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

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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

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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

first time we showed that Cys has direct or indirect roles in cellulose classification, either alone or in connection with the other amino acids as dipeptides in cellulase categorization. The count of Cys and Cys-Asp reported as an important factor in 100% and the count of Cys-Ala in 80% of weighing algorithms. The result of decision tree algorithms also clearly confirmed that Cys has significant role in cellulase classification.

Keywords: Cellulase, Attribute Weighting, Decision Tree Algorithms, Bioinformatics.

Abstract No.58

The Enhancement of Surface Hydrophobicity by Calcium Ion may have Significant Contribution in cell Death Inducing Activity of Human Calprotectin

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As calcium and zinc-binding protein complex, calprotectin (MRP8/14) is abundant in cytosolic fraction of human neutrophils. Calprotectin is a multifunctional protein with broad spectrum of activities, including antimicrobial property and apoptosis inducing activity. This protein is significantly elevated in serum and body fluids of patients with various inflammatory conditions, suggesting that this protein plays significant function influencing the inflammatory processes. In this study calprotectin was purified from human neutrophils, using a two-step ion exchange chromatography. The apoptosis inducing activity of this protein was examined against two leukemia cancer cell lines, using 3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium bromide (MTT) assay. Furthermore, to explore role of calcium binding on surface hydrophobicity of calprotectin, fluorescence study was performed. As shown, calcium binding induces conformational changes and increases the solvent exposed hydrophobic surfaces of human calprotectin, making the protein prone to aggregation. Since the early aggregates have an intrinsic ability to impair fundamental cellular processes by interacting with cellular membranes, consequently, calcium binding to calprotectin may lead to the formation of a toxic folding variant of this protein with sticky (hydrophobic) surface which may interact with plasma membrane to kill cells. This study may suggest contribution of the exposure of surface hydrophobicity by calcium ion, in the pathway of apoptosis inducing activity of human calprotectin.

Keywords: Calprotectin, Calcium, Surface Hydrophobicity, Aggregation, Fluorescence Study.

Abstract No.59

Interaction of [Pd(phen)(n-pr-dtc)]Br with DNA of Calf Thymus

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Cis-diamminedichloroplatinum(II) (cisplatin) is used in the clinical treatment of several types of human cancers[1]. Various strategies have been used to reduce the major toxicity of cisplatin. One of these strategies is to develop new compounds capable of reducing these toxicities[2].thus in this study we prepared 1,10-phenanthroline-n-propyldithiocarbamatopalladium(II) bromide, [Pd(phen)(n-pr-dtc)]Br,and characterized by spectroscopic techniques such as UV-Vis,FT-IR,1HNMR and nonspectroscopic techniques like conductivity measurements, elemental analysis and decomposition temprature.Studies of antitumor activity of this complex against human cell tumor lines(k562) have been carried out. It shows IC50 value lower than that of cisplatin.The interaction of the complex has been studied with DNA of calf thymus (CT-DNA) at 300K and 310K using UV-Vis isothermal titration method in 25 mM Tris-HCl buffer of pH=7.0. This complex can denature CT-DNA at very lower concentrations (~ 100 μM). The concentration of this complex in the midpoint of transition, [L]1/2, are 0.078 and 0.064mM at 300 and 310K respectively. The mode of binding of the complex to CT-DNA, has been investigated by ultraviolet spectroscopy. The result of these studies indicate that [Pd(phen)(n-pr-dtc)]Br complex exhibit cooperative binding with DNA. In the interaction studies between the [Pd(phen)(n-pr-dtc)]Br complex with CT-DNA, several binding parameters such as, K (the apparent binding constants, are 46.68 and 58.45 mM^{-1} at 300 and 310 K, respectively), n (the Hill coefficients, are 2.15 and 2.93 at 300 and 310K respectively), g (the number of binding sites per 1000 nucleotides, is 5 at 300 and 310 K), n (the ratio of the concentration of bound metal complex to the total DNA concentration) and m (a measure of the metal complex ability to denature DNA, are 207.30 and 223.78 $(kJ/mol)(mmol/L)^{-1}$ at 300 and 310 K respectively). Thermodynamic parameters such as (conformational stabilities of DNA in the absence of metal complex, are 15.10 and 14.00 kJ/mol at 300 and 310 K, respectively), (the heat needed for DNA denaturation in the absence of metal complex, is 47.98 kJ/mol)