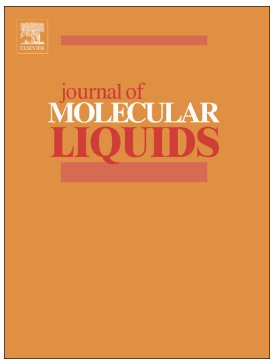

Synthesis, structural characterization, molecular docking and DNA binding studies of copper complexes

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of copper complexes

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Abstract

Azo pyrazolones and their copper(II) complexes were characterized by elemental analyses, IR, ^{1}H NMR, UV-Visible and magnetic measurements as well as thermal analysis and X-ray diffraction. The molar conductance measurements proved that all the complexes are non electrolytes. IR spectra showed that the ligands (**HL_n**) acts as a monobasic bidentate ligand by coordinating *via* the nitrogen atom of the pyrazole ring (-HN-N=) and oxygen atom of the deprotonated -OH group moiety, thereby forming a square planar chelating ring with bidentate acetate group. Analytical data revealed that all the complexes exhibited 1:1 (metal-ligand) ratio. The Thermal decomposition of the complexes revealed the outer water molecules and acetate group as well as the end product is CuO. The thermodynamic parameters of the ligands (**HL_n**) and their Cu(II) complexes are calculated using Coats–Redfern and Horowitz-Metzger methods. The optimized bond lengths, bond angles and the calculated quantum chemical parameters for the ligands (**HL_n**) and their Cu(II) complexes (**1-3**) were investigated. The calf thymus DNA binding activity of the ligands (**HL_n**) and their Cu(II) complexes were studied by absorption spectra and viscosity measurements. Molecular docking was used to predict the binding between the ligands and the receptor of 2a91-hormone of prostate cancer and 3hb5-oxidoreductase receptor of breast cancer.

Keywords: Copper complexes; Molecular Structure; Molecular docking; DNA binding.

1. Introduction

Pyrazole-derived ligands have been interesting compounds over the last decades because of their unusual structural features, coordination chemistry and remarkable physical and chemical properties [1]. Pyrazoles are potential imidazole mimics and can serve in the development of ligand systems that resemble active sites of metalloenzymes [2]. The design and synthesis of novel pyrazole-containing complexes