



## Synthesis, characterization, DNA and HSA interactions of Cu(II) and Ni(II) complexes with 9,10-Phenanthrenequinone p-toluichydrazone

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### ABSTRACT

The new complexes of Cu(II) and Ni(II) of a tridentate Schiff base ligand derived from 9,10-phenanthrenequinone and p-toluic hydrazide have been synthesized and characterized by elemental analysis, electrical conductometry, FT-IR, Mass, NMR and UV–Vis. The DFT calculations were carried out at B3LYP/6-31G\*(d) level for the determination of the optimized structures of these compounds. Their binding behavior with fish salmon-DNA (FS-DNA) and human serum albumin (HSA) were comprehensively studied by different methods, including electronic absorption spectroscopy, fluorescence spectra, thermal denaturation experiments, and molecular docking examinations. Fluorescence and absorption spectra were investigated in order to estimate the binding parameters. The analysis of fluorescence data at different temperatures were done in order to estimate the thermodynamics parameters of interactions of ligand and its complexes with DNA and HSA. The experimental results show that the compounds can bind to FS-DNA and HSA and the major binding mode is groove binding. Molecular docking study for DNA indicated that these compounds bind to the minor groove of DNA. Furthermore, the results of molecular docking calculation and competitive binding experiments represent the binding of these compounds with the hydrophobic residues located in the subdomain IB of HSA. In addition, they can exhibit good binding propensity to HSA. The molecular docking results kept in good consistence with experimental data.

**Key words:** 9,10-Phenanthrenequinone, p-toluyil hydrazone, DFT calculation, DNA & HSA interaction, docking calculation.