A time course of enzyme activity assays, SDS-page analysis and K_m and V_{max} determination, the zymogram examinations were performed for more characterization of the enzyme.The enzyme purification and the protein structure identification are in progress.

Key words: Protease, enzyme activity, tyrosine.

Abstract No.127

Molecular dynamics study of lysozyme C in various conditions: temperature, pressure, salts, alcohol,

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Lysozyme with 129 residues and 14.7 KDa Molecular weight is an enzyme, EC 3.2.1.17 with hydrolase activity acts as antibacterial in human saliva. It is widely distributed in the human body including: tissues, exocrine secretions, and circulating cells and considered as an important component of innate immune system against bacteria. Lysozyme has a total of four intra molecular disulfide bonds, take part in tertiary structure stability. We have used molecular dynamics simulation to study the mechanism of thermal stability in lysozyme focusing on secondary structures elements. In the present work Gromacs Version 3.3.3, installed on ubuntu linux Version 8.10 package under ffgmx force field was used as simulation media. Lysozyme coordinate was obtained from RCSB protein data bank with PDB ID: 2W1M the protein was equilibrated in a cubic box with (4.94*4.32*5.07) nm dimensions. Energy minimization was carried out using steep integrator and fmax were chosen 1000 for 1000 step. Molecular dynamics with all-bond constrain for 200ps and then with no constrain were done for up to 4ns. Our findings show that lysozyme has transition temperature, 47-77°C. There is about 10% increase in gyration radius in this transition state, which is swelling like state of lysozyme. produced by thermal denaturation. The change in hydrodynamic radius is deduced from direct salt bridge analysis shows thermal denaturation promotes by increased positive-positive repulsive forces during with temperature. A solvent-protein and protein-protein hydrogen bond alteration caused by heating is not determinately, in protein denaturation. Hydrogen bonds break down take place upon melting temperature (67°C). The results show that the four disulfide bonds of lysozyme remain unchanged during simulation and even at higher temperatures over melting point and resist structural distortion.

Key words: molecular dynamics, Lysozyme, denaturation, structural distortion.

Abstract No.128

The interaction mode between DNA and salen-Co(III) N,N′-dipyridoxyl (1,4-butanediamine) Shiff-base complex

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Interaction of cationic metal complexes of Schiff bases, as a new agent in order to study anticancer characteristics and analytical application with DNA has been developed. The cationic metalocomplexes bind to DNA through a series of following interactions: (i) electrostatic forces, (ii) hydrophobic interactions with minor and major grooves, (iii) hydrogen bonding, and (iv) π-stacking interactions associated with the interaction of aromatic heterocyclic groups between the base pairs. It is valuable to understand the type of interactions involved between the complex and DNA sites.

In this work, we studied the interaction of new salen-co(III) of N,N′-dipyridoxyl (1,4-butanediamine) Schiff-base complex with DNA by melthing temperature, fluorescence spectrometry and gel electrophoresis techniques. This salen-Co(III) complex shows increase in melting temperature when bound to native calf thymus-DNA (CT-DNA). The intersection point of the binding isotherm indicated a binding site size of 3 bp per bound complex molecule in Tris–HCl buffer. Upon adding the new salen-Co(III), the electrophoretic mobility of pTZ57R DNA plasmid becomes slower for both super coiled and open circular forms without any structural changes in DNA. The experimental results showed that the salen-Co(III) complex bound to DNA by intercalative mode.

Key words: Schiff bases, anticancer, melting temperature, structural change.
