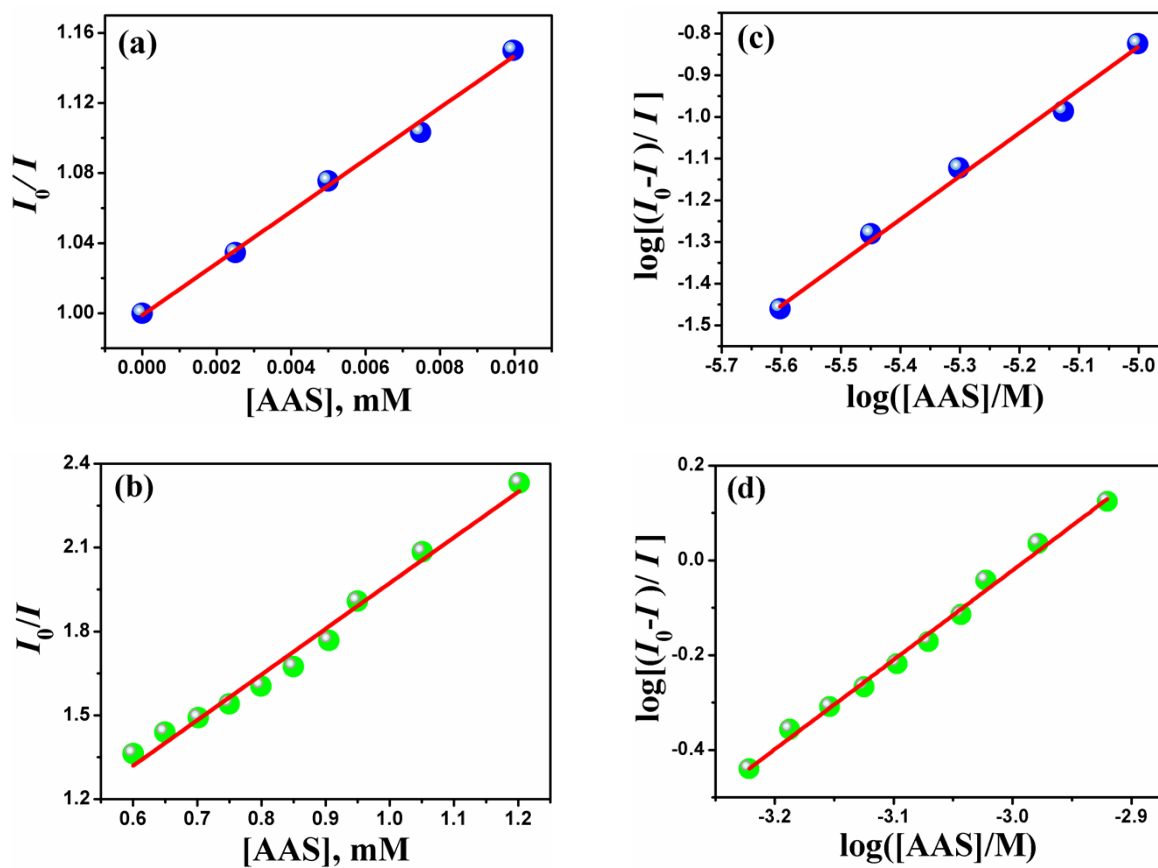
Fig. S5: (a) and (b) are Stern-Volmer plot of region I and III respectively; (c) and (d) are modified Stern-Volmer plot of region I and III respectively at 298 K, [BSA] = 3.0 µM
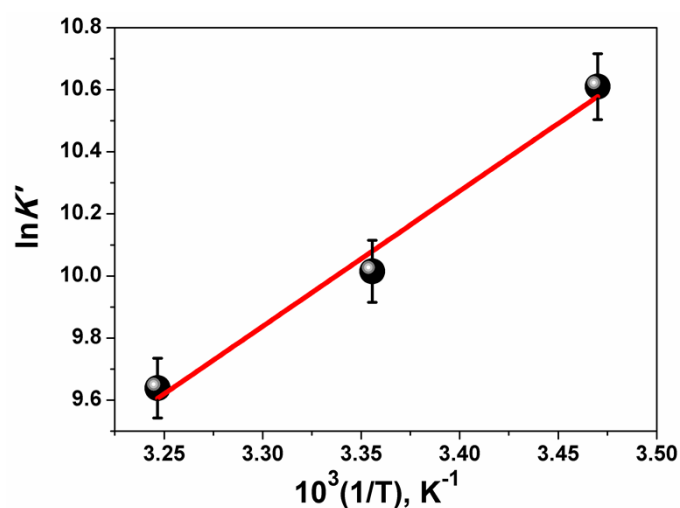

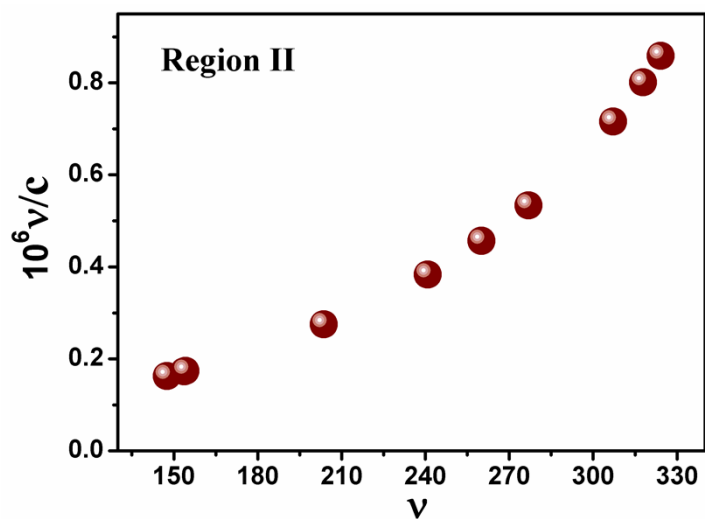Fig S6: Van't-Hoff plot for region I of BSA-AAS system, [BSA] = 3.0 µM.

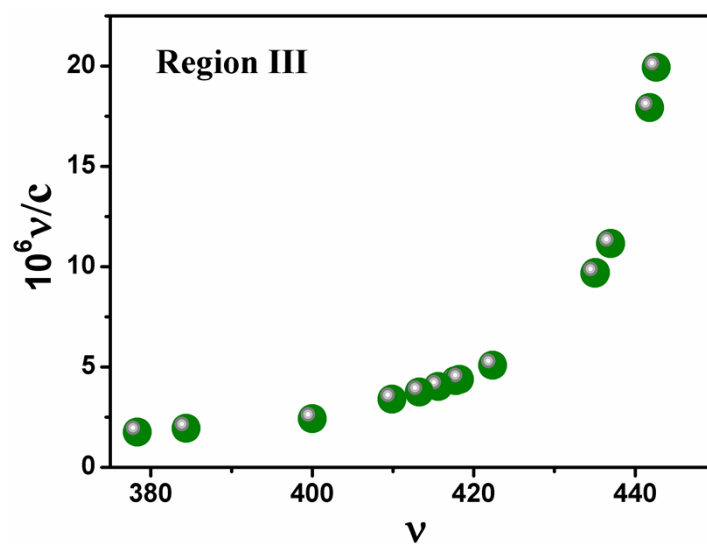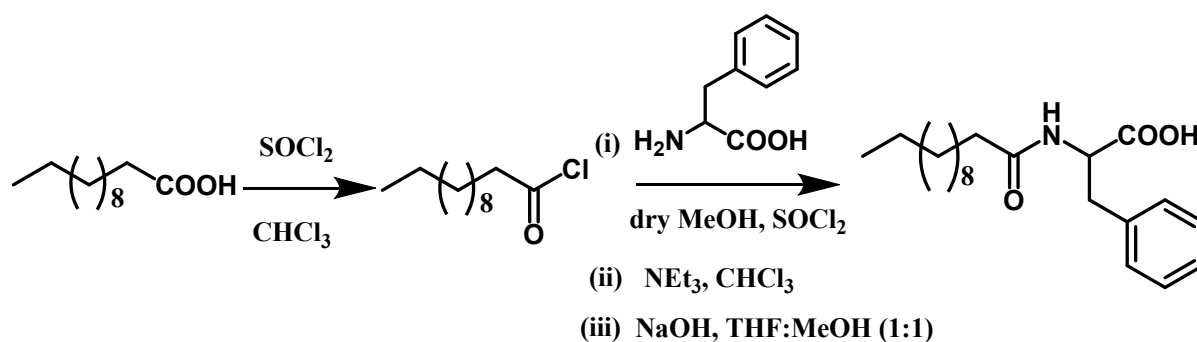Fig. S7: Scatchard plot for region II of BSA-AAS system at 298 K, [BSA] = 3.0 μM.

Fig. S8: Scatchard plot for region III of BSA-AAS system at 298 K, [BSA] = 3.0 μM.

Scheme S1: Synthetic route of N-dodecanolphenylalanine

Table S1: Stern-Volmer quenching constant and modified Stern-Volmer association constant for the first three regions of BSA-AAS system at 298 K.

Region	$10^3 \, K_{SV}$, M^{-1}	K_a, M^{-n}	R[a]	ΔG, kJ mol^{-1}
I	14.8 ± 0.05	2.23×10^4	0.9921	-24.81 ± 1.61
II	0.31 ± 0.02	1.34	0.9758	-0.73 ± 0.11
III	1.63 ± 0.07	4.39×10^5	0.9933	-32.19 ± 0.93

[a] R is correlation coefficient for the K_a values

Table S2: Stern-Volmer quenching constant, modified Stern-Volmer association constant and thermodynamic parameters at different temperatures for region I of BSA-AAS system

Temperature, K	$10^4 K_{SV}$, M^{-1}	$10^4 K_a$, M^{-n}	R^a	ΔH^o, kJ mol^{-1}	ΔS^o, J mol^{-1} K^{-1}	ΔG^o, kJ mol^{-1}
288	1.89 ± 0.1	4.05	0.9855			-25.40 ± 2.16
298	1.48 ± 0.05	2.23	0.9921	-36.21 ± 4.19	-37.69 ± 1.41	-24.81 ± 1.61
308	1.33 ± 0.03	1.54	0.9977			-24.68 ± 0.86

[a] R is correlation coefficient for the K_a values

Table S3: Secondary structural content of BSA in the absence and presence of AAS at 298 K.

[AAS]/[BSA]	% α-helix	% β-sheets	% β-turn	% Random coil
0	64.2	7.2	12.3	17.2
10	59.9	8.1	12.8	19.1
20	58.2	8.4	13.1	19.8
50	54.8	9.3	13.5	21.3
100	50.6	10.6	14.2	23.6
200	38.5	14.4	16.3	29.8