

Synthesis, Characterization, Computational Study, Antimicrobial Evaluation, in Vivo Toxicity Study of Manganese (II) and Copper (II) Complexes with Derivative Sulfa-drug

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Abstract : The synthesis, characterization and comparative biological study of manganese (II) and copper (II) complexes with an heterocyclic ligand used in pharmaceutical field (Scheme 1), were reported. Two kinds of complexes were obtained with derivative sulfonamide, $[M(L)_2(H_2O)_2].H_2O$ and $[M(L)_2(Cl)_2]3H_2O$. These complexes have been prepared and characterized by elemental analysis, FAB mass, ESR magnetic measurements, FTIR, UV-Visible spectra and conductivity. Their stability constants have been determined by potentiometric methods in a water-ethanol (90:10 v/v) mixture at a 0.2 mol l⁻¹ ionic strength (NaCl) and at 25.0 ± 0.1 °C using Sirko program. DFT calculations were done using B3LYP/6-31G(d) and B3LYP/LanL2DZ. The antimicrobial activity of ligand and complexes against the species *Escherichia coli*, *P. aeruginosa*, *Klebsiella pneumoniae*, *S. aureus*, *Bacillus subtilisan*, *Candida albicans*, *Candida tropicalis*, *Saccharomyces*, *Aspergillus fumigatus* and *Aspergillus terreus* has been carried out and compared using agar-diffusion method. Also, the toxicity study was evaluated on synchesis complexes using Mice of NMRI strain.

Keywords : hetterocyclic ligand, complex, stability constant, antimicrobial activity, DFT, acute and genotoxicity study

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