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 filteration, 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 CO_2/ionic liquid biphasic system were obtained. Molecular dynamic simulation clearly showed that in supercritical CO_2, 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 CO_2. By analysis of root mean square deviation it was found that the enzyme has more native and stable conformation in supercritical CO_2/ionic liquid system than in supercritical CO_2. This result is in agreement with experimental observations about the stability of the enzyme in supercritical CO_2/ionic liquid system. Moreover, based on radius of gyration values, it is concluded that enzyme has a more compact and active conformation in supercritical CO_2/ionic liquid system than that in supercritical CO_2. Root mean square fluctuations of enzyme flexible residues including α5 and α10 helixes are highly reduced by adding Ionic liquid molecules to supercritical CO_2. Although α-helix and β-sheet content of the enzyme in supercritical CO_2 reduced to some extent, they almost remained unchanged in supercritical CO_2/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 CO_2.

Keywords: Supercritical CO_2, 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