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Synthesis, Spectral Characterization and Computed Optical Analysis of Potent Triazole Based Compounds

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Abstract

Biologically active triazole Schiff base ligand (**L**) and metal complexes [Fe(II), Co(II), Ni(II), Cu(II) and Zn(II)] are reported herein. The ligand acted as tridentate and coordinated towards metallic ions via azomethine-N, triazolic-N moiety and deprotonated-O of phenyl substituents in an octahedral manner. These compounds were characterized by physical, spectral and analytical analysis. The synthesized ligand and metal complexes were screened for antibacterial pathogens against *Chromohalobacter salexigens*, *Chromohalobacter israelensi*, *Halomonas halofila and Halomonas salina*, antifungal bioassay against *Aspergillus niger* and *Aspergellus flavin*, antioxidant (DPPH, phosphomolybdate) and also for enzyme inhibition [butyrylcholinesterase (BChE) and acetylcholinesterase (AChE)] studies. The results of these activities indicated the ligand to possess potential activity which significantly increased upon chelation. Moreover, vibrational bands, frontier molecular orbitals (FMOs) and natural bond analysis (NBO) of ligand (**1**) were carried out through density functional theory (DFT) with B3lYP/6-311++G (d,p) approach. While, UV-Vis analysis was performed by time dependent TD-DFT with B3lYP/6-311++G (d,p) method. NBO analysis revealed that investigated compound (**L**) contains enormous molecular stability owing to hyper conjugative interactions. Theoretical spectroscopic findings showed good agreement to experimental spectroscopic data. Global reactivity descriptors were calculated using the energies of FMOs which indicated compound (**L**) might be bioactive. These parameters confirmed the charge transfer phenomenon and reasonable correspondence with experimental bioactivity results.

Keywords: Metals based triazole, Antimicrobial, Antioxidant, Enzyme Inhibition Studies, Frontier Molecular Orbital, Global Reactivity Descriptors.

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