Research Article

Synthesis, Spectroscopic Characterization and Biological Activities of Transition Metal Complexes Derived from a Tridentate Schiff Base

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A new series of Cu (II), Ni (II), Co (II) and Zn (II) complexes have been synthesized from the Schiff base derived from 4-hydroxy-3-methoxybenzylidene-4-aminoantipyrine and 2-aminophenol. The structural features have been determined from their elemental analysis, magnetic susceptibility, molar conductance, Mass, IR, UV-Vis, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$ and ESR spectral studies. The redox behavior of the copper complex has been studied by cyclic voltammetry. The data confirm that the complexes have composition of ML_2 type. The electronic absorption spectral data of the complexes propose an octahedral geometry around the central metal ion. All the metal complexes with DNA structure were guided by the presence of inter-molecular C-H $\cdots$ O and C-H $\cdots$ N hydrogen bonds. The biological activity of the synthesized compounds were tested against the bacterial species such as *Bacillus subtilis*, *Staphylococcus aureus*, *Proteus vulgaris* and fungal species such as *Candida albicans* by the well-diffusion method.

1. Introduction

Schiff bases are regarded as “privileged ligands” due to their ability to form complexes with a wide range of transition metal ions yielding stable and strongly colored metal complexes. Some of them have been shown to reveal attractive physical, chemical properties and potential biological activities [1, 2]. In azomethine derivatives, the C=N linkage is essential for biological activity; several azomethines were reported to possess important antibacterial [3–5], antifungal [6, 7], anticancer [8], and diuretic activities [9]. With the rising occurrence of deep mycosis, there has been increasing emphasis on the screening of new and more effective antimicrobial drugs with low toxicity. Schiff bases and their complexes were recently established to have significant antitumor and biological activity [10, 11]. In recent years, a great deal of interest in the transition metal complexes of 4-aminoantipyrine and its derivatives have been extensively examined due to their diverse biological properties as antifungal, antibacterial [12], analgesic, sedative, antipyretic, anti-inflammatory [13], anticonvulsant agents [14] and greater DNA binding ability [15]. This

prompted us to synthesize a novel series of heterocyclic Schiff bases containing the antipyrinyl moiety. The present study reports the synthesis, characterization, and antimicrobial studies of transition metal complexes containing tridentate Schiff base derived from 4-hydroxy-3-methoxybenzylidene-4-aminoantipyrine and 2-aminophenol. The structure of the complexes is elucidated using elemental analyses, magnetic moment, Mass, IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, ESR and molar conductance. The biological activity of the Schiff base and their metal complexes is reported.

2. Experimental

2.1. Materials and Methods. 4-Aminoantipyrine, 4-hydroxy-3-methoxybenzaldehyde and 2-aminophenol were obtained from Sigma. Metal chlorides were purchased from Merck. All chemicals used were of AR grade. Solvents were purified and distilled before use. Molar conductivity was determined using Systronic Conductivity Bridge with a dip type cell using freshly prepared 10^{-3} M solutions in DMSO at RT. The IR spectra were recorded in KBr pellet on a Perkin-Elmer

SCHEME 1: Schematic route for the synthesis of Schiff base ligand (HL).

783 spectrometer in the range $4000\text{--}400\text{ cm}^{-1}$. UV-Visible spectra of the complexes were recorded on Perkin Elmer Lambda EZ201 spectrophotometer in DMSO solution. ^1H -NMR spectra was recorded on a JEOL FX-90X instrument using CDCl_3 as a solvent and TMS as an internal standard. The RT magnetic measurements were carried out using Guoy balance and the diamagnetic corrections were made using Pascal's constant.

2.2. Synthesis of Schiff base Ligand (HL). 4-hydroxy-3-methoxybenzylidene-4-aminoantipyrine was prepared by the condensation of 4-hydroxy-3-methoxybenzaldehyde and 4-aminoantipyrine as reported earlier [16]. 4-hydroxy-3-methoxybenzylidene-4-aminoantipyrine (2 mmol) and 2-aminophenol (2 mmol) were taken in ethanol (50 mL) solvent. To this mixture, 1 g of anhydrous potassium carbonate was added and then refluxed for 10 hrs. The resulting solution was concentrated on a water bath and allowed to cool at 0°C for $\sim 24\text{ h}$. The solid product formed was separated by filtration and washed thoroughly with EtOH and then dried *in vacuum*. (Yield: 64%) (Scheme 1).

2.3. Synthesis of Metal (II) Complexes. A solution of metal (II) chloride (2 mmol) in ethanol (25 mL) was stirred with an ethanolic solution (50 mL) of the Schiff base (4 mmol). The above mixture was magnetically stirred for 2 h. Then the solution was reduced to one-third on a water bath. The solid

complex precipitated was filtered off and washed thoroughly with ethanol and dried *in vacuo*.

2.4. In Silico Studies on DNA and Metal Complexes. On the basis of literature evidences [17, 18], we have selected the DNA sequence and it was subjected into DNA sequence to structure web server [19] for generating the three-dimensional structure of DNA based on experimental fiber-diffraction studies [20]. The structure of metal complexes was drawn using ChemDraw Ultra10.0 program [21] and three-dimensional structure of metal complexes was prepared by using Discovery studio 3.1 [22]. The DNA-metal complex interaction was studied using Patch dock web server [23]. The PyMol stand-alone program [24] was used to visualize the interaction between DNA Structure and metal complexes. HBAT [25], hydrogen bond analysis tool was used to analyze the strong and weak hydrogen bonds present between DNA and metal complexes. In this in-house developed program, the standard hydrogen bond distance ($\text{H}\cdots\text{A}$) and angle ($\text{X-H}\cdots\text{A}$) was set as $2.8\text{ \AA}$ and 90° , respectively.

2.5. Biological Activity. The biological activities of synthesized Schiff Base and its Cu (II), Co (II), Ni (II) and Zn (II) complexes have been studied for their antibacterial and antifungal activities by *well diffusion* test using Mueller-Hinton Agar (MHA) and Sabouraud Dextrose Agar (SDA). The antibacterial and antifungal activities were done at $60\text{ }\mu\text{g/mL}$ concentrations in DMF solvent using bacteria (*S. aureus*, *B. subtilis*, and *P. vulgaris*) and fungi (*C. albicans*) at the minimum inhibitory concentration (MIC) method. These bacterial strains were incubated for 24 h at 37°C and fungi strains were incubated for 48 h at 37°C . Standard antibacterial (tetracycline) and antifungal drug (amphotericin) was used for comparison under similar conditions. Activity was determined by measuring the diameter of the zone showing complete inhibition (mm).

3. Results and Discussion

3.1. Characterization of Schiff Base Ligand. The analytical data for the ligand and their complexes together with some physical properties are summarized in Table 1. The magnetic susceptibilities of the complexes at room temperature are consistent with octahedral geometry around the central metal ion. The low conductance of the complexes supports the non-electrolytic nature of the metal complexes.

3.2. Mass Spectra. Mass spectra provide an essential clue for elucidating the structure of compounds. The ESI mass spectra of the ligand and its copper complex were recorded and used to compare their stoichiometry composition. The Schiff base displays the prominent molecular ion peak (M^+) at $m/z = 428$ and weak isotopic peak at $(\text{M}^+ + 1)\text{ } m/z = 429$ (Figure 1). The base peak appears at $m/z = 200$ corresponding to $[\text{C}_{11}\text{H}_{12}\text{N}_4]^+$. The other fragments give the peaks at 136, 93 and 77. The mass spectrum of copper complex shows the molecular ion peak at $m/z = 923$ due to $(\text{CuC}_{50}\text{H}_{46}\text{N}_8\text{O}_6)^+$ (Figure 2). The complex underwent demetallation to form

TABLE 1: Physical and analytical data of the synthesized Schiff base and its complexes.

Compound	Empirical formula	Yield (%)	Colour	Found (Calcd) (%)				Formula weight	(λM) Ohm ⁻¹ cm ² mol ⁻¹ × 10 ⁻³	μ _{eff} (B.M.)
				M	C	H	N			
HL	C ₂₅ H ₂₄ N ₄ O ₃	64	Brown	—	69.97 (70.08)	5.21 (5.64)	12.95 (13.07)	428.4	—	—
CuL ₂	CuC ₅₀ H ₄₆ N ₈ O ₆	58	Dark Brown	6.76 (6.88)	64.89 (65.02)	5.14 (5.02)	12.02 (12.13)	923.1	2.6	1.88
NiL ₂	NiC ₅₀ H ₄₆ N ₈ O ₆	56	Brown	6.07 (6.45)	65.42 (65.70)	4.87 (5.07)	12.12 (12.26)	913.5	1.6	2.97
CoL ₂	CoC ₅₀ H ₄₆ N ₈ O ₆	62	Red	6.14 (6.42)	65.35 (65.72)	4.75 (5.07)	12.05 (12.26)	913.3	1.9	4.38
ZnL ₂	ZnC ₅₀ H ₄₆ N ₈ O ₆	56	Yellow	7.10 (7.22)	65.20 (65.42)	4.99 (4.85)	12.17 (12.31)	920.2	1.8	Diamagnetic

FIGURE 1: Mass spectrum of Schiff Base Ligand (HL).

FIGURE 2: Mass spectrum of the CuL₂ complex.

SCHEME 2: M = Cu (II), Ni (II), Co (II) and Zn (II).

the original molecular weight of the Schiff base ligand, gave fragment ion peak at $m/z = 428$.

3.3. IR Spectra. The IR spectra of ligand shows a broad band for the $-OH$ group at $3450-3050\text{ cm}^{-1}$. The absence of this peak in all the spectra of the complexes shows the deprotonation of the $-OH$ group upon complexation. The spectrum of ligand shows the characteristic $-C=N$ bands in the region $1570-1510\text{ cm}^{-1}$, which are shifted to lower frequencies in the spectra of all the complexes ($1560-1490\text{ cm}^{-1}$) representing the involvement of azomethine nitrogen in coordination to the metal ion [26–28]. Accordingly, the ligand acts as a tridentate chelating agent bonded to the metal ion via the two nitrogens ($-C=N$) and one phenolic oxygen atom (2-aminophenol) of the Schiff base. Assignment of the proposed coordination sites is further supported by the appearance of medium bands at $510-500$ and $570-550\text{ cm}^{-1}$, which could be attributed to $\nu(M-N)$ and $\nu(M-O)$ respectively [29].

The proposed structure of the Schiff base complexes is shown in Scheme 2.

3.4. 1H -NMR and ^{13}C -NMR Spectra. The 1H NMR spectrum of ligand (HL) in $CDCl_3$ provides the following signals: phenyl as multiplet at $6.91-7.49\text{ ppm}$, $=C-CH_3$ at 2.46 ppm ,

FIGURE 3: ^1H -NMR spectrum of Schiff Base Ligand (HL). FIGURE 4: ^1H -NMR spectrum of ZnL_2 .

$-\text{N}-\text{CH}_3$ at 3.11 ppm, $\text{OH}-$ group in benzaldehyde moiety at 6.35 ppm and $\text{C}-\text{CH}=\text{N}-$ protons at 9.66 ppm. The peak at 10.52 ppm is attributable to the phenolic $-\text{OH}$ group present in the 2-aminophenol (Figure 3). The absence of this peak noted for the zinc complex proves the loss of the $-\text{OH}$ proton due to complexation. The azomethine proton signal in the spectrum of the zinc complex is moved downfield compared to the free ligand, suggesting deshielding of the $>\text{C}=\text{N}$ group due to coordination with metal ion (Figure 4).

In the ^{13}C -NMR spectrum (Figure 5), the azomethine carbon signal has appeared at 161 ppm. The pyrazolone ring carbon attached methyl carbon ($-\text{CH}_3$) and pyrazolone ring nitrogen attached methyl carbon ($>\text{N}-\text{CH}_3$) peaks have been observed in the expected range at 10.2 and 35.9 ppm. In addition, the methoxy methyl carbon ($-\text{O}-\text{CH}_3$) appears at 55.9 ppm. The aromatic carbon signals are seen at 108–157 ppm range depending on their electronic environment.

3.5. Electronic Spectra. The electronic spectra can often give quick and dependable information about the ligand and arrangements in the transition metal complexes. The UV-Vis spectrum of the copper complex shows three bands, which are assigned as an intraligand charge-transfer band (25090 cm^{-1}), ligand-to-metal charge-transfer band (23980 cm^{-1}) and a $d-d$ band (15120 cm^{-1}) which is due to $^2E_g \rightarrow ^2T_{2g}$ transition. This $d-d$ band strongly favors an octahedral geometry around the metal ion. It is further supported by the magnetic susceptibility value ($1.88\text{ }\mu\text{B}$). The nickel complex reveals three $d-d$ bands at 13305, 15299, and 23520 cm^{-1} which are assigned as $^3A_{2g} \rightarrow ^3T_{2g} (F)$, $^3A_{2g}$

FIGURE 5: ^{13}C -NMR spectrum of Schiff Base Ligand (HL). FIGURE 6: The cyclic voltammetry of the CuL_2 complex.

$(F) \rightarrow ^3T_{1g} (F)$ and $^3A_{2g} (F) \rightarrow ^3T_{1g} (P)$ transitions, respectively, being characteristic of an octahedral geometry supported by its magnetic susceptibility value ($2.97\text{ }\mu\text{B}$). The cobalt complex indicates three absorption bands at 17789, 16457, and 11477 cm^{-1} , which are assigned as $^4T_{1g} (F) \rightarrow ^4T_{2g} (F)$, $^4T_{1g} (F) \rightarrow ^4A_{2g} (F)$ and $^4T_{1g} (F) \rightarrow ^4T_{1g} (F)$ transitions, respectively. The band at 11467 cm^{-1} confirms the octahedral geometry, which is also supported by its magnetic susceptibility value ($4.38\text{ }\mu\text{B}$) [30–32].

3.6. Cyclic Voltammetry. Cyclic voltammetry is the most popular technique for studying electrochemical reactions. The cyclic voltammogram of the CuL_2 complex in DMSO solution (from 0.6 to -0.6 V potential range) shows a well defined redox active corresponding to the formation of the Cu(II)/Cu(III) couple at $E_{\text{pa}} = 0.197\text{ V}$ and the associated anodic peak at $E_{\text{pc}} = 0.152\text{ V}$ (Figure 6). This couple found to be reversible with $\Delta E_p = 0.04\text{ V}$ and the ratio of anodic to cathodic peak currents ($I_{\text{pc}}/I_{\text{pa}} = 1$) corresponding to

FIGURE 7: ESR spectrum of copper complex at Room Temperature.

FIGURE 8: ESR spectrum of copper complex at liquid nitrogen temperature.

a simple to one-electron process. The complex also shows a reversible peak in the negative region characteristic of the Cu(II) $\rightarrow$ Cu(I) couple at $E_{pc} = -0.082$ V with the associated anodic peak at $E_{pa} = -0.076$ V for Cu(I) $\rightarrow$ Cu(II) oxidation.

3.7. EPR Spectra. The EPR spectrum of copper complex provides information, important in studying the metal ion environment. The EPR spectra were recorded in DMSO at RT (room temperature) and LNT (liquid nitrogen temperature) (Figures 7 and 8). The spectrum of the copper complex at RT showed one intense absorption band in the high field and was isotropic due to the tumbling motion of the molecules. However, this complex at LNT showed well resolved peaks with low field region. The copper complex exhibited the g value of 2.36 and g value of 2.08. These values indicate that the Cu (II) lies predominantly in the $d_{x^2-y^2}$ orbital, as was evident from the value of the exchange interaction term G , estimated from the expression:

$$G = g_{\parallel} - \frac{2.0023}{g_{\perp}} - 2.0023. \quad (1)$$

TABLE 2: Shape complementarity score of DNA-Metal complexes.

S. No	Metal Complexes	Shape-Complementarity score
(1)	DNA-CoL ₂	4032
(2)	DNA-CuL ₂	3724
(3)	DNA-NiL ₂	3884
(4)	DNA-ZnL ₂	4122

FIGURE 9: Structure of DNA Molecule (Display: PyMol).

It is reported that $g_{\parallel}$ is 2.4 for copper-oxygen bonds, 2.3 for copper-nitrogen bonds. For mixed copper-nitrogen and copper-oxygen systems, there is a small difference in the point of symmetry from octahedral geometry [33]. For the present copper complex, the $g_{\parallel}$ value (2.36) is between 2.3–2.4. This shows that the complex contains mixed copper-nitrogen and copper-oxygen bonds. If $G > 4.0$, the local tetragonal axes are aligned parallel or only slightly misaligned. If $G < 4.0$, significant exchange coupling is present and the misalignment is appreciable. The observed value for the exchange interaction parameter for the copper complex ($G = 4.5$) suggests that the local tetragonal axes are aligned parallel or slightly misaligned, and the unpaired electron is present in the orbital. This result also indicates that the exchange coupling effects are not operative in the present complex [34].

3.8. In Silico DNA-Metal Complex Interaction. The structure of DNA is displayed in Figure 9. The Patch dock web server [23] was used to study the interaction between DNA and metal complexes. One hundred docking conformations were generated for each metal complex with its DNA molecule. For each docking results, the best solution was inferred by highest value of shape complementarity score (Table 2). The shape-complementarity score of four complexes was computed using Patch dock web server [23] and the results

TABLE 3: Inter-molecular hydrogen bonds present in DNA-CoL₂.

Type	Donor	Donor atom	Acceptor	Acceptor atom	d (H...A) (Å)	D (X...A) (Å)	q (X-H...A) (°)
C-H...N	CoL ₂	C	Adenine	N6	2.068	3.054	148.8
C-H...N	CoL ₂	C	Adenine	N6	2.251	3.160	139.1
C-H...N	CoL ₂	C	Adenine	N7	1.307	1.749	93.07
C-H...N	CoL ₂	C	Adenine	N6	2.473	3.121	118.6
C-H...N	CoL ₂	C	Adenine	N7	2.273	3.103	133.8
C-H...O	CoL ₂	C	Adenine	O2P	2.640	3.656	154.6
C-H...O	CoL ₂	O	Adenine	O2P	2.943	3.191	96.02
C-H...O	CoL ₂	C	Adenine	O1P	1.253	1.934	113.2
C-H...O	CoL ₂	C	Guanine	O2P	1.390	2.013	109.7
C-H...O	CoL ₂	C	Thymine	O4	1.187	2.122	141.6

TABLE 4: Inter-molecular hydrogen bonds present in DNA-CuL₂.

Type	Donor	Donor atom	Acceptor	Acceptor atom	d (H...A) (Å)	D (X...A) (Å)	q (X-H...A) (°)
C-H...O	CuL ₂	C	Thymine	O4	2.949	3.479	110
C-H...N	CuL ₂	C	Adenine	N7	2.859	3.657	129.7
C-H...N	CuL ₂	C	Adenine	N7	2.839	3.445	114.8
C-H...O	CuL ₂	C	Adenine	O2P	2.762	3.688	142.3
C-H...O	CuL ₂	C	Adenine	O1P	2.877	3.650	127.6
C-H...O	CuL ₂	C	Adenine	O2P	2.741	3.366	115.9
C-H...O	CuL ₂	C	Adenine	O5	2.459	3.351	170.3
C-H...N	CuL ₂	C	Adenine	N7	2.504	3.352	165.9
C-H...N	CuL ₂	C	Adenine	N6	2.328	2.926	114.1
C-H...N	CuL ₂	C	Adenine	N6	2.872	3.480	116.7
C-H...O	CuL ₂	C	Adenine	O1P	2.597	2.939	98.01
C-H...N	CuL ₂	C	Adenine	N6	2.810	3.262	105.8
C-H...N	CuL ₂	C	Adenine	N7	2.203	3.015	132
C-H...N	CuL ₂	C	Adenine	N6	2.192	2.951	126.8
C-H...N	CuL ₂	C	Adenine	N6	2.709	2.935	91.53
C-H...O	CuL ₂	C	Adenine	O1P	2.445	2.861	102

TABLE 5: Inter-molecular hydrogen bonds present in DNA-NiL₂.

Type	Donor	Donor atom	Acceptor	Acceptor atom	d (H...A) (Å)	D (X...A) (Å)	q (X-H...A) (°)
C-H...O	NiL ₂	C	Thymine	O4	2.943	3.760	131.6
C-H...O	NiL ₂	C	Adenine	O2P	2.899	3.651	126.1
C-H...O	NiL ₂	O	Guanine	O1P	1.745	2.387	121.1
C-H...O	NiL ₂	O	Guanine	O2P	2.008	2.874	149.0
C-H...O	NiL ₂	C	Adenine	O2P	2.951	3.177	92.36
C-H...O	NiL ₂	C	Adenine	O2P	2.902	3.622	125.4
C-H...O	NiL ₂	C	Thymine	O4	2.343	2.963	115.7
C-H...O	NiL ₂	C	Guanine	O2P	1.755	2.692	144.8
C-H...O	NiL ₂	C	Adenine	O2P	2.880	3.115	92.68
C-H...O	NiL ₂	C	Thymine	O4	2.514	3.028	108.8
C-H...N	NiL ₂	C	Adenine	N6	2.885	3.905	161.5

TABLE 6: Inter-molecular hydrogen bonds present in DNA-ZnL₂.

Type	Donor	Donor atom	Acceptor	Acceptor atom	d (H...A) (Å)	D (X...A) (Å)	q (X-H...A) (°)
C-H...N	ZnL ₂	C	Adenine	N6	2.437	3.450	153.6
C-H...N	ZnL ₂	C	Adenine	N7	2.711	3.471	126.2
C-H...N	ZnL ₂	C	Adenine	N7	2.619	2.960	97.09
C-H...N	ZnL ₂	C	Adenine	N6	2.646	3.433	128.3
C-H...N	ZnL ₂	C	Adenine	N7	2.444	2.960	107.0
C-H...O	ZnL ₂	C	Adenine	O2P	2.943	3.270	97.5
C-H...O	ZnL ₂	C	Adenine	O2P	2.853	3.270	102.5
C-H...O	ZnL ₂	C	Guanine	O5	2.982	3.802	134.6
C-H...O	ZnL ₂	C	Guanine	O3	2.790	3.539	127.6
C-H...O	ZnL ₂	C	Adenine	O2P	1.746	2.389	114.5
C-H...O	ZnL ₂	C	Thymine	O4	2.619	3.645	162.9
C-H...N	ZnL ₂	C	Adenine	N6	2.479	2.919	103.7
C-H...N	ZnL ₂	C	Adenine	N7	2.660	3.302	118.7
C-H...O	ZnL ₂	C	Thymine	O4	2.974	3.480	109.8

TABLE 7: Statistics of inter-molecular hydrogen bonds present between DNA and metal complexes.

Metal complexes	N-H...O	O-H...O	N-H...N	O-H...N	C-H...O	C-H...N	N-H...S	O-H...S	C-H...S
DNA-CoL ₂	0	0	0	0	5	5	0	0	0
DNA-Cu L ₂	0	0	0	0	7	9	0	0	0
DNA-NiL ₂	0	0	0	0	10	1	0	0	0
DNA-Zn L ₂	0	0	0	0	7	7	0	0	0

reveal that DNA with Cu-complex possesses the lowest shape-complementarity score compared to other three complexes. From the molecular docking results (Figure 10), the best solution was selected and it was processed into HBAT [25] or Hydrogen Bond Analysis Tool for computing the possible inter-molecular hydrogen bonds present between DNA and metal complexes. HBAT [25] results explain that two inter-molecular C-H...O and C-H...N hydrogen bonds played a crucial role for the stability of all metal complexes with DNA. The details of inter-molecular C-H...O and C-H...N interactions were given in Tables 3–6. However, in all four complexes did not contain other inter-molecular hydrogen bonds such as N-H...O, O-H...O, N-H...N, O-H...N, N-H...S, O-H...S, C-H...S, C-H... π , N-H... π and O-H... π . Figure 11 and Table 7 explain the statistics of various possible weak inter-molecular hydrogen bonds present between DNA and metal complexes.

In order to understand the stability of metal complex with DNA, we have used two parameters such as “shape complementarity score” and “number of inter-molecular hydrogen bonds”. Patch dock and HBAT analysis results suggested that the interaction between DNA and Cu-complex is more stable (Low shape complementarity score and more number of weak intermolecular hydrogen bonds) rather than others. All the four complexes are binding to “Major groove” portion of DNA and hence they are called as “Major groove binders”.

3.9. Antimicrobial Activity. Standard antibacterial agents were used for the comparative studies. The disc concentration levels are under National Committee for Clinical Laboratory Standards (NCCLS) column. The results of the antibacterial agents were given in the Table 8. From this data, it has been found that all the compounds showed various significant inhibitory activity [35, 36] against five MTCC human pathogenic of microbial species namely *S. aureus*, *B. subtilis*, *P. aeruginosa*, *P. vulgaris* and *C. albicans*. The antibacterial activity of the tested compounds some of may have dose dependent and it may found to be good activity at 40 and 60 μ L concentrations.

4. Conclusion

A new series of transition metal complexes were synthesized from the Schiff base ligand derived from 4-aminoantipyrine, 4-hydroxy-3-methoxybenzaldehyde and 2-aminophenol. The structural features were derived from their elemental analyses, Mass spectroscopy, IR, UV-vis, NMR, ESR spectral analyses and conductivity measurements. Cyclic voltammogram of copper complex in DMSO show well defined quasi-reversible one electron transfer process corresponding to the formation of the couple. The data of the complexes suggested an octahedral geometry for the metal complexes. The results of *in silico* DNA-metal complex

FIGURE 10: Molecular docking results DNA-metal complex interaction (a) DNA- CoL_2 , (b) DNA- CuL_2 , (c) DNA- NiL_2 and (d) DNA- ZnL_2 complex. [Color codes: Ligand: Yellow, Representation: Stick, Display: PyMol].

TABLE 8: Antimicrobial activity data for the Schiff base and their metal complexes.

Compounds	<i>B. subtilis</i>			<i>S. aureus</i>			<i>P. vulgaris</i>			<i>C. albicans</i>		
	20 μL	40 μL	60 μL	20 μL	40 μL	60 μL	20 μL	40 μL	60 μL	20 μL	40 μL	60 μL
HL	10	12	14	11	13	18	—	—	9	12	14	15
CuL_2	—	10	11	8	11	12	10	11	13	9	12	13
NiL_2	9	13	15	9	14	16	—	9	11	9	13	15
CoL_2	10	11	13	8	12	13	10	12	14	9	11	13
ZnL_2	10	12	15	8	13	15	10	12	14	9	12	14
Tetracycline (Antibacterial agent)	14	19	23	13	16	21	15	18	24	—	—	—
Amphotericin (Antifungal agent)	—	—	—	—	—	—	—	—	—	15	19	21

Zone of inhibition (diameter in mm).

FIGURE 11: Statistics of various possible weak intermolecular hydrogen bonds present between DNA and metal complexes.

interaction reveal that all the complexes can interact with DNA. The Schiff base coordinates through its two azomethine nitrogen and phenolic oxygen. The Schiff base behaves as a tridentate ligand. The results of antimicrobial screening explored that metal complexes are potentially active against bacterial cells rather than fungal cells.

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