

## Synthesis, Characterization, Biological Activity and DFT Studies of Cyclic Benzaldehyde Derivative Schiff Base Ligands and its Cu(II) and Zn(II) Metal Complexes

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### Structured Abstract

**Background:** Schiff base compounds are the topic of significant study due to their pharmacological activity and tendency to form complexes with almost all transition metals. Primary amines condense with carbonyl compounds to form Schiff bases. This study synthesised three Schiff base ligands: 2-hydroxybenzaldehyde (L1), 3-hydroxybenzaldehyde (L2), and 5-bromo-2-hydroxybenzaldehyde (L3) with o-phenylenediamine. Two metal complexes, namely Cu(II) and Zn(II) were synthesized and tested for their antibacterial activity.

**Methods:** Three Schiff base ligands were synthesized by mixing o-phenylenediamine in ethanol solvent and refluxed for 3 hours. The metal complexes were synthesized by mixing ligands with copper and zinc chlorides. The metal complexes were synthesized under reflux for 4 hours. All Schiff base ligand and metal complexes were characterised by melting point, elemental analysis, FTIR, UV-Vis, and <sup>1</sup>H NMR. DFT approaches were used to determine determined HUMO-LUMO gap of the ligands. The ligands and metal complexes were tested in vitro against Gram-positive and Gram-negative bacteria, *S. mutans*, MRSA 43300, and TDB35.

**Results:** Infrared spectral measurements showed that ligand and metal complexes' C=N bond at wavelength 1582 to 1618 cm<sup>-1</sup>. In UV-Vis spectra, ligands and metal complexes exhibit  $\pi \rightarrow \pi^*$  transitions at 207-295 nm and  $n \rightarrow \pi^*$  transitions at 281-394 nm. The ligands and metal complexes had hydrogen protons of CH=N bond at 708-956 ppm in <sup>1</sup>H NMR. The melting point of Schiff base ligands was lower than that of metal complexes. The HOMO-LUMO energy gap determined the stability order of the ligands, and DFT showed that L2 at 0.14197 eV was more stable than L3 and L1 at 0.13664 eV. The inhibition zones of the ligand and its metal complexes show that most complexes are more effective against bacteria than the free ligand. ZnL1(H<sub>2</sub>O) inhibited *S. mutans* zones the most, while ZnL2(H<sub>2</sub>O) inhibited MRSA 43300 zones the most. The synthesised Schiff base ligands and metal complexes did not inhibit Gram-negative bacteria TDB35.

**Conclusion:** This study synthesized and characterized all Schiff base ligands and metal complexes by elemental analysis, FTIR, UV-Vis, and <sup>1</sup>H NMR. Compounds with metal have better antibacterial action than free ligand.

**Keywords:** Schiff base, UV-Vis, <sup>1</sup>H NMR, DFT, antibacterial activity

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