

and (the entropy of DNA denaturation by metal complex, is 0.11 KJ/mol.K at 300K) have been determined. Also gel filtration results had shown that binding of the complex with DNA is strong enough that not readily break from DNA.

Keywords: Palladium(II) Complex, DNA-binding, Dithiocarbamate, Gel filtration, Binding Parameters, Thermodynamic Parameters.

Abstract No.60

Glucose Interaction with Carbon nanotube as a Theoretical Investigation

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Since Carbon nanotubes (CNTs) have unique properties, discovery of CNTs in 1991 by Ijima demonstrated a new way for researches in study of molecules, especially biomolecules. Many investigations have been done about Single walled carbon nanotubes (SWCNTs) interaction with biomolecules, such as DNA, proteins and sugars. Results of these studies revealed the many secrets of biomolecules, but interaction of SWCNT with biomolecules especially sugar still rises many questions. Hence, we carried out the theoretical investigation about α -D-glucose and β -D-glucose interaction with SWCNT by molecular mechanic method (MM), using OPLS force field. Also we carried out quantum mechanics (QM) study using density functional theory (DFT) at theoretical level of B3LYP, wherein physical properties have been described using this method by compare between energy interaction, atomic charge and dipole moment. We believe that our results are helpful for drug design and drug delivery.

Keywords: Carbon nanotube, Theoretical Investigation, Density Functional Theory.

Abstract No.61

Enzyme Stability in Supercritical CO₂/ionic Liquid System, Insights from Molecular Dynamic Simulation

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In this paper, new findings about enzyme microenvironment in supercritical CO₂/ionic liquid biphasic system were obtained. Molecular dynamic simulation clearly showed that in supercritical CO₂, enzyme and ionic liquid molecules form a supramolecular-like structure. Ionic liquid molecules do as a coating layer and protect enzyme from denaturing condition in supercritical CO₂. By analysis of root mean square deviation it was found that the enzyme has more native and stable conformation in supercritical CO₂/ionic liquid system than in supercritical CO₂. This result is in agreement with experimental observations about the stability of the enzyme in supercritical CO₂/ionic liquid system. Moreover, based on radius of gyration values, it is concluded that enzyme has a more compact and active conformation in supercritical CO₂/ionic liquid system than that in supercritical CO₂. Root mean square fluctuations of enzyme flexible residues including α 5 and α 10 helices are highly reduced by adding Ionic liquid molecules to supercritical CO₂. Although α -helix and β -sheet content of the enzyme in supercritical CO₂ reduced to some extent, they almost remained unchanged in supercritical CO₂/ionic liquid. At the molecular level, the results of this research reasonably confirmed that the use of ionic liquid molecules is an efficient method for stabilizing enzymes in supercritical CO₂.

Keywords: Supercritical CO₂, Molecular Dynamic Simulation.

Abstract No.62

A Computational Study on Single Walled Carbon Nanotube Interaction with Sphingomyelin

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The combination of single-walled carbon nanotubes (SWCNTs) with biologically important structures is particularly intriguing since it opens the door to novel biotechnology and nanotechnology applications. So, the interaction between SWCNTs and neuron membrane is a subject of intense current interest. On the other hand, over the past decade or so, there has been increasing interest in the use of SWCNTs in neuroscience study due to the excellent electrical conduction properties, chemical, mechanical and thermal stability, and discernible

biocompatibility properties of this material. Hence nanoneuroscience is a recently coined term describing the convergence of the existing but different worlds of nanotechnology, neurobiology that a large body of research is emerging that hints at the potential applications of nanotechnology in neuroscience. In present investigation, applying molecular mechanic (MM) method with OPLS, force field and quantum mechanics (QM) method using density functional theory (DFT) with B3LYP keyword- we carried out a theoretical study on SWCNTs interaction with sphingomyelin as one of the most important components of the neuron membrane. We study about physical properties of this interaction. Hence, we have investigated places of interaction and electrical properties of this interaction. The result shows that the interaction of sphingomyelin with SWCNT has minimum value of interaction energy and structural stability in solvent. Since physical properties of this system are important for nanoneuroscience practical applications, the present study opens the door to nanoneuroscience.

Keywords: Nanoneuroscience, Sphingomyelin, SWCNT, DFT.

Abstract No.63

Real-Time Differential Scanning Fluorimetry of Quorum Sensing-Mediated Proteolytic Activity in Selected Bacterial Pathogens

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Cellular communication between bacterial pathogens is established through the release of autoinducers upon reaching a certain population density. This mechanism, called quorum sensing (QS), allows synchronization and downstream expression of associated virulence genes leading to an efficient and effective establishment and survival within the host. In bacterial pathogens, several proteases are reportedly secreted during QS and play major roles during

pathogenesis. Aversion of this process is very crucial in order to prevent further damage within the host and can be achieved by anti-quorum sensing (AQS) usually by molecules produced as secondary metabolites from certain plant species. This study developed a real-time proteolytic activity assay by differential scanning fluorimetry using the high-resolution melt (HRM) program of the Rotor-Gene cyclor and the fluorescent dye Flamingo Pink™ based on the principle of substrate protein stability. QS-mediated proteolytic activity from expressed gelE, sspA and apr gene products of *Enterococcus faecalis*, *Staphylococcus aureus* and *Pseudomonas aeruginosa*, respectively, were analyzed with high-precision based on their real-time enzymatic effect on substrate protein stability measured as fluorescence by Flamingo Pink which undergoes dramatic fluorescence enhancement in the presence of denatured protein – a reflection of the thermodynamic state of the protein substrate during enzymatic digestion. A remarkable decrease in fluorescence was observed when bromofenone, an AQS molecule, was added during bacterial culture. The levels of expressed protease gene products were also confirmed by real-time quantitative PCR of the gene transcripts. The developed protocol demonstrates precise detection and measurement of proteolytic activity mediated by the QS signaling pathway. This technique enables rapid screening of AQS molecules such as from plant extracts, and can therefore be applied as a tool for discovery of drugs with potential antimicrobial activity.

Keywords: Fluorescence, Quorum Sensing, Protease, Protein Stability.

Abstract No.64

A Theoretical Investigation on Oxaliplatin Interaction with β -Lactoglobulin

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Bovine β -Lactoglobulin (BLG) as the most important whey protein in milk, is a globular protein belonging to the lipocalin family. According to the crystal structure, BLG comprises predominantly a β -sheet configuration containing nine antiparallel β -strands from A to I. Many investigations have been done about BLG interaction with material for various applications, such as fatty acid, Vitamins and Drugs. But