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Molecular docking, photocatalytic activity and biomedical investigations of some metal complexes

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ABSTRACT

Metal(II)–(furfural-L-his) complexes with a potentially bidentate furfural-L-his have been synthesized. Furfural-L-his and its Co/Ni/Cu/Zn(II)–(furfural-L-his) complexes have been optimized by DFT. The structural features were determined from their elemental analyses, molar conductance, magnetic, UV–Vis, IR, mass, ^{1}H NMR and EPR spectral studies. On the basis of electronic spectral data and magnetic measurements, suitable geometry has been proposed for each complex. The redox behaviour of Cu(II)–(furfural-L-his) complex has been studied by cyclic voltammetry. Thermal decomposition profiles are consistent with the proposed formulation of Co/Ni/Cu/Zn(II)–(furfural-L-his) complexes. PXRD studies reveal that furfural-L-his and Zn(II)–(furfural-L-his) complex are of nanomeric structure. SEM images of furfural-L-his exhibit flake-like morphology. Photodegradation of methylene blue dye indicates that they are photocatalyticaly efficient. NBO and NPA shown considerable reduction in the formal charge on metal ions. Docking analysis with EGFR and cyclooxygenase-2 receptor has been performed to find the best binding energy. Antimicrobial, antioxidant and anti-inflammatory activity against standard at variable concentrations revealed that the Co/Ni/Cu/Zn(II)–(furfural-L-his) complexes show enhanced antimicrobial, free radical scavenging and anti-inflammatory activities as compared to furfural-L-his. Furfural-L-his and Cu(II)–(furfural-L-his) complex have been tested against human ovarian cancer cells, which showed that Cu(II)–(furfural-L-his) complex exhibited promising anticancer activity.

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1. Introduction

Medicinal inorganic chemistry offers additional opportunities for the design of therapeutic agents not accessible to organic compounds (Faria et al., 2004; Hambley, 2007; Orvig & Abrams, 1999). The inclusion of biologically active ligands into metal complexes deals much scope for the design of novel drugs with improved targeted activity. Studies on metal complexes indicate that new mechanisms of action are favourable when combining the bioactivity of ligand with properties inherent to the metal, leading to the possibility of overcoming current drug resistance pathways.

Overproduction of activated oxygen species is considered to be the major contributor to oxidative damage of biomolecules such as DNA, lipids and proteins, thereby expedite cancer, aging, inflammation and neurodegenerative diseases (Basu et al., 2007). The caliber of antioxidants has motivated scientists to search for the interdependence of compounds for improving antioxidant activity and cytotoxicity (Wheate et al. 2010). Even though secure platinum-based chemotherapeutic compounds have been efficiently used against wider range of subsets of cancer, but still several side effects such as nephrotoxicity and cytotoxicity are the major drawbacks (Clarke et al., 1999). There have been rapid developments in inorganic research to find out new and more efficacious metal-based chemotherapeutic drugs in recent years (Criado et al., 2003; Mishra et al., 2020). Amon the metal ions, copper complexes have shown remarkable efficiency in antioxidant (Johnson & Dhanaraj, 2020; Marzano et al., 2009) and anticancer studies (Azuara & Gomez, 2010). There is a great deal of interest in the synthesis and characterization of transition metal chelates of heterocyclic compounds.

L-histidine (L-his) is one of the proteinogenic amino acids (Deschamps et al., 2003). It serves as a strong metal–ion binder in biological systems such as enzymes and proteins (Spencer et al., 2000). The complexing ability of L-his with transition metal ions is reported in the literature (Amr et al., 2005; Azuara & Gomez, 2010; Beinert, 1977; Marzano et al., 2009; Spiro, 1980). Recognizing the importance of Schiff base metal complexes as antioxidants and anticancer agents, we synthesized and characterized Co(II), Ni(II), Cu(II) and Zn(II)–(furfural-L-his) complexes of Schiff base derived from the condensation of furfural with L-his. The coordination ability and behaviour of the synthesized compounds were investigated by spectral characterization methods and thermogravimetric analysis. In addition to this, theoretical calculations using DFT and molecular docking analysis were performed for the compounds.

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