Supplementary Information

Interaction of bovine serum albumin (BSA) protein with mixed anionic-cationic surfactants and resultant structure

Debasish Saha,[a] Debes Ray,[a] Sugam Kumar,[a] Joachim Kohlbrecher,[b] and Vinod K. Aswal*[,a, c]

[a]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India

[b]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, CH-5232 PSI Villigen, Switzerland

[c]Homi Bhabha National Institute, Mumbai 400 094, India

*Email: vkaswal@barc.gov.in

Theory of Dynamic Light Scattering

The dynamic light scattering measures the temporal fluctuation in scattering light intensity at a specific angle using a monochromatic light. The signal generated by diffusing particles can be analyzed by the normalized intensity autocorrelation function $g^2(\tau)$[1,2]

$$g^{(2)}(\tau)=\frac{\langle I(t)I(t+\tau)\rangle}{\langle I(t)\rangle^2} \quad \text{(S1)}$$

where $I(t)$ is the scattered light intensity at time t and $I(t+\tau)$ the scattered intensity at time t plus delay time τ. The normalized intensity correlation function is related to the normalized filed autocorrelation function by the Siegert relation

$$g^{(2)}(\tau)=1+\beta\left|g^{(1)}(\tau)\right|^2 \quad \text{(S2)}$$

where β is the spatial coherence factor and depends on the alignment and detection optics.

The field autocorrelation function for a dilute system of monodisperse particles is represented by

$$g^1(\tau)=\exp(-\Gamma\tau) \quad \text{(S3)}$$

where Γ is the average decay rate of $g^1(\tau)$ and extracted from the monomodal fit. The diffusion coefficient (D_a) and the wave vector q are related to Γ as $\Gamma=D_aq^2$

For a suspension of polydisperse particles, the field autocorrelation function is modified to

$$g^1(\tau)=\int_0^\infty G(D_a)\exp(-D_aq\tau)dD_a \qquad \text{(S4)}$$

where $G(D_a)$ is the distribution of particles with different diffusion coefficients about the mean value. The mean value of the diffusion coefficient (D_m) and polydispersity index (PI) are calculated by using the cumulant analysis method.[3] Including the cumulant analysis, Eq. (4) can be simplified to

$$g^1(\tau)=\exp\left[-D_mq^2\tau+\frac{\mu_2\tau^2}{2}\right] \qquad \text{(S5)}$$

where PI is calculated from the ratio of variance (μ_2) to the square of the mean of the decay rate ($\Gamma_m=D_mq^2$). The corresponding effective hydrodynamic radius (r_h) is calculated using Stoke-Einstein equation.[4]

Schematic of the DLS instrument (SZ100, Horiba)

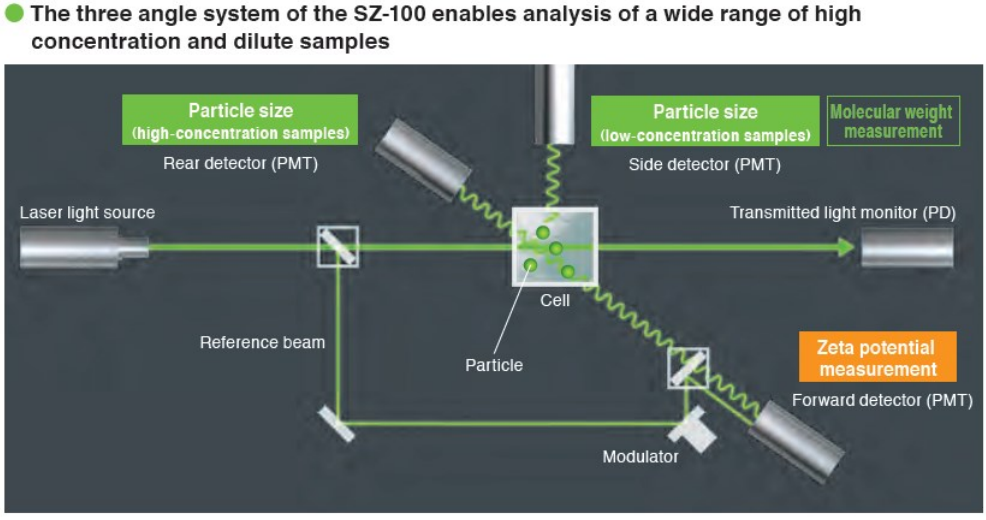

Fig. S1. Schematic of the DLS instrument (SZ100, Horiba) used for the measurements of transmission (0° scattering angle) and auto correlation function (173° scattering angle).

SANS of 1wt% BSA-SDS rich mixed surfactant complexes

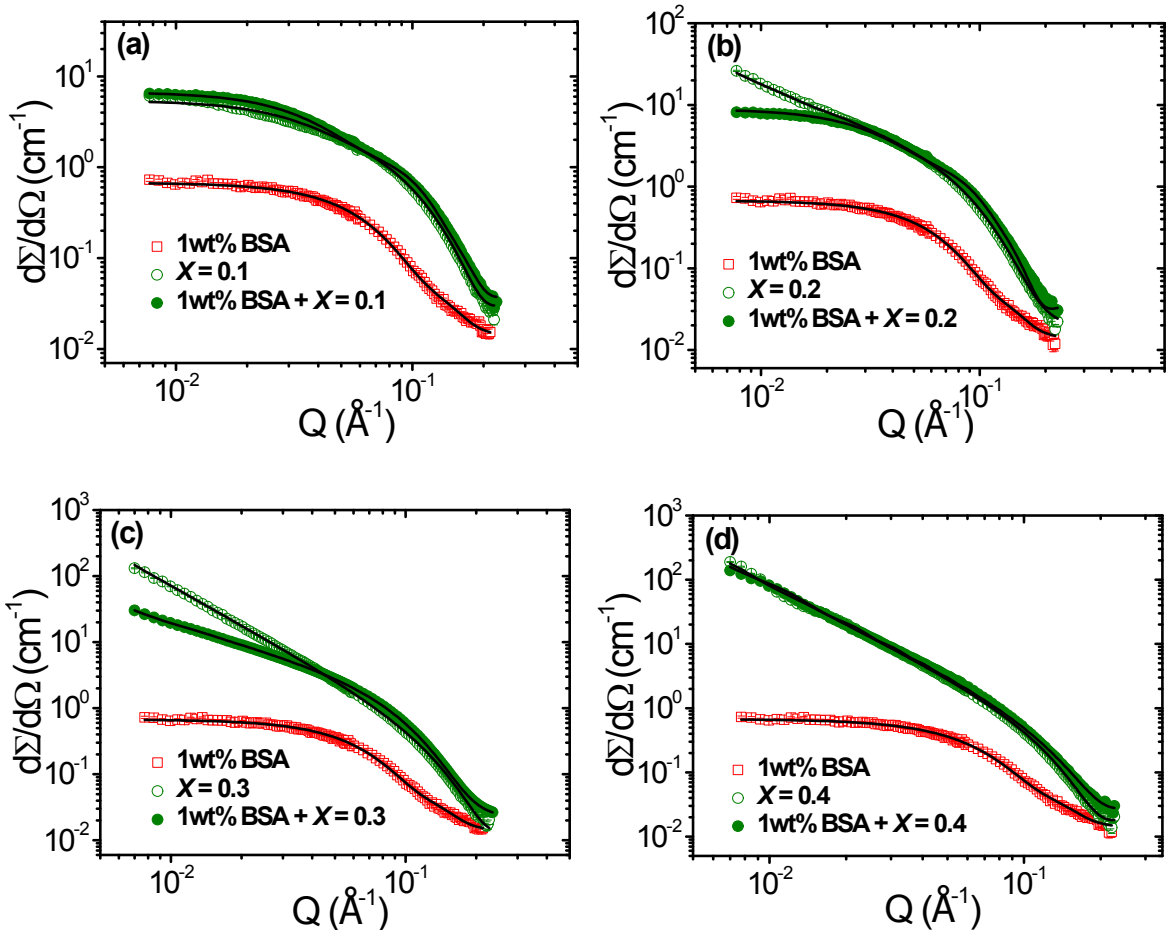

Fig. S2. SANS profile of 1 wt% BSA with SDS rich mixed surfactant (*X*= 0.1-0.4 and total 50 mM concentration) at pH=7.0 and 0.2 M NaCl in D_2O. For comparison SANS profiles of pure protein and corresponding mixture of surfactants are also plotted. The significant change in the scattering profiles in the lower Q region of mixed surfactant systems (particularly for *X*=0.2 and 0.3) on addition of BSA suggests the participation of BSA in the resultant complex formation.

SANS of 1wt% BSA-DTAB rich mixed surfactant complexes

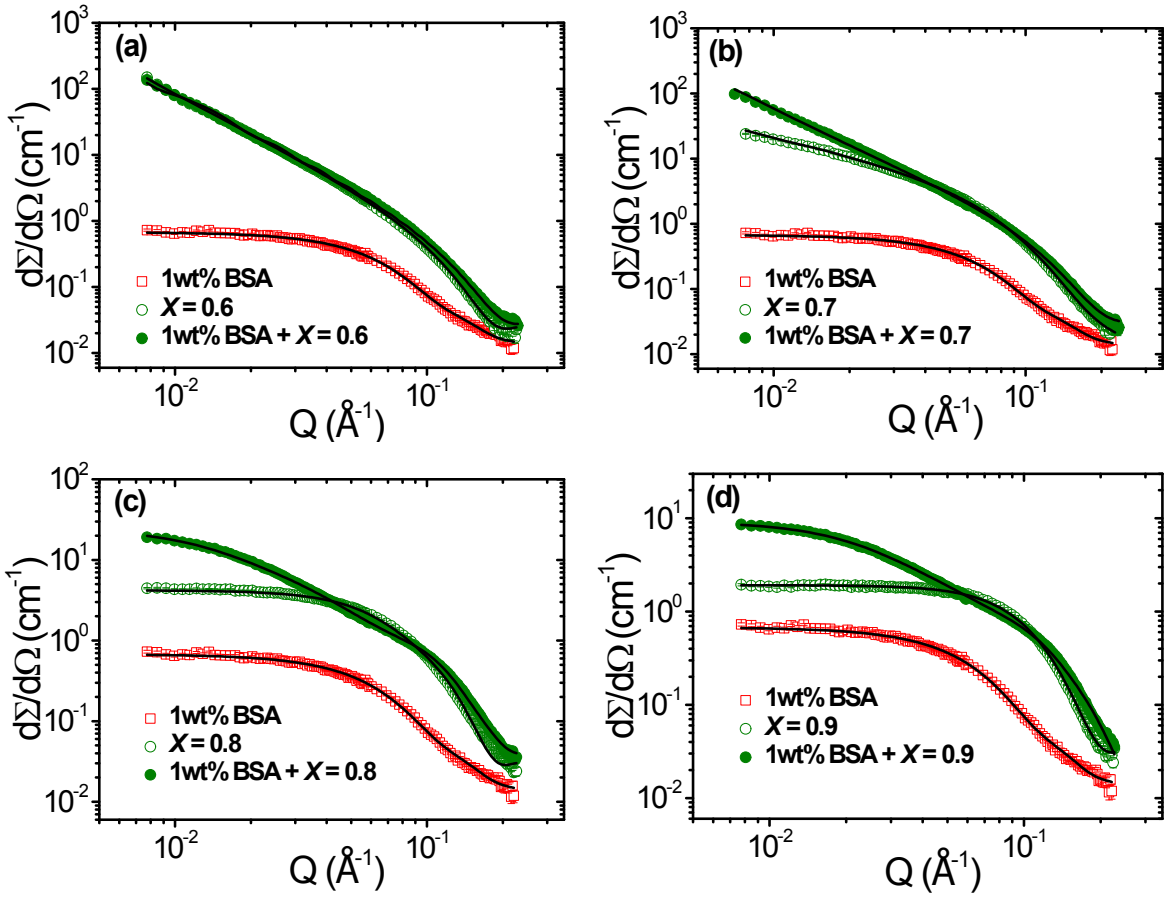

Fig. S3. SANS profile of 1 wt% BSA with DTAB rich mixed surfactant (X= 0.6 - 0.9 and total 50 mM concentration) at pH=7.0 and 0.2 M NaCl in D_2O. For comparison SANS profiles of pure protein and corresponding mixture of surfactants are also plotted. The significant change in the scattering profiles in the lower Q region of mixed surfactant systems (particularly for X=0.7, 0.8 and 0.9) on addition of BSA suggests the participation of BSA in the resultant complex formation.

SANS of 1wt% BSA with equimolar mixture of SDS-DTAB

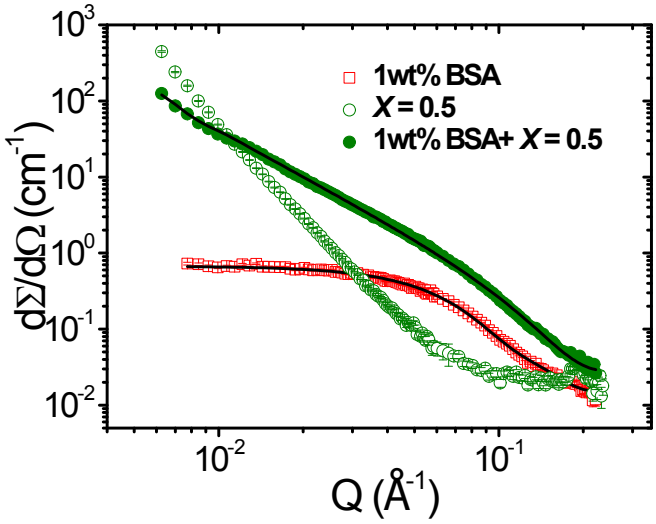

Fig. S4. SANS profile of 1 wt% BSA with equimolar mixture of SDS-DTAB surfactants (total 50 mM concentration) at pH=7.0 and 0.2 M NaCl in D_2O. For comparison SANS profiles of pure protein and equimolar mixture of surfactants are also plotted. The significant change in the scattering profile of mixed surfactant system on addition of BSA suggests the participation of BSA in the resultant complex formation.

References

1 *Dynamic Light Scattering: Applications of Photon Correlation Spectroscopy*, Springer US, 1st edn., 1985.

2 P. A. Hassan, S. Rana and G. Verma, *Langmuir*, 2015, **31**, 3–12.

3 D. E. Koppel, *J. Chem. Phys.*, 1972, **57**, 4814–4820.

4 P.N. Pusey and R.J. Tough, *Adv. Colloid Interface Sci.*, 1982, **16**, 143–159.