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Topic of Research: Synthesis, Spectral Characterization, DFT calculations and Antibacterial activities of Schiff's Base Complexes of Transition Metals

Findings

The Ph.D. thesis titled **"Synthesis, Spectral Characterization, DFT Calculations, and Antibacterial Activities of Schiff's Base Complexes of Transition Metals"** delves into the synthesis, characterization, computational analysis, and antibacterial assessment of novel Schiff base ligands and their transition metal complexes. A series of these novel ligands were synthesized through the condensation of 2-amino-4-chlorophenol with p-dimethylaminobenzaldehyde, o-vanillin, and 3,5-di-tert-butyl-2-hydroxybenzaldehyde, followed by complexation with Co(II), Ni(II), Cu(II), and Zn(II) ions. The synthesized compounds were characterized using various analytical and spectroscopic techniques, including FTIR, NMR, UV-vis, ESI/MS, XRD, and elemental and thermal analysis. DFT calculations were conducted to explore the electronic structure, stability, and molecular properties of the compounds. Molecular docking simulations were performed to examine the binding interactions between the compounds and target bacterial proteins. The antibacterial activities of the compounds were tested against various bacterial strains. This study underscores the potential of these Schiff base metal complexes as antimicrobial agents and offers insights into their structure-activity relationships and potential pharmaceutical applications. The thesis is comprised of six chapters. The first chapter provides a literature review of various Schiff base ligands derived from 2-amino-4-chlorophenol, o-vanillin, 4-dimethylaminobenzaldehyde, and 3,5-di-tert-butyl-2-hydroxybenzaldehyde, along with their metal complexes, which exhibit promising antimicrobial, anti-inflammatory, and anticancer properties. The second chapter presents a comprehensive examination of the experimental methodologies employed in the synthesis and characterization of the Schiff base ligand and its transition metal complexes, as well as computational methodologies, such as density functional theory (DFT) calculations,

molecular dynamics (MD) simulations, and molecular docking analyses. The remaining four chapters detail the synthesis, characterization, and biological evaluation of novel Schiff base transition metal complexes, along with computational studies to gain insights into their electronic structure, stability, and potential mode of action.