Human serum albumin (HSA) is an abundant plasma protein that can transport various drugs and small molecules in the blood circular system. This study was designed to investigate the binding of three Schiff base complexes with HSA using Docking and molecular dynamics simulation approaches. The potential affinity of these Schiff bases to DNA has been previously reported, hence, the results of this study can be useful for improving the pharmacokinetic efficiency of these drugs.The Topology file of Schiff bases were calculated at DFT/B3LYP/6-31G** level using Gaussian 03 package. A molecular docking using AutoDock 4 is applied to investigate the binding of these compounds to the HSA.The lowest docking energy structure from each cluster was selected. The results show that in contrast to the most drug-like compounds that usually bind to either site I (subdomain IIA) or site II (subdmain IIIA), these compounds bind to subdomain IB(siteIII).The residues within a maximum distance of 3.9 Å to the ligands are Leu115, Val116, Arg117, Met123, Tyr138, Glu141, Ile142, Tyr161,Leu182, Leu185 and Arg186. The hydroxyl group of Tyr161 and the guanidino group of Arg117 are within hydrogen bonding distance with these complexes.The energy minimum conformations from each cluster were applied as the initial structures in the 14 ns molecular dynamics simulations using GROMACS 4.5.5 software package.The position fluctuations of the ligands located inside subdomain IB were explored, and the stable binding modes of the three ligands were determined. Furthermore, the results revealed the main differences in binding modes of these complexes .

Keywords: Human Serum Albumin, Schiff Base, Docking, Simulation.

Abstract No.56

Activatory and Inhibitory Behavior of Various Concentration of NiO and CdTe Nanoparticles on Horseradish Peroxidase Activity at Different Temperatures

Nayere Bahamin, Behzad Shareghi, Parisa Nooraei, Sadegh Farhadian, Somayeh Asgari*

Department Of Biology, Shahrekord University, Shahrekord, IR
(E-mail: nayere.bahamin@gmail.com)

Nanoparticles are in interest of scientists because of their exclusive properties. Data on biological effects show that NPs can be toxic to bacteria, algae, invertebrates and fish species, as well as mammals. Peroxidases (EC 1.11.1.7) are a group of oxidoreductases that catalyse the reduction of peroxides. Peroxidase activity has been identified in plants, microorganisms and animals, where peroxidases play important rols. In this study effect of NiO and CdTe nanoparticles on the activity of horseradish peroxidase (HRP) has been investigated. In the prescence of NiO nanoparticles, the lower consentrations (up to 0.05 mM) inhibit the enzyme activity in the noncompetitive manner, but higher concentration (up to 0.5 mM) stimulated it, that may be because of obtain more flexibility under this condition. Also thermostability studies shown that Tm of the enzyme decreased about 10 degrees in the presence of NiO nanoparticles. All of CdTe nanoparticles concentrations stimulated the enzyme activity at 25 and 35 °C, in which lower concentration more effective. Noncompetetive inhibition for 0.1 and 0.5 mM of CdTe nanoparticles concentration was observed at 45 °C. Also CdTe nanoparticles decreased Tm of HRP about 22 degrees. So the behavior of these nanoparticles on kinetic of HRP not only dose and time dependent but temperature would affect this manner.

Keywords: Horseradish Peroxidase, Kinetic, Thermostability, NiO Nanoparticles, CdTe Nanoparticles.

Abstract No.57

The Application of Bioinformatics Algorithms in Amino Acid-based Cellulase Classification

Narges Shamabadi [1], Mohammad Ali Tajick Ghanbary [2], Faezeh Hosseinzadeh [3], Mansour Ebrahimi [1]*

1. Bioinfromatics Research Group, Green Research Center, University of Qom, IR
2. Department of Plant Protection, College of Agronomic Sciences, Sari Agriculture and Natural Resources University, Sari, IR
3. Laboratory Of Biophysics And Molecular Biology, Institution Of Biophysics And Biochemistry, University Of Tehran, Tehran, IR
(E-mail: ariasamin@yahoo.com)

Cellulose is the most abundant renewable natural biological resource which makes up about 45% of the dry weight of wood. Cellulose lineal polymer composed of D-glucose subunits linked by β-1,4 glycosidic. It is resistance to degradation, so its enzymatic hydrolysis is important in industry. Cellulolytic enzymes generally classified as Endoglucanase, Exoglucanase and Celobiohydrolase. All of which are extracellular, so they perform their roles out of cell.The mentioned classic classification categorized cellulase enzymes based on chemical properties according to cleavage mechanisms. In this article, we tried to make a sequence-based classification to determine appropriate borders for cellulase classification.To identify the main determining protein attributes to represent each kind, attribute weighting and decision tree models applied to dataset of 296 cellulase sequences of different microorganisms (894 protein attributes for each sequence). For the