

SUPPLEMENTARY MATERIAL TO
Synthesis, characterization, thermal, theoretical and antimicrobial studies of Schiff base ligand and its Co(II) and Cu(II) complexes

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CHARACTERISATION DATA FOR THE LIGAND AND ITS Co AND Cu COMPLEXES

Ligand L. Yield: 82 %; m.p.: 215 °C, Anal. Calcd for C₁₀H₁₈N₈: C, 47.98; H, 7.25; N, 44.77 %. Found: C, 47.76; H, 7.17; N, 44.62 %; IR (cm⁻¹): 3277 ring (NH), 1690 (C=N), 1560 (C=NH); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 2.9 (3H, s, methyl); 3.3 & 3.6 (6H, 2s, methylene); 9.8 (1H, s, NH); UV-Vis (DMSO, λ_{max} / nm): 235, 350.

[Co(L)Cl₂] (**1**). Yield: 77 %, m.p.: >250 °C, Anal. Calcd.: C, 31.60; H, 4.77; N, 29.48; Co, 15.5 %. Found: C, 31.47; H, 4.89; N, 29.35; Co, 15.28 %; IR (cm⁻¹): 3347, 3186 (NH₂), 1641 (C=N), 418 (M–N), 369 (M–Cl); UV-Vis (DMSO, λ_{max} / nm): 620, 581; μ_{eff} (μ_B): 4.25.

[Cu(L)Cl₂] (**2**). Yield: 76 %; m.p.: >250 °C, Anal. Calcd: C, 31.22; H, 4.71; N, 29.12; Cu, 16.52 %. Found: C, 31.09; H, 4.59; N, 29.25; Cu, 16.38 %. IR (cm⁻¹): 3362, 3156 (NH₂), 1628 (C=N), 434 (M–N), 371 (M–Cl); UV-Vis (DMSO, λ_{max} / nm): 850–950; μ_{eff} (μ_B): 1.93.

TABLE S-I. IR stretching frequencies (ν / cm⁻¹) of the ligand and its metal complexes

Compound	ν					
	C=N	C=NH	Ring NH	NH ₂	M–N	M–Cl
C ₁₀ H ₁₈ N ₈ L	1690	1560	3277	–	–	–
[Co(L)Cl ₂] (1)	1641	–	–	3347, 3186	418	369
[Cu(L)Cl ₂] (2)	1628	–	–	3362, 3156	434	371

TABLE S-II. Electronic spectral data and magnetic moment values

Compound	λ _{max} / nm	Band assignments	μ _{eff} / μ _B
C ₁₀ H ₁₈ N ₈ L	235, 350	π → π* π*	–
[Co(L)Cl ₂] (1)	620, 581	⁴ A ₂ → ⁴ T ₁ (F); A ₂ → ⁴ T ₁ (P)	4.25
[Cu(L)Cl ₂] (2)	850–950	d–d envelope	1.93

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TABLE S-III. Chemical reactivity parameters of the ligand **L**

E_{total} / Hartree	-829.9286
$\Delta E_{\text{HOMO-LUMO}}$ / eV	6.17757
Ionisation potential, eV	5.88260
Electron affinity, eV	-0.29497
Chemical hardness, eV	3.08878
Electronegativity, eV	2.7938
Chemical potential, eV	-2.7938
Global softness, eV ⁻¹	0.16187
Electrophilicity index, eV	1.26349
Dipole moment, Debye*	3.3672

TABLE S-IV. The polarizability (α), the first-order hyperpolarizability (β_{tot}) and their components for the ligand and urea

Cmpd.	$\langle\alpha\rangle$ (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}	5.223
Urea	-21.5925	8.375	15.892	1.3729×10^{-31}	1

TABLE S-V. The zone of inhibition (mm) of ligands and its metal complexes; amount of substance: 100 μg ; solvent used DMSO

Compound	Species					
	Bacterial species Std. (ciprofloxacin)				Fungal species Std. (clotrimazole)	
	Gram +		Gram -			
	<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
[CoLCl ₂]	29	29	33	37	26	28
[CuLCl ₂]	20	18	25	17	27	09
Standard	38	34	36	40	16	11

* 1 D $\approx 3.33564 \times 10^{-30}$ C m

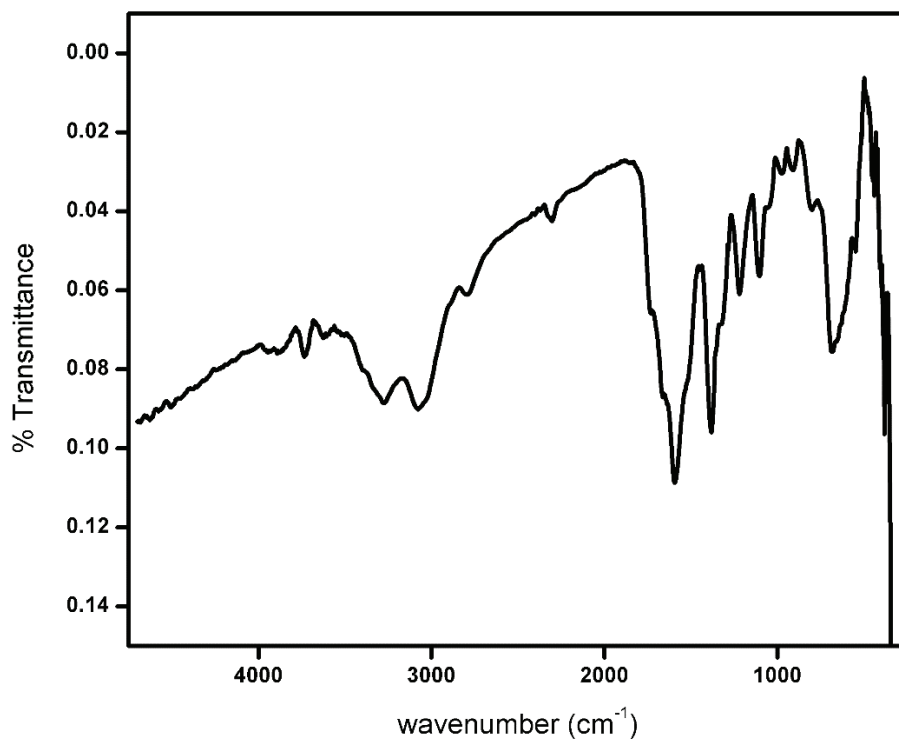
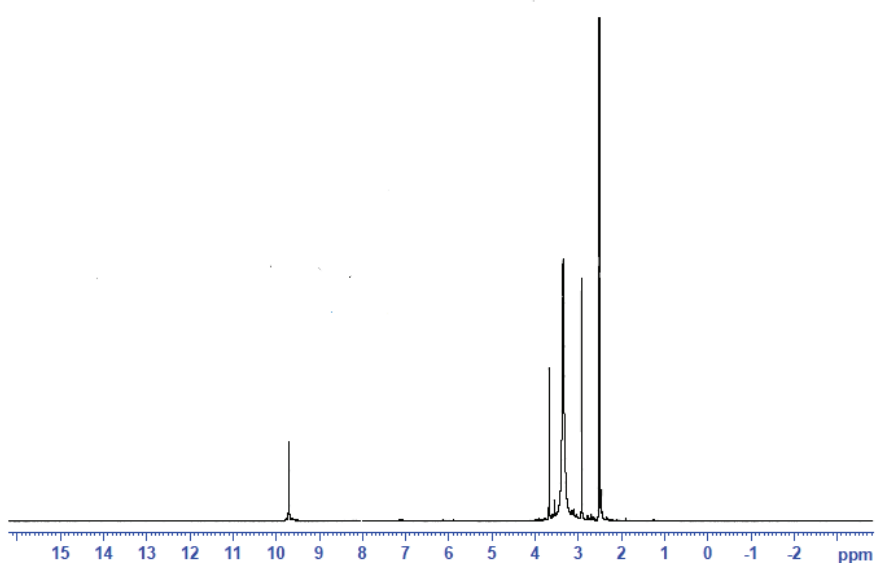


Fig. S-1. FTIR spectrum of the Schiff base ligand L.

Fig. S-2. ¹H-NMR spectrum of the Schiff base ligand L.

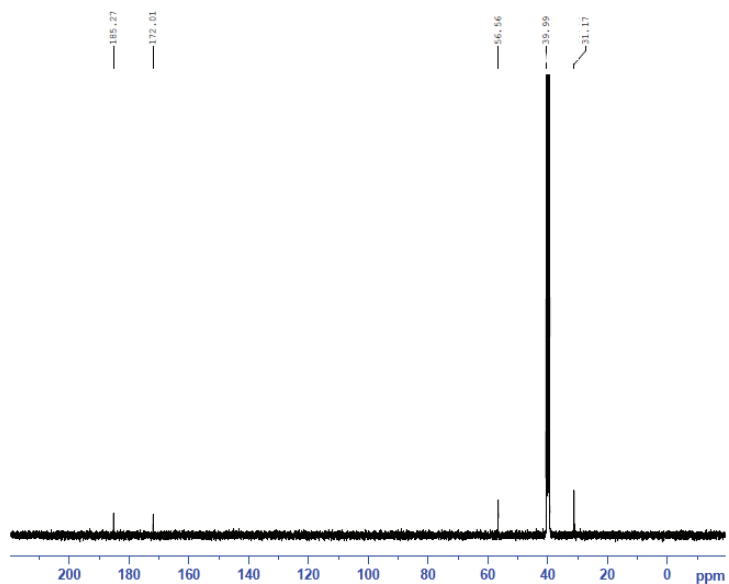
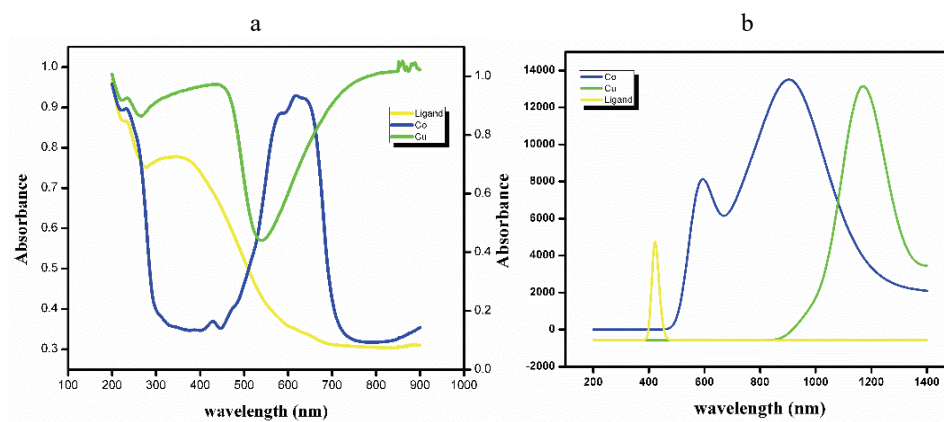
Fig. S-3. ^{13}C -NMR spectrum of the Schiff base ligand L.

Fig. S-4. Electronic spectrum of the Schiff base ligand L and its Co(II) and Cu(II) complexes: a – experimental; b – calculated.

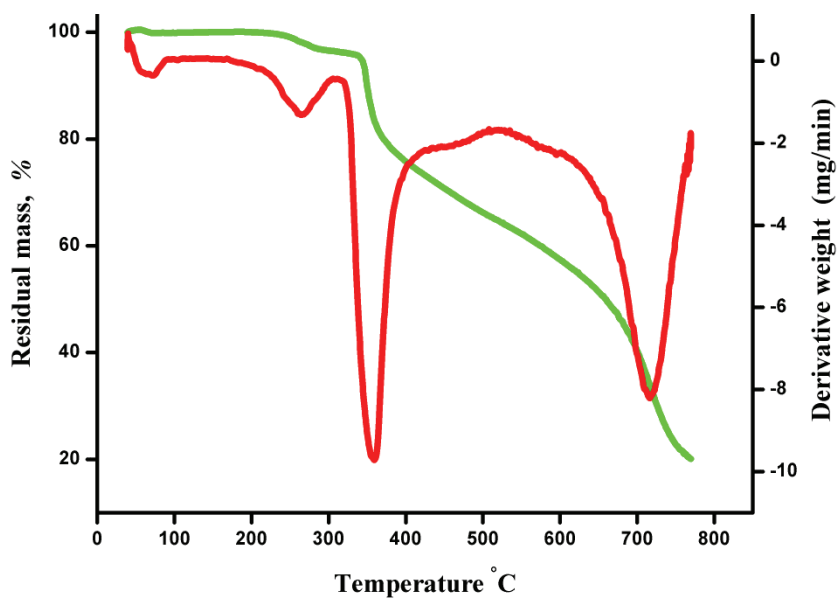


Fig. S-5. Thermogram of the Co(II) complex 1.

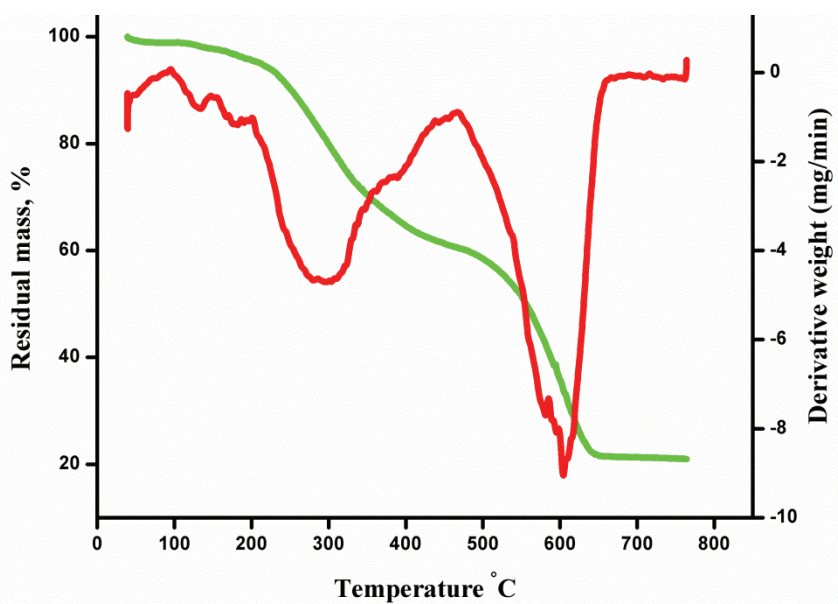


Fig. S-6. Thermogram of the Cu(II) complex.

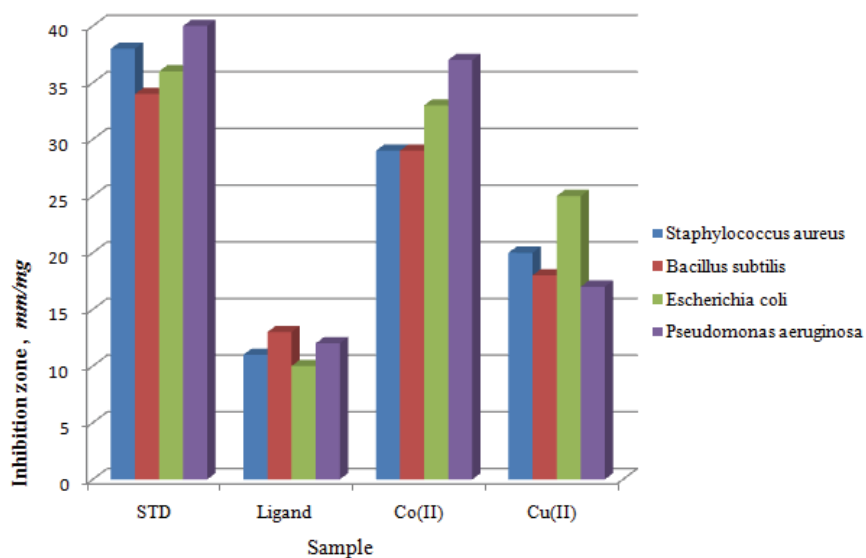


Fig. S-7. Antibacterial activity of the Schiff base ligand and its metal complexes.

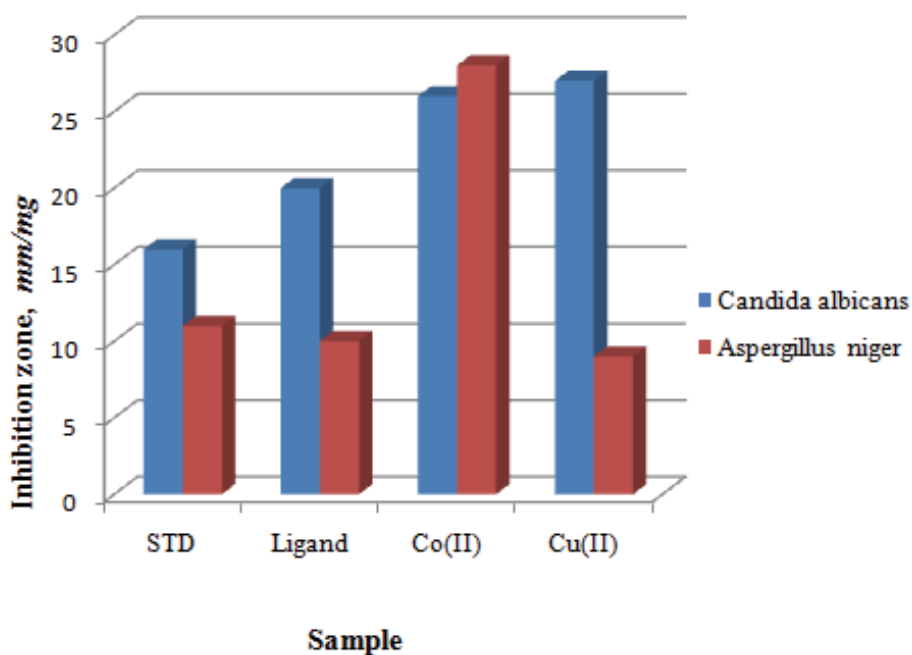


Fig. S-8. Antifungal activity of the Schiff base ligand and its metal complexes.