Coordination of manganese (II) and copper (II) complexes with derived imidazole ligand: Synthesis, Characterization, antimicrobial activity, DFT, molecular docking acute and subacute toxicity

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Abstract

The synthesis, characterization and comparative biological study of manganese (II) and copper (II) complexes with heterocyclic ligand used in pharmaceutical field, were reported. $[M(L)_2(Cl)_2(H_2O)_2]\ nH_2O$ stoichiometric was found for metronidazole complexes. These complexes have been prepared and characterized by elemental analysis, FAB mass, ESR magnetic measurements, FTIR, UV-Visible spectra and conductivity. The antimicrobial activity of ligand and complexes against the species *Escherichia coli*, *P. aeruginosa*, *Klebsiella pneumoniae*, *S. aureus*, *Bacillus subtilis*an, *Candida albicans*, *Candida tropicalis*, *Saccharomyces*, *Aspergillus fumigatus* and *Aspergillus terreus* has been carried out and compared using agar-diffusion method.

DFT calculations were done using B3LYP/6-31G(d) and B3LYP/LanL2DZ in order to calculate the vibrational properties, NBO charges, global chemical reactivity indices and to illustrate the frontier molecular orbitals FOM. The molecular docking studies were performed against different targets to study the molecular interactions and to predict the antibacterial, antifungal active sites

The acute toxicity study revealed that the manganese complex is not toxic at 2000 mg/kg dose orally administrated. LD50 for copper complex was determined using graphical method. No significant differences in the body weights between the control and the treated groups of both rat sexes in subacute toxicity study using for manganese complex. Hematological and clinical blood chemistry analysis revealed no toxicity effects of the manganese complex.

Keywords: Heterocyclic ligand, Complex, Characterization, Antimicrobial activity, Molecular docking, *in vivo* toxicity study.

Communications Affichées

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