

oligomerization are different but eventually they give rise to the same type of oligomeric species.

**Keywords:** Superoxide dismutase 1 (SOD1), Aggregation, ALS, Neurodegenerative Disease.

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**Abstract No.123**

**Application of Hollow fiber-Supported Liquid-Phase Microextraction Coupled with HPLC for the Determination of some Chiral Drug Enantiomers-Protein Binding**

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A hollow fiber liquid-phase microextraction technique coupled with high-performance liquid chromatography was employed for determination and evaluation of the binding characteristics of drugs to human serum albumin (HSA). Enantiomers of Donepezil and Lorazepam were investigated as a model system. After optimization of some influencing parameters on microextraction, the proposed method was used for calculation of the target drug distribution coefficient between n-octanol and the buffer solution as well as study of drug-HSA binding in physiological conditions. The developed method shows a new, improved and simple procedure for determination of free drug concentration in biological fluids and the extent of drug-protein binding.

**Keywords:** Hollow Fiber, HSA, Donepezil, Lorazepam Enantiomer, Binding.

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**Abstract No.124**

**Chemometric Studies of Hemoglobins from the Caspian Sea Sturgeon (*Acipenser persicus* and *Acipenser stellatus*) by n-dodecyl Trimethylammonium Bromide**

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Variety of hemoglobin (Hb) forms in fish is usually well adapted to the different ecological conditions or various habitats. In the current study, Hbs from two Sturgeon species of the Southern Caspian Sea Basin were investigated. After extraction and separation of hemoglobin from whole blood, we showed that although both species have variable Hbs with different isoelectric points, their dominant Hbs purified by ion-exchange on CM-cellulose chromatography. The dominant Hbs from these blood fishes were utilized for further experiments. In this study, the behavior of Hbs during the denaturation and process by n-dodecyl trimethylammonium bromide (DTAB) is investigated. In chemometric study, the interaction of DTAB as a cationic surfactant under variable concentrations, with the purified dominant hemoglobins (Hbs) was investigated using UV-visible absorption and circular dichroism (CD) spectra. The analysis of the obtained spectral data using singular value decomposition (SVD), Simple-to-use interactive self-modeling mixture Analysis (SIMPLISMA), evolving factor analysis (EFA) and multivariate curve resolution-alternative least square (MCR-ALS) as well-known chemometric techniques. The chemometric resolution techniques were used to determine the number of the components and mole fractions of the oxidized Hbs that donate the evidence for the existence of three different molecular components including native (N), intermediate (I) and denatured (D) in sturgeon Hbs. According to the distribution of intermediates broaden in a range of DTAB concentrations, the aggregation state of Hbs are slightly reduced from *Acipenser stellatus* to the *Acipenser persicus*. The results demonstrate a significant relationship between stability of fish hemoglobins and habitat depths.

**Keywords:** Sturgeon Hemoglobins, Intermediates, Chemometric Analysis, Aggregation.

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**Abstract No.125**

**The Concept of Hyperfold and Its Application to Evidence Theoretical Protein Fold Prediction**

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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 Dempster-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.

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#### 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 ( $\mu\text{M}$  vs.  $\text{mM}$ ) critical micelle concentrations and possess slower (ms vs.  $\mu\text{s}$ ) monomer to micelle kinetics. The structure of the gemini surfactants studied is  $[\text{HOCH}_2\text{CH}_2\text{-CH}_3\text{-CH}_3(\text{CH}_2)_{15}\text{-N}^+(\text{CH}_2)_s\text{-N}^+\text{-CH}_3\text{-CH}_2\text{CH}_2\text{OH,}-(\text{CH}_2)_{15}\text{CH}_3] \cdot 2\text{Br}^-$  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.

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#### 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 °C. The interaction was analyzed by UV/Vis, fluorescence 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 fluorescence emission intensity was gradually decreased with increasing the metal concentration. Circular dichroism showed that the ellipticity 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.