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SYNTHESIS, SPECTRAL CHARACTERIZATION AND ENHANCED ANTIBACTERIAL ACTIVITY OF CO (II) AND CU (II) SCHIFF BASE COMPLEXES: A MOLECULAR DOCKING APPROACH

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ABSTRACT

The novel Schiff base ligand(L) (Z)-4-1-((3-methylpyridine-2-yl) imino) ethyl) Phenol was synthesised using 2-amino-3-picoline with p-hydroxy acetophenone. The corresponding coordination metal complexes were made using the synthesized ligands. Further, the synthesized ligands and the metal complexes (L-Co(II), L-Cu(II))were examined using several analytical techniques like FT-IR, 1H-NMR, UV-Vis spectroscopy, thermogravimetric analysis (TGA), elemental analysis, molar conductivity, mass spectrometry, and magnetic susceptibility measurements. The structural and electronic properties of the ligands and their complexes were completely analysed, and the geometries of the metal chelate were clarified using magnetic and spectroscopic data. The metal complexes formed exhibited distinct characteristics that indicated their potential value in applications requiring coordinated metal-ligand frameworks. In addition, Molecular docking studies have been conducted to see how well the metal complexes bind to proteins like DNA gyrase and riboflavin biosynthesis. The study shows that the cobalt complex attaches to DNA gyrase with a score of -7.13 kcal/mol whereas the copper complex binds to riboflavin enzyme more effectively with a score of -8.59 kcal/mol. These results are promising for using metal complexes to fight microorganisms. This work also helps to develop bioactive coordination compounds and supports Sustainable Development Goal 3, which is about having good health and well-being, by looking for effective antimicrobial agents that can help people have good health and well-being. The metal complexes are important for this goal because they can be used to make medicines that are effective against microorganisms.

Keywords: Schiff Base; Magnetic Susceptibility; Spectroscopic Data, Biological Activity; Molecular Docking.
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INTRODUCTION

Schiff bases, known for their ability to form stable coordination complexes with diverse metal ions[1]They have long been a cornerstone of coordination chemistry.[2] These compounds are synthesized through the condensation of alkyl amines with aldehydes/ketones, offering versatility in both structure and functionality.[3] The resulting ligands exhibit unique electronic and steric properties, making them valuable in applications such as catalysis, material science, medicinal chemistry, and enzyme mimetics.[4] Schiff base complexes are used in many different medical applications. Since Rosenburg created cisplatin as an anticancer drug in 1965, the use of metal complexes in cancer treatment has undergone significant modification. However, cisplatin's limited range of action, adverse side effects, and toxicity restricted its use. The researchers were motivated to investigate alternative metal complexes with better properties by the limitations of cisplatin. Because of its uses in bioinorganic systems, the coordination chemistry of Schiff base complexes[5] containing oxygen and nitrogen donors has also caught the attention of biochemists.[6] It has been widely recognised that many biological processes rely on heterocyclic compounds such as the purine and pyrimidine bases found in both DNA and RNA. Among them, five-membered N-heterocycle compounds, notably triazoles ($C_2H_3N_3$) and their derivatives, as well as tetrazole (CH_2N_4), are attracting a significant interest.[7] Triazoles exist in two distinct types, namely, 1,2,3-triazoles and 1,2,4-triazoles. Their three nitrogen heteroatoms, grouped in five-membered ring configurations, set them apart. Derivatives of 1,2,4-triazole are considered an important class of compounds with antimicrobial, antibacterial, anticancer, anti-inflammatory, and antiviral properties,

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which possess a wide range of biological, agricultural, industrial, and environmental applications. It has been observed that the growth of the field of study of heterocyclic compounds and their derivatives, which are extensively distributed in nature and utilized in a range of sectors, such as paint, medicine, and cosmetics, has recently increased interest in these molecules.[8] In general, Schiff base ligands obtained from aromatic precursors possess improved stability and reactivity due to their conjugated systems and donor atoms.[9] Despite extensive studies on Schiff base complexes, limited reports exist on the combined spectroscopic, biological, and molecular docking evaluation of ONO donor ligands derived from p-hydroxy acetophenone and 2-amino-3-picoline, highlighting a significant gap in the literature. Therefore, the present study aims to synthesize, characterize, and evaluate ligand using p-hydroxy acetophenone and 2-amino-3-picolin. The precursors were chosen because of their complementing steric and electronic characteristics: 2-amino-3-picoline provides a nitrogen donor site, which improves the ligand's coordination ability, while p-hydroxy acetophenone contributes electron-donating hydroxyl groups. FT-IR, NMR, UV-Vis spectroscopy[10] Complexes were characterized using various analytical techniques, including FT-IR, NMR, and UV-Vis spectroscopy.[11] and thermogravimetric analysis were among the analytical and spectroscopic methods used to thoroughly characterize the resulting L and its L-Co(II) and L-Cu(II) complexes. To learn more about the complexes' physicochemical characteristics, their geometry, electronic structure, and coordination behavior were examined.[12] In order to investigate these complexes' potential as antibacterial agents, their biological activity was also assessed. It is well recognized that L-metal ion coordination improves biological efficacy by changing the steric and electronic environment, which facilitates improved contact with microbial targets. By improving our knowledge of their coordination behaviour and investigating their useful uses in materials science and medicine, this work perfectly correlates with Sustainable Development Goal (SDG-3: Good Health and Well-being) by exploring metal complexes with potential antibacterial applications.

EXPERIMENTAL

Material and Methods

In the current study, all chemicals and solvents was analytical grade, and they didn't require any further purification. Metal salts were purchased from standard suppliers.

Synthesis of Para-Hydroxy Acetophenone + 2-amino 3-picoline Schiff Base Ligand

A solution of 4-hydroxyacetophenone (1.36 g, 0.01 moles) was produced in 50 mL of methanol, as was a separate solution of 2-amino-3-picoline (5 mL, 0.01 moles). A magnetic stirrer was used to completely mix these two solutions in a 250 mL RB flask. For an hour, the mixture was refluxed in a water bath. The solvent evaporated, leaving behind a brown solid substance. Filtration was used to gather the solid, which was then cleaned three times with hot water and methanol, vacuum-dried, and recrystallized from methanol. The compound has a melting point of 90–92°C and a 67% yield.

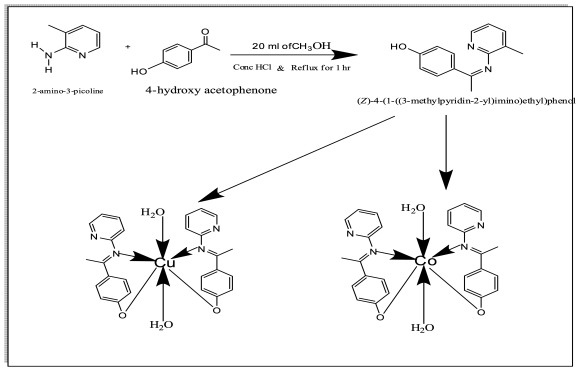
Synthesis of the L-Co (II) and L-Cu (II) Complexes

A 250 mL flask with a circular bottom was constructed and cleaned completely. 50 mL of 50% methanol was used to dissolve 1.361 g (0.01 moles) of ligand before it was added to the flask. The necessary quantities of copper and cobalt sulfate salts (0.01 moles each) dissolved independently in 25 mL of water, were then added to the combination. 5 mL of 0.2 M sodium acetate (NaOAc) solution were added to the solution after it had refluxed for thirty minutes. After that, refluxing was maintained for two more hours. Light blue and pale-yellow metal complexes were formed as a result of gradual evaporation at room temperature. After filtering, these complexes underwent a thorough methanol and hot water wash before being dried in a vacuum desiccator. The schematic representation of the preparation of the Schiff base is given in Scheme-1.

General Procedure

The elemental composition of the synthesized ligand (L) and its metal complexes was determined using Elemental analysis. The experimental values were compared with the theoretically calculated values to confirm the purity and composition of the synthesized compounds. The analytical data for carbon, hydrogen, nitrogen, and metal content are summarized in Table-1. Upon complexation with cobalt and

copper, the elemental composition of the resulting metal complexes, CoL_2X_2 and CuL_2X_2, showed values consistent with the expected molecular formulas.



Scheme-1: Schematic Representation of L and its L-Co (II) and L-Cu (II) Complexes

The slight deviations observed between the calculated and experimental values may be attributed to experimental errors or instrumental limitations. However, the overall agreement between the theoretical and found values confirms the successful formation of the L and its L-Co(II) and L-Cu(II) complexes.

Table-1: Elemental Analysis Data for L and L-Co(II), L-Cu(II) Complexes

Molecular formula	Carbon%		Hydrogen%		Nitrogen%		Metal%	
	Calc.	Found	Calc.	Found	Calc.	Found	Calc.	Found
$L=C_{14}H_{14}N_2O$	74.33	73.84	6.19	6.76	12.38	13.12	-	-
CoL_2X_2	61.43	60.49	5.85	6.05	10.23	9.87	10.75	10.45
$[CuL_2]2X$	60.91	61.25	5.85	5.58	10.15	10.75	11.51	11.79

Detection Method

A Fison EA 1108 analyser was used to do elemental analysis. A Gallen Kamp hot stage melting point equipment was used to determine the melting points. A Perkin Elmer 598 Spectrophotometer was used to record the FTIR spectra, which covered the frequency range of 4000–400 cm^{-1}. Using an AV-400 MHz spectrometer and DMSO-D_6 and $CDCl_3$ solvents, the 1H NMR studies were carried out in ambient circumstances. At RT and LNT, ESR spectra of the metal complexes were acquired on a Bruker ESP 300E spectrometer. A Thermo Spectronic Heylos Spectrophotometer was used to measure the compound's UV spectra. Using DMSO as the solvent, UV spectral analysis was conducted. The VSM-155 vibrating sample magnetometer for applied research operates at field strengths between 0.3 and 0.8T. The saturated moment of 99.9 % ultra-pure nickel is used to calibrate the VSM. A Seiko device was used to create the TG and DTA curves.

Analytical Discussion

Table-2: Physical & Analytical Data for L and Metal Complexes

Molecular formula	$C_{14}H_{14}N_2O$(L)	CoL_2X_2	(Cu. L_2)2X
Molecular weight in grams	226	546.90	551.55
Color	Brown	Light Blue	Pale Yellow
Yield (%)	67	71	74
Melting point (^oC)	90-92	315-317	267-271

RESULTS AND DISCUSSION

IR Studies

The infrared (IR) spectra of the L and its L-Co(II) and L-Cu(II) complexes were compared to identify the coordination sites and bonding interactions within the complexes. The significant IR spectral frequencies and their corresponding assignments are summarised in Table-3. A well-known band at 1633 cm^{-1} in the spectrum of the L was attributed to the ν(C=N) stretching vibration of the imine group. Upon complexation, this band shifted to 1615 cm^{-1} and 1608 cm^{-1} for L-Co (II) and L-Cu (II) complexes,

respectively. This shift to lower wavenumbers confirms the presence of imine coordination with the metal ions.[13], likely due to reduced electron density in the C=NC=NC=N group upon metal binding. The ν(OH) stretching and bending vibrations of the phenolic group appeared at 3420 cm^{-1} and 1352 cm^{-1} in the L spectrum[14] and the complex's spectra remain unchanged[1]. This implies that the coordination mechanism was not facilitated by the phenolic OH group. New bands observed at 470–419 cm^{-1} and 530–562 cm^{-1} in the spectra of the L-Co and L-Cu Complexes were designated to ν(M−N) and ν(M−O) stretching frequencies.[15]

It supports the presence of metal-nitrogen and metal-oxygen bonds. A band in the L spectra at 1405–1410 cm^{-1} was identified as ν(C=C) stretching vibrations, and ν(C=N) stretching in the pyridine ring as another band at 1590 cm^{-1}. The pyridine nitrogen atom's participation in coordination with the metal ions was demonstrated by the complexes' shift in the pyridine C=NC=NC=N stretching vibration to 1582 cm^{-1}. Both the L and the complexes showed a faint band at about 2910 cm^{-1}, which was attributed to ν(C−H) stretching frequencies. Furthermore, the complexes' spectra showed large bands at 3210 cm^{-1} and 3225 cm^{-1}, which were ascribed to the coordinated water molecules' ν(OH) stretching vibrations.[16] The spectral analysis supports the proposed coordination mode of the L with cobalt (II) and copper (II) ions through the azomethine nitrogen and pyridine nitrogen atoms.[14] The suggested structures of the complexes are illustrated in Scheme-1.

Table-3: FT-IR Analysis of L and its Metal Complexes

Compound	OH(Water)	OH(Phenolic)	C=N	M-O	M-N
L	---	3420	1633	---	---
L-Co	3210	3420	1615	530	470
L-Cu	3225	3420	1608	562	419

NMR Studies

The 1H NMR spectra of the L and its L-Co (II) and L-Cu (II) complexes were analysed to confirm the structure and coordination behaviour. The obtained data are summarised in Table-4. In the 1H NMR spectrum of the ligand, a singlet at 2.51 ppm[17] was assigned to the methyl protons attached to the azomethine (C=NC=NC=N) group, while another singlet at 2.06 ppm[18] corresponded to the methyl protons of the picoline moiety. A multiplet found in the region 6.83–8.33 ppm was attributed to the aromatic protons of the pyridine and phenyl ring. A prominent singlet at 13.71 ppm was assigned to the hydroxyl proton attached to the phenyl ring. In the 1H NMR spectrum of the L-Co(II) complex, the signal due to the methyl protons attached to the azomethine group shifted downfield to 2.62 ppm, indicating the de-shielding effect caused by the bond through the nitrogen atom[19] of the imine group.[20] The methyl protons of the picoline moiety showed a slight shift from 2.06 ppm. From 2.05 ppm in the ligand to 2.05 ppm in the cobalt complex.

The hydroxyl group did not take part in coordination, as evidenced by the slight change in the phenolic hydroxyl proton signal, which was detected in the ligand at 13.71 ppm, to 13.80 ppm. The influence of variations in electron density on complex formation was reflected in the minor shift of the multiplet attributed to aromatic protons to 6.93–8.23 ppm. A coordinated water molecule was also detected in the cobalt complex by a new singlet at 3.37 ppm.

The de-shielding effect caused by coordination through the azomethine nitrogen was confirmed by the shift of the signal for the methyl protons linked to the azomethine group to 2.60 ppm in the 1H NMR spectrum of the copper (II) complex.[21] The ligand's hydroxyl proton signal, which was measured at 13.71 ppm, slightly changed to 13.79 ppm, further indicating that the phenolic group is not involved in coordination. The transfer of ring electrons toward the metal ion is probably what caused the aromatic proton multiplet to change to 6.81–8.28 ppm. In the copper complex, the methyl protons of the picoline moiety showed a change from 2.06 ppm in the ligand to 2.01 ppm.[10]

A new singlet at 3.25 ppm in the copper complex spectrum confirmed the presence of a coordinated water molecule. The observed shifts and new signals in the 1H NMR spectra confirm the coordination of the ligand to L-Co(II) and L-Cu(II) ions through the azomethine nitrogen and the involvement of coordinated water molecules, while the phenolic OH group remained non-coordinated.

Table-4: NMR-Spectral Data for L and their Metal Complexes

Compound	H_3C-C=N	Ar-H	CH_3	Ar-OH
L	2.51	6.83-8.33	2.06	13.71
L-Co	2.62	6.93-8.23	2.05	13.80
L-Cu	2.60	6.81-8.23	2.01	13.79

UV Studies

The electronic absorption spectra of the ligand and its L-Co and L-Cu complexes were recorded and compared with the spectra of the corresponding aqueous $Co^{2+}$and Cu^{2+} ions. The spectral data are presented in Table-5. The shift is attributed to a minor covalent interaction between the vacant 3D orbitals of the metal ions and the ligand orbitals, resulting in partial delocalisation and a consequent reduction in interelectronic repulsion.[22] Additionally, increased nuclear shielding due to electron drift from the ligand to the metal contributes to the observed changes. For the free ligand, a band at 304 nm corresponds to ligand-centred electronic transitions. Upon coordination, new charge transfer bands appear at 320 nm for the L-Co (II) complex and 337 nm for the L-Cu (II) complex, indicating ligand-to-metal charge transfer. Additional bands in the region 372–327 nm for the metal complexes further confirm charge transfer transitions.[23] Based on these spectral observations, a tetrahedral geometry is proposed for the cobalt (II) and copper (II) complexes.[13] The electronic transitions provide strong evidence for the coordination behaviour and the structural arrangement of the complexes.[24,25]

Table-5: UV- Spectral Data for Metal Complexes

Compound	λmax of metal ions in nm	λmax of complex in nm	λmax of L
L-Co	319	320	304
L-Cu	336	337	304

Thermogravimetric Studies

The cobalt complex exhibited thermal stability up to 200°C**,** while the copper complex was stable up to 154°C. In the first stage, the loss of two coordinated water molecules occurred between 200 and 357°C for the L-Co complex, and 154–295°C for the copper complex, indicating an endothermic dehydration process. The second stage corresponded to the exothermic decomposition of the ligand moiety, occurring within the range 460–525°C for cobalt and 406–535°C for copper complexes. Above 525°C and 535°C, the final solid residues were identified as cobalt oxide (CoO) and copper oxide (CuO)**,** respectively.[9] These findings confirm the thermal stability and decomposition pathways of the complexes. The attained data are given in Table-6.

Table-6: TG-DTA -Spectral Data for Metal Complexes

S. No.	Complex X=H_2O	Molecular weight in grams	Weight of the complex taken in mgs	Stage	Temperature range during weight loss in ^oC	Probable assignment
1	(CoL_2X_2)	546.90	7.40	1 2 3	200-357 400-525 Above 525	Loss of $2H_2O$ Loss of 2L molecules Remaining residue corresponding to CoO
2	(CuL_2X_2)	551.55	7.40	1 2 3	154-295 406-535 Above 535	Loss of $2H_2O$ Loss of 2L molecules Remaining residue corresponding to CuO

VSM (Vibrational Spin Magnetometer)

The magnetic susceptibility measurements using a Vibrating Sample Magnetometer (VSM) provided insights into the geometry and magnetic behavior of the metal complexes. The cobalt complex exhibited magnetic moment values in the range of 4.6–6.3 B.M, indicative of a high-spin octahedral geometry**.** Potential magnetic exchange interactions between cobalt centres are suggested by the observed

discrepancies. Magnetic moment values for the copper complex varied from 2.5 to 3.7 B.M., which is in line with the idea that Cu (II) complexes contain a single unpaired electron. The data support an octahedral geometry for the coordination environment by confirming the copper complex's monomeric nature and the lack of metal-metal interactions.[26]

Conductivity Studies

The non-electrolytic character of the complexes was shown by conductometric tests conducted at 27 ± 2°C in DMF (~10^{-3} M). For the cobalt complex, the molar conductance was 20 Ω^{-1} cm² mol^{-1}, while for the copper complex, it was 22 Ω^{-1} cm^2 mol^{-1}. The lack of ionic dissociation is confirmed by these low conductance values, which imply that the complexes are neutral in solution.

ESR Studies

The Schiff base ligand's copper and cobalt complexes' electrical surroundings, shape, and bonding properties can all be better understood by analysing their Electron Spin Resonance (ESR) spectra. The ESR spectra for the Cu (II) complex 49 were captured in DMF at ambient temperature and at liquid nitrogen temperature (LNT). With different values for the parallel (g‖g_\parallel‖) and perpendicular (g⊥g\perpg⊥) components, the spectra showed anisotropic behaviour. The pattern g‖>g⊥>2.0023g_\parallel > g_\perp > 2.0023g‖>g⊥>2.0023 was followed by the observed g-values, suggesting that the unpaired electron is located in the dx^2-y^2 orbital of the Cu (II) ion.[27] This demonstrates that a deformed octahedral geometry is present, which is explained by the Jahn-Teller distortion frequently seen in Cu (II) complexes. Furthermore, the G-value greater than 4 suggests the absence of significant metal-metal interactions, indicating that the complex exists in a mononuclear form in the DMF medium. The ESR data also highlight the covalent nature of the Cu-N and Cu-O bonds within the complex. The low g‖g_\parallel‖ value and the orbital reduction parameter (K) support strong ligand-metal interactions and partial covalency.[28] In the case of the Co (II) complex, the spectrum confirms a high-spin octahedral geometry around the cobalt centre. Although cobalt ESR spectra are generally less resolved due to the d^7 configuration, the observed anisotropy suggests the unpaired electrons are localised in the t_2g orbitals, consistent with a covalent metal-ligand bonding framework. Overall, the ESR results for both complexes confirm their structural integrity, electronic configurations, and mononuclear nature, with strong L-metal covalent interactions and distorted coordination geometries in the Cu (II) complex.

Biological Applications

The antibacterial activity of the synthesized Schiff base ligand and its L-Co(II) and L-Cu(II) complexes was evaluated using the disc diffusion method against *Escherichia coli* and *Bacillus subtilis.*[3] To evaluate the broad-spectrum effectiveness of the produced compounds, these strains were chosen as representative models of Gram-positive and Gram-negative bacteria, respectively.[29] The compounds were tested at different concentrations, and the zones of inhibition were measured after 24 h of incubation. When compared to the free ligand, the metal complexes showed noticeably stronger antibacterial activity. The results show that, in comparison to the ligand, the metal complexes have significantly higher antibacterial activity.[13] Among the complexes, the Co (II) and Cu (II) complexes showed enhanced inhibition against both bacterial strains. This increase in activity upon complexation can be due to the chelation effect, which decreases the polarity of the metal ion by partially sharing its positive charge with the ligand's donor atoms. This increases the lipophilicity of the complexes, allowing them to pass through the lipid membranes. of microorganisms and thereby improving their biological efficacy.[30] Furthermore, the results demonstrate that the complexes are more effective against *Escherichia coli* compared to *Bacillus subtilis*, indicating selective antibacterial behaviour. The observed trend suggests that metal coordination plays a crucial role in modulating the biological properties of Schiff base ligands. All experiments were done in triplicate, and the average data were used for analysis.

Molecular Docking Analysis

A computational method called molecular docking helps with drug discovery and design by predicting interactions between small molecules (ligands) and target proteins.[31] In order to assess the binding processes and efficiency of DNA gyrase and riboflavin biosynthesis enzymes, this work focuses on

docking interactions with different ligands and metal complexes. A type II topoisomerase necessary for transcription and DNA replication is DNA gyrase (PDB: 1KZN). Developing antibacterial medicines requires an understanding of possible inhibitors' binding to DNA gyrase. Using the software AutoDock 1.5.7, the study examines binding interactions that are typified by hydrophobic interactions, van der Waals forces, and hydrogen bonds. Since copper (Cu) can improve binding efficiency by creating coordination bonds and changing the electrical environment of the active site, the impact of metal complexes like Cu and Co on these interactions is being investigated. At the same time, Co's coordination geometry may alter binding stability. The study also investigates the riboflavin biosynthesis enzyme (PDB: 3EX8), which is essential for the metabolism of riboflavin (vitamin B2).[32] Interactions between ligands and this enzyme can disclose inhibitory mechanisms important for the development of antimicrobials. L-Co complexes may cause conformational changes that impact the binding mode, whereas L-Cu complexes may boost binding affinity through coordination stability. All things considered, molecular docking helps with the logical design of new medicinal treatments by shedding light on L-protein interactions and the function of metal complexes. The drug development pipeline can be enhanced by combining docking with experimental validation, which will help find new molecules with better pharmacological characteristics. The molecular docking analysis was performed to study the interaction between the L and L- (Co and Cu) complexes. The target proteins, DNA gyrase subunit B (1KZN) and riboflavin biosynthesis enzyme (3EX8), obtained from the protein data bank, were isolated from the source of *E. coli* and *Bacillus subtilis,* respectively. Figures-13 to 15 illustrates the formation of interactions between the DNA gyrase B (1KZN) with L, Cu-complex and Co-complex, respectively. As can be seen from Fig.-13, the L molecule forms two hydrogen bonds between the GLU58 and GLN135 by the bond distances of 2.07 Aº and 1.95 Aº, respectively. Hydrophobic interactions or alkyl interactions between the L molecule and enzyme are MET166 and LYS162, with a total docking score of -4.78 Kcal/mol, were noticed.

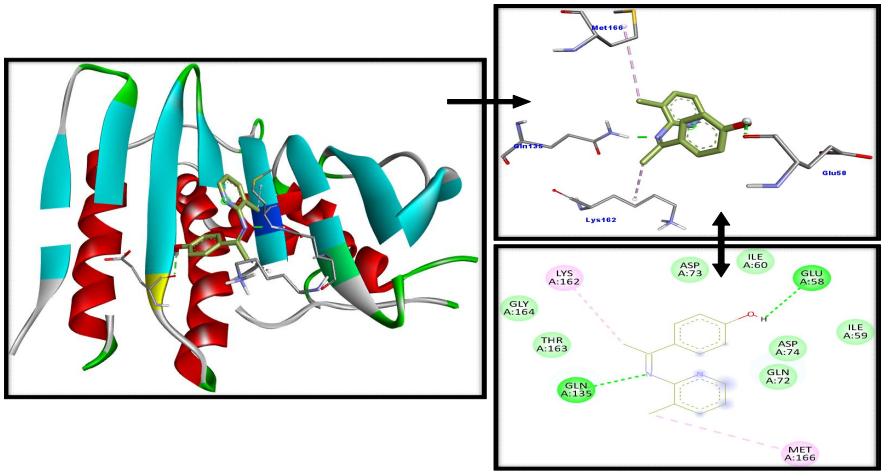


Fig.-1: Study of Molecular Docking Interactions between L with DNA Gyrase B (1KZN)

Figure-2 demonstrates the docking interaction between the DNA gyrase B (1KZN) and the L-Cu complex with the total average binding energy of -6.45 Kcal/mol. The complex molecule interacts with HIS116 in the form of two hydrogen bonds at distances of 2.16 Aº and 1.98 Aº. Furthermore, ILE27 and HIS38 interact with metal complexes through the alkyl interactions.

Figure-3 illustrates the various interactions among the amino acids of protein with the L-Co complex, one hydrogen bond between the oxygen of the complex with the hydrogen of the LYS212 at a distance of 2.82 Aº. Some other hydrophobic interactions were found, such as GLU181, ASP210, ARG209, and GLU185; the total average binding energy of the system of -7.13 Kcal/mol was noticed. The attained results confirmed that the molecular docking interactions are more in the L-Co complex with DNA gyrase B (1KZN) than in L-Cu and L. Similarly, Figures-4 to 6 illustrates the molecular docking interactions between Riboflavin biosynthesis protein rib D (3EX8) with L, Cu and Co complexes.

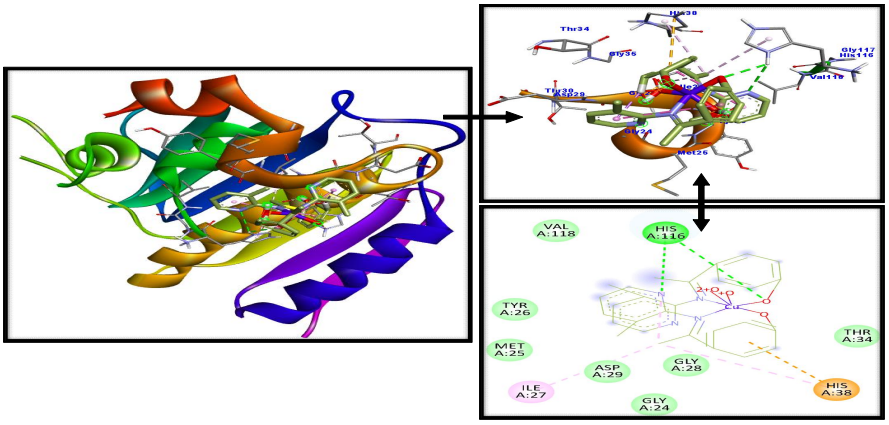


Fig.-2: Study of Molecular Docking Interactions Between the L-Cu Complex with DNA Gyrase B (1KZN)

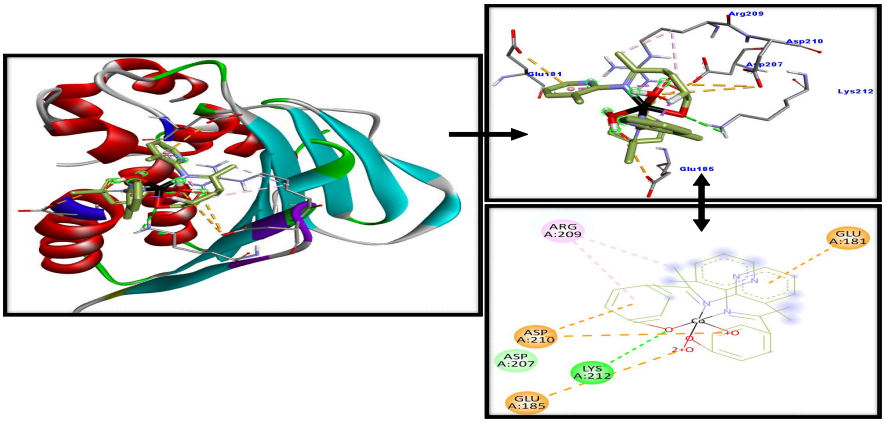


Fig.-3: Study of Molecular Docking Interactions Between L-Co Complex with DNA Gyrase B (1KZN)

Figure-4 demonstrates the interactions between the L with the 3EX8 protein; three hydrogen bonds, such as ARG176, GLU290, and SER167, were observed by the bond distances of 2.001 Aº, 1.817 Aº, and 2.982 Aº, respectively.

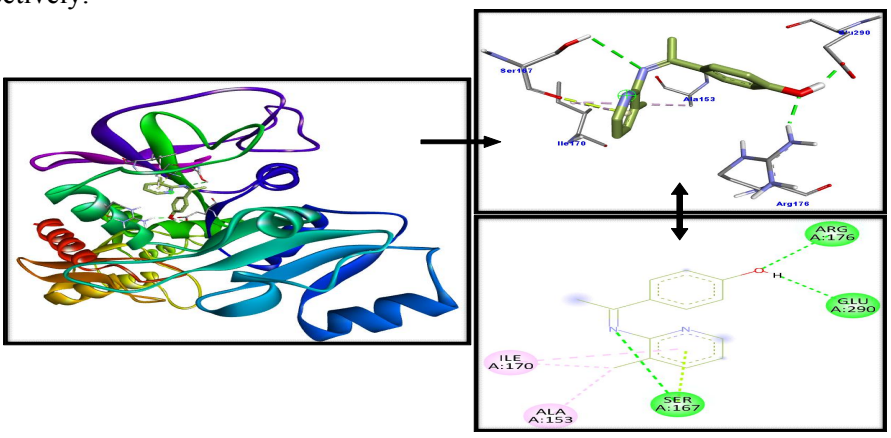


Fig.-4: Study of Molecular Docking Interactions Between L with Riboflavin Biosynthesis Protein Rib D (3EX8)

Hydrophobic interactions such as ILE170 and ALA153 are formed between the amino acids of 3EX8, and the total docking score for the system was -5.5 Kcal/mol. Figure-5 demonstrates the interactions of 3EX8 with the L-Cu complex; the ligand formed two hydrogen bonds with the HIS139 of 3EX8 by the bond distances of 2.73 Aº and 2.45 Aº. Three hydrophobic interactions, namely GLU135, ARG142, and LYS357, were noticed in the system.

The average binding energy of the complex with 3EX8 was found to be -8.59 Kcal/mol. The complex of L-Co (Fig.-6) interacts with the 3EX8 protein and forms only hydrophobic interactions, such as HIS76,

HIS49, AVL106, PRO24, and CYS74, with an average binding energy of -5.59 Kcal/mol.[34] From the attained results, the L-Cu complex showed more binding interactions with the 3EX8 protein than the L and L-Co complexes. Moreover, the molecular docking study consists of experimental results that L-Co has more interactions with 1KZN (E. coli, zone of inhibition of 125 mm) than L-Cu (85 mm). Similarly, L-Cu showed more interactions with 3EX8 (B. subtilis, zone of inhibition of 165 mm) than L-Co (120 mm).

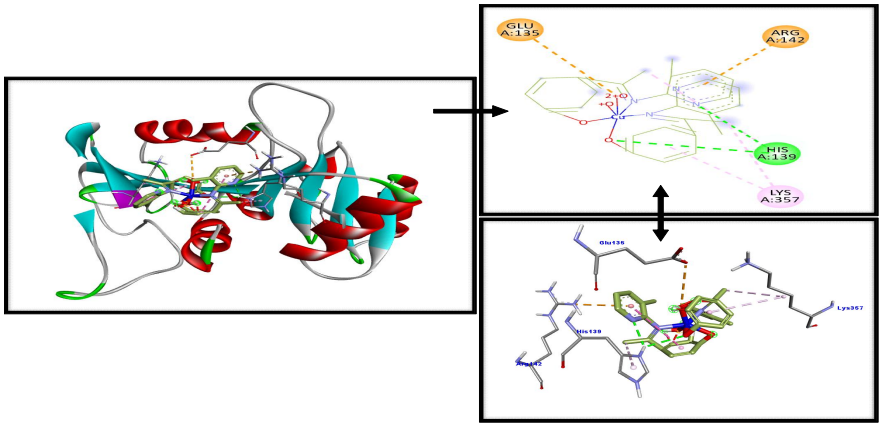


Fig.-5: Study of Molecular Docking Interactions between L-Cu Complex with Riboflavin Biosynthesis Protein Rib D (3EX8)

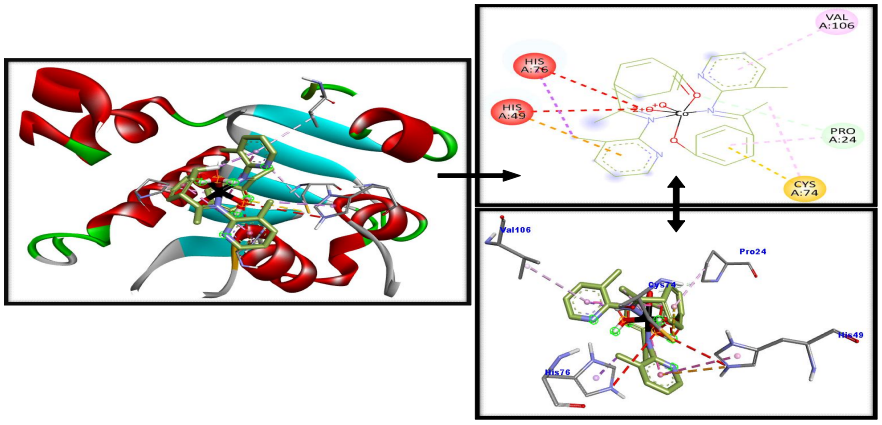


Fig.-6: Study of Molecular Docking Interactions between L-Co Complex with Riboflavin Biosynthesis Protein Rib D (3EX8)

CONCLUSION

The synthesis and comprehensive characterisation of the novel Schiff base L and its L-Co and L-Cu complexes reveal their potential as multifunctional materials. Structural and spectroscopic analyses confirm stable coordination through azomethine and pyridine nitrogen atoms, while thermal and magnetic studies highlight their unique properties. The enhanced antibacterial activity of the metal complexes compared to the free ligand underscores the significance of metal-ligand interactions in biological efficacy. The findings provide valuable insights into the coordination chemistry of Schiff bases and pave the way for their application in antibacterial agents and other advanced materials. Future studies will focus on exploring their catalytic and environmental applications to further expand their utility. Molecular Docking was performed to determine the ligand and metal complexes with protein molecules from the attained results cobalt complex shows the highest docking score among the copper complex when interacting with *E. coli* -7.13kcal/mol. Similarly, the copper complex showed the highest docking score when interacting with *B.substillus* -8.59kcal/mol. This study contributes to Sustainable Development Goal 3 by advancing the development of Schiff base metal complexes with potential anticancer activity, thereby supporting the discovery of more effective and targeted therapeutic agents.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

The present work is related to *SDG-3: Good Health and Well-being*. All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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REFERENCES

1. C. Jayabalakrishnan and K. Natarajan, *Synthetic and Reactive Inorganic and Metal-Organic Chemistry*, **31**, 983 (2001), https://doi.org/10.1081/SIM-100105255.
2. H. Kargar, M. Fallah-Mehrjardi and K. S. Munawar, *Coordination Chemistry Reviews*, **501**, 215587 (2024), https://doi.org/10.1016/j.ccr.2023.215587.
3. N. R. Gosu, C. H. Yadav, K. R. Reddy, V. Losetty, R. R. Kothinti and S. Sampath, *Polyhedron*, **255**, 116954(2024), https://doi.org/10.1016/j.poly.2024.116954.
4. A. I. Osman, A. Ayati, P. Krivoshapkin, B. Tanhaei, M. Farghali, P.-S. Yap and A. Abdelhaleem, *Coordination Chemistry Reviews*, **514**, 215900 (2024), https://doi.org/10.1016/j.ccr.2024.215900.
5. M. Mir and B. Banik, *Inorganic Chemistry Communications*, **174**, 113987(2025), https://doi.org/10.1016/j.inoche.2025.113987
6. F. M. Elantabli, S. M. El-Medani, A. Al-Anazi, M. R. Shehata, M. Haukka and R. G. Mohamed, *Journal of Molecular Structure*, **1330**,141511(2025), https://doi.org/10.1016/j.molstruc.2025.141511
7. M. A. Mir and B. K. Banik, *Inorganic Chemistry Communications*, **174**, 113987(2025), https://doi.org/10.1016/j.inoche.2025.113987
8. S. İpekbayrak, Y. K. Karabulut, Z. Ş. Turhan, E. S. Yigittekin and E. Yildiz, *Journal of Molecular Structure*, **1334**, 141758 (2025), https://doi.org/10.1016/j.molstruc.2025.141758
9. C. J. Dhanaraj and M. Jebapriya, *Journal of Molecular Structure*, **1220**, 128596(2020), https://doi.org/10.1016/j.molstruc.2020.128596
10. Z. Çetin and B. Dede, *Journal of Molecular Liquids*, **380**, 121636(2023), https://doi.org/10.1016/j.molliq.2023.121636
11. C. H. Yadav and A. Mallibabu, *Journal of Medicinal Chemistry Sciences*, **5**, 1018(2022), https://doi.org/10.26655/JMCHEMSCI.2022.6.15
12. G. N. Reddy, V. Losetty and C. H. Yadav, *Journal of Molecular Structure*, **1282**, 135161(2023), https://doi.org/10.1016/j.molstruc.2023.135161
13. *Al-Zahraa Journal for Health and Medical Sciences*, https://zjhms.alzahraa.edu.iq/, (accessed April 25, 2026).
14. T. Saritha and P. Metilda, *Journal of Saudi Chemical Society*, **25**, 101245(2021), https://doi.org/10.1016/j.jscs.2021.101245
15. U. P. S. Prabhakar, G. Periyasami and P. Karthikeyan, *Inorganic Chemistry Communications*, **159**, 111796(2024), https://doi.org/10.1016/j.inoche.2023.111796

16. V. Losetty, C. H. Yadav, K. Aswini, C. B. Kumar and K. Sivakumar, *Journal of Molecular Structure*, **1254**, 132393 (2022), https://doi.org/10.1016/j.molstruc.2022.132393
17. A. R. M. Sikkander, M. Meena, H. Yadav, N. Wahi and V. V. Lakshmi, *Journal of Applied Organometallic Chemistry*, **4**, 145(2024), https://doi.org/10.48309/jaoc.2024.433120.1154
18. C. H. Yadav and A. M. Babu, *Research Journal of Pharmacy and Technology*, **14**, 5175(2021), https://doi.org/10.52711/0974-360X.2021.00900
19. S. M. E. Khalil, H. S. Seleem, B. A. El-Shetary and M. Shebl, *Journal of Coordination Chemistry*, **55**, 883(2002), https://doi.org/10.1080/0095897022000002213
20. P. Middya, R. M. Gomila, A. Frontera and S. Chattopadhyay, *Polyhedron*, **267**, 117362(2025), https://doi.org/10.1016/j.poly.2024.117362
21. M. Nagoor Meeran, C. H. Yadav and A. Z. Hussain, *International Journal of Applied Pharmaceutics*, **14**, 163(2022), https://doi.org/10.22159/ijap.2022.v14ti.47
22. H. S. Awes, A. L. El-Ansary, S. A. Abdel-Latif, S. Abdel-Khalik and S. M. Abbas, *Journal of Molecular Structure*, **1325**, 140993(2025), https://doi.org/10.1016/j.molstruc.2024.140993
23. Anuradha, S. Kumari and D. D. Pathak, *Tetrahedron Letters*, **56**, 4135(2015), https://doi.org/10.1016/j.tetlet.2015.05.049
24. A. O. Sarıoğlu, B. Türkmenoğlu, D. T. Kahraman, S. Güler, B. Sürmelihindi and M. H. Morcali, *Journal of Molecular Structure*, **1325**,140907(2025), https://doi.org/10.1016/j.molstruc.2024.140907
25. T. Alorini, I. Daoud, A. N. Al-Hakimi and F. S. Alminderej, *Journal of Molecular Structure*, **1276**, 134785 (2023), https://doi.org/10.1016/j.molstruc.2022.134785
26. V. Losetty, M. Dhanalakshmi, S. Devanesan, M. S. AlSalhi, P. Prabu, C. H. Yadav, U. Chalapathi and S.-H. Park, *Inorganic Chemistry Communications*, **170**, 113338(2024), https://doi.org/10.1016/j.inoche.2024.113338
27. N. Sarkar, P. K. Bhaumik and S. Chattopadhyay, *Polyhedron*, **115**, 37(2016), https://doi.org/10.1016/j.poly.2016.04.013
28. A. R. M. Sikkander, H. Yadav and M. Meena, *Advanced Journal of Chemistry Section A*, **7**, 501 (2024), https://doi.org/10.48309/ajca.2024.443156.1490
29. D. I. Tofiq, H. Q. Hassan and K. A. Abdalkarim, *Arabian Journal of Chemistry*, **14**, 103429 (2021), https://doi.org/10.1016/j.arabjc.2021.103429
30. M. Dhanalakshmi and V. Losetty, *Journal of Water Process Engineering*, **70**, 106933(2025), https://doi.org/10.1016/j.jwpe.2025.106933
31. V. Losetty, S. Devanesan, M. S. AlSalhi, P. P. Velu, D. Muthupillai, K. A. Kumar and S. K. Lakkaboyana, *Environmental Science and Pollution Research*, **31**, 55562(2024), https://doi.org/10.1007/s11356-024-34872-9
32. S. A. Elseginy and M. M. Anwar, *ACS Omega*, **7**, 1150(2022), https://doi.org/10.1021/acsomega.1c05732

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