Abstract

The major goal of this investigation is to examine the head group and chain-length effect of the binding of N-acyl amino acid surfactants (NAASs) with globular proteins e.g., BSA, HSA and pepsin. The objective is to understand the mechanism of surfactant binding and to provide a general structure of the protein/surfactant complex at low surfactant concentrations. For this, a detailed study of the protein-surfactant interactions using fluorescence and circular dichroism spectroscopy was carried out. The thermodynamics of the binding process was also investigated in order to understand the driving force for surfactant binding. The thesis consists of six chapters. **Chapter 1** provides a brief overview of the current status of research in the area of protein-surfactant interaction, highlighting the serum albumins (SAs) and pepsin structure and their interaction with drug, fatty acid and other common surfactants, such as SDS, CTAB etc. In **Chapter 2,** the general synthesis of NAASs and the methods used to characterize the protein/surfactant complex have been described. **Chapter 3** describes and discusses the results of the experimental measurements on the interaction of BSA with different NAASs. It was found that when the head-group hydrophobicity increased the binding becomes stronger. However, the polar amino acid side chain at the surfactant head group reduced the binding affinity. An effect of amide hydrogen bonding on the surfactant binding to BSA was also observed. In **Chapter 4,** results of the binding studies on the interactions NAASs with HSA are discussed and are compared with those of BSA. **Chapter 5** discusses the solution behavior of pepsin under various conditions as well as its interaction with two amino acid-based cationic surfactants (3-hexadecylecarbamoyl–2–hydroxypropyl)trimethylammonium chlorides (C16-CAR) and (3-hexadecylecarbamoyl–2–propyl)-trimethylammonium chlorides (C16-PTAC). It has been shown that pepsin is most stable in pH 5, but it partially denatured in pH 8. Also in pH 7 it undergoes amyloid fibril formation at room temperature. The cationic surfactants were observed to interact strongly with pepsin at all pH > 2. **Chapter 6** summarizes the work carried out in the thesis and also gives the general conclusions drawn from the results described in chapters 3-5. A substantial head group effect on the protein-surfactant interactions was observed in the cases of BSA, HAS and pepsin proteins.

Keywords: Protein, fluorescence, circular dichroism, calorimetry, amino acids, carnitine, surfactants.