Indole-derived water-soluble N, O bi-dentate ligand-based mononuclear transition metal complexes: *in silico* and *in vitro* biological screening, molecular docking and macromolecule interaction studies

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Abstract

A novel tryptophan-derived Schiff base ligand (potassium (E)-2-((4-chloro-3-nitrobenzylidene)amino)-3-(1H-indol-3-yl)propanoate) and a series of its transition metal complexes of the types [ML_2] and [$ML(1,10\text{-phen})_2$]Cl where M = Cu(II), Co(II), Ni(II) and Zn(II) were prepared. They were analyzed by various spectral and physicochemical studies. The XRD data were also used to determine the average lattice parameters and crystalline size of the compounds. All the synthesized compounds were tested against a series of five bacterial and fungal strains. The obtained results showed that the biological activity of free ligand was increased on complexation. PASS online software predicts the various biological activities of ligand such as enzyme inhibitor, antiviral, analgesic and antituberculosis. The *in silico* theoretical prediction of synthesized compounds is also deliberated by Swiss ADME predictor which gives the properties of molecular hydrophobicity (log P), topological polar surface area (TPSA) and oral bioavailability score. The binding energy of the docked molecule with macromolecules 1BNA and 3EQM is also determined by using Hex 8.0 software. The ligand has the least binding energy score which signifies that the potential of binding is greater in the receptor. Moreover, the interactions of complexes with DNA have been explored by electronic absorption titration, fluorescence emission titration, viscosity measurements and gel electrophoresis.