three types of states. channels are classified according to the type of ion for which the channel is selective, e.g. K+ channels, Na^+ channels, Cl^- channels. Voltage gated cation (Na , K) channels are responsible for the generation and propagation of action potential in neurological signal transmission . K1 selective channels are widely spread in all organisms and have the ability to conduct K1 ions at near diffusion limit. The KcsA channel shares sequence and structure similaritieswith all members of the K1 channel family.We have used geometry optimization ,molecular mechanics simulations to calculate the relative binding energies of Na and K in the KcsA ion channel .We investigated the complex of na and k ions with ion channels in different tempreture (300, 305, 310, 315) and calculated potential energy of these molecule in force fields MM, AMBER, BIO (charmm) and OPLS. Maximom potential energy of comlex of Na^+ ion channels with MONTE CARLO and OPLS method at T=300 K is 3614.84 kcal/mol .

Keywords: Molecular mechanic, KcsA ion channel, OPLS, AMBER, Hyperchem.

Abstract No.220

The Study of Glucose Interference on Interaction of Doxorubicin and Hemoglobin

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Hemoglobin (Hb) is the iron containing oxygen transport metalloprotein in the red blood cells. Quaternary structure and the associated subunit interaction property of tetrameric Hb confers it the regulatory property when small ligands such as metabolites or drugs bind to it and modulate the functional activity of this important protein. Protein-Drug interactions play an important role in a variety of biological processes and disease treatment.Doxorubicin (DOX) is a very effective anti-tumor drug that is effective in the treatment of solid tumors. It has been suggested that on reduction DOX reacts directly with oxyHb. It seems the role that Hb plays in disposition of DOX or its interaction with the drug is important. The direct interaction of this protein with drugs may also affect its functionally important structural conformation.Binding of some ligands to Hb induce alterations in the structure and function of this protein. However, competitive binding displayed by different ligands may result from allosteric effects.Hemoglobin exposure to plasma glucosecauses glycation of hemoglobin in a non-enzymatic glycationpathway. Normal levels of glucose produce a normal amount of glycated hemoglobin. As the average amount of plasma glucose increases, the fraction of glycated hemoglobin increases in a predictable way. In this study, hemoglobin was incubated with doxorubicin and with different concentrations of glucose and was studied by uv-visible spectroscopy technique. Observations showed a hyperchromic effect upon Hb treatment by doxorubicin, however this effect was reliefed through glycation in elevated concentrations of glucose.

Keywords: Hemoglobin, Doxorubicin, Glycation, Ultraviolet Spectroscopy.

Abstract No.221

Purification and Biochemical Characterization of Anacidic Metalloprotease from Serratia sp. HR-1

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Proteases are used in a great variety of commercial sectors.An acidic extracellular protease produced by anisolate from soilsamples was purified to homogeneity in three steps including ammonium sulfate precipitation, SP-Sepharose cation-exchange and Sephacryl S-200 size exclusion chromatography. The purified protease exhibited an apparent molecular mass of 50 kDa either by SDS-PAGE or gel filtration chromatography. It was found as a cold-adapted acidic protease with optimumtemperature and pH of 30-35 °C and 4.0, respectively. The protease showed 24% of its initial activity after incubation at 50 °C for 60 min, which indicates a relatively low thermostability. The enzyme was classified as a metalloprotease according to its unaffected function in the presence of inhibitors: Aprotinin, E-64, Chymostatin, Pefabloc SC, Pepstatin, Leupeptin, Bestatinand Antipain-dihydrochloride and its complete inhibition by 10 mM of EDTA. Althoughthe enzyme was identified as a metalloprotease, no significant effect of 1,10-phenanthroline on caseinolytic activity showed Zi+2independency of the protein. No inhibitory function of Phosphoramidon, as a thermolysin-like metalloprotease inhibitor, revealed that the purified protease is not a member of M4 family of metallopeptidases. In overall, regarding tothe acidic properties and low temperature stability of the protease, it proposed that the purified acidic metalloprotease can be an ideal choice for applications in food industry especially in cheese making.

Keywords: Metalloprotease, Serratiasp.HR-1, Acidic Protease, Protease Inhibitors.
