

and the stereochemical quality of protein structures and molecular dynamics simulation of the refined models was performed. The structural analysis showed the key features of IceA1 relative to IceA2 that may illustrate their different potentiality for interaction with possible ligands or inhibitors.

**Keywords:** Helicobacter Pylori, IceA, Peptic Ulcer Disease, Comparative Modeling.

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**Abstract No.84**

**Suicide Inactivation of Horseradish Peroxidase by Aminophenol Using Voltametric Method**

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Horseradish peroxidase (HRP) is the enzyme which catalysis the oxidation of variety of molecules in the presence of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) and used as a label in biosensors. In such biosensors, HRP detect the biological reaction (e.g. antigen-antibody), which essentially is applicable for determination of desired analyte. The use of peroxidase substantially increases the sensitivity of this method. In this report, we studied the reaction of HRP with o-aminophenol (o-AP) as a substrate. The oxidation of o-AP is owing to the presence of two functional groups, OH and NH<sub>2</sub>, which undergo hydrolysis of o-AP and produce the reactive soluble intermediates such as 0-quinone imine. Finally this intermediate is changed into 2-aminophenoxazine-3-one. In order to identify the effect of o-AP on inactivation of peroxidase, we used cyclic voltammetry and glassy carbon as working electrode. After optimization of the results, it was revealed that to get the maximum efficiency of enzyme, the optimum concentration for H<sub>2</sub>O<sub>2</sub> and o-AP must be less than 10 and 2 mM, respectively.

**Keywords:** Horseradish peroxidase, Aminophenol, Hydrogen peroxide, Cyclic Voltammetry.

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**Abstract No.85**

**Protein Structure and Function in Different Surface Nanoparticle: Applications in Biological Area and Biomedicine**

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The conformational changes of glucose oxidase (GOx) in the negative charge colloidal gold nanoparticles (NC-GNPs), positive charge colloidal gold nanoparticles (PC-GNPs), mercaptopurine:GNPs and 11-mercaptopundecanoic acid:GNPs as a hydrophobic and hydrophilic GNPs was investigated by various spectroscopic techniques including UV-Vis absorption, fluorescence and circular dichroism (CD) spectroscopies. Moreover, the fluorescence quenching constant and binding parameters after the formation of the GOx:GNPs conjugates follows by Stern-Volmer (S-V) plots. Size and charge of NC-GNPs and PC-GNPs was determined by zeta sizer and zeta potential analyzer, which their size and charge are 83.7 nm (-16.4 mV) and 90.4 nm (+8.44 mV) respectively. Also GOx activity and amount of protein adsorption on GNPs was determined. The results showed that NC-GNPs have least conformational changes for GOx at both secondary and tertiary structure levels. And hydrophobic-GNPs with the minimum protein adsorption have a maximum conformational change

**Keywords:** Negative Charge Colloidal Gold Nanoparticles, Positive Charge, CD Spectroscopy, Glucose Oxidase.

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**Abstract No.86**

**Interaction Studies Between a [(phen)Pd μ-(S2CNH(CH2)3NHCS2)Pd(phen)](NO3)2 anti-Tumor Complex and Calf Thymus DNA**

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Palladium(II) complexes are very interesting candidates for alternative platinum-based drugs, because the coordination geometry and complex forming processes of palladium(II) are very similar to those of platinum(II). Thus we focused on the interaction of calf thymus DNA (CT-DNA) with a new palladium(II) anticancer complex of formula [(phen)Pd μ-(S2CNH(CH2)3NHCS2)Pd(phen)](NO3)2 (where phen is 1,10-phenanthroline and S2CNH(CH2)3NHCS2 is propylenbis(dithiocarbamate)). This interaction was studied by spectroscopic techniques such as UV-Vis and fluorescence in 30mM

Tris-HCl buffer solution (pH=7.0) containing 20 mM sodium chloride at 300 and 310K. 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. There is a set of 6 binding sites (g) for the complex on the DNA with positive cooperativity in binding.  $n$ , the Hill coefficient (as a criterion of cooperativity) find out to be 5.6 at 300 K and 7.3 at 310 K, respectively.  $K_{app}$  the apparent equilibrium constant are  $21.4 \text{ mM}^{-1}$  and  $39.3 \text{ mM}^{-1}$  at 300 and 310K respectively. The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ( $[L]_{1/2}$ ), is decreased by improving temperature, from 0.25 mmol/L at 300K to 0.28 mmol/L at 310K. The conformational stability of DNA in the interaction with ligand ( $\Delta G^\circ \text{ H}_2\text{O}$ ) determined to be 32.5 kJ/mol and 35.7 kJ/mol at 300 and 310 K, respectively. Presence of ligand led to less stability of the DNA. Values for  $m$ , (a measure of ligand strength for DNA denaturation) are 121 and 153 (kJ/mol). $(\text{mmol/L})^{-1}$  at 300 and 310 K, respectively. Enthalpy of DNA denaturation by the complex ( $\Delta H^\circ$  coformation or  $\Delta H^\circ$  denaturation) in the range of 300 and 310 K is find out to be 42.2 kJ/mol. In addition, the calculated entropy ( $\Delta S^\circ \text{ H}_2\text{O}$ ) of DNA denaturation by complex is -0.23 kJ/mol at 300 K. The negative value of entropy change is related to the more disorder of denatured DNA with respect to the native DNA. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The gel chromatograms obtained from Sephadex G-25 column experiments showed that the binding of metal complex with DNA is so strong that it does not readily break.

**Keywords:** Thermodynamic Parameters, Spectroscopic Techniques, Anti-Tumor, DNA-Binding, Palladium (II) Complex.

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**Abstract No.87**

**Spectroscopic Studies on the Thermodynamic and Thermal Denaturation of the CT-DNA Binding with [Pd(en)(dppz)](NO<sub>3</sub>)<sub>2</sub>**

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The development of new metal complexes which can selectively interact with nucleic acid is of much current interest. During recent years, the interest for metal complexes containing planar extended polyaromatic ligands has increased tremendously, mainly for their usage as probes capable to utilize the nucleic acid structures and as DNA-molecular light

switches. Many efforts have been directed towards the design of complexes containing modified bpy or phen ligands that bind DNA primarily via-base pair intercalation. In this study, we report the results of investigation of interaction between calf thymus DNA (CT-DNA) and [Pd(en)(dppz)](NO<sub>3</sub>)<sub>2</sub> complex (where en is ethylenediamine and dppz is dipyrido[3,2-a:2',3'-c]phenazine). Electronic absorption, fluorescence titration and gel filtration experiments were employed to determine the thermodynamic parameters, binding parameters and the mode of binding between this complex and DNA in Tris-HCl buffer solution containing 20mM sodium chloride (pH=7.0) at 300 and 310 K. 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 above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ( $[L]_{1/2}$ ), is 0.046 mmol/L at 300 K and 0.045 mmol/L at 310 K. The conformational stability of DNA in the interaction with ligand ( $\Delta G^\circ \text{ H}_2\text{O}$ ) determined to be 485.5 kJ/mol and 385.2 kJ/mol at 300K and 310K respectively. There is one set of 5 binding sites (g) for the complex on the DNA (per 1000 nucleotides) with positive cooperativity in binding.  $n$ , the Hill coefficient (as a criterion of cooperativity) find out to be 4 at 300 K and 6 at 310 K respectively.  $K_{app}$  the apparent equilibrium constant are  $14.37 \text{ mM}^{-1}$  and  $18.9 \text{ mM}^{-1}$  at 300 and 310 K, respectively. Presence of complex led to less stability of the DNA. Values for  $m$ , (a measure of ligand strength for DNA denaturation) are 162 and 155 (kJ/mol). $(\text{mmol/L})^{-1}$  at 300 and 310 K, respectively. Enthalpy of DNA denaturation by the complex ( $\Delta H^\circ$  coformation or  $\Delta H^\circ$  denaturation) in the range of 300 and 310 K is find out to be 42.1 kJ/mol. In addition, the calculated entropy ( $\Delta S^\circ \text{ H}_2\text{O}$ ) of DNA denaturation by complex is 0.12 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The gel chromatograms obtained from Sephadex G-25 column experiments showed that the binding of metal complex with DNA is so strong that it does not readily break.

**Keywords:** Thermodynamic Parameters, Spectroscopic Studies, Anti-Cancer, Palladium (II) Complex, DNA-Binding.

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**Abstract No.88**

**Comparative Structural Analysis of two forms (m1/m2) of p55 Domain of Helicobacter Pylori Vacuolating Toxin**

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