Spectroscopic, SOD, anticancer, antimicrobial, molecular docking and DNA binding properties of bioactive VO(IV), Cu(II), Zn(II), Co(II), Mn(II) and Ni(II) complexes obtained from 3-(2-hydroxy-3-methoxybenzylidene)pentane-2,4-dione

A Sakthivel [1], B Thangagiri [1], N Raman [2], J Joseph [3], Ramu Guda [4], Mamatha Kasula [4], L Mitu [5]

Affiliations + expand

PMID: 32794423 DOI: 10.1080/07391102.2020.1801508

Abstract

Novel macrocyclic Schiff base complexes [[ML]X; where M = Cu(II), Co(II), Ni(II), Zn(II), Mn(II) and VO(IV); L = macrocyclic ligand; X = Cl_2 and SO_4^{2-}] have been synthesized and characterized by microanalytical, ^1H, ^{13}C NMR, IR, Mass, UV-Vis, EPR spectral studies, as well as conductivity data. All the complexes exhibit square-planar geometry except vanadium complex. Magnetic susceptibility measurements and high conductance data reveal the monomeric and electrolytic nature of the complexes. Electronic absorption, cyclic voltammetry, viscosity measurements have been carried out on the interaction of the complexes with DNA. The results suggest that the complexes bind to DNA by intercalation *via* the aromatic ring of the macrocycle into the base pairs of DNA. Using gel electrophoresis experiment in the presence and absence of oxidant (H_2O_2) the nuclease cleavage activity of the complexes has been performed on plasmid DNA. The results demonstrate that most of the complexes have promising superoxide dismutase (SOD)-mimetic activity. The *in vitro* cytotoxicity of ligand and its complexes has also been evaluated against human breast and colon carcinoma cells. Binding interactions and energies of ligand and its metal complexes $[ML]^{2+}$ (M = VO(IV), Mn(II), Co(II), Ni(II), Cu(II), Zn(II)) against the receptors EGFR and HER2 are performed using the Auto dock module. Consequently, it is found that the ligand is strong inhibitor for EGFR and HER2 while [VOL]SO_4 is good inhibitor for EGFR and [ZnL]Cl_2 is moderate inhibitor for HER2. The antimicrobial activity of the ligand and its complexes against bacteria *Salmonella typhi*, *Staphylococcus aureus*, *Escherichia coli* and *Bacillus subtilis* and fungi *Aspergillus niger*, *Aspergillus flavus*, *Candida Albicans* and *Rhizoctonia bataicola*. The complexes have higher activities than the macrocyclic free Schiff base. Communicated by Ramaswamy H. Sarma.

Keywords: DNA cleavage; SOD; antimicrobial activities; intrinsic binding constant.