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Molecular docking, structural characterization, DFT and cytotoxicity studies of metal(II) Schiff base complexes derived from thiophene-2-carboxaldehyde and L-histidine

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ABSTRACT

Co(II), Ni(II), Cu(II) and Zn(II) complexes of Schiff base ligand (thio-L-his) derived from thiophene-2-carboxaldehyde (thio) with L-histidine (L-his) were synthesised. The thio-L-his and its metal complexes have been optimized and quantum chemical parameters are calculated using density functional theory. Despite several donor sites in the synthesised thio-L-his, the coordination with metal ion occurred through azomethine nitrogen and carboxylate oxygen as evidenced by elemental analyses, fourier transform infrared, mass and nuclear magnetic resonance spectral analysis. The electronic spectral data together with magnetic measurements suggest tetrahedral for Co(II) and Zn(II)-(thio-L-his) and square planar geometries for Ni(II) and Cu(II)-(thio-L-his) complexes, respectively. Molecular docking has been performed to predict the binding energy between thio-L-his and complexes with Epidermal Growth Factor and Cyclooxygenase-2 receptors. The efficiency of metal complexes as promising candidates for the photodegradation of methylene blue has been established in the present study. The comparative in vitro antimicrobial activities against various pathogens with reference to known antibiotics and antioxidant activity against standard control at variable concentrations revealed that the metal complexes show enhanced antimicrobial and free radical scavenging activities as compared to free thio-L-his. In vitro anticancer activity of the Cu(II)-(thio-L-his) was assayed against human ovarian cancer cells, showed that the complex exhibited promising anticancer activity on PA1 cell line.

1. Introduction

Due to the large variety of available metals and the ability to tune the reactivity and structure of the metal complexes by their organic ligand spheres, coordination chemistry comprises a large body of current inorganic research, especially design of compounds with bioactivity [1]. In general, the nature of metal ion and its oxidation states, types, number of ligands and isomers can utilize a critical influence on the biological activity of transition metal complex systems [2]. As an understanding of these factors affecting biological activity, enables the design of metal complexes with specific medicinal properties. Transition metal complexes obtained from Schiff base have still received a great deal of attention worldwide in view of their potential biological significance [3]. Cancer is a malignant neoplasm; broad group of diseases caused by abnormal and uncontrolled cell proliferation and become the major cause of death globally [4]. The efforts have been directed over the years to overcome severe side effects of chemotherapy [5] as a result of generation of free radicals and reactive O_2 species. Therefore, the attention has been focused towards designing the drug molecules with antioxidant and anticancer activities to scavenge free radicals and reactive O_2 species to reduce and avoid side effects of chemotherapy while destroying tumour cells [6]. Even though 70% of all cancer patients receive cisplatin during cancer treatment, nephrotoxicity and drug resistance are **the major side effects** associated with platinum based drugs. Research based on non-platinum based metallochemo therapeutic drug molecules will reduce the cytotoxicity [7] activities. Thiophene moiety compounds manifest a wide range of biological properties such as

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