Abstract No.172

Effects of Structural Constraints on Thermodynamic Parameters of Protein Unfolding

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Important thermodynamic parameters including denaturant equilibrium m values (meq) and heat capacity changes (ΔCp) 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 ΔSASA and ultimately on meq and ΔCp based on in silico methods. Changes of SASA upon computationally simulated unfolding were calculated for a set of 45 proteins with known meq and ΔCp values and the effect of crosslinks on ΔSASA of unfolding was investigated. The results were used to predict the meq of denaturation for guanidine hydrochloride and urea, as well as ΔCp 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, Denaturant 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 this 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, Denaturant 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(vmax), michaelis-menten constant(km), catalytically constant(kcat)} 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 ofreduced sugar (maltose) was determined spectrophotometrically at 620 nm. Using kinetic data for Lineweaver–Burk plots, Km and Vmax 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