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Synthesis and Antibacterial Studies of New Benzimidazole Schiff Base Ligands and its Cu(II) and Zn(II) Complexes

Ameer Haqeem Mohd Nasharuddin[a], Karimah Kassim[ab*]

Structured Abstract

Background: Benzimidazole is a heterocyclic aromatic organic compound with the chemical formula $C_7H_6N_2$. It is one of the most promising moieties with a variety of biological functions and is present in many clinically beneficial medications. Research has explored the potential uses of benzimidazole-based compounds in various therapeutic areas due to the fact that the benzimidazole structure meets the fundamental design criteria in pharmaceutical chemistry. This study utilized newly synthesized benzimidazole Schiff base ligands and their Cu(II) and Zn(II) complexes to investigate their antibacterial properties and potential applications as antibacterial agents on *Staphylococcus aureus* as Gram-positive and *Escherichia coli* as Gram-negative bacteria.

Methods: The ligands L1 and L2 were synthesized through condensation reactions between 2-(aminomethyl) benzimidazole with 2,4-dihydroxybenzaldehyde and 3-hydroxybenzaldehyde, respectively, while the complexes were formed by reacting ligands with metal acetates in a 2:1 molar ratio under reflux. The synthesized compounds were characterized using CHNS elemental analysis, melting point detection, FT-IR spectroscopy, ^{1}H NMR spectroscopy, and Density Functional Theory (DFT) analysis. Antibacterial activity was evaluated using the disc diffusion method against *Staphylococcus aureus* (Gram-positive) and *Escherichia coli* (Gram-negative).

Results: Two synthesized ligands and four metal complexes were obtained with satisfactory yields. CHNS analysis confirmed the compositions matched theoretical values. FT-IR spectra showed shifts in azomethine (C=N) bands, confirming nitrogen coordination to the metal centers. ^{1}H NMR spectroscopy verified the structures of the ligands. Antibacterial studies showed that the Cu(II) and Zn(II) complexes exhibited significantly better antibacterial activity than the ligands, demonstrating their potential as effective antimicrobial agents. The DFT analysis showed that L1 had a higher energy gap (4.91 eV) compared to L2 (4.907 eV), indicating higher chemical stability and lower reactivity.

Conclusion: In conclusion, this study successfully synthesized and characterized new benzimidazole Schiff base ligands and their Cu(II) and Zn(II) complexes. The findings highlight the enhanced antibacterial properties of metal complexes, suggesting their potential as candidates for developing new antimicrobial agents.

Keywords: Benzimidazole, 2-(aminomethyl) benzimidazole, Characterized, Density Functional Theory (DFT), Antibacterial Activity.

*Correspondence: karimah@uitm.edu.my

[a] School of Chemistry & Environment, Faculty of Applied Sciences, Universiti Teknologi MARA, Shah Alam, Malaysia

[b] Centre of Chemistry Synthesis and Polymer Technology, Institute of Science (IOS), Universiti Teknologi MARA, Shah Alam, Malaysia