



## Spectral, DFT, molecular docking and antibacterial activity studies of Schiff base derived from furan-2-carbaldehyde and their metal(II) complexes

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**Abstract:** Metal(II) complexes of cobalt(II) (1), copper(II) (2), nickel(II) (3), and zinc(II) (4) with Schiff base ligand derived from furan-2-carbaldehyde were synthesized and elucidated by IR, electronic, mass, <sup>1</sup>H NMR, and magnetic susceptibility measurements. Using DFT-based optimization of structures, bond length, bond angle, HOMO-LUMO energy gaps, and molecular electrostatic potential maps (MEP) of ligand and complexes 1-3 were theoretically calculated at the B3LYP/LANL2DZ level of theory. HOMO-LUMO energy gap was calculated which allowed the calculation of comparable properties like chemical hardness, chemical inertness, and chemical potential. The Ni(II) and Cu(II) complexes showed potent inhibition against all the bacterial strains. In comparison with antibacterial activity, molecular docking studies were carried out with protein receptor SEC2 (PDB: 1STE) in *Staphylococcus aureus*.

**Keywords:** Furan-2-carbaldehyde, Metal complexes, DFT, Antibacterial, Molecular docking.

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### INTRODUCTION

The Schiff base ligands with nitrogen and oxygen donor atoms act as good chelating agents for the transition and non-transition metal ions. The azomethine (-CH=N-) linkage present in Schiff base ligands and its metal (II) complexes show a wide range of biocidal activities such as antibacterial (1) antifungal (2) anti-inflammatory

(3) anticancer, anti-diabetic (4), and antitumor activities. Furthermore, the interactions of these complexes with DNA have gained much attention due to their possible applications as new therapeutic agents (5-7). The high affinity for the chelation of the Schiff bases towards the transition metal ions is utilized in preparing their complexes in the solid form (8-10). The tractability of Schiff base ligands can be

enhanced by hydrogenation of (C=N) bands, and they should thus coordinate metal ions more easily. For these explanations, condensed Schiff bases have newly expanded significant consideration (11). Herein we report the synthesis and characterization of furan-2-ylmethylidene-hydrazinylidene-ethyl-phenol [AF], which is derived from 2-[(1E)-1-hydrazinylidene-ethyl] phenol and 2-furancarboxaldehyde and its metal(II) complexes.

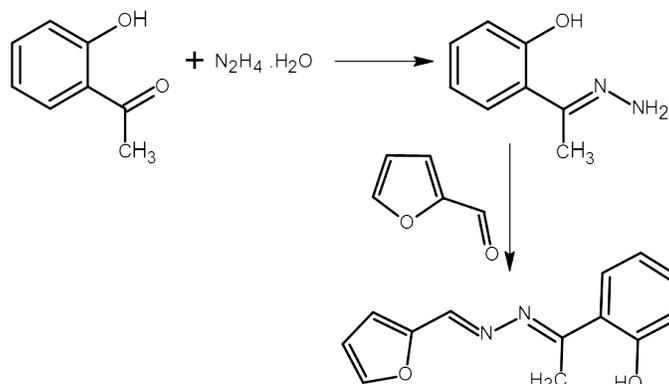
## EXPERIMENTAL

All the chemicals used were of analytical grade and were as procured. The reagent grade chemicals 2-hydroxyacetophenone, hydrazine hydrate, 2-furancarboxaldehyde, and metal(II) salts were purchased from Sigma-Aldrich and used without further purification. The melting point had been recorded on an electro-thermal melting factor apparatus and are uncorrected. <sup>1</sup>H-NMR spectra were recorded on a Bruker 400 MHz spectrometer at IISc, Bangalore, and Karnataka, INDIA. The chemical shifts have been proven in  $\delta$  values (ppm) with tetramethylsilane

(TMS) as an internal standard. LC-MS changed into acquired the usage of a C-18 column on Shimadzu, LCMS 2010A, Japan. The FT-IR spectra of the compounds were taken as KBr pellets (100 mg), the usage of Shimadzu FT-IR spectrometer. Magnetic susceptibility has been measured at 35 °C through the Gouy technique.

### Synthesis of 2-[(1E)-1-[(2E)-(furan-2-ylmethylidene) hydrazinylidene] ethyl] phenol [AF]

The Schiff base ligand was prepared by refluxing 2-hydroxyacetophenone (4.02 g, 0.02 mol) and hydrazine hydrate, each dissolved in 30 mL ethanol with continuous stirring. The stirring was continued for 3 h and to obtain the white product. A solution of the isolated 2-[(1E)-1-hydrazinylidene ethyl]phenol (2.7g 0.02 mol) in 10 mL ethanol was then refluxed with an ethanolic solution of furan-2-carbaldehyde (1.8 g, 0.02 mol) for 5 h after adding 1 mL of glacial acetic acid (Scheme 1). The obtained solid product was filtered off, washed several times with methanol and recrystallized from hot methanol, and dried over anhydrous CaCl<sub>2</sub>.



**Scheme 1:** Synthesis of Schiff base ligand AF .

Yield: 78%; M.p.: 178–180 °C, Anal. Calc. for C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub> = C(68.41%) H(5.30%) and N(12.27%), Found: C(67.11%) H(5.68%) and N(11.94%), LC-MS: m/z 228 [M+1].

### Synthesis of metal complexes

Ethanolic solution of metal(II) chlorides [Co(II), Ni(II), Cu(II) and Zn(II)] (2 mmol) added in drops to an ethanolic solution of the ligand (AF) (4 mmol) and the mixture was refluxed on a water bath for 3–4 h. The solid complexes obtained was filtered, washed with hot ethanol and dried in vacuum over anhydrous calcium chloride.

**Co(II) Complex [1]:**- Pale yellow solid, yield: 61%. Mp: > 300 °C. Anal. C(53.44%), H(3.79%), Co(10.09%), N(9.59%), Cl(12.13%), Found: C(53.62%), H(4.03%), Co(10.44%), N(10.21%), Cl(11.82%), 23  $\lambda\text{m cm}^{-2} \Omega^{-1} \text{mol}^{-1}$ .

**Ni(II) Complex [2]:**- Light green solid, yield: 53%. Mp: > 300 °C Anal. C(52.37%), H(3.61%), Ni(10.21%), N(8.89%), Cl(12.05%), Found: C(52.62%), H(3.91%), Ni(10.44%), N(9.22%), Cl(12.63%), 21  $\lambda\text{m cm}^{-2} \Omega^{-1} \text{mol}^{-1}$ .

**Cu(II) Complex [3]:-** Dark brown solid, yield: 55%. Mp: > 300 °C Anal. C(55.12%), H(4.19%), Cu(12.11%), N(8.66%), Cl(13.22%), Found: C(55.41%), H(4.51%), Cu(11.81%), N(8.05%), Cl(13.87%),  $28 \text{ } \mu\text{m cm}^{-2} \Omega^{-1} \text{ mol}^{-1}$

**Zn(II) Complex [4]:-** Light cream solid, yield: 62%. Mp: > 300 °C Anal. C(51.43%), H(4.16%), N(8.12%), Zn(9.12%), Cl(10.18%), Found: C(51.92%), H(3.83%), Zn(8.78%), N(8.73%), Cl(10.51%),  $21 \text{ } \mu\text{m cm}^{-2} \Omega^{-1} \text{ mol}^{-1}$ .

## Biological studies

### Antibacterial assay

The obtained compounds were screened *In-vitro* against *S. aureus*, *B. Subtilis*, and *S. Pneumonia* (gram-positive) *P. aeruginosa* and *K. pneumonia* (gram-negative) bacterial strains by using disc diffusion method (12, 13). Ciprofloxacin was used as a standard for the current study with a concentration of about 10  $\mu\text{g}/\text{disc}$ . Sterile molten Muller and Hynton agar cooled to 45 °C was injected with different strains. Fresh inocula containing  $\sim 100 \text{ cells mL}^{-1}$  were used. Homogeneously, the inoculums were transferred on to a molten agar media with sterile cotton swabs by disease-free technique. A Whatman, no 2 filter paper disc of 6 mm diameter containing 200  $\mu\text{L}/\text{disc}$  of sample, was placed over the inoculated medium. The plates were left uninterrupted at room temperature for two hours and incubated at 37 °C for 24 h. Zone inhibition was measured with the zone reader scale.

### In-silico docking studies

HEX 8.0 docking software in support with the discovery visualizer studios were used to perform interaction studies with protein receptor SEC2 (PDB: 1STE) in *Staphylococcus aureus* obtained from RCSB protein data bank (14).

## RESULTS AND DISCUSSION

The metal (II) complexes are soluble in DMSO, DMF, and are sparingly soluble in chloroform. The complexes are stable at room temperature. The elemental analysis data of the ligand [AF] and its metal complexes [Co(II), Ni(II), Cu(II) and Zn(II)] indicate that the metal to ligand ratio is 1:2.

### <sup>1</sup>H NMR and Mass spectra

To identify the structure of free ligand AF, the resonance signals at  $\delta$  12.12,  $\delta$  7.11–7.75,  $\delta$  3.52–3.81, and  $\delta$  2.75–2.95 ppm are due to OH, Ar-protons,  $-\text{CH}_2$ , and  $-\text{CH}_3$ , respectively. The

sharp peak at 8.08 ppm corresponding to ( $-\text{CH}=\text{N}-$ ) proton is shifted towards the upper field, which proves the formation of coordination bond between the metal and imine nitrogen. The deprotonation of OH proton has been observed in the spectrum of Zn(II) complex, which supports the phenolic oxygen atom was coordinated with metal ions and <sup>1</sup>H NMR spectra of ligand AF and Zn(II) complex provided in the supplementary file.

The mass spectrum of ligand (AF) shows (Fig. 3) a well-defined molecular ion peak at  $m/z$  288, which is equivalent with (M+ 1), was proposed molecular formula weight of ligand. The molecular ion peaks of the Cu(II), Co(II) Ni(II) and Zn(II) complexes were appeared at  $m/z$  of 588.93, 584.31, 584.07 and 590.79 respectively, which are equivalent to the stoichiometric ratio of 1:2 (M:L) type. Further, the observed molecular mass in all the spectra of the prepared complexes are in consistency with their proposed molecular structures.

### IR spectra

The ligand AF showed the characteristic band at  $3334 \text{ cm}^{-1}$  due to stretching vibrations of OH group and the absorption bands of 2920, 1590, 1298, 916 and  $1357 \text{ cm}^{-1}$  are due to Ar-CH, C=N, C-O, N=N and  $-\text{CH}_3$  respectively (15). The OH stretching vibrations have disappeared with complexation in the metal (II) complexes, indicating coordination through the OH group. Additional support by the  $\nu(\text{C-O})$  stretching shifted to the lower frequency at  $1245\text{--}1253 \text{ cm}^{-1}$ . The C=N band also shifted lower frequency by  $1512\text{--}1589 \text{ cm}^{-1}$  indicating coordination of azomethine nitrogen (16, 17). The new IR bands witnessed in the range at  $570\text{--}522 \text{ cm}^{-1}$  in the spectra of the metal complexes suggest the presence of M-O bonding in their structure, and M-N bands are tentatively assigned to absorptions in the regions  $443\text{--}499 \text{ cm}^{-1}$  (18).

### Electronic spectra

The electronic spectra of the ligand AF and their metal complexes are set in Table 1. The uncoordinated ligand showed two absorptions bands at 250, 290 nm due the  $\pi \rightarrow \pi^*$ ,  $n \rightarrow \pi^*$ , for (C=N) groups respectively (19, 20), and for the metal complexes, the bands appeared clearly in the range of 460 to 785 nm due to the  $\pi \rightarrow d_x^2 - y^2$  and /or  $(\pi \sigma) \rightarrow d_x^2 - y^2$  LMCT transition in all complexes (21-23).

**Table 1:** UV-Visible Bands of the AF and their metal complexes.

| Compound  | Solvent | $\lambda_{\max}$ in ( $\text{cm}^{-1}$ ) | Transition   | Magnetic moment (BM) | Geometry             |
|-----------|---------|--|--|----------------------|----------------------|
| Co(II)-AF | DMF     | 16,150<br>20,270                         | ${}^4\text{T}_{1g}(\text{F}) \rightarrow \text{A}_{2g}(\text{F})$<br>${}^4\text{T}_{1g}(\text{F}) \rightarrow {}^4\text{T}_{1g}(\text{P})$   | 4.81                 | Octahedral           |
| Ni(II)-AF | DMF     | 10,354<br>17,556<br>23,712               | ${}^3\text{A}_{2g}(\text{F}) \rightarrow {}^3\text{T}_{2g}(\text{F})$<br>${}^3\text{A}_{2g}(\text{F}) \rightarrow 3\text{T}_{1g}(\text{F})$<br>${}^3\text{A}_{2g}(\text{F}) \rightarrow {}^3\text{T}_{1g}(\text{P})$ | 3.11                 | Octahedral           |
| Cu(II)-AF | DMF     | 13,478-<br>14,331                        | ${}^2\text{E}_g \rightarrow {}^2\text{T}_{2g}$   | 1.92                 | Distorted Octahedral |
| Zn(II)-AF | -       | -  | -  | -                    | Diamagnetic complex  |

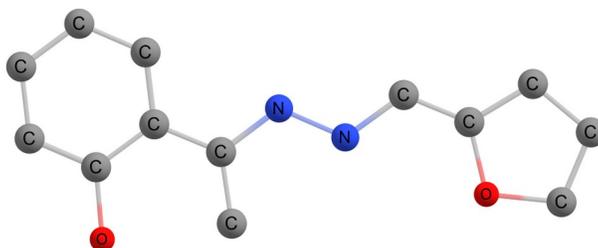
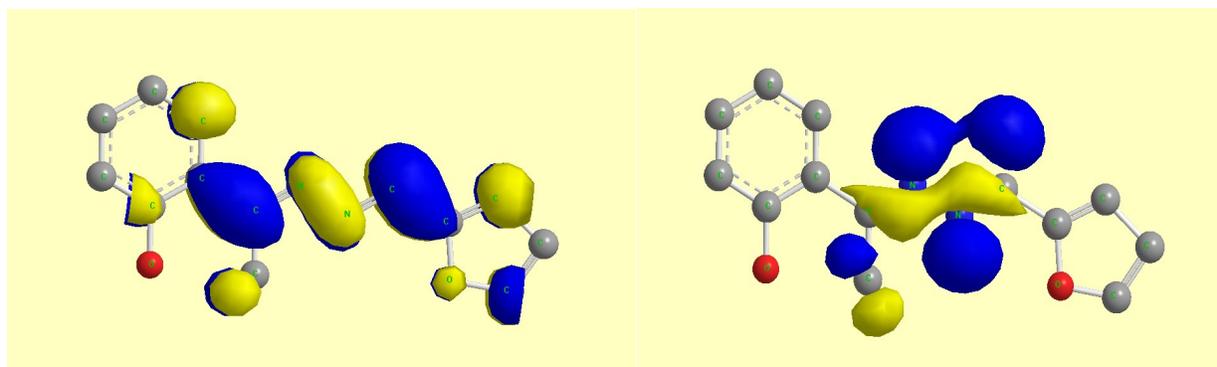
**Computational studies**

The calculations, optimized geometry of ligand, Co(II), and Ni(II) complexes are carried out with Gaussian 09 software using B3LYP/6-311, +G(d,p)(5D, 7F) basic set in the gas phase (24).

**Frontier molecular orbital analysis (FMOs) and Molecular electrostatic potential (MEP)**

In FMOs, the HOMO act as donor and LUMO as electron acceptor between the occupied and unoccupied molecular orbitals are shown in Figures 1 and 4. The energy gap  $\Delta E$  of HOMO-LUMO for the ligand is 0.917 eV, in which HOMO

orbital is delocalized on the nitrogen atom and  $\text{CH}_3$  group while the LUMO orbital is occupied on phenyl and thiophene rings (25). The energy gaps  $\Delta E$  of Co(II) and Ni(II) complexes are 2.311 and 2.778 eV. In HOMO orbitals for Co(II) and Ni(II) complexes are mainly delocalized on corresponding metal ions and thiophene and phenyl rings. Whereas in LUMO, electrons are concentrated on nitrogen, methyl group, and some part of metal ions. These tell us the chemical reactivity and stability of the ligand and their corresponding metal (II) complexes (26).

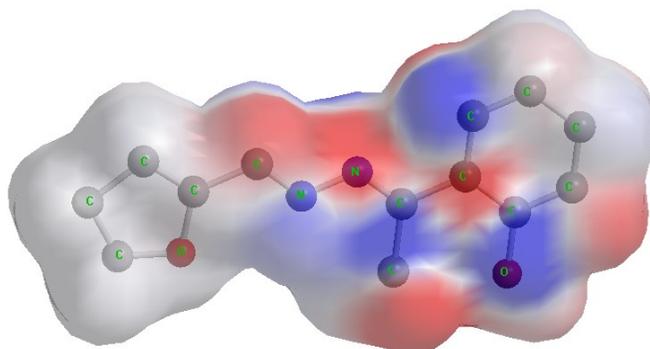
**Figure 1:** Optimized geometry of schiff base AF.**Figure 2:**  $E_{\text{LUMO}}-E_{\text{HOMO}}$  [-4.820 eV and -3.903 eV] molecular Schiff base AF.**Molecular electrostatic potential (MEP)**

MEP relates to the chemical reactivity and electronegativity by the electron and proton of

the molecules (Figure 5). Red color shows the negative electrostatic potential and mostly contains on the nitrogen and methyl moiety,

whereas the blue color represents the positive electrostatic potential contains on the phenyl and OH group of the molecule. The potential shows

the oxygen is nucleophilic center nitrogen acts as an electrophilic center and gives molecular interactions in the compounds (27).



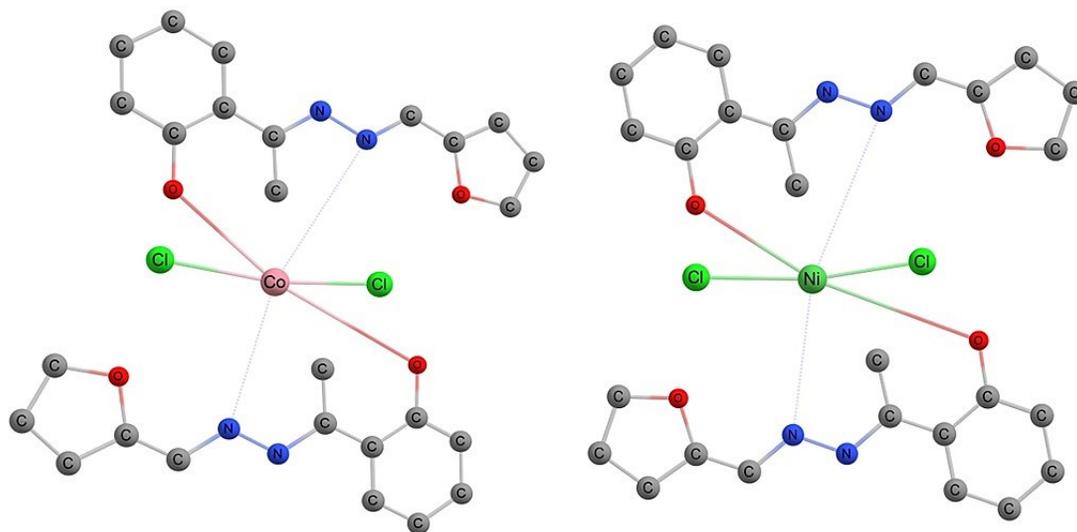
**Figure 3:** Molecular electrostatic potential (MEP) of ligand

**Table 2:** Selected parameters of Schiff base AF.

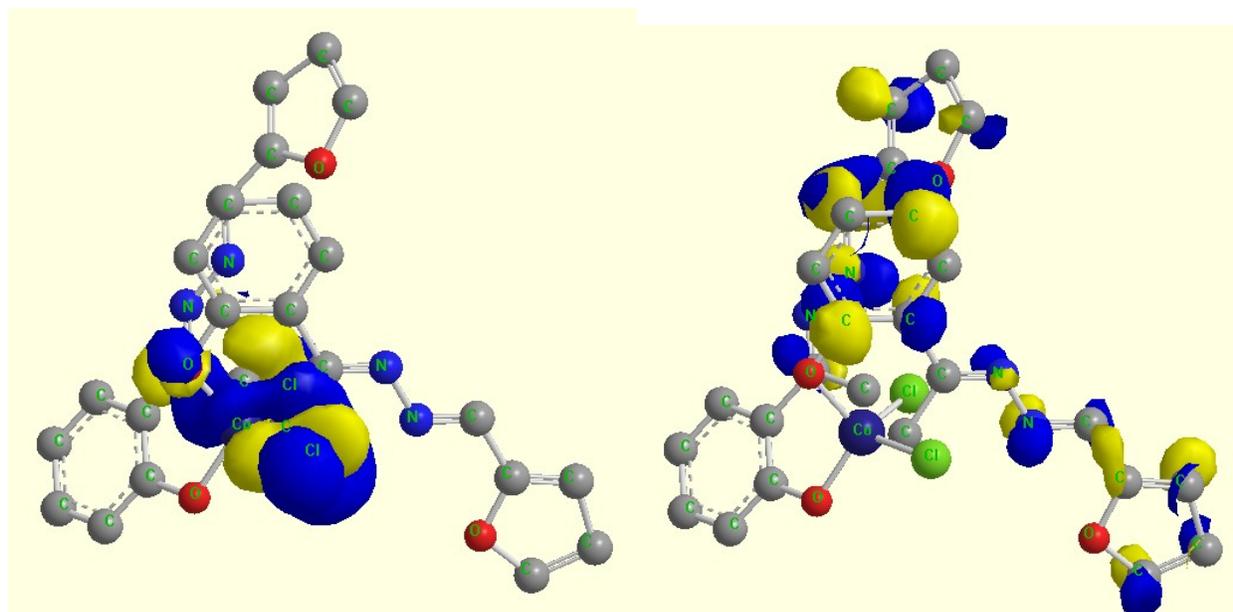
| Bond               | Bond length (Å) | Angle (°)         | Dihedral angle (°) |
|--------------------|-----------------|-------------------|--------------------|
| <b>C(8)-C(10)</b>  | 1.540           | N(9)-C(8)-C(10)   | 119.999            |
| <b>N(9)-N(11)</b>  | 1.352           | C(8)-N(9)-N(11)   | 120.000            |
| <b>N(11)-C(17)</b> | 1.244           | N(9)-N(11)-C(17)  | 120.000            |
| <b>C(12)-O(13)</b> | 1.410           | O(13)-C(12)-C(14) | 110.999            |
| <b>C(12)-C(14)</b> | 1.324           | O(13)-C(12)-C(17) | 124.499            |
| <b>C(12)-C(17)</b> | 1.540           | C(14)-C(12)-C(17) | 124.500            |
| <b>O(13)-C(15)</b> | 1.410           | C(12)-O(13)-C(15) | 104.000            |

The energy gaps  $\Delta E$  of Co(II) and Ni(II) complexes are 2.311 and 2.778 eV. In HOMO orbitals for Co(II) and Ni(II) complexes are mainly delocalized on the corresponding metal ions and thiophene and phenyl rings. Whereas in LUMO, electrons are concentrated on nitrogen, the methyl group, and some part of metal ions.

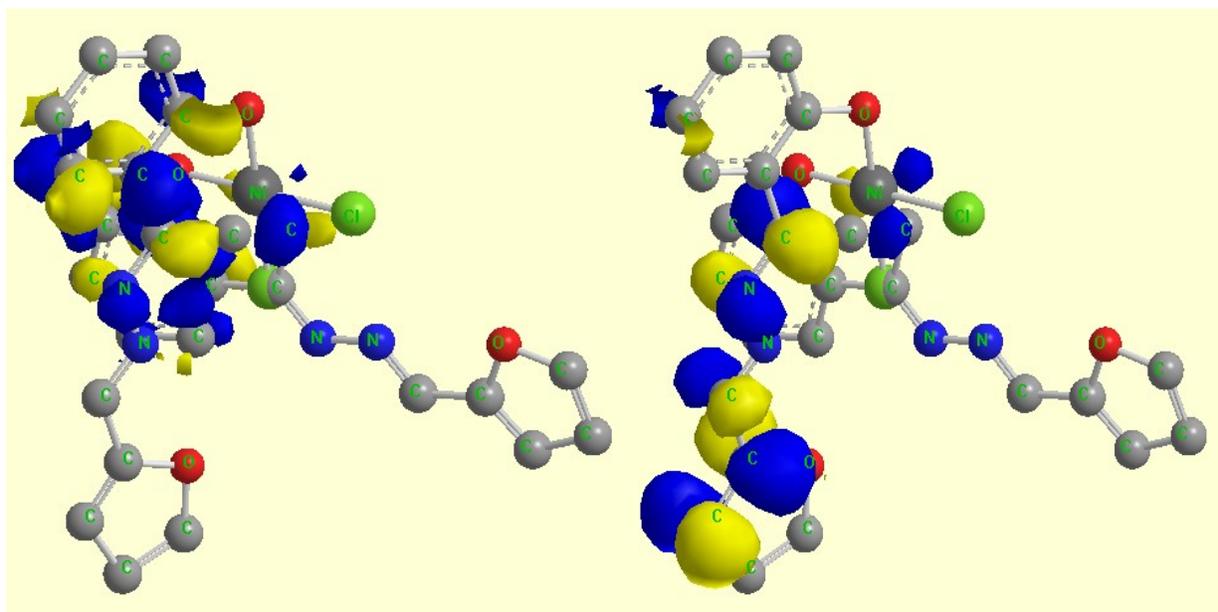
These tell us the chemical reactivity and stability of the ligand and their corresponding metal Co(II) and Ni(II) complexes and represented in Figures 5 and 6, and for Cu(II) and Zn(II) complexes were represented in supplementary file (28).



**Figure 4:** Optimized geometry of Co(II) and Ni(II) complexes.



**Figure 5:**  $E_{\text{LUMO}}-E_{\text{HOMO}}$  [-4.951 eV and -2.631eV] molecular orbitals of Co(II) complexes.



**Figure 6:**  $E_{LUMO}-E_{HOMO}$  [-8.811eV and -6.033 eV] molecular orbitals of Ni(II) complexes.

### Biological studies

#### Antibacterial activity

The obtained results of the antibacterial assay of synthesized compounds have given in Table 3. The Ni(II) and Cu(II) complexes showed potent inhibition against all the bacterial strains, in which *B. subtilis* and *K. pneumonia* showed the

highest activity towards these cell lines. On the other hand, Co(II) complex showed promising activity towards gram-negative bacterial strains of *P. aeruginosa* and *B. subtilis*. While the ligand AF and Zn(II) showed the least activity towards all the bacterial strains (29, 30).

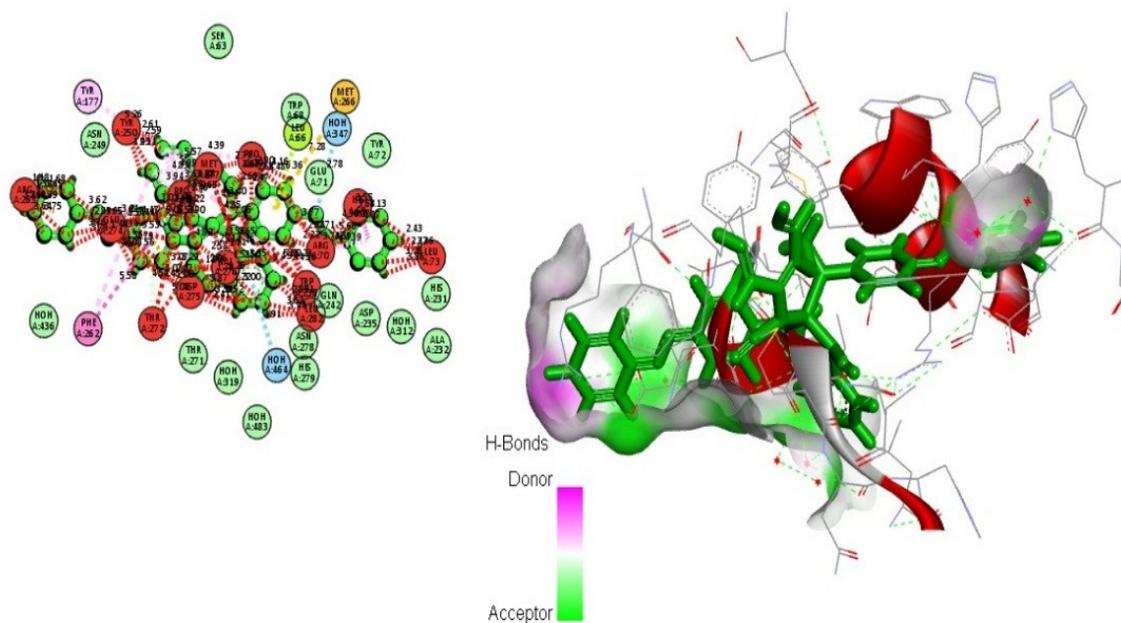
**Table 3:** Antibacterial data of AF and their metal complexes.

| Compounds     | <i>P.aeruginosa</i> | <i>K. pneumonia</i> | <i>B. subtilis</i> | <i>S. pneumonia</i> | <i>S. aureus</i> |
|---------------|---------------------|---------------------|--------------------|---------------------|------------------|
| AF            | 6                   | 8                   | 9                  | 8                   | 7                |
| Co(II)        | 12                  | 13                  | 15                 | 13                  | 13               |
| Ni(II)        | 15                  | 18                  | 19                 | 15                  | 12               |
| Cu(II)        | 15                  | 18                  | 20                 | 17                  | 16               |
| Zn(II)        | 12                  | 13                  | 15                 | 11                  | 13               |
| Ciprofloxacin | 16                  | 19                  | 22                 | 18                  | 17               |

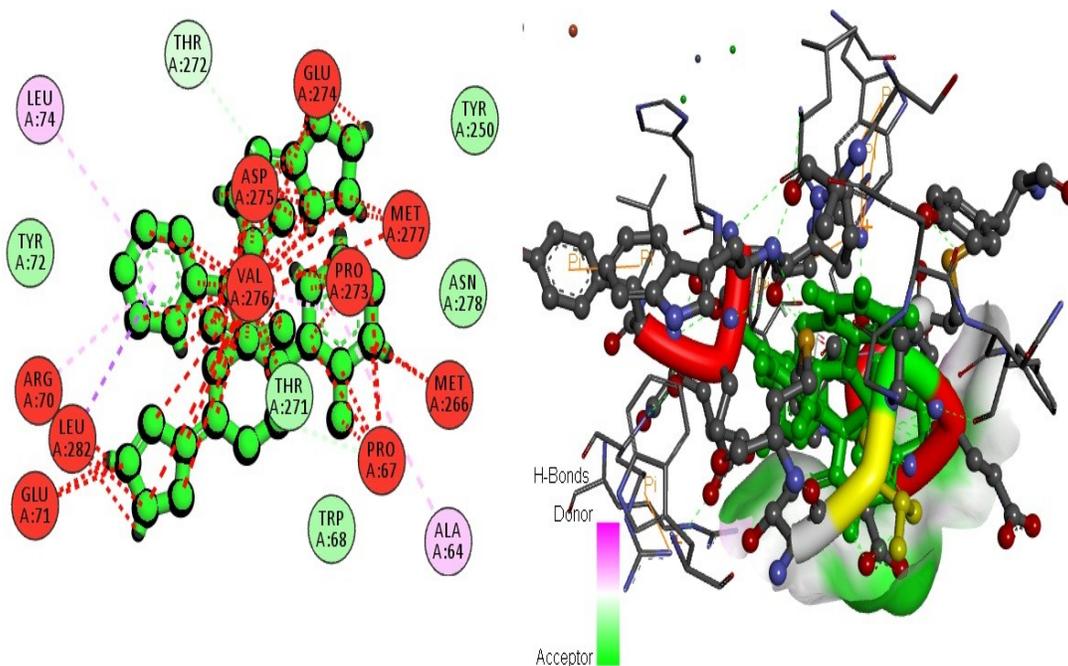
#### Molecular docking

In accordance with antibacterial activity, it is significant to carry out *in silico* docking studies. The protein receptor SEC2 (PDB: 1STE) in *Staphylococcus aureus* revealed that the excellent docking interactions with different amino acids and E-total score (31). The Ni(II) complex showed excellent binding affinity towards enzyme receptor 1STE of -287.16

kcal/mol, while Co(II) and Cu(II) complexes also exhibit good binding interactions docking score of -257.11 and -222.99 kcal/mol. But the ligand, AF, showed the least binding interactions of -155.73 kcal/mol. The ligand and the receptor interactions involve binding with different amino acids like His6, Phe20, Thr136, Ser165, Phe167, Glu198, Phe200, Val236, Thr237, Leu250, and Leu253.



**Figure 7:** 3D and 2D binding interactions of Co(II) complex with PDB: 1STE.



**Figure 8:** 3D and 2D binding interactions of Ni(II) complex with PDB: 1STE.

## CONCLUSION

The synthesized compounds were characterized by spectral and analytical data. The bidentate nature of ligand indicates the bonding through (-OH) and (C=N) groups. The Co(II), Ni(II)

complexes suggest the octahedral geometry and the Cu(II) complex exhibits The theoretical study using DFT/B3LYP supports experimental pieces of evidence of the binding sites of the ligand, geometry and the stability of the complexes. *B. subtilis* and *K. pneumonia* showed the highest

activity towards Ni(II) and Cu(II) complexes, The docking study revealed that Co(II) and Cu(II) complexes showed binding interaction with several amino acid residue of the protein receptor SEC2 (PDB: 1STE) in *Staphylococcus aureus*.

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## Spectral, DFT studies, molecular docking and antibacterial activity of Schiff base derived from furan-2-carbaldehyde and their metal (II) complexes

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### Supplementary Figures

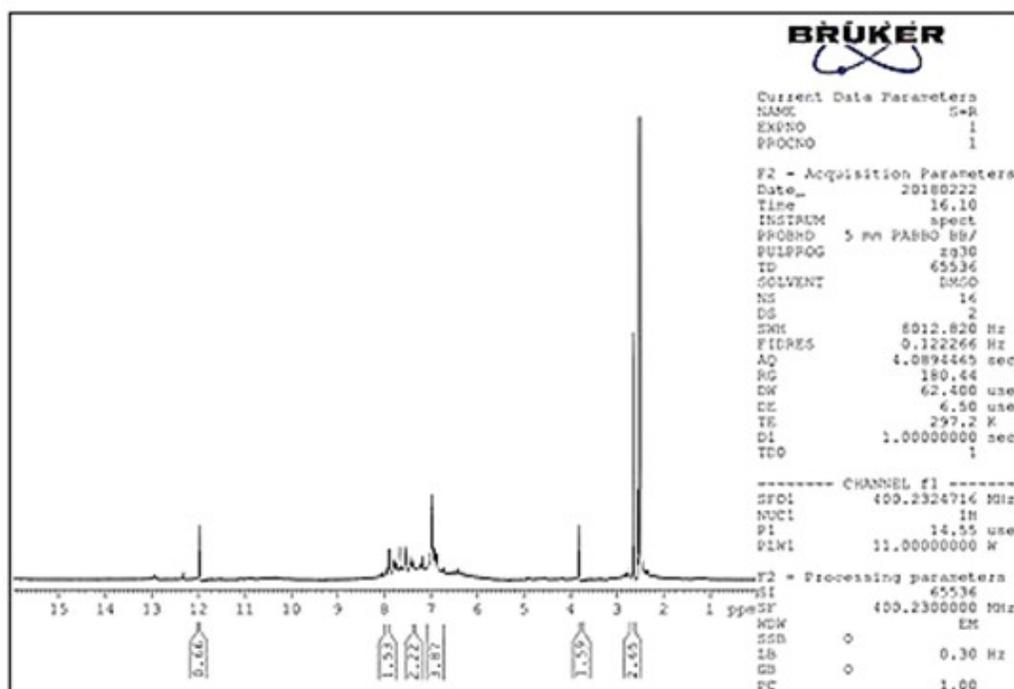


Figure S1: <sup>1</sup>H NMR spectrum of AF.

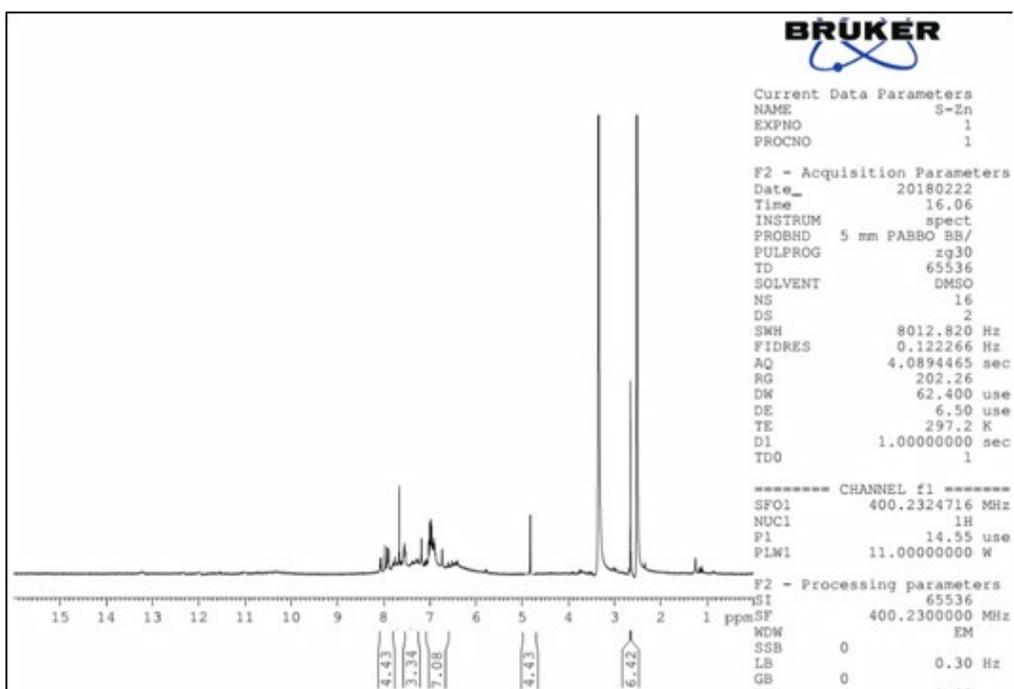


Figure S2: <sup>1</sup>H NMR of Zn(II) complex.

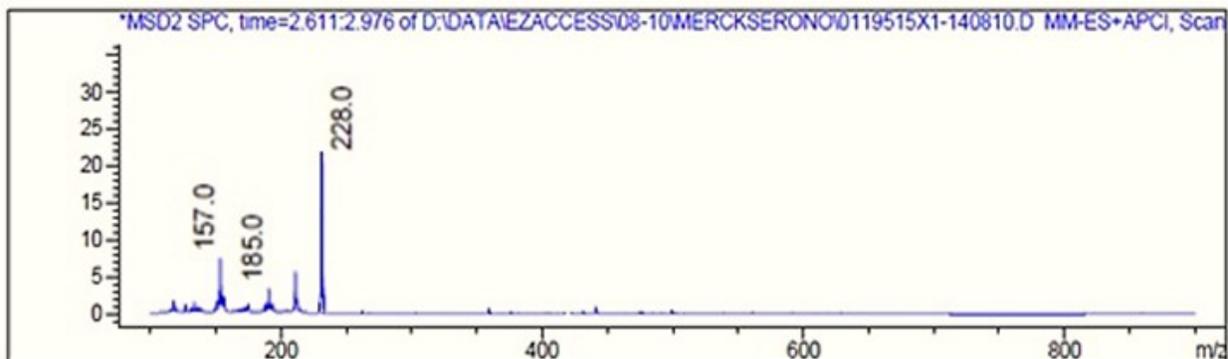


Figure S3: LCMS spectrum of Ligand AF.

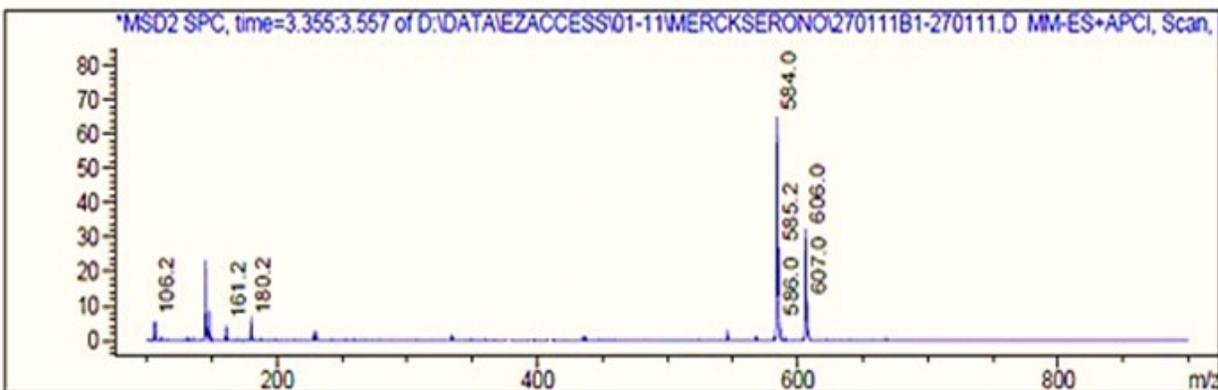


Figure S4: LCMS spectrum of Ni(II) complex .

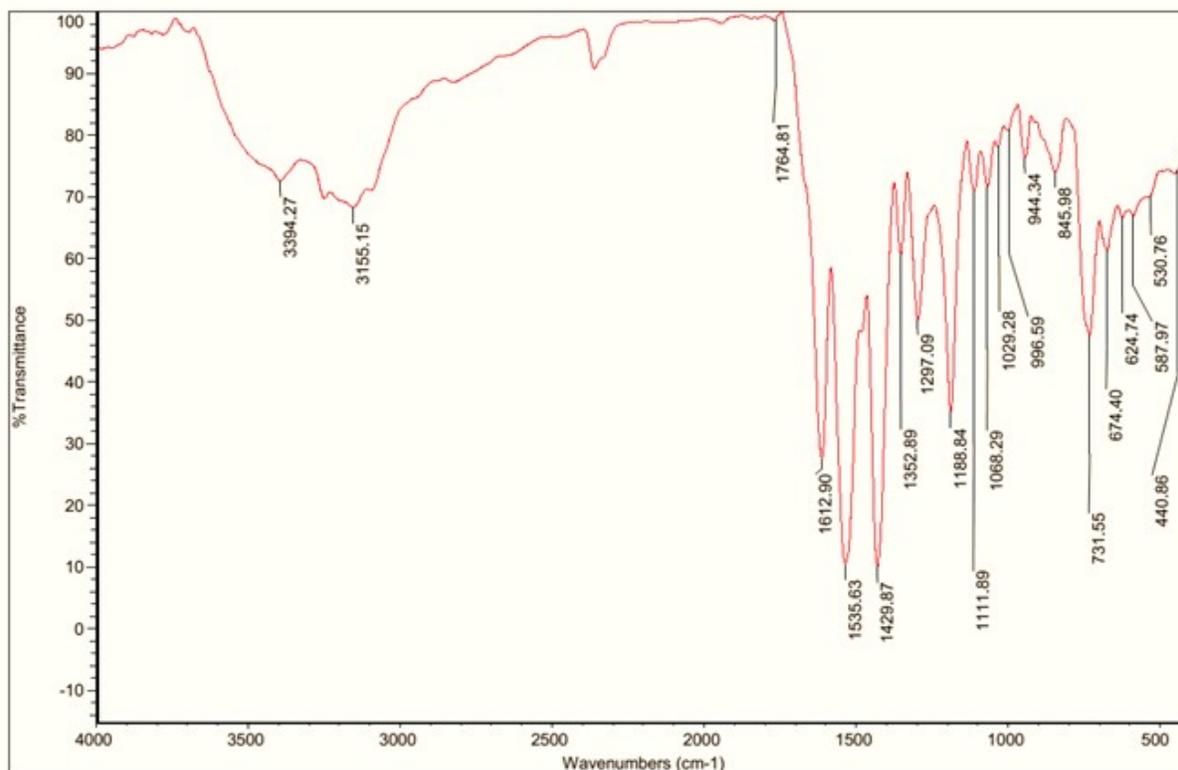


Figure S5: FT-IR Spectrum of Ligand AF .

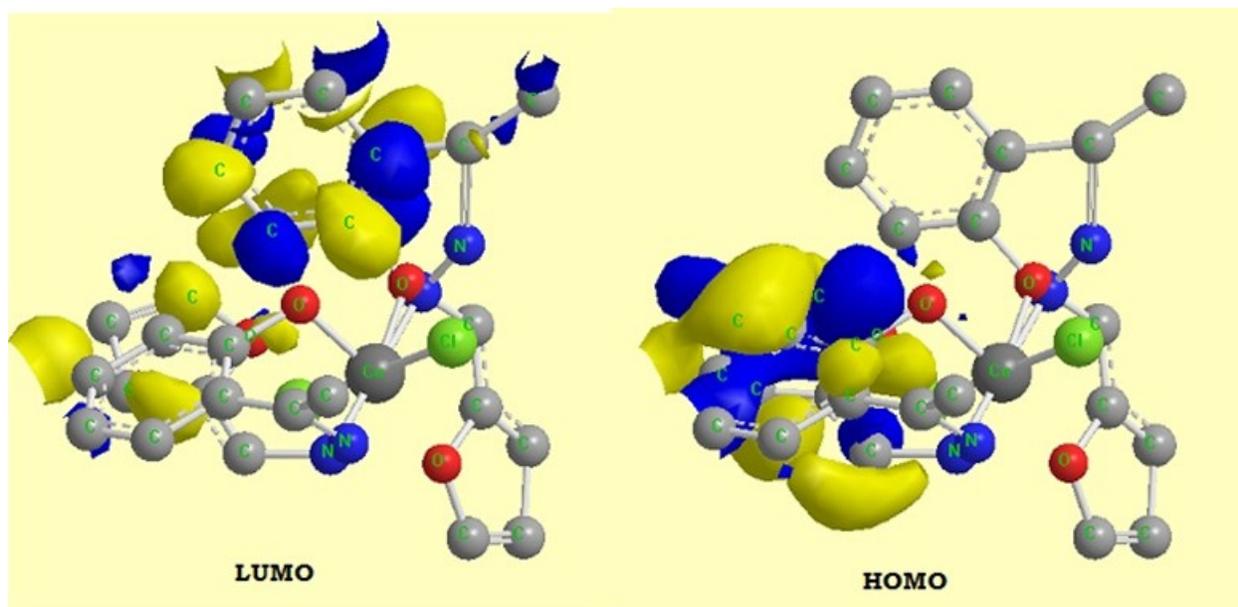
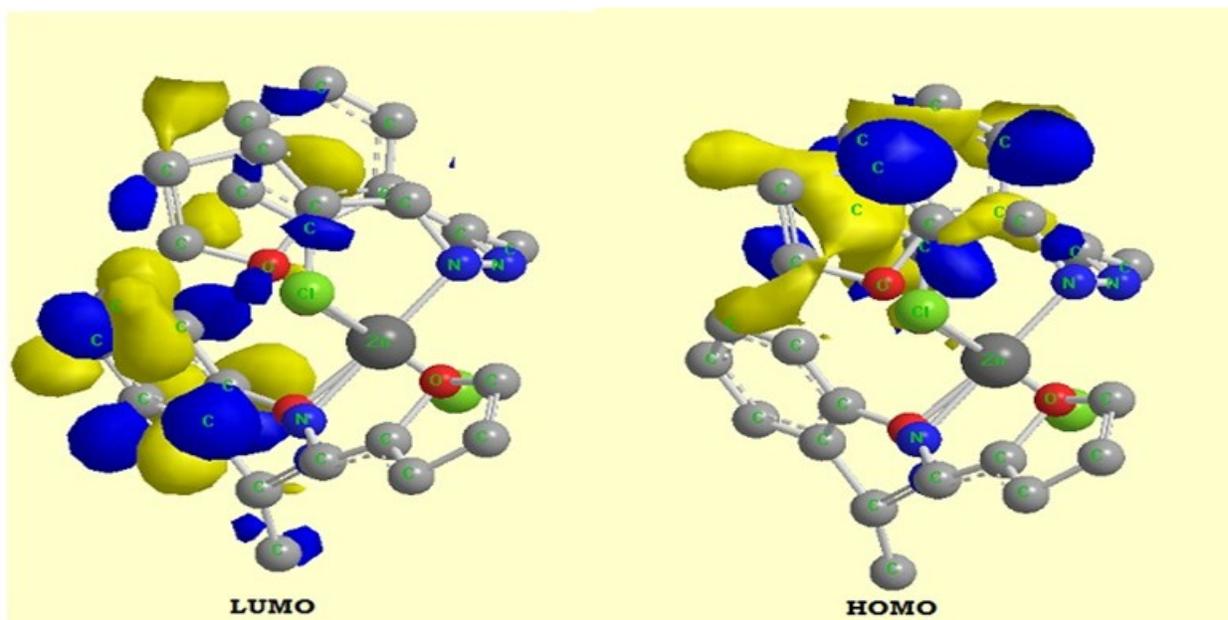


Figure S6:  $E_{LUMO}-E_{HOMO}$  [-5.114 eV and -2.231eV] molecular orbitals of Cu(II) complexes.



**Figure S7:**  $E_{\text{LUMO}}-E_{\text{HOMO}}$  [-6.221 eV and -4.241eV] molecular orbitals of Zn(II) complexes.