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Design, Structural Analysis, Computational Modelling and Antibacterial Assessment of Schiff Base Metal Complexes

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ABSTRACT: The Schiff base ligand 2-(((5-aminonaphthalen-1-yl)imino)methyl)-4-chlorophenol(2ANIM4C) and its metal complexes with Co(II), Cu(II) and Zn(II) ions were successfully synthesized. Schiff base metal complexes are known for their significant roles in biomedical applications. The synthesized ligand and its metal complexes were characterized through both physical methods and various spectroscopic techniques, including ultraviolet-visible (UV-Vis) spectroscopy, Fourier-transform infrared (FTIR) spectroscopy and nuclear magnetic resonance (NMR) spectroscopy. Additionally, three-dimensional molecular modelling was employed to propose the structural configuration of the 2ANIM4C ligand. The ligand and its metal complexes were evaluated for their pharmacological activities, particularly antibacterial and antifungal properties, using the disc diffusion assay. The results indicate that both the free ligand and its metal complexes exhibit promising bioactivity, highlighting their potential for development as therapeutic agents.

KEYWORDS: Schiff base, Ligand, Metal complexes, Spectroscopy, Antibacterial activity

I. INTRODUCTION

The formation of Schiff bases, first described by Hugo Schiff in 1864, involves a condensation reaction between a primary amine and a carbonyl compound—typically an aldehyde or ketone—resulting in the formation of an imine (-HC=N) functional group[1]. Due to their ease of synthesis, structural versatility, and ability to coordinate metal ions, Schiff bases have become crucial ligands in coordination chemistry[2]. Depending on the nature of the carbonyl and amine precursors, these compounds can function as mono-, bi-, or tridentate ligands, enabling the formation of stable complexes with transition metals such as cobalt, copper, and zinc[3].

The coordination of Schiff bases with metal ions significantly influences their physicochemical and biological properties. Metal complexes derived from Schiff bases often exhibit enhanced biological activities compared to the free ligands, attributed to the synergistic interaction between the ligand framework and the metal centre[4]. These complexes have shown promising potential in a wide range of biomedical applications, including their use as antibacterial, antifungal, and anti-parasitic agents[5].

Moreover, Schiff base metal complexes have been extensively investigated as model systems for studying enzyme-substrate interactions and metal ion transport in biological systems[6]. Some have been employed in therapeutic and diagnostic applications such as radiopharmaceuticals, artificial oxygen carriers, and biosensors due to their unique electronic and structural properties[7]. In addition to their biomedical relevance, they also serve as efficient catalysts in various organic reactions[8].

In the present study, a novel Schiff base ligand was synthesized through the condensation of 5aminonaphthalene-1-amine with 4-chlorosalicylaldehyde. The resulting ligand was further complexed with Co(II), Cu(II), and Zn(II) ions. The ligand and its metal complexes were characterized using various spectroscopic techniques. Their antibacterial activity was evaluated against selected bacterial strains to assess their potential as therapeutic agents.





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II. METHODOLOGY

2.1 Reagents used

The reagents used in the synthesis were 1,5-diaminonaphthalene, 5-chlorosalicylaldehyde, and metal salts such as zinc chloride (ZnCl₂), copper(II) chloride (CuCl₂·2H₂O), and cobalt(II) chloride (CoCl₂·6H₂O), all procured from Precision Company. Ethanol was used as the solvent, and calcium chloride (CaCl₂) served as the desiccant for storing the final products.

2.2Synthesis of Schiff Base Ligand

The Schiff base ligand, 2-(((5-amino naphthalen-1-yl)imino)methyl)-4-chlorophenol, was synthesized via a condensation reaction between 1,5-diaminonaphthalene and 5-chlorosalicylaldehyde in an equimolar ratio (1:1)[9]. Specifically, 0.39 g (0.1 mol) of 1,5-diaminonaphthalene was dissolved in 25 mL of ethanol, and separately, 0.39 g (0.1 mol) of 5-chlorosalicylaldehyde was also dissolved in 25 mL of ethanol. Both solutions were mixed in a 100 mL round-bottom flask, and the total volume was adjusted to 50 mL using ethanol as the solvent. The reaction mixture was stirred continuously and heated gently on a water bath or hotplate for approximately 3 hours to facilitate the condensation process. During this time, the formation of the imine (Schiff base) linkage occurred with the elimination of water. After heating, the resulting mixture was allowed to stand undisturbed in a beaker at room temperature for one week, allowing the ethanol to slowly evaporatecompletely. Upon solvent evaporation, an orange-red solid precipitate of the Schiff base ligand was obtained. The solid product was carefully collected, washed with cold ethanol to remove any unreacted starting materials or impurities, and dried thoroughly at room temperature or under vacuum. The final product was then weighed and stored in a desiccator for further use and characterization. The reaction mechanism for the formation of the Schiff Base Ligand are shown in the Figure - 1



Fig. 1Reaction mechanism for the formation of the Schiff Base Ligand

2.3Synthesis of Schiff base metal complex

The metal complexes of the Schiff base ligand 2-(((5-aminonaphthalen-1-yl)imino)methyl)-4-chlorophenol (2ANIM4C) were synthesized by reacting the ligand with metal(II) chloride salts in a 1:2 molar ratio (metal salt : ligand)[10]. For this purpose, metal chlorides such as $ZnCl_2$, $CuCl_2$, and $CoCl_2$ (0.1 mM in 25 mL ethanol) were each mixed with 0.2 mM of the Schiff base ligand dissolved in 25 mL ethanol. The resulting solution (total volume 50 mL) was subjected to reflux with constant stirring on a water bath for 2 hours to ensure complete complexation. After refluxing, the solution was allowed to cool naturally to room temperature. The resulting solid precipitates of the metal complexes were formed and then filtered, washed thoroughly with cold ethanol to remove any unreacted ligands or impurities, and dried at room temperature. Theyield of each [M(2ANIM4C)₂] complex (where M = Zn(II), Cu(II), or Co(II)) was recorded. All the synthesized metal complexes were found to be coloured, stable, and were stored in a desiccator over anhydrous calcium chloride (CaCl₂) to prevent moisture absorption. The synthesized Schiff base metal complex are displayed in Figure – 2





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M = Co, Cu, Zn

Fig. 2 Schiff base metal complex

III. EXPERIMENTAL RESULTS

3.1 FTIR Analysis

FTIR (Fourier Transform Infrared) spectroscopy was employed to investigate the interactions between the Schiff base ligand and its metal complexes by monitoring the shifts in vibrational frequencies[11]. This technique helps in identifying the functional groups involved in coordination and provides valuable insights into the bonding between the ligand and metal ions. The FTIR spectra of both the Schiff base ligand and the Schiff base metal complexes exhibit distinct differences, reflecting the changes in molecular structure upon complexation. The resulting spectra were analyzed to observe any shifts or changes in the characteristic absorption bands of the ligand, which indicate the coordination of metal ions. The following figure shows the FTIR graphs for both the Schiff base ligand and its corresponding metal complexes, highlighting these spectral variations.



Fig. 3 Schiff base ligand FT-IR result





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3.2 UV Analysis

The UV-Vis absorption spectra of the Schiff base ligand and its metal complexes (Cu²⁺, Zn²⁺, Co²⁺) reveal significant shifts in absorption bands, indicating the coordination of the ligand with metal ions. The ligand exhibits absorption bands at 263, 315 and 357 nm, corresponding to $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ transitions[12, 13, 14]. Upon complexation, the metal complexes show shifts in their absorption bands, with copper, zinc and cobalt complexes exhibiting bands at 239-318 nm, 222-365 nm and 221-361 nm, respectively. These shifts confirm the interaction between the Schiff base ligand and metal ions, which alters the electronic structure of the ligand, thereby modifying its UV-Vis absorption properties.



Fig. 5UV-VIS graph of Schiff base Ligand (2ANIM4C)





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Fig. 6 UV-VIS graph of Schiff base Copper Ligand [Cu (2ANIM4C)]



Fig. 7UV-VIS graph of of Schiff base Zinc Ligand [Zn (2ANIM4C)]





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Fig. 8 UV-VIS graph of Cobalt base Ligand [Co (2ANIM4C)]

3.3 Antibacterial Activity

The antibacterial and antifungal activities of the synthesized Schiff base ligand and its metal complexes with Cu(II), Zn(II), and Co(II) ions were evaluated using the agar diffusion method[15]. The antimicrobial performance was tested against two Gram-negative bacteria (Escherichia coli, Pseudomonas aeruginosa), one Gram-positive bacterium (Staphylococcus aureus), and two fungal strains (Aspergillus niger, Aspergillus flavus). Sterile discs impregnated with the test samples were placed on the inoculated agar plates and incubated at 37 °C for 24 hours. The zones of inhibition, measured in millimeters, indicated the compounds' effectiveness in suppressing microbial growth.

The Schiff base ligand exhibited moderate to good antibacterial activity, especially against E. coli and S. aureus, with inhibition zones measuring 22 mm and 20 mm, respectively. Upon metal complexation, the antimicrobial activity generally improved. Among the metal complexes, the Cu(II) complex demonstrated the highest antibacterial activity, showing inhibition zones of 23 mm against E. coli and 21 mm against S. aureus. The Zn(II) and Co(II) complexes also showed significant activity, though slightly lower than the Cu(II) complex.

In contrast, the antifungal activity was relatively weaker. The Schiff base ligand showed moderate inhibition against Aspergillus niger and Aspergillus flavus with zones of 17 mm and 16 mm, respectively. However, the metal complexes, especially the Zn(II) complex, exhibited minimal to no antifungal effect. The Cu(II) and Co(II) complexes showed some activity against the fungal strains, with inhibition zones ranging from 10 mm to 12 mm.Overall, the Schiff base ligand and its metal complexes, particularly those with Cu(II) and Co(II), demonstrated promising antibacterial properties, suggesting their potential as antimicrobial agents. However, their antifungal efficacy appears limited, warranting further structural modifications for broader antimicrobial applications.





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Fig. 9Zone of inhibition for Schiff base ligand and its Cu(II), Zn(II), and Co(II) metal complexes against selected bacterial strains

IV. CONCLUSION

In the present study, an efficient synthetic route was employed for the preparation of the Schiff base ligand, 2-(((5-aminonaphthalen-1-yl)imino)methyl)-4-chlorophenol. Its corresponding metal complexes with Co(II), Cu(II), and Zn(II) ions were successfully synthesized and thoroughly characterized using various analytical techniques. Based on the spectral and analytical data, the metal complexes are proposed to adopt a distorted square planar or tetrahedral geometry, depending on the nature of the central metal ion. The biological evaluation revealed that the metal complexes exhibited significantly enhanced antibacterial activity compared to the free Schiff base ligand. This increase in activity may be attributed to the coordination of the ligand with metal ions, which likely enhances the complexes' ability to interact with microbial cells. Overall, the results indicate that these Schiff base metal complexes have promising potential as antimicrobial agents.

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