spectroscopic technique. A series of spectrofluoremetric titration experiments were designed and data sets were collected. These data (with concentration in first mode, emission wavelengths in second mode and excitation wavelengths as third mode) were arranged in a bilinear (augmented data) and trilinear (cube data) data matrix and then, analyzed using multivariate curve resolution-alternating least squares (MCR-ALS) and parallel factor analysis (PARAFAC). Using best fit MCR-ALS and PARAFC models, the pure concentration and spectral (excitation and emission spectra) profiles were achieved. The estimation of binding affinity, binding stoichimetry and site-site interaction were made with high accuracy.

Keywords: Bovine Serum Albumin, Serotonin, Fluorescence Spectra, Chemometrics.

Abstract No.38

Pulsed Field Gradient NMR Study on Micellization Process of Sodium Dodecyl Sulfate in The Presence of Protein

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Pulsed field-gradient (PFG) NMR spectroscopy has become the method of choice for measuring diffusion in solutions in both chemical and biological systems. Diffusion can be used to map intermolecular interactions that play an important role in both chemical and biochemical systems.In this work, using the Bruker 400 NMR spectrometer, we have investigated the changes in the SDS diffusion coefficients in the presence and absence of the protein. The Self-diffusion coefficients of SDS, were measured by the PFG-NMR technique.In 1D H-NMR spectrum of SDS, the peak with the highest intensity was selected and the surfactant self-diffusion coefficient was obtained from the decrease in the height of this peak with increasing the strength of the applied gradient. The intensity of this peak was found to obey the Stejskal–Tanner relation:= (1)where γ is the proton magnetogyric ratio, g isthe field gradient strength and A0 is a fitting parameter. Measurement of the self-diffusion coefficients of a component in solution gives a population-weighted average of this component in its different states. These states include free and protein-bound states. The measured self-diffusion coefficient (Dobs) of a component corresponds to: (2)where Pf and Pb are the free and bound fractions of surfactant, respectively, and Df and Db are the self-diffusion coefficients of the surfactant in the free and bound states, respectively. Values of the self-diffusion coefficient against the total concentration of SDS for systems made up of SDS/D2O, SDS/Protein (0.1 wt.%) /D2O has been provided.The rearrangement of Eq.2 gives: (3)where Cb is the concentration of protein-bound SDS and Ctot is the total SDS concentration in the solution. Isotherm bindings were obtained by applying Eq.3 to the self-diffusion coefficient data for the SDS/Protein system. Finally, the thermodynamic parameters of protein/SDS interactions were obtained.

Keywords: PFG-NMR, Self-diffusion, Protein, SDS.

Abstract No.39

Homocysteinylation of Bovine Pancreatic Insulin, Importance of C-Terminal Beta Chain In Structural Stability and Protein Aggregation

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Homocysteine thiolactone (HCTL) which is a cyclic thioester of homocysteine, showing high reactivity, toward lysine residues of proteins, leading to protein damages and induction of immune responses. As reported before, C-terminal B-chain of insulin plays a critical role in stability and structural integrity of this glucose regulating hormone. In this study HCTL was used to modify the only Lysine residue (Lys29) of insulin on its C-terminal B-chain. Different spectroscopic instruments were applied to study effect of homocysteinylation on structure of this protein.The obtained results suggest a marked structural alteration in insulin structure with predominant conversion of a-helical to b-sheet structure in the presence of increasing concentration of this cyclic thioester. Also the gross structural change of insulin induced by HCTL was followed with an aggregation event, suggesting the importance of Lys29 of C-terminal B-chain in protein stability and structural integrity. Moreover this study may have important implications regarding to the structural consequences of possible exposure of insulin to HCTL, particularly during hyperhomocysteinemia.

Keywords: Insulin, Homocysteine Thiolactone (HCTL), Structural Lteration, Aggregation.
