

first time we showed that Cys has direct or indirect roles in cellulose classification, either alone or in connection with the other amino acids as dipeptides in cellulase categorization. The count of Cys and Cys-Asp reported as an important factor in 100% and the count of Cys-Ala in 80% of weighing algorithms. The result of decision tree algorithms also clearly confirmed that Cys has significant role in cellulase classification.

Keywords: Cellulase, Attribute Weighting, Decision Tree Algorithms, Bioinformatics.

Abstract No.58

The Enhancement of Surface Hydrophobicity by Calcium Ion may have Significant Contribution in cell Death Inducing Activity of Human Calprotectin

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As calcium and zinc-binding protein complex, calprotectin (MRP8/14) is abundant in cytosolic fraction of human neutrophils. Calprotectin is a multifunctional protein with broad spectrum of activities, including antimicrobial property and apoptosis inducing activity. This protein is significantly elevated in serum and body fluids of patients with various inflammatory conditions, suggesting that this protein plays significant function influencing the inflammatory processes. In this study calprotectin was purified from human neutrophils, using a two-step ion exchange chromatography. The apoptosis inducing activity of this protein was examined against two leukemia cancer cell lines, using 3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium bromide (MTT) assay. Furthermore, to explore role of calcium binding on surface hydrophobicity of calprotectin, fluorescence study was performed. As shown, calcium binding induces conformational changes and increases the solvent exposed hydrophobic surfaces of human calprotectin, making the protein prone to aggregation. Since the early aggregates have an intrinsic ability to impair fundamental cellular processes by interacting with cellular membranes, consequently, calcium binding to calprotectin may lead to the formation of a toxic folding variant of this protein with sticky (hydrophobic) surface which may interact with plasma membrane to kill cells. This study may suggest contribution of the exposure of surface hydrophobicity by calcium ion, in the pathway of apoptosis inducing activity of human calprotectin.

Keywords: Calprotectin, Calcium, Surface Hydrophobicity, Aggregation, Fluorescence Study.

Abstract No.59

Interaction of [Pd(phen)(n-pr-dtc)]Br with DNA of Calf Thymus

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Cis-diamminedichloroplatinum(II) (cisplatin) is used in the clinical treatment of several types of human cancers[1]. Various strategies have been used to reduce the major toxicity of cisplatin. One of these strategies is to develop new compounds capable of reducing these toxicities[2].thus in this study we prepared 1,10-phenanthroline-n-propyldithiocarbamatopalladium(II) bromide, [Pd(phen)(n-pr-dtc)]Br, and characterized by spectroscopic techniques such as UV-Vis, FT-IR, ¹H NMR and nonspectroscopic techniques like conductivity measurements, elemental analysis and decomposition temperature. Studies of antitumor activity of this complex against human cell tumor lines (K562) have been carried out. It shows IC₅₀ value lower than that of cisplatin. The interaction of the complex has been studied with DNA of calf thymus (CT-DNA) at 300K and 310K using UV-Vis isothermal titration method in 25 mM Tris-HCl buffer of pH=7.0. This complex can denature CT-DNA at very lower concentrations (~ 100 μM). The concentration of this complex in the midpoint of transition, [L]_{1/2}, are 0.078 and 0.064 mM at 300 and 310K respectively. The mode of binding of the complex to CT-DNA, has been investigated by ultraviolet spectroscopy. The result of these studies indicate that [Pd(phen)(n-pr-dtc)]Br complex exhibit cooperative binding with DNA. In the interaction studies between the [Pd(phen)(n-pr-dtc)]Br complex with CT-DNA, several binding parameters such as, K (the apparent binding constants, are 46.68 and 58.45 mM⁻¹ at 300 and 310 K, respectively), n (the Hill coefficients, are 2.15 and 2.93 at 300 and 310K respectively), g (the number of binding sites per 1000 nucleotides, is 5 at 300 and 310 K), n (the ratio of the concentration of bound metal complex to the total DNA concentration) and m (a measure of the metal complex ability to denature DNA, are 207.30 and 223.78 (kJ/mol)(mmol/L)⁻¹ at 300 and 310 K respectively). Thermodynamic parameters such as (conformational stabilities of DNA in the absence of metal complex, are 15.10 and 14.00 kJ/mol at 300 and 310 K, respectively), (the heat needed for DNA denaturation in the absence of metal complex, is 47.98 kJ/mol)

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