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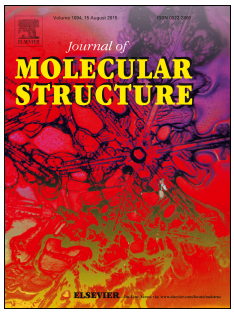

Structural, thermogravimetric, B3LYP and biological studies on some heterocyclic thiosemicarbazide copper (II) complexes and evaluation of their molecular docking

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Structural, thermogravimetric, B3LYP and biological studies on some heterocyclic thiosemicarbazide Copper (II) complexes and evaluation of their molecular docking

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Abstract

Two copper (II) complexes of ligands H_2L^1 and H_2L^2 have been prepared and investigated. The ligands were prepared by the individually addition of picolinic acid hydrazide and 2-(2-aminothiazol-4-yl) acetohydrazide into benzoyl isothiocyanate. The results of analytical and spectroscopic equipments revealed that H_2L^1 act as monobasic bidentate with square planner environment. While H_2L^2 behaves as monobasic tetradentate with Oh geometry. The geometries of ligands and their complexes being carefully studied using Jaguar 9.1 program based on the density functional theory (DFT) to predict properties of materials performed by the hybrid density functional method B3LYP. Additionally, thermal degradation data were evaluated to determine the kinetic and thermodynamic parameters by different methods. Moreover, the anti-oxidant (using DPPH and SOD methods), and anti-bacterial activities of the compounds have been studied. Furthermore, the docking study of ligands and their complexes were applied against gram-positive *S. Aureus*, negative *E. Coli* bacterial and *C. Albicans* fungal strains by Schrödinger suite program using XP glide protocol.

Keywords: Thiosemicarbazide, Cu(II) complexes, spectral characterization, thermal degradation, anti-bacterial activity, Molecular docking.

1. Introduction:

Heterocyclic thiosemicarbazide compounds and their metallic coordination compounds have a biological and pharmacological potencies [1, 2] because their flexibility [3] as well as existence of soft (S) and hard (N) donor atoms [4]. Moreover, the Cu(II) complexes exhibit bactericidal activity and they are demonstrate as therapeutic drugs [5-7] as a result of formation of stable coordinated compound with thiosemicarbazide moieties [8]. Also, Cu(II) complexes react as an active catalyst for atom transfer radical cyclisation [9].

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