Abstract No.69

Role of Osmolytes in The Stabilization of Bovine Pancreatic Ribonuclease A at Different pH values

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Bovine pancreatic ribonuclease A (RNase A, EC 3.1.27.1) is composed of 124 amino acids (molecular mass 13686 Da), among which basic residues (10 Lys, four Arg and four His) prevail over acidic residues (five Glu and five Asp), making the protein definitely basic, with a pI of 9.3. The protein's secondary structure consists of three α-helices and seven β-strands, and the molecule contains four disulphide bonds(26–84, 40–95, 58–110 and 65–72) that contribute, in particular the two terminal ones (26–84 and 58–110), to the remarkable stability of the protein.It catalyzes the cleavage of P-O5′ bonds in RNA on the 3′side of pyrimidine to form cyclic 2′,5′-phosphates. In their study of the effect of osmolytes (Butandiol, Butanol, Glycerol at pHs 1.5 and 3.3) by spectrophotometric techniques on thermal stability of enzymes in terms of Tm (the midpoint of the transition curve), have reported Butandiol, Butanol destabilizes RNase A at pH=1.5 and 3.3 and byincreasing concentration of Glycerol at pH 1.5 increases enzyme stability.Polyols are co-solvents that are used to protect organisms from denaturation by harsh environmental stresses. Glycerol stabilize ribonuclease A, not by interacting with that directly but by altering the solvent properties of the surrounding water and hence the protein–solvent interaction. As a rule, branching of the hydrocarbon portion of the alcohols tends to reduce their effectiveness as protein denaturants. The glycerols are found to be less effective than the corresponding alcohols, suggesting that increased polarity or hydrogen-bonding capacity is of secondary importancewhen compared with the effects of increasing hydrocarbon content.

Keywords: Bovine Pancreatic Ribonuclease A, Polyols, Osmolytes, Butandiol, Butanol, Glycerol.

Abstract No.70

Theoretical Investigation of Stability of a Di-Copper(I) Macrocyclic Complex as a Model for Active Site of Tyrosinase Enzyme

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Tyrosinase is a widespread dinuclear copper enzyme present in microorganisms as well as in plants and mammals. It is able to oxidize most phenols to the corresponding catechols and, eventually, o-quinones. Most of the information about the electronic structure and mechanism of tyrosinase action has been obtained from structural and functional models. In this work the di-copper(I) complex of a 20-membered [2+2] macrocyclic Schiff base ligand with three nitrogen donors is chosen to model the real tyrosinase. The activation of tyrosinase enzyme is accomplished by binding an O_2 molecule as a bridged ligand between two Cu(II)-(Hys)3 complex. Also, the similar active state of model complex has been shown before. All DFT calculations were performed by B3LYP hybrid-GGA functional and SBKJC basis set which included effective core potentials for inner shell of heavy atoms. Then the electronic structure, HOMO-LUMO energy gap, Mulliken charges, and relative stability of model complex, tyrosinase active site, and their oxidized state are calculated and discussed.

Keywords: Tyrosinase, Enzyme, Active Site, Stability, Model Complex, DFT.

Abstract No.71

Interaction of Bisdemethoxycurcumin and Diacetylbisdemethoxycurcumin with β-lactoglobulin: Spectroscopic and Molecular Dynamics Simulation Studies

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This study demonstrates the interactions of bisdemethoxycurcumin (BDMC) and diacetylbisdemethoxycurcumin (DABC) as the bioactive constituents of turmeric with bovine β-lactoglobulin (BLG) variant B using fluorescence, circular dichroism (CD), molecular docking, and molecular dynamics simulation methods. The binding constant for formation of BLG-BDMC and BLG-DABC complexes were $8.99 \pm 0.1 \times 10^4$ M^{-1} and $1.87 \pm 0.1 \times 10^2$ M^{-1}, respectively. The distance between BLG and BDMC was obtained based on Förster`s theory of non-radiative energy transfer. The secondary structure contents of BLG in the presence of ligands were obtained by analysis of CD spectra. Molecular docking studies revealed