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The continuous protein tertiary structure space has many unknowns. Protein function is related to its chemical reaction with surrounding environment including other proteins. On the other hand, this depends on the spatial shape and tertiary structure of protein and folding of its constituent components in space. In current computational biology, assigning a protein to a fold class is a complicated and controversial task and can be more challenging in the much harder task of correct identification of protein domain fold solely through using extracted information from protein sequence. In this context, the concept of hyperfold and interlaced folds are introduced for the first time in the current study. A novel approach is proposed that is featured by the Demster-Shafer theory of evidence, as a generalization of the Bayesian theory of subjective probability, which makes it possible to represent and manage incomplete knowledge through the bodies of evidence and uses Dempster's rule of combination to combine them. These bodies of evidence were obtained on the basis of different functional domain properties as well as the sequential evolution information. The classification architecture thus developed was applied for identifying protein folds among the 27 SCOP (Structural Classification of Proteins) fold patterns. Compared with the existing predictors tested by a similar stringent benchmark data set, our approach may achieve the most successfully prediction results.

Keywords: Computational Biology, Protein Folding, Hyperfold, Dempster's Rule.

Abstract No.126

CD and Fluorescence Spectroscopies on Interactions of Gemini Surfactants and cationic Proteins at high pH

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Gemini surfactants have two polar head groups and two hydrocarbon tails. Compared to conventional surfactants, geminis have much lower (μM vs. mM) critical micelle concentrations and possess slower (ms vs. μs) monomer ßà micelle kinetics. The structure of the gemini surfactants studied is [HOCH2CH2-,CH3-,CH3(CH2)15-N+-(CH2)s-N+-CH3,-CH2CH2OH,-(CH2)15CH3]·2Br- where s=4, 5 or 6. Our objective is to reveal the effect of these cationic gemini surfactants on the structure and stability of two model proteins: Ribonuclease A (RNase A) and Hen Egg White Lysozyme (HEWL). At alkaline pH, where these proteins lose their net positive charge, fluorescence and CD spectroscopies show that they do interact with gemini surfactants and three different Protein•Gemini complexes are observed. Based on the results, we conclude that these cationic gemini surfactants neither interact strongly with nor severely destabilize these well folded proteins in physiological conditions and we advance that they can serve as useful membrane mimetics for studying interactions between membrane components and positively charged proteins.

Keywords: Gemini Surfactant, Ribonuclease A, Lysozyme, Fluorescence Spectroscopy, Circular Dichroism Spectroscopy.

Abstract No.127

Spectroscopic Studies on the Interaction of Chromium Oxide (Cr (VI)) with Chromatin in Solution

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Chromium compounds are well known as human carcinogens, but their molecular mechanism is not fully understood. The objective of the study was to investigate the interaction of chromium oxide (Cr (VI)) with soluble chromatin using spectroscopic techniques. Nuclei was prepared from rat liver and after brief digestion with MNase, the soluble chromatin was treated with different concentration of chromium oxide for 45 min at 23 ºC. The interaction was analyzed by UV/Vis, florescence and CD spectroscopy. The results showed that the binding of chromium oxide to chromatin reduces the absorbances at 210, 230 and 260 nm producing hypochromicity. The florescence emission intensity was gradually decreased with increasing the metal concentration. Circular dichroism showed that the elliplicity of chromatin was increased at negative extremes 209 and 222nm corresponding to proteins whereas it is decreased at positive extreme 275 nm (DNA), suggesting that induction of structural changes in chromatin upon metal binding. From the results it is concluded that chromium oxide binds to the DNA and histones in soluble chromatin and proceeds it into compaction.

Keywords: Chromium Oxide, Metals, Chromatin, Spectroscopic Techniques.
