Abstract No.50

The effects of Wet Cupping on the Structure and Function of Extracted Hemoglobin from Diabetic Volunteers

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Cupping is one of the most treating methods used in traditional medicine for controlling blood sugar in people with diabetes mellitus. The aim of present study is evaluating the effects of wet-cupping on changes in molecular structure and function of human hemoglobin (Hb).In the present study, Hb was extracted from blood samples of healthy non-diabetic and diabetic volunteers who were/were not experienced cupping.The Bradford method was used to determine the concentration of hemoglobin solution and then SDS-PAGE electrophoresis was used to determine the purity of the samples. The intrinsic fluorescence spectroscopic studies in the wavelength range of 300-500nm were performed to represent the conformational changes of extracted Hb. For determining the changes in structure and amount of accessible hydrophobic groups of extracted Hb, the extrinsic fluorescence emission with the ANS probe were accomplished.The location of the emission peak in intrinsic fluorescence spectrum didn't change but there was a decrease in the peak's intensity in diabetic sample that may be as a result of conformational changes near the tryptophan residue. While the intensity of the peak in diabetic Hb samples after cupping was increased a bit.Although the effect of cupping in different individuals according to age, sex, blood sugar levels and nutritional requirements can vary which may be concluded that the wet cupping can reduce the side effects of diabetes on Hb molecule.

Keywords: Cupping, Diabetes, Hemoglobin, Fluorescence Spectroscopy.

Abstract No.51

Comparison of Molecular Dynamic Simulation of Full Length and Truncated Insulin Aggregation

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Theoretical studies can be useful to get information about the details protein misfolding and aggregation that lead to diseases such as Alzheimer's and type II diabetes. Molecular dynamics simulation on full length and truncate insulin was conducted for 10 to 16ns in solvent (water) and vacuum condition at acidic pH (2), and high temperatures (345 K and 500 K). Presence of salt was studied with inclusion of NaCl and KCl (2 M). Potential energy (U) and RMSD output were analyzed, as well as secondary structure percent of structures. DSSP, Stride, PALSSE, STICK, P-SEA, XTLSSTR were used to determine secondary structures percentages. During simulation time, potential energy of all cases did not show significant changes. RMSD of truncated insulin run increased more than other conditions to about 20A°. Beta sheet structures percentage of full-length insulin in the presence of NaCl reached 40%, however for truncated insulin increase up to 20% was observed. In almost all cases, the alpha structures percentage reduced and beta structures, unstructured parts, turn and bend increased. These results can be further proof on the fact that insulin probably unfold and then refold before getting aggregate beta structures. This study has also shown that the presence of salt, especially NaCl, can be effective in insulin fibrillation. Furthermore, it appears that five residues of the C-terminal the B chain is very effective and very important in insulin misfolding.

Keywords: Aggregation, Secondary Structure, Insulin, Simulation.

Abstract No.52

Optimization of Acid (HCl) Hydrolysis of Date Palm Leaf to Produce Bioethanol

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Increase in global energy demand has caused oil prices to reach record levels in recent times.High oil prices together with concerns over CO2 emissions have resulted in renewed interests in renewable energy . In recent years bioethanol has been recognized as a potential alternative to petroleum-derived transportation fuels. In this study, optimization of bioethanol production from Date Palm Leaf investigated with effect of

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 70C0 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 $[Pd(phen)(FIT)]NO_3$, 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 $[Pd(FIT)2]NO_3$, 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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