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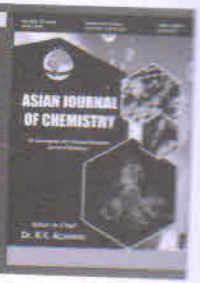

Cobalt(III), Nickel(II) and Copper(II) Complexes of Schiff Base Ligand 5-Methoxy-2-[(*E*)-{[2-(thiophen-2-yl)ethyl]imino}methyl]phenol: Synthesis, Characterization, Biological Applications and Docking Studies

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Schiff base ligand, 5-methoxy-2-[(*E*)-{[2-(thiophen-2-yl)ethyl]imino}methyl]phenol (LH) and its cobalt(III), nickel(II) and copper(II) metal complexes *viz.*, $Co(L)_3$, $Ni(L)_2$, $Cu(L)_2$ were synthesized and characterized. The structure of the ligand was established from the X-ray diffraction studies including other conventional techniques *viz.*, FT-IR, UV-visible, ^1H NMR, ^{13}C NMR and Mass studies. Complexes of the ligand LH were confirmed through FT-IR, UV-visible and CHN analysis. The ligand (LH) and its metal complexes were evaluated for their antimicrobial and antidiabetic potential, supported by a comprehensive computational molecular docking study. Docking simulations demonstrated strong and favourable binding interactions of the ligand and its complexes with major antimicrobial proteins, DNA gyrase and cytochrome P450 14α-sterol demethylase, as well as antidiabetic targets, α-amylase and α-glucosidase, thereby supporting the experimental findings. The antimicrobial activity was assessed using the agar well diffusion method against bacterial strains *Staphylococcus aureus* and *Escherichia coli*, and fungal strains *Aspergillus flavus* and *Pichia anomala*. Antidiabetic activity was evaluated through *in vitro* α-amylase and α-glucosidase inhibition assays. The results indicated that both the ligand and its metal complexes exhibited moderate to good antibacterial and antifungal activities. However, in antidiabetic studies, the $Cu(L)_2$ complex showed negligible inhibitory activity, while the remaining complexes displayed appreciable effects. Among all the tested compounds, the $Co(L)_3$ complex emerged as the most promising antidiabetic agent, exhibiting significant inhibition of both α-amylase and α-glucosidase enzymes. Overall, the experimental antimicrobial and antidiabetic outcomes showed strong agreement with the molecular docking results, underscoring the reliability of computational predictions in rationalizing the biological behaviour of the synthesized compounds.

Keywords: Schiff base ligand, Metal complexes, Antimicrobial, Antidiabetic activity, Computational molecular docking.