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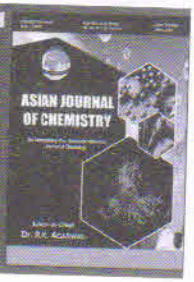

Synthesis, Characterisation and *in silico* Evaluation of Imidazole-Based Schiff Base Transition Metal(II) Complexes with Antioxidant and Antidiabetic Potential

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In this work, few transition metal(II) complexes of Cu^{2+}, Co^{2+}, Ni^{2+} and Zn^{2+} were synthesised with imidazole-based Schiff base ligand, (*E*)-*N*-(4-chlorobenzo[*d*]thiazol-2-yl)-1-(1*H*-indole-3-yl)methanimine. These complexes were characterised by mass, NMR and FT-IR spectroscopies. The NMR and FT-IR spectral data confirmed coordination of the azomethine nitrogen and sulphur atoms with the metal centers. The physico-chemical properties, drug-likeness parameters and pharmacokinetic behaviour of the imidazole-based Schiff base ligand and its metal(II) complexes were predicted using the SwissADME web server. Bioactivity prediction and PASS analysis further validated the favourable drug-like characteristics of both the free ligand and its metal(II) complexes. Molecular docking studies were carried out using AutoDock Vina against selected biological targets, including an antioxidant enzyme (PDB ID: 1HD2), ferritin (PDB ID: 1FHA) and α-amylase (PDB ID: 2QV4). The docking results demonstrated strong binding affinities and significant intermolecular interactions with the active sites of the target proteins, thereby supporting the multifunctional therapeutic potential of the synthesized metal complexes. Notably, the compounds exhibited pronounced antioxidant and antidiabetic activities, underscoring their promise as effective bioactive agents. Overall, these findings suggest that the synthesized Schiff base metal(II) complexes represent promising candidates for further development as multifunctional therapeutic agents.

Keywords: Schiff base ligand, Pharmacokinetics, Bioactivity, Antioxidant activity, Antidiabetic activity, Drug-likeness evaluation.