Research Article

Biomedical application studies of Schiff base metal complexes containing pyridine moiety: molecular docking and a DFT approach

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Abstract

Co/Ni/Cu/Zn(II) Schiff base complexes with furfural-MAP derived from furfural and 6-methyl-2-aminopyridine have been synthesized and characterized. Quantum chemical parameter calculations of the furfural-MAP and its complexes have been investigated by DFT. The structural characterization have been carried out from their elemental analyses, molar conductance, magnetic, UV–Vis, IR, mass, ^{1}H NMR and EPR. On the basis of spectral data and magnetic measurements, suitable geometries have been proposed for each complex. Redox behaviour of [Cu(II)-(furfural-MAP)$_2$Cl$_2$] has been studied by cyclic voltammetry. Thermal behaviour of [Cu(II)-(furfural-MAP)$_2$Cl$_2$] is consistent with proposed formulation. Powder XRD studies reveal that the compounds are of nanomeric structures. SEM micrograph of furfural-MAP exhibit flake like morphology. NBO, NPA revealed the furfural-MAP to metal charge transfer in complexes. Docking analysis has been performed to identify the interaction between synthesized compounds and active site of EGFR. Antimicrobial activities against various pathogens with reference to known antibiotics and antioxidant activity against standard at variable concentrations exhibit that the metal complexes show remarkable antimicrobial and free radical scavenging activities. In vitro anticancer activity of [Cu(II)-(furfural-MAP)$_2$Cl$_2$] has been studied against human ovarian cancer cells, which exhibit promising anticancer activity. Furthermore, cytotoxicity of [Cu(II)-(furfural-MAP)$_2$Cl$_2$] has been analyzed against L929 cells.

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