

help to rational design of novel PI3Ks inhibitors with preferred activities.

**Keywords:** 4D-QSAR, CoMFA, CDOCKER, Molecular Dynamic Simulation, Phosphoinositide-3-Kinase (PI3K) Inhibitors.

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**Abstract No.284**

**Hydrophilicity of Ionic Liquids Plays Important Role on Choline Oxidase Electron Transferring**

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Room-temperature ionic liquids (RTILs) and their related nano-composites attracted considerable attention because of their desirable properties and potential applications in biomolecular immobilization, biocatalysis, electrochemical biosensors and bioreactors. In the present report, six different nano-composites containing the same amine functionalized multi-walled carbon nanotubes (NH<sub>2</sub>-MWCNTs) but different room temperature ionic liquids (RTILs) were prepared. Then, the efficiency of these nano-composites as supporting materials for studying the electrochemistry and electrocatalysis of choline oxidase (ChOx) as a model enzyme were compared. The corresponding cyclic voltammetric and amperometric data showed that the electrocatalytic activity and the electroanalytical performance of immobilized ChOx depend on the degree of hydrophilicity of RTILs used in the applied nano-composite. The higher stability (180 days), more enzyme loading (6.56 M cm<sup>-2</sup>), lower detection limit (3.85 μM) and wider linear range (0.005-0.8 mM) were obtained for the most hydrophilic RTIL (1-allyl-3-methylimidazolium bromide).

**Keywords:** Nanocomposite, Choline Oxidase, Electron Transfer, Functionalized Carbon Nanotubes, Ionic-Liquid, Choline.

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**Abstract No.285**

**Chemical Modification of Antibody Using Gold Nanoparticles Bearing Luminol**

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Gold nanoparticles (GNPs) are very attractive labels due to their special physical and chemical properties such as ease of synthesis, simplicity of conjugation and excellent biocompatibility. Because of these advantages they can be used as the carrier for a large number of markers and bio-catalysts. In the present work, at first luminol was attached to GNPs then the modified GNPs were chemically bound to antibody as a secondary antibody (Ab2-GNPs). The characteristics of chemically modified antibody were investigated by three methods including: UV-Vis spectroscopy, chemiluminescence emission and ELISA (Enzyme linked immuno-sorbance assay). The native antibody showed a UV-Vis absorbance at 521 nm wavelength. But after chemical modification it has a broad peak along with 10 nm red shift compared to GNP. In second method, Ab2-GNPs were added to Ab1-Ag (primary antibody (Ab1) bonded to antigen (Ag)), after washing, chemiluminescence emission was recorded in 425 nm. High chemiluminescence emission shows antibody preserves its function in conjugation with GNP-Luminol. Preservation of antibody function has been proved by ELISA method too. This bio-composite proposed for diagnostic and medical usage, due to its praiseworthy detection limit of antigen in this immuno-sensors (14 pg/ml).

**Keywords:** Gold Nanoparticles, Chemiluminescence, Immuno Sensor, Antibody Function, Antigen Detection.

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**Abstract No.286**

**Fine Structural Analysis of Human Serum Albumin**

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Human serum albumin is the most abounding protein in human blood plasma. It plays essential roles such as maintaining pH level and osmotic pressure in blood. This protein possesses a particular adequacy to bind to a great number of various endogenous and exogenous compounds. This article outlines different features of HAS and its multifunction eligibility. These studies can be obtained by pH metery, ligand binding, UV spectroscopy, fluorescence spectroscopy and CD techniques. The results compared and discussed based on data

achieved by these methods. Statistical analysis has been revealed at least six fine individual structures for HSA. Each structures present individual and exclusive function. It can be concluded that, albumin unique features and functions are due to its switching capability to different possible fine structures with the lowest energy exchange.

**Keywords:** Human Serum Albumin, Fine Structures, Structural And Functional Alteration.

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**Abstract No.287**

**Mixed Quantum Mechanical/ Molecular Mechanical (QM/MM)  
Study of the S-nitrosylation Reaction 4-phenyl-3-  
Furoxan carbonitrile as Inhibition of Thioredoxin Glutathione  
Reductase (TGR)**

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Combined quantum mechanics/molecular mechanics (QM/MM) methods allow computations on chemical events in large molecular systems. We present a theoretical study of a mechanism for the S-nitrosylation Reaction 4-phenyl-3-furoxan carbonitrile or furoxan belongs to an oxadiazole-2-oxide class whose therapeutic effects are largely due to their inhibition of thioredoxin glutathione reductase (TGR) for the control of schistosomiasis bases in QM/MM calculations at the DFT RB3LYP/6-31G+(d)//SCC-DFTB AMBER level. The activity of the oxadiazole 2-oxides was associated with a donation of nitric oxide. We first attempted to dock inhibitor in the active site of enzyme available in the Protein Data Bank, (PDB codes: 3H4K), to see how intact inhibitor would bind. Since our interest was focused on the region where reaction should take place, all molecules that might potentially be involved in the mechanism of nucleophilic attack, namely furoxan, residues Cys159, and nearby water molecules, were treated by QM, while the rest of the protein, as well as the bulk water, were treated by traditional molecular mechanics. As soon as a preliminary minimization of complex was carried out on TGR using the hybrid QM/MM potential, migration of the Cys159 to the carbon 3 furoxan was observed. We were quite surprised by this outcome, while the formation of the tetrahedral intermediate might be a reasonable explanation for location of the initial nucleophilic attack shows this mechanism: The potential

energy of the system with respect to the initial state ( $\Delta U$ ) along the minimum energy reaction path (MERP) is also reported with the 3D structures of relevant intermediates. The results are consistent with the available experimental data and provide new insight into the detailed mechanism of this important reaction.

**Keywords:** Quantum Mechanic, Molecular Mechanical, Thioredoxin, Glutathione Reductase.

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**Abstract No.288**

**Effect of Glycine, as Chemical Chaperone, on Catalase  
Glycation by Glucose**

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Oxidative mechanisms are thought to have a major role in several biological phenomena, including cataract formation and diabetic complications. Glycation of catalase, as a powerful antioxidant enzyme, by glucose alters its structure and function and increases the risk of cataract formation in diabetic patients. Glycine is a chemical chaperones that inhibit protein glycation and stabilize them against thermal and chemical denaturation. Therefore, we investigated the effects of this chemical chaperone on catalase glycation. Catalase solution, pH 7.4, was incubated separately with glucose in the presence or absence of glycine at 37°C in a shaker incubator. The aliquots were collected every week and stored at -80°C. Then, they were analyzed by fluorescence spectroscopy, circular dichroism spectroscopy (CD) and polyacrylamide gel electrophoresis (PAGE). The activity of catalase in each sample was also determined. Structure and activity of catalase were changed due to the glycation with glucose. Glycation caused an increase in the fluorescence emission and electrophoretic mobility and a decrease in the alpha helix content and catalase activity. Glycine inhibited this phenomenon and the fluorescence emission, alpha helix content, electrophoretic mobility and activity of catalase were closed to the normal values. Our results indicated a decrease in the catalase glycation by glucose in the