

acid (HCl) hydrolysis in different concentrations, different times and different temperatures. In this study we used different concentrations such as 100%, 50%, 12/5%, 6/25%, 3/125% and 1/562% of HCl in different times such as 70, 100 and 115 centigrade and different temperatures such as 24 hours, 5 hours, 1 hour and 15 minutes that we optimized on Date Palm Leaf. We used of Lane-Eynons way to measurement of sugar percentage. Highest percentage of sugar(50%) obtained at concentration of 3/12% HCl at 70°C and time was 24 hours. Results exhibit, Palm wastes are very good for optimization in bioethanol production and acid(HCl) hydrolysis on this biomass has great effect in separating of sugar that can be changed into the bioethanol.

Keywords: Optimization, Date Palm Leaf, Bioethanol, Acid Hydrolysis.

Abstract No.53

Synthesis, Characterization, Cytotoxic and HSA Binding Studies of Palladium (II) Complex of Phenanthroline Derivative

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Serum albumins are abundantly found in blood plasma and are often termed transport proteins. They are circulated in the body several times and act as carriers for numerous exogenous and endogenous compounds. The most popularly studied albumins are bovine serum albumin (BSA) and human serum albumin (HSA). Both BSA and HSA have very high conformational adaptability to a great variety of ligands. Two main approaches have been adopted in the ligand-protein binding studies. In this work, an antitumor complex of formula [Pd(phen)(FIT)]NO₃, where phen is 1,10-phenanthroline and FIT is phenanthroline derivative, has been synthesized and characterized by spectroscopic methods such as UV-Visible, IR and ¹H-NMR as well as conductivity measurements and chemical analysis. This new complex has been interacted with HSA using UV-visible isothermal titration method in Tris-HCl buffer solution containing 10 mmol/L sodium chloride (pH=7.4) at 300 and 310K. It can denature HSA at very low concentrations (~10 μM). In addition, this water soluble complex has been tested for their in vitro anti-tumor activity against chronic

myelogenous leukemia cell line, K562. They show Cc50 values lower than that of cisplatin.

Keywords: Phenanthroline Derivative, Human Serum Albumin, Palladium Complex, Cytotoxicity.

Abstract No.54

Study on the Interaction of Palladium (II) Complex of Phenanthroline Derivative with Human Serum Albumin by Ultraviolet-visible Spectroscopic Methods

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Studies into the interactions between drugs and human serum albumin (HSA) are extremely important for drug discovery, since HSA behaves as a carrier for external drugs and internal biological molecules. In this study, we report synthesis of novel Pd(II) complex of formula [Pd(FIT)₂]NO₃, where FIT is phenanthroline derivative (see figure1). This complex has been characterized by spectroscopic methods such as ultraviolet-visible, infrared and ¹H-NMR as well as conductivity measurements and chemical analysis. This complex has been interacted with HSA (Human Serum Albumin) using UV-visible isothermal titration method in Tris-HCl buffer solution containing 10 mM sodium chloride (pH=7.4) at 27 and 37°C. The above compound can denature the protein at very low concentrations (~100 μM).

Keywords: HSA, Pd(II) Complex, Isothermal Titration, Phenanthroline Derivative.

Abstract No.55

Docking and Molecular Dynamics Simulation Study on Interaction of some Schiff Base Complexes with Human Serum Albumin

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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 (subdomain IIIA), these compounds bind to subdomain IB (site III). 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 catalyze the reduction of peroxides. Peroxidase activity has been identified in plants, microorganisms and animals, where peroxidases play important roles. In this study effect of NiO and CdTe nanoparticles on the activity of horseradish peroxidase (HRP) has been investigated. In the

presence of NiO nanoparticles, the lower concentrations (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. Noncompetitive 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