

Abstract No.172

Effects of Structural Constraints on Thermodynamic Parameters of Protein Unfolding

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Important thermodynamic parameters including denaturation equilibrium m values (m_{eq}) and heat capacity changes (ΔC_p) can be predicted based on changes in Solvent Accessible Surface Area (SASA) upon unfolding. Crosslinks such as disulfide bonds influence the stability of the proteins by decreasing the entropy gain as well as reduction of SASA of unfolded state. The aim of the study was to develop mathematical models to predict the effect of crosslinks on Δ SASA and ultimately on m_{eq} and ΔC_p based on *in silico* methods. Changes of SASA upon computationally simulated unfolding were calculated for a set of 45 proteins with known m_{eq} and ΔC_p values and the effect of crosslinks on Δ SASA of unfolding was investigated. The results were used to predict the m_{eq} of denaturation for guanidine hydrochloride and urea, as well as ΔC_p for the studied proteins with overall error of 20%, 31% and 17%, respectively. The results of the current study were in close agreement with those obtained from the previous studies.

Keywords: Protein Stability, Disulfide Bonds, Crosslinks, Heat Capacity Changes, Denaturation M value.

Abstract No.173

Bioinformatic Analysis and Molecular Modeling of DOF Domain Proteins

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DOF domain proteins belonging to Zinc Finger family are a group of plant transcription factors with highly conserved DNA-binding domain. They are associated with plant-specific phenomena including: light and defense responses, seed germination, dormancy and flowering time. Purification of DOF domain proteins for solving their structures still remains a big challenge as these proteins bind tightly to their

putative DNA sequences. In the absence of experimentally solved structure for protein, comparative modeling can reliably predict the three dimensional (3D) structure based on known 3D structure of one or more template proteins. Since 3D structure of this group of proteins has not been determined experimentally, in the current investigation we used comparative modeling approach in order to predict a 3D-model for these proteins. To this end, Erythroid transcription factor (GATA1) was selected as the template. The models were generated using SWISS-MODEL server. The models were used to calculate binding free energy for DOF-DNA complex. In this study MM-PBSA/GBSA methods implemented in AMBER package were applied for this purpose. The results were analyzed and compared among different DOF domain proteins. The result of this work could give useful information in designing novel DOF domain protein with desired affinity to DNA and further experimental design.

Keywords: Protein Stability, Disulfide Bonds, Crosslinks, Heat Capacity Changes, Denaturation M value.

Abstract No.174

Effects of Static Magnetic Field on Activity of Immobilized α -amylase on Silica Gel

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In this study, α -amylase was immobilized on silica gel via adsorption with glutaraldehyde in the presence and absence of magnetic field and was compared with free enzyme. The α -amylase (free enzyme) and the enzymatic reaction (immobilized and free enzyme) were treated by 13mT magnetic field for 100 min and 1.5 min, respectively, at 25°C compared with the control sample which was not exposed to the magnetic field and characteristics including activity, kinetic parameters {maximum velocity (v_{max}), Michaelis-Menten constant (K_m), catalytic constant (k_{cat})} in different pH (6, 6.5, 6.9, 7.6) were investigated. The highest activity of free enzyme was obtained at pH 6.9 while this value was shifted to pH 6.5 for immobilized enzyme. The amount of reduced sugar (maltose) was determined spectrophotometrically at 620 nm. Using kinetic data for Lineweaver-Burk plots, K_m and V_{max} values were calculated from the slopes of the curve. Results showed that the activity of the free enzyme decreased in the presence of magnetic field and in the case of enzymatic reactions the reduction rate in the presence of magnetic field was

more than other modes, and immobilization activity in the presence of magnetic field also showed enhancement. K_m for immobilized α -amylase was found to be higher than that of the free enzyme, which may be due to interparticle diffusional mass transfer restrictions.

Keywords: Static Magnetic Field, α -Amylase, Enzyme Immobilization, Kinetic Parameters.

Abstract No.175

Interaction of Cu(II) Phthalocyanine and Porphyrazines with Plasmid DNA and Their Antibacterial Properties

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Multiple resistances to antibiotics are a growing public health issue that is compounded by the inability of the pharmaceutical industry to generate new strains of antibiotics to combat infections. Identification of new antibacterial agents and exploitation of new approaches for the drug-resistant bacteria is in great demand. Among the novel developed antibacterial agents, porphyrin complexes have attracted much attention. Phthalocyanines differ from porphyrins by having nitrogen atoms link the individual pyrrole units. Tetrapyrrolineporphyrazines are phthalocyanine aza analogs in which four pyridine moieties formally substitute four benzene moieties in the macrocycle. The tetramethylated quaternized forms of tetrapyrrolineporphyrazines (tmtppa) are tetra-positively charged and hence water soluble. In this study, the antibacterial effect of an anionic phthalocyanine Cu(PcTs) and two cationic tetrapyrrolineporphyrazine including [Cu(2,3-tmtppa)]⁴⁺ and [Cu(3,4-tmtppa)]⁴⁺ complexes towards *Staphylococcus aureus* and *Escherichia coli* growth were investigated. In addition, their interaction with plasmid DNA was studied using spectroscopic and gel electrophoresis methods. The results indicated that both porphyrazines have significant antibacterial properties against the Gram negative and the Gram positive bacteria. but, Cu(PcTs) has a very weak antibacterial effect. Gel retardation assay implied that [Cu(2,3-tmtppa)]⁴⁺ (the figure is shown) and [Cu(3,4-tmtppa)]⁴⁺ degrade plasmid DNA and Cu(PcTs) causes no retardation in movement of the plasmid. Stern-Volmer dynamic quenching constant, binding constant and number of binding sites for interaction of the complexes with plasmid DNA were measured using analyzing of the fluorescence and absorption spectroscopic data. The

results indicated interaction of [Cu(2,3-tmtppa)]⁴⁺ and [Cu(3,4-tmtppa)]⁴⁺ with plasmid are more stronger than Cu(PcTs).

Keywords: Interaction, Phthalocyanine, Tetrapyrrolineporphyrazine, Antibacterial properties.

Abstract No.176

Applying a Bi-chaperone System to Prevent Insulin Aggregation

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The aggregation of insulin is a big medical- and biotechnological challenges, therefore in this study a Bi-chaperone system consisting of alpha-crystallin (α -Crs) and beta-casein (β -CN) with different molar ratios were applied to prevent insulin aggregation spectroscopically. These two proteins are amphiphilic, each contains distinct polar and non-polar regions in their primary structures. While polar domain of α -Crs is highly electropositive, the counterpart domain in β -CN is strongly electronegative. The results of both fluorescence study and native gel electrophoresis confirmed a non-covalent interaction between α -Crs and β -CN. Consequently the synergistic chaperoning operation observed in Bi-chaperone system can be explained with the possible electrostatic interactions between its chaperone components through their polar/charged domains. Furthermore, the results of this study may provide useful information to identify potential interacting molecular partners for α -Crs chaperone.

Keywords: Alpha-crystallin, Beta-casein, Aggregation, Chaperone activity, Bi-chaperone system.

Abstract No.177

Caseoperoxidase: Novel Peroxidase-Like Nano-Artificial Enzyme

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