

SUPPLEMENTARY MATERIAL TO

Synthesis, Characterization, Thermal and Antimicrobial studies of Schiff base ligand and its Co(II) and Cu(II) complexes.

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Table S1. IR stretching frequencies of the ligand and their metal complexes in cm⁻¹

Compound	$\nu(\text{C}=\text{N})$	$\nu(\text{C}=\text{NH})$	Ring $\nu(\text{NH})$	$\nu(\text{NH}_2)$	$\nu(\text{M}-\text{N})$	$\nu(\text{M}-\text{Cl})$
$\text{C}_{10}\text{H}_{18}\text{N}_8$ L	1690	1560	3277	-	-	-
$[\text{Co}(\text{L})\text{Cl}_2]$ (1)	1641	-	-	3347 3186	418	369
$[\text{Cu}(\text{L})\text{Cl}_2]$ (2)	1628	-	-	3362 3156	434	371

Table S2. Electronic spectral data and magnetic moment values

Compounds	λ_{max} (nm)	Band assignments	μ_{eff} BM
$\text{C}_{10}\text{H}_{18}\text{N}_8$ L	235 350	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$	-
$[\text{Co}(\text{L})\text{Cl}_2]$ (1)	620 581	${}^4\text{A}_2 \rightarrow {}^4\text{T}_1$ (F) ${}^4\text{A}_2 \rightarrow {}^4\text{T}_1$ (P)	4.25
$[\text{Cu}(\text{L})\text{Cl}_2]$ (2)	584	${}^2\text{B}_{1g} \rightarrow {}^2\text{A}_{1g}$	1.73

Table S3. Chemical reactivity parameters of the ligand L

E_{total}	-829.9286
$\Delta E_{\text{HOMO-LUMO}}$	6.17757
Ionisation Potential (IP)	5.88260
Electron Affinity (EA)	-0.29497
Chemical Hardness (η)	3.08878
Electronegativity (χ)	2.7938
Chemical Potential (μ)	-2.7938
Global Softness (S) eV^{-1}	0.16187
Electrophilicity index (ω)	1.26349
Dipole moment (Debye)	3.3672

Table S4. The polarizability (α), the first – order hyperpolarizability (β_{tot}) and their components for the ligand and urea.

	$\langle\alpha\rangle$ (a.u)	$\Delta\alpha$ (a.u)	β_{tot} (a.u)	β_{tot} (esu)	$\beta_{\text{tot}} / \beta_{\text{tot(urea)}}$
Ligand	-107.78	31.36	82.99	7.17026×10^{-31}	2.1558
Urea	20.3	30.5	38.5	3.326×10^{-31}	1

Table S5. The zone of inhibition (mm) of ligands and their metal complexes

Compounds	Bacterial species				Fungal species	
	Std (Ciprofloxacin)				Std (Clotrimazole)	
	Gram + ve		Gram - ve			
	<i>S.aureus</i>	<i>B.subtilus</i>	<i>E.coli</i>	<i>P.aeruginosa</i>	<i>C.albicans</i>	<i>A.niger</i>
L	11	13	10	12	20	10
[Co LCl ₂]	29	29	33	37	26	28
[CuLCl ₂]	20	18	25	17	27	09
Standard	38	34	36	40	16	11

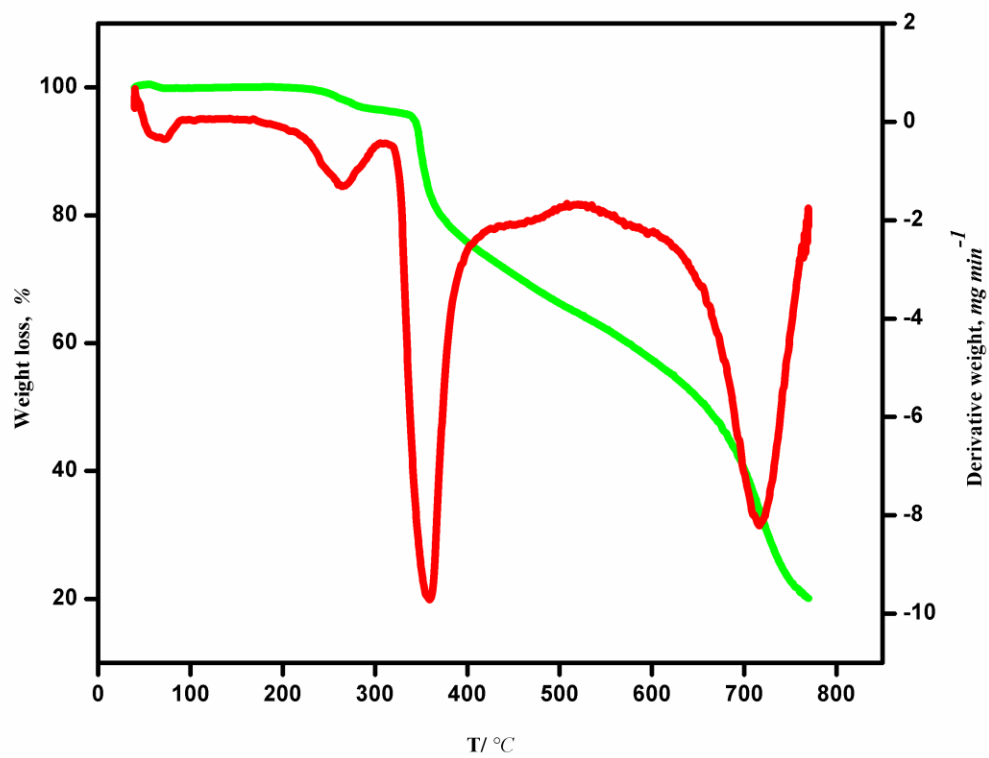


Fig. S1 Thermogram of Co(II) complex 1

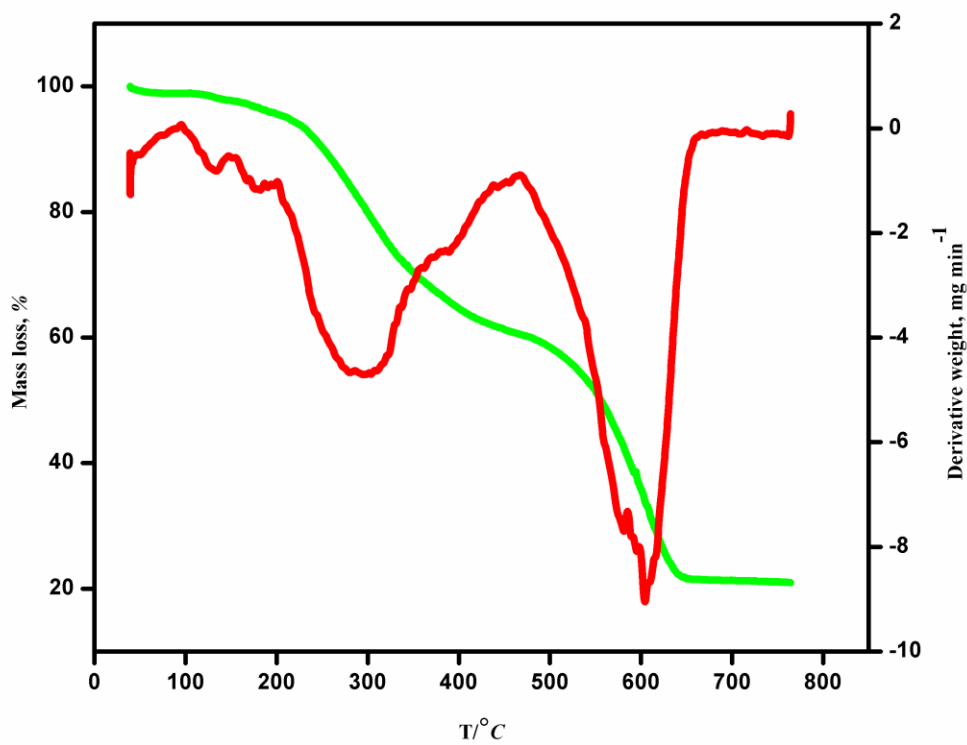


Fig. S2 Thermogram of Cu(II) complex 2

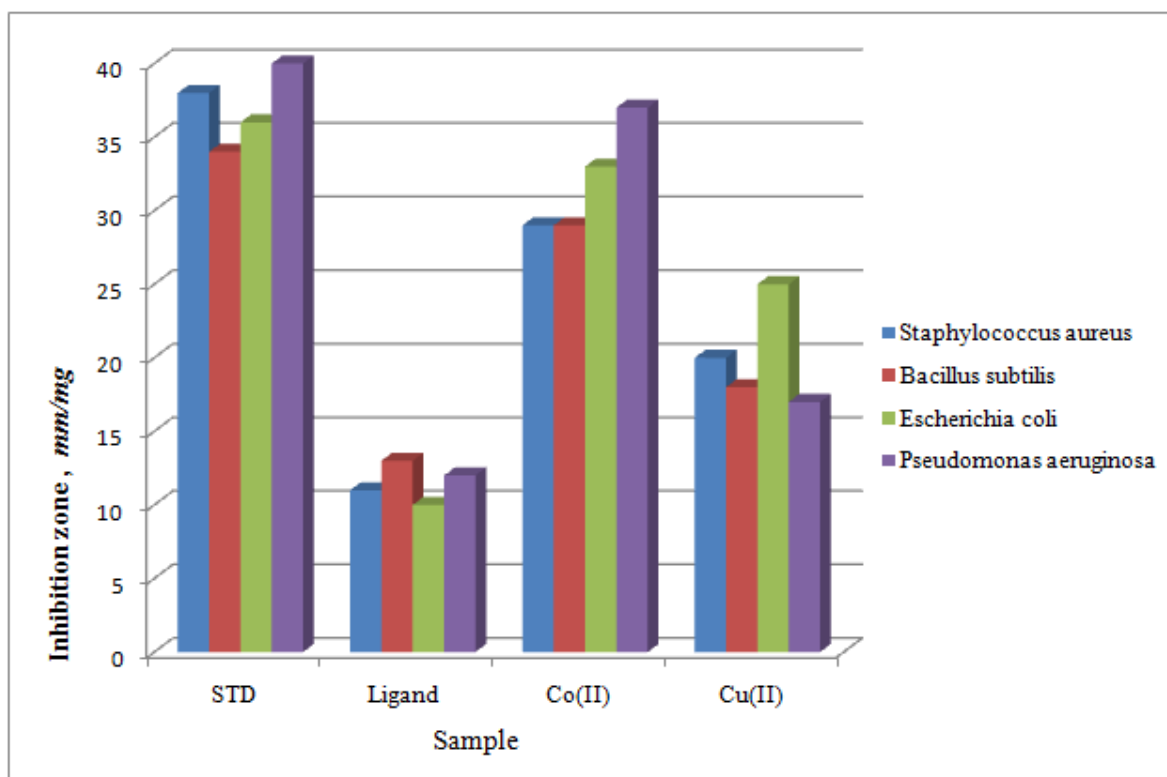


Fig.S3 Antibacterial activity of the Schiff base ligand and their metal complexes

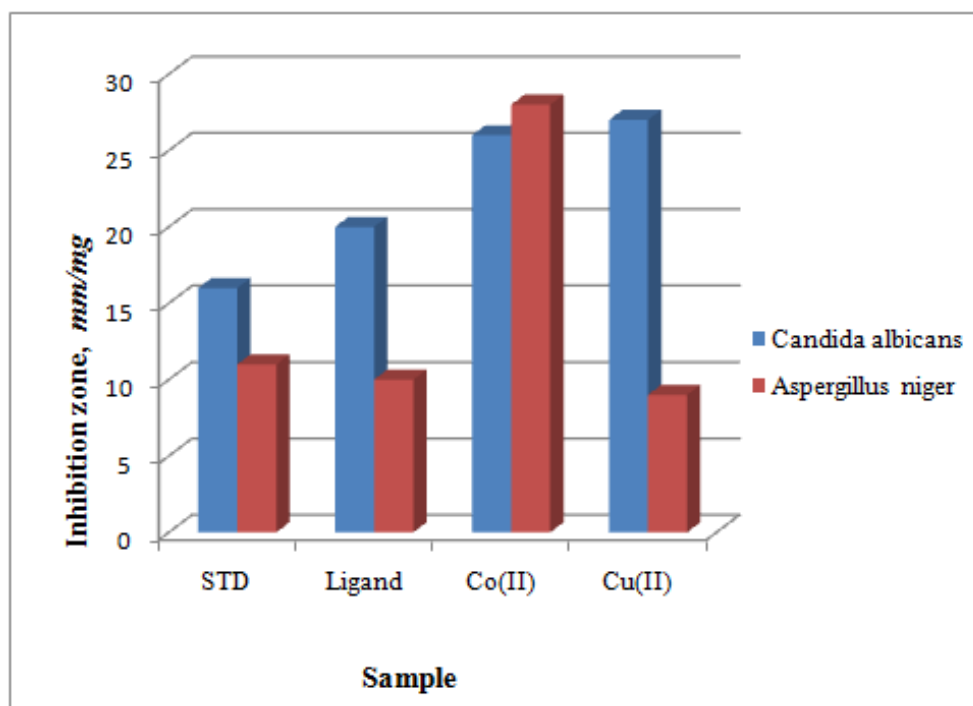


Fig.S4 Antifungal activity of the Schiff base ligand and their metal complexes