Surface Active Ionic Liquid Cholinium Dodecylbenzenesulfonate: Self-Assembling Behaviour and Interaction with Cellulase

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Supporting information

Annexure 1.

1. The Adsorption efficiency of surfactant at air-water interface is estimated by measuring pC_{20} using the relation (1)

$$pC_{20} = -\log C_{20} \quad \text{.....(1)}$$

where, C_{20} is the concentration needed to reduce the surface tension of the solvent (water in the present case) by 20mN.m^{-1}. The higher pC_{20} value indicates high adsorption efficiency of the surfactant[1].

2. The effectiveness of surface tension reduction is the other parameter that measures the adsorption efficiency of a surfactant, denoted by π_{CMC} and calculated using the relation (2).

$$\pi_{CMC} = \gamma_{H_2O} - \gamma_{CMC} \quad \text{.....(2)}$$

where γ_{H_2O} stands for the surface tension of the pure water and γ_{CMC} stands for the surface tension of the solvent medium at CMC[1].

3. The amount of surfactants adsorbed at the interface is estimated from relative surface excess concentration (Γ_{max}).The values Γ_{max} of at the CMC have been calculated using Gibbs adsorption Eq. 3 from the least-squares slope of the γ versus log C plot.

$$\Gamma_{max} = -\frac{1}{nRT}\frac{\partial\gamma}{\partial \ln C} \quad \text{.....(3)}$$

Where "$\partial\gamma/\partial \ln C$'' is the slope of $\gamma - \ln C$ the plot in the pre-*CMC* region.[5-7] and n is Gibbs adsorption coefficient. In the current paper, it is used 2 due to ionic dissociation of [Chol]DBS in an aqueous medium[1].

4. The minimum area occupied by monomers at the interface was calculated using equation 4.

$$A_{min} = \frac{10^{16}}{\Gamma_{max}.N_A} \quad \text{.....(4)}$$

Where N_A is Avogadro number and the factor of 10^{16} arises as a conversion factor of the area from nm^2 to $Å^1$.

5. Gibbs free energy of micellization :

$$\Delta G^o_{mic} = (1+\beta)RT \ln X_{cmc} \text{.....(5)}$$

Where β is the 1-α and α has been calculated from conductivity measurement. α is the ratio of the slope of the post-CMC region and pre-CMC region[1].

6. Gibbs Free energy of adsorption[1]:

$$\Delta G^o_{ad} = \Delta G^o_{mic} - \frac{\pi_{CMC}}{\Gamma_{\max}} \text{.....(6)}$$

7. Enzyme activity (IU):

$$1U = \frac{C}{M \times t \times V} \text{.....(7)}$$

The c= concentration of sugar released, *M* is molecular weight of sugar, t is a time of incubation and *V* is the volume of enzyme used[2].

8. Kaputinskii equation:

$$U_L = -K\frac{v|z^+|z^-|}{r^+r^-}\left(1-\frac{d}{r^+r^-}\right)\text{-------(1)}$$

Where UL, z, r, and ν, represent the lattice enthalpy, ion charges, radii and stoichiometric coefficient (e.g. 2 for NaCl) respectively. The terms K and d, are salt specific constants[3].

Annexure 2.

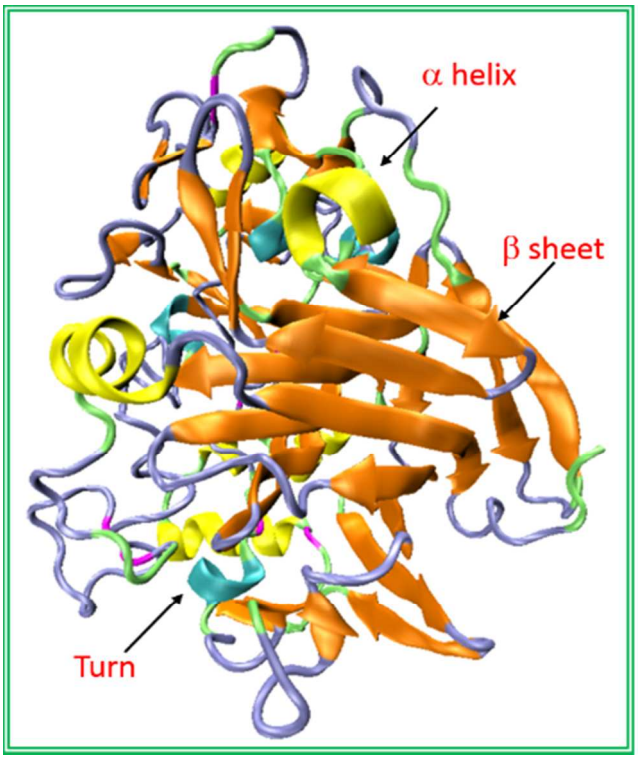

Figure S1. A model of cellulase from *Trichoderma reesei* (fungi) based on template 1EGN PDB85 file using Visual Molecular Dynamic software.

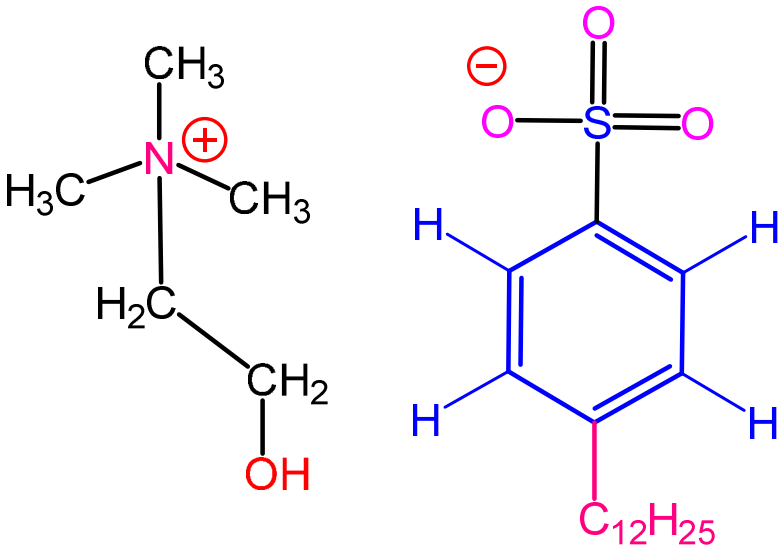

Figure S2. Chemical structure of Cho[DBS].

The ^{1}H NMR spectrum of synthesized Cho[DBS] was recorded in deuterated DMSO using a Brüker 200 MHz spectrometer. Before measurement, Cho[DBS] was dried in vacuum oven.

^{1}HNMR 200 MHz: Cho[DBS]. In DMSO-d_6 Chemical shift value for proton (δ_H) in ppm: 7.517(d, 2H of –S-C=C**H**-), 7.100 (d, 2H of C–C=C**H**-), 3.818 (m, 2H of N-CH_2-C**H**$_2$-O), 3.390 (t, 2H N-C**H**$_2$-CH_2-O), 3.097 (s, 9H of 3× -C**H**$_3$), 1.429 (m),1.170 (m), 0.800 (m), 0.684 (t) of –C_{12}**H**$_{25}$.

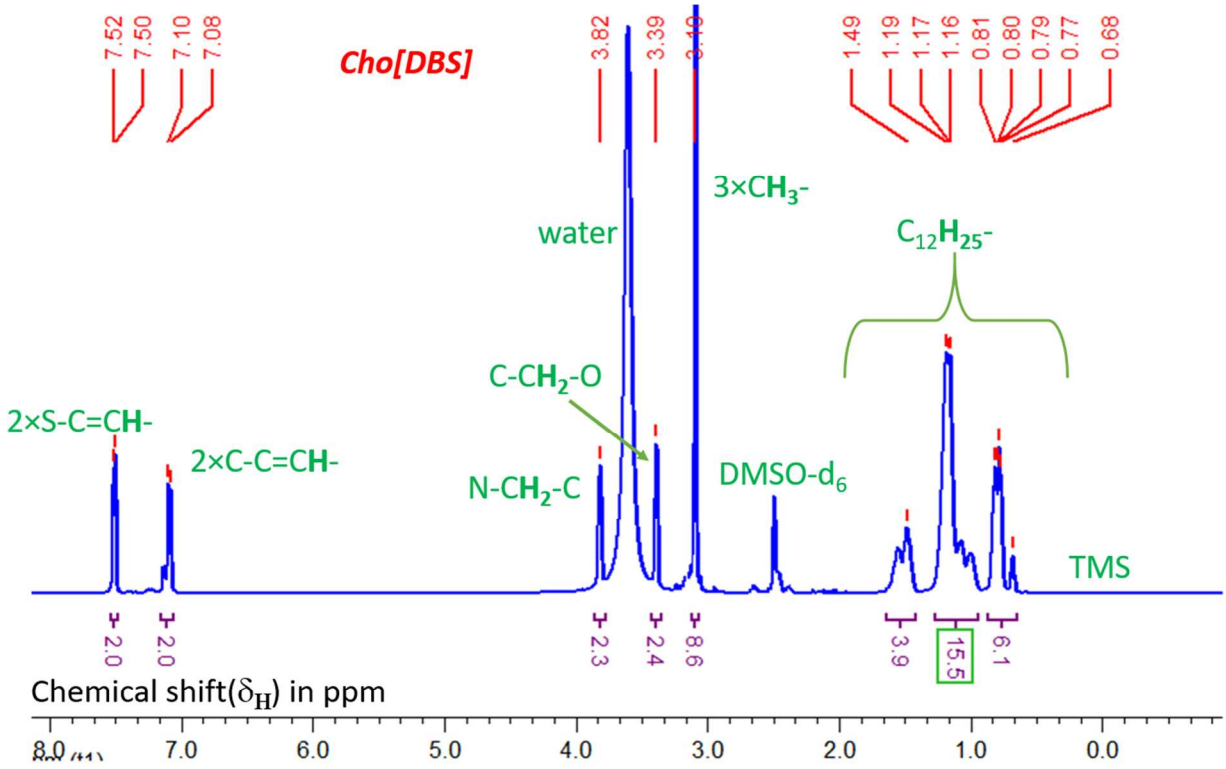

Figure S3. ^{1}HNMR spectrum at 200MHz Cho[DBS] in DMSO-d_6

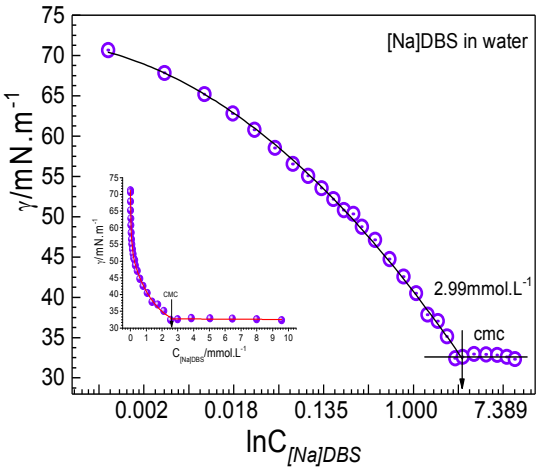

Figure S4. Polynomial reduction in surface tension of water as function of Na[DBS] in aqueous medium at 298.15 K. (CMC= 2.9 mmol.L^{-1})

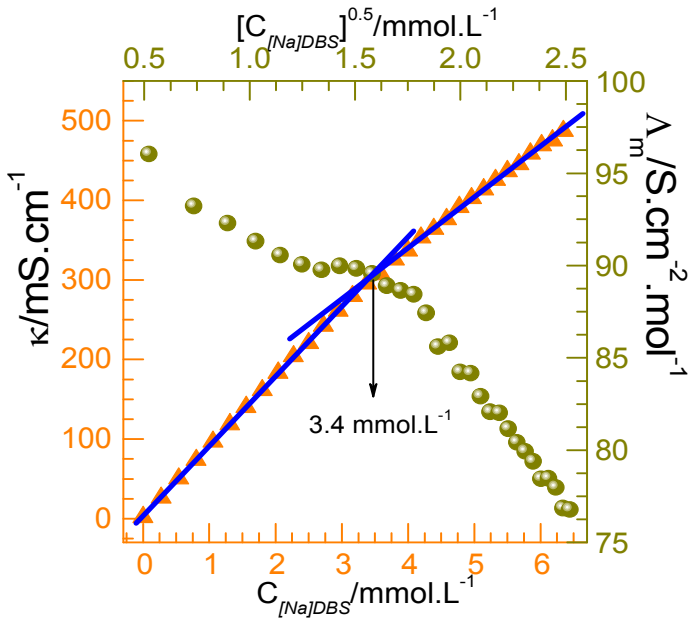

Figure S5. Specific and Molar conductance of [Na]DBS at 298.15K in aqueous medium (CMC= 3.4 mmol.L^{-1})

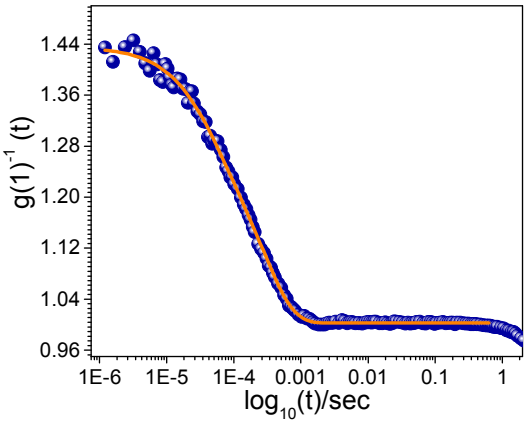

Figure S6. Autocorrelation function of cellulase in Cho[DBS] solution.

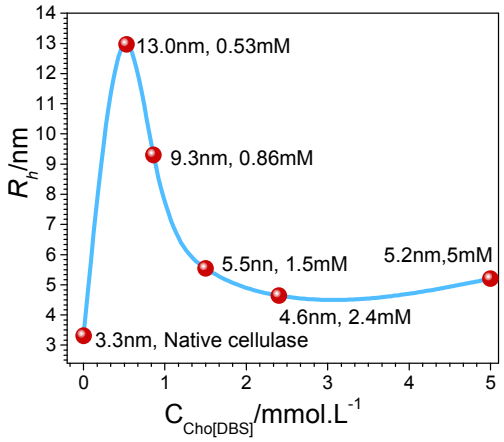

Figure S7. Variation in the size of cellulase with concentration of Cho[DBS].

Reference:

1. Gehlot, P. S.; Rao, K. S.; Bharmoria, P.; Damarla, K.; Gupta, H.; Drechsler, M.; Kumar, A., Spontaneous Formation of Multiarchitecture Vesicles of [C8mim]Br + [Na]DBS in Aqueous Medium: Synergic Interplay of Electrostatic, Hydrophobic, and pi-pi Stacking Interactions. *J Phys Chem B* **2015,** *119*, 15300-9.

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3. Kapustinskii, A., Lattice energy of ionic crystals. *Quarterly Reviews, Chemical Society* **1956,** *10*, 283-294.