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Title of thesis: Interaction of Gemini Surfactants with Amino Acids and their Effect Proteins in Aqueous Medium

## ABSTRACT

**CHAPTER 1** This is the introductory chapter which covers the scope and objective of the proposed work. Various aspects of the work have been explained. An up to date literature survey has been presented to illustrate the work being carried out in this field. Thus, clearly emphasizes the need of the work.

**CHAPTER 2** Experimental methods and chemicalsused in the present investigations along with the calibrations of the apparatus have been detailed out and are presented in the second chapter. Quenching mechanism, binding constant, number of binding site and different thermodynamic parameter have been measured at different temperatures for protein and gemini interaction.

**CHAPTER 3** In thischapter describes the effects of amino acids on the cmc of imidazolium bashed ionic liquid type gemini surfactant ($[C_{12}\text{-}4\text{-}C_{12}im]Br_2$)in the aqueous solution were studied by conductivity, surface tension measurement. The conductivity results show that the micellization of $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$depends on their nature of amino acids additive and temperature. For the three amino acids, Trp, Tyr and Phe, hydrophobicity play an important role during the micellization process of $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$. The cmc of $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$in the presence and absence of amino acids at different temperature decrease with the increase of temperature. The quenching behavior of $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$were also studied with the Trp, Tyr and Phe by using fluorescence spectroscopy.

**CHAPTER 4** The interactions of cationic dodecyl betainategemini (DBG) surfactant with lysozyme was studied by fluorescence, time resolved fluorescence, UV-visible, circular dichroism, and molecular docking methods. The results showed that the DBG quenched the fluorescence of lysozyme through static quenching mechanism as confirmed by time resolved spectroscopy. The Stern-Volmer quenching constant ($K_{sv}$) and relevant thermodynamic parameters such as enthalpy change ($\Delta H$), Gibbs free energy change ($\Delta G$) and entropy change

(ΔS) for interaction system were calculated at different temperatures. The results revealed that hydrophobic forces played a major role in the interactions process. The results of synchronous fluorescence, UV-visible and CD spectra demonstrated that the binding of DBG with lysozyme induces conformational changes in lysozyme. Moreover, the molecular modelling results shows the possible binding sites in the interaction system.

**CHAPTER 5** In this chapter we reporting the interaction of ionic liquid type gemini surfactant, 1,4-bis(3-dodecylimidazolium-1-yl) butane bromide ($[C_{12}\text{-}4\text{-}C_{12}im]Br_2$) with lysozyme by using fluorescence, UV-visible, time resolved fluorescence, Fourier transform infrared (FT-IR) spectroscopy techniques in combination with molecular modelling and docking method. The steady state fluorescence spectra suggested that the fluorescence of lysozyme was quenched by $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$ through static quenching mechanism as confirmed by time resolved fluorescence spectroscopy. The binding constant for lysozyme-$[C_{12}\text{-}4\text{-}C_{12}im]Br_2$ interaction have been measured by UV-visible spectroscopy and found to be $2.541 \times 10^5\ M^{-1}$. The FTIR results show conformational changes in the secondary structure of lysozyme by the addition of $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$. Moreover, the molecular docking study suggested that hydrogen bonding and hydrophobic interactions play a key role in the protein-surfactant binding. Additionally, the molecular dynamic simulation results revealed that the lysozyme-$[C_{12}\text{-}4\text{-}C_{12}im]Br_2$ complex reaches an equilibrium state at around 3 ns.

**CHAPTER 6** The interactions of imidazolium bashed ionic liquid type cationic gemini surfactant ($[C_{12}\text{-}4\text{-}C_{12}im]Br_2$) with HSA was studied by fluorescence, time resolved fluorescence, UV-visible, circular dichroism, and molecular docking methods. The results showed that the $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$quenched the fluorescence of HSA through dynamic quenching mechanism as confirmed by time resolved spectroscopy. The Stern-Volmer quenching constant ($K_{sv}$) and relevant thermodynamic parameters such as enthalpy change (ΔH), Gibbs free energy change (ΔG) and entropy change (ΔS) for interaction system were calculated at different temperatures. The results revealed that hydrophobic forces played a major role in the interactions process. The results of synchronous fluorescence, UV-visible and CD spectra demonstrated that the binding of $[C_{12}\text{-}4\text{-}C_{12}im]Br_2$with HSA induces conformational changes in HSA. Moreover, the molecular modelling results shows the possible binding sites in the interaction system.