

## Studies on nucleic acid/protein interaction, molecular docking and antimicrobial properties of mononuclear nickel(II) complexes of piperazine based Schiff base



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### ABSTRACT

The mononuclear nickel(II) complexes (**1–3**) of ligands bappz [1,4-bis(3-aminomethyl)piperazine] and its Schiff bases L<sup>1</sup> with 5-methyl salicylaldehyde; and L<sup>2</sup> with 5-bromosalicylaldehyde have been synthesized and characterized. The single crystal X-ray study showed that the complex **1** crystallized in the orthorhombic Pbc<sub>a</sub> space group with distorted square planar geometry. The ligands and their nickel(II) complexes presented good binding propensity to bovine serum albumin protein (BSA). The strong binding interaction of the prepared complexes with calf thymus DNA (CT-DNA) was confirmed by absorption, fluorescence, circular dichroism spectral analysis and molecular docking studies in the order as follows: **3** > **2** > **1**. The Schiff bases and their Ni(II) complexes were also screened for antimicrobial activity. All the complexes exhibited higher antimicrobial activity than free ligands.

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Continued interest on the development of DNA binding agents has been driven by the goals for obtaining novel antitumor drugs, DNA sequencing agents and DNA conformation probes [1]. The interaction of drugs and their compounds with blood plasma proteins especially with serum albumin has involved in the transport of metal ions and metal complexes of drugs through the blood stream, is of increasing interest. Nickel is an important transition metal and its coordination compounds display interesting binding properties with proteins and nucleic acids [2]. The N- and O-containing ligands and their nickel(II) complexes have become important due to their wide biological activity anti-HIV activities etc. Bappz ligand molecule provides two pendant aminopropyl arms and two tertiary amines incorporated in the six-membered piperazine ring, which induces some sort of strain especially in the middle chelate ring when the two N-donor atoms of piperazine bind with Ni<sup>2+</sup> ion [3]. Schiff bases derived from the salicylaldehyde and its derivatives are well known as polydentate ligands, coordinating in deprotonated or neutral forms. Schiff base complexes possess suitable biometric properties that can mimic the active sites and hence they have wide applications in as illness treatment, biochemical reactions and also as biological regulators [4].

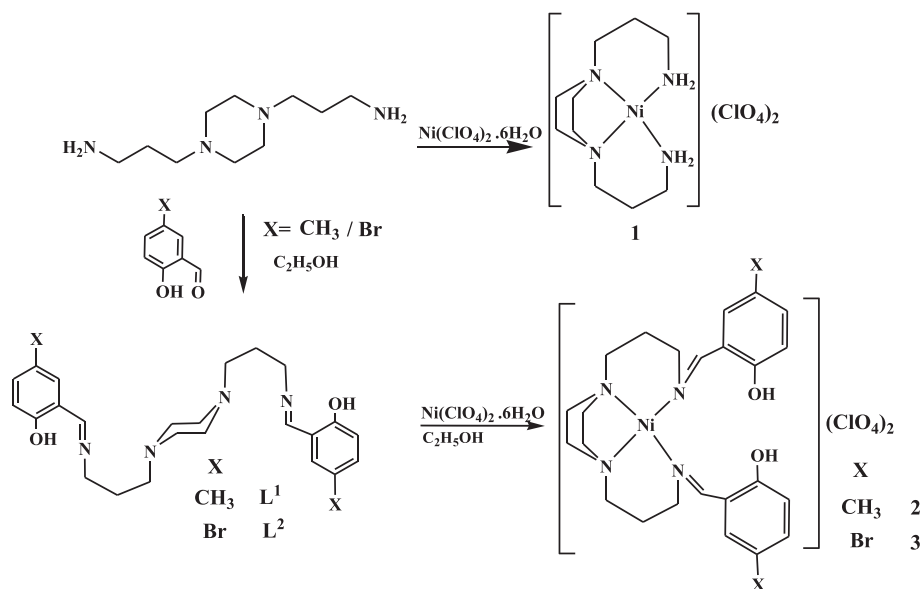
Recently our research group reported that the mononuclear copper(II) complexes using Schiff base ligands L<sup>1</sup> [N, N'-bis(2-hydroxy-5-methylbenzyl)-1,4-bis(3-iminopropyl) piperazine] and L<sup>2</sup> [N,

N'-bis(2-hydroxy-5-bromobenzyl)-1,4-bis(3-iminopropyl)piperazine] have molecular motion between N<sub>4</sub> and N<sub>2</sub>O<sub>2</sub> compartments on varying pH and have good DNA interaction properties [5]. In order to study the change in molecular motion and DNA binding properties due to nickel(II) atoms, in this paper we have reported the synthesis (Scheme 1) of mononuclear nickel(II) complexes ([Ni(bappz)](ClO<sub>4</sub>)<sub>2</sub> [6], [NiL<sup>1</sup>](ClO<sub>4</sub>)<sub>2</sub> [7] and [NiL<sup>2</sup>](ClO<sub>4</sub>)<sub>2</sub> [8]) of ligands bappz, Schiff bases L<sup>1</sup> and L<sup>2</sup> (Scheme 1), respectively were synthesized and characterized by elemental analysis, IR, UV–visible, and ESI-mass spectroscopy. The preparation of ligands and their crystal structure were reported in our previous work [5].

The X-ray crystallographic analysis [9] of complex **1** (ORTEP diagram with 30% thermal probability ellipsoids shown in Fig. 1, crystallographic data are listed in Table 1 and selected bond angle and bond distances are given in Table S1) shows that, the structure of the complex [Ni(bappz)](ClO<sub>4</sub>)<sub>2</sub> (**1**) consists of monomeric isolated [Ni<sup>II</sup>(bappz)]<sup>2+</sup> cations and two perchlorate counter anions in which one of the carbon atoms (C13) is disordered over two positions with an occupancy ratio of 0.62 (2):0.38 (2). The sum of the different angles around the Ni atoms is 359.98° indicating slightly distorted square-planar geometry around the metal atom. The distortion may conveniently be measured by the trans angles that are ideally 180° for a square-planar complex and 109.5° in a tetrahedral complex. The average N–M–N angles for the present Ni<sup>II</sup> (173.9°) complex are larger than those for the already reported Cu<sup>II</sup> (165.6°) complex with the same ligand [10]. The Ni–N(2) and Ni–N(15) distances (average 1.913 Å) are shorter than the Ni–N(6) and Ni–N(9) distances (average 1.930 Å) are mainly due to

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**Scheme 1.** The synthetic pathway of the complexes.

the different states of hybridization of nitrogen atom and/or the ring strain [11] due to the boat conformation of inner piperazine unit. The non-coordinating perchlorate anions have a distorted tetrahedral structure, as indicated from their bond angles. In cif check report, the low ratio (43%) of the Ratio of Observed to Unique Reflections might be from the poor crystallinity of the complex.

The intermolecular Ni...Ni separation is 7.547 (2) Å, a value which does not permit any kind of bridging between the nickel atoms. Fig. S1 shows the packing of the molecule in a lattice, which is stabilized by the H-bonding interactions between the oxygen of the anion with the piperazine ring hydrogen. The intramolecular hydrogen bonds are also observed between the amino groups and nearer perchlorate O atoms (2.267 Å), which help in stabilizing the crystal structure.

The FT-IR spectrum of nickel(II) complexes (**2** and **3**) showed the broad peak at 3423–3450  $\text{cm}^{-1}$  is assigned to the phenolic  $\nu(\text{OH})$  group [12]. The ligands and complexes showed a sharp band in the region of 1620–1650  $\text{cm}^{-1}$  due to the presence of  $\nu(\text{C}=\text{N})$  [13]. The

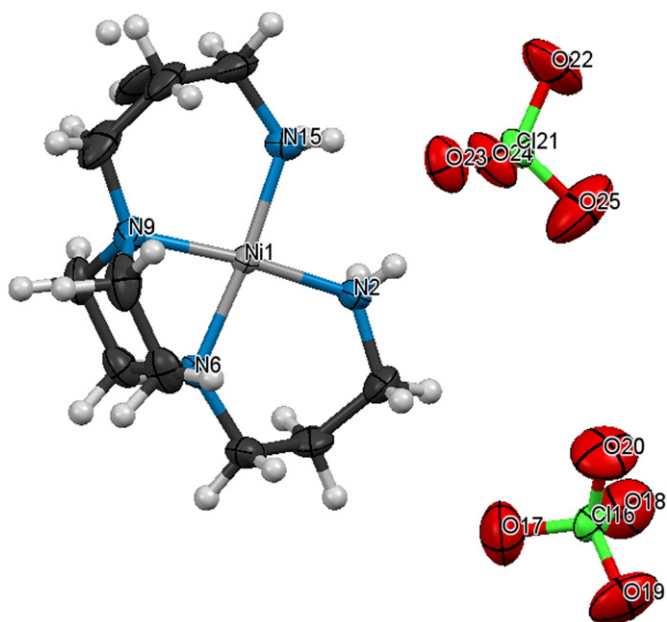
effective Schiff base condensation was confirmed by the disappearance of the  $\nu(\text{C}=\text{O})$  peak at 1680  $\text{cm}^{-1}$ . All nickel(II) complexes showed a strong band around 1000–1100  $\text{cm}^{-1}$  and a sharp band in the region around 625  $\text{cm}^{-1}$  is due to the antisymmetric stretch and antisymmetric bend of the perchlorate ions respectively [14].

The absorption spectral data for Schiff base ligands and their complexes in DMF solution shows the peaks in the UV region of 270 nm to 278 nm are obtained due to  $\pi \rightarrow \pi^*$  transition of coordinated ligands, broad and slightly intense bands between 384 and 396 nm due to ligand–metal charge transfer associated with the nitrogen and oxygen donors [15]. The visible spectra display the absorption bands below 670 nm assigned to the spin allowed d–d transitions, which have a low-spin  $d^8$  nickel(II) ion in a square-planar environment [16].

Electron spray ionization (ESI) mass data of complex **2** (Fig. S2) shows the molecular ion peak at  $m/z$  694.2 (5), which is assignable to

**Table 1**  
Crystallographic data and structure refinement parameters for complex **1**.

	1
Empirical formula	$\text{C}_{10} \text{H}_{24} \text{Cl}_2 \text{N}_4 \text{Ni O}_8$
Formula weight	457.94
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system, space group	Orthorhombic, Pbc <sub>a</sub>
<i>a</i> (Å)	14.4352(11)
<i>B</i> (Å)	15.4172(12)
<i>c</i> (Å)	16.1779(13)
$\alpha$ (°)	90
$\beta$ (°)	90
$\gamma$ (°)	90
Volume (Å <sup>3</sup> )	3600.4(5)
<i>Z</i> , calculated density ( $\text{mg m}^{-3}$ )	8, 1.690
Absorption coefficient ( $\text{mm}^{-1}$ )	1.421
<i>F</i> (000)	1904
Crystal size (mm)	0.18 × 0.15 × 0.12
Theta range for data collection (°)	2.31 to 25.50
Limiting indices, <i>h, k, l</i>	−17 ≤ <i>h</i> ≤ 17, −18 ≤ <i>k</i> ≤ 18, −19 ≤ <i>l</i> ≤ 19
Reflections collected/ unique	21,459/3355
<i>R</i> <sub>int</sub>	0.0998
Data/restraints/parameters	3355/0/234
Goodness-of-fit on <i>F</i> <sup>2</sup>	0.819
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> 1 = 0.0523, <i>wR</i> 2 = 0.1272
<i>R</i> indices (all data)	<i>R</i> 1 = 0.1158, <i>wR</i> 2 = 0.1575
Largest difference peak and hole/ $\text{e}^{-}\text{Å}^{-3}$	0.629 and −0.499



**Fig. 1.** ORTEP view of the molecular structure and atom labeling scheme of complex **1**.

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