Supporting Information

Spectroscopic Investigation of Binding Interaction of a Membrane Potential Molecule in Various Supramolecular Confined Environments: Contrast Behavior of Surfactant Molecules to Relocate or Release of Probe between Nanocarriers and DNA Surface

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1. Circular Dichroism (CD) Measurements:

Figure S1: Circular Dichroism spectra of CT DNA in presence of (a, b) LDS 698, (c) SDS, (d) CTAB and (e) TX-100.

2. Isothermal Titration Calorimetry (ITC):

A microcalorimeter of Microcal ITC_{200} , was used for isothermal titration calorimetric (ITC) measurements. We have tried our best to perform ITC experiments to gain better information regarding the interaction of LDS 698 with micelles and DNA molecules. We have performed the experiments to obtain satisfactory results in all possibilities (using LDS 698 in syringe and surfactant or DNA in cell and vice versa). We are unable to fit the obtained results using instrumental software to get the binding energy or stoichiometry of the complex formed between dye and surfactant micelles or DNA molecules. The ITC profiles between LDS-698 (syringe) and surfactant micelles or DNA molecules (cell) are given below:



Figure S2: Isothermal titration calorimetry profiles of (a) SDS, (b) CTAB, (c) TX-100 and (d) DNA (in cell) with LDS 698 (in syringe).



Figure S3: Variation of nonradiative rate constant (k_{nr}) with increasing concentration of surfactant.



Figure S4: Variation of nonradiative rate constant with concentration of CT DNA in aqueous buffer solution.



Figure S5: Time-resolved decay plots of LDS-698 in (a) 100 mM SDS, (b) 100 mM CTAB, (c) 100 mM TX-100 and (d) 1 mM DNA as a Function of temperature. (Inset Shows the Variation of Steady State Emission Intensity as a Function of Temperature).



Figure S6: Absorption and emission spectra of LDS 698 in 10 mM SDS solution (black line) and 10 mM SDS solution in presence of 1 mM CT DNA.



Figure S7: Temperature dependent CD profiles of CT DNA.



Figure S8: Variation of UV-vis absorption spectra of LDS 698 in (a) SDS micelles, (b) SDS-CT DNA solution, (c) CT DNA and (d) CT DNA-TX100 solution.



Figure S9: Variation of emission profiles of LDS 698 in (a) SDS micelles, (b) SDS-CT DNA solution, (c) CT DNA and (d) CT DNA-TX100 solution.