

Supplementary Information

An Innovative Schiff-Base Colorimetric Chemosensor for the Selective Detection of Cu^{2+} ions and its applications

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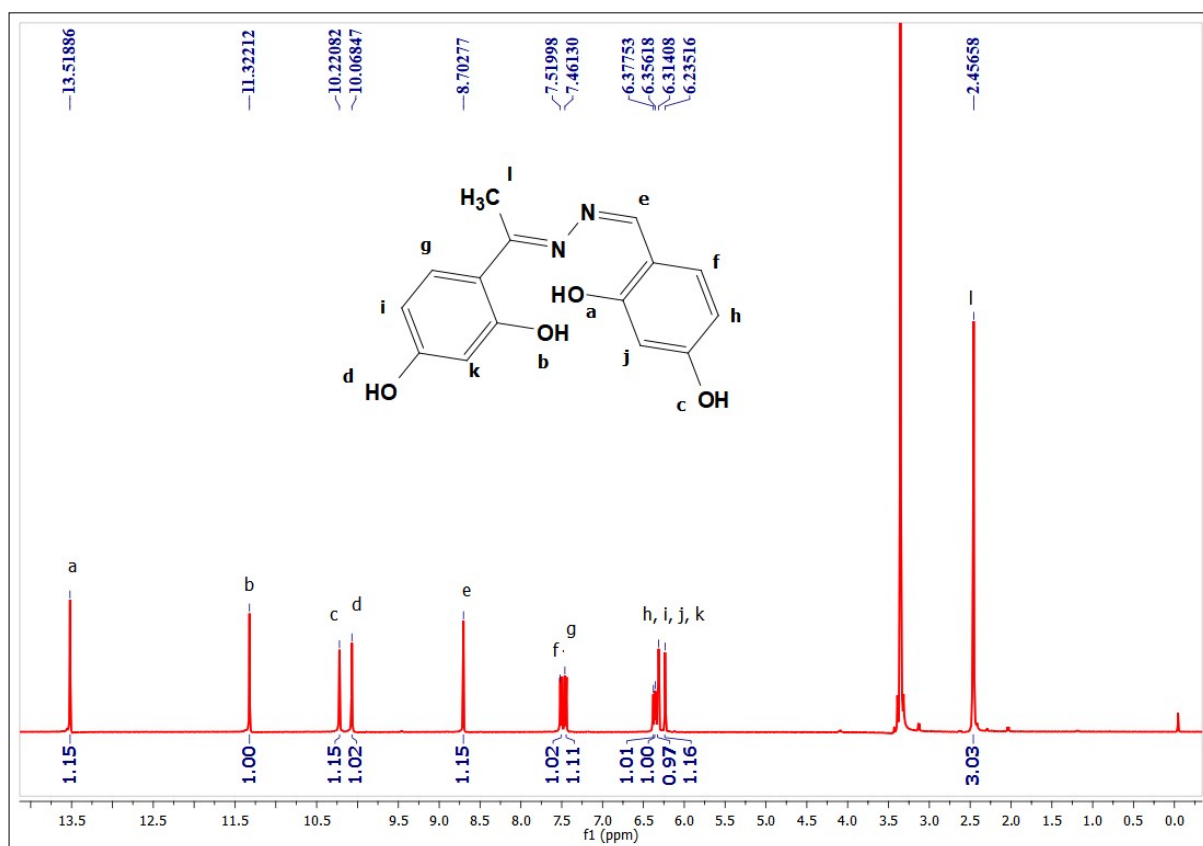


Figure S1. ¹H NMR of compound L in (DMSO-*d*₆, 400 MHz)

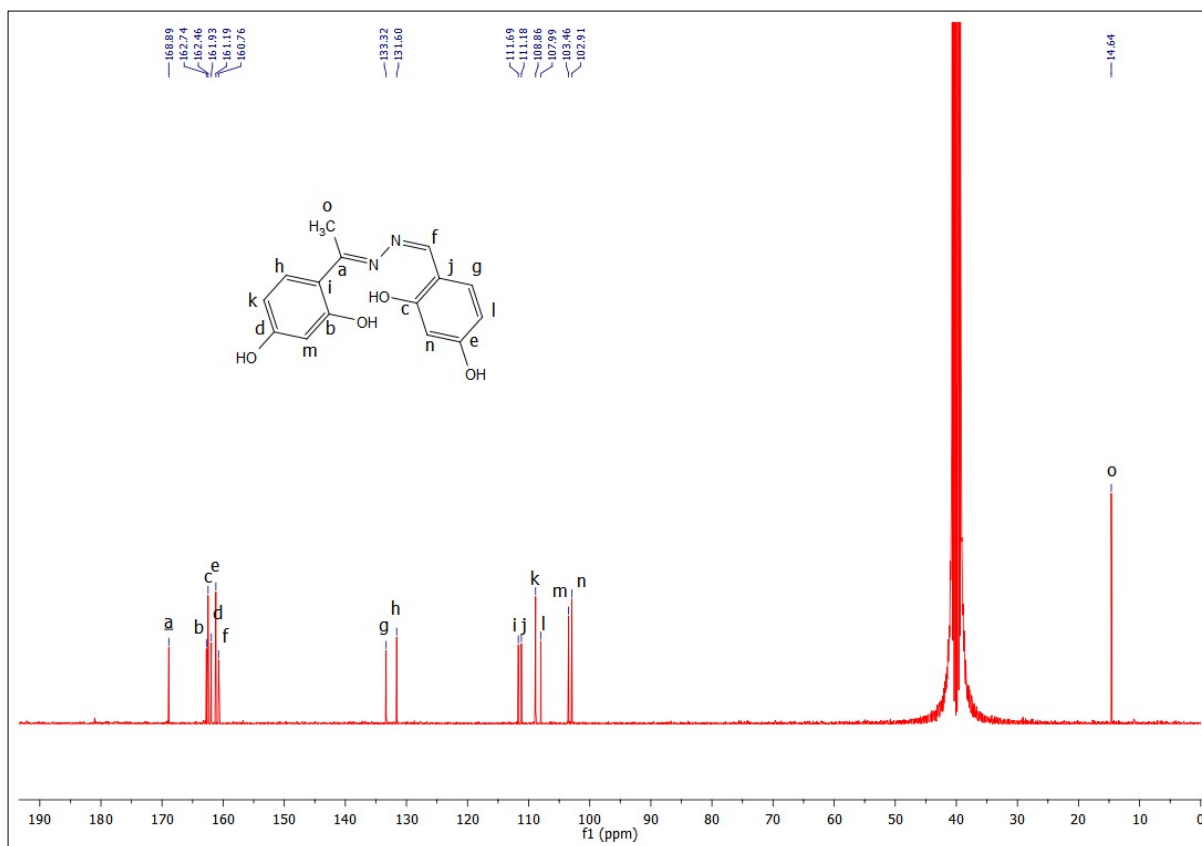
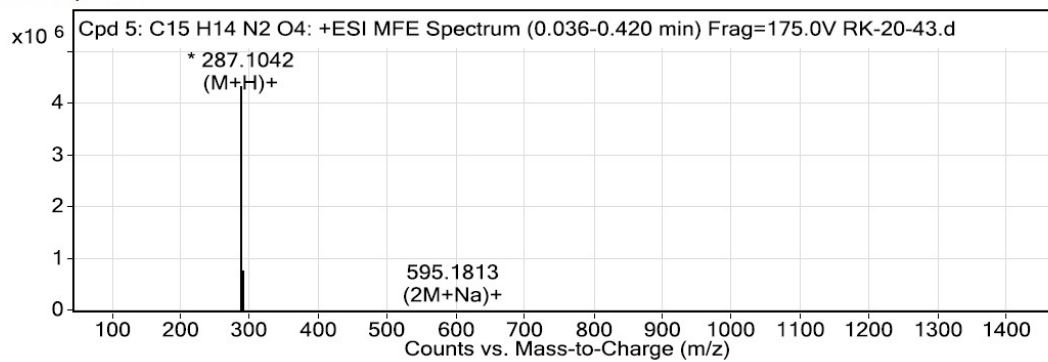


Figure S2. ^{13}C NMR of compound L in ($\text{DMSO-}d_6$, 100 MHz)

MFE MS Spectrum



MFE MS Zoomed Spectrum

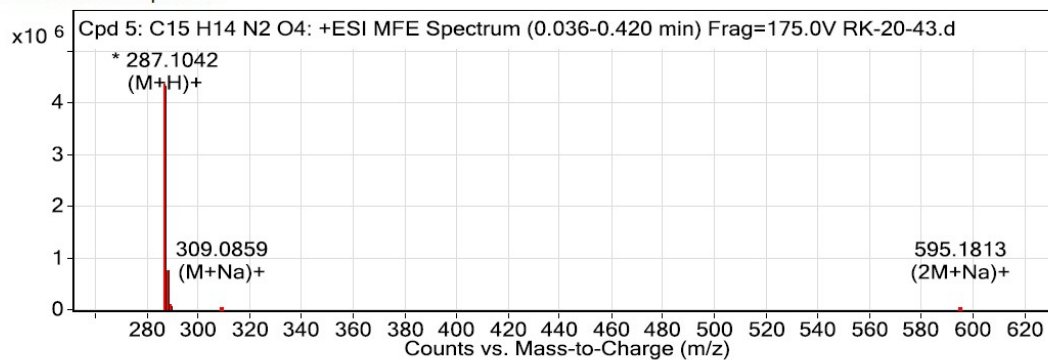


Figure S3. HRMS data of compound L

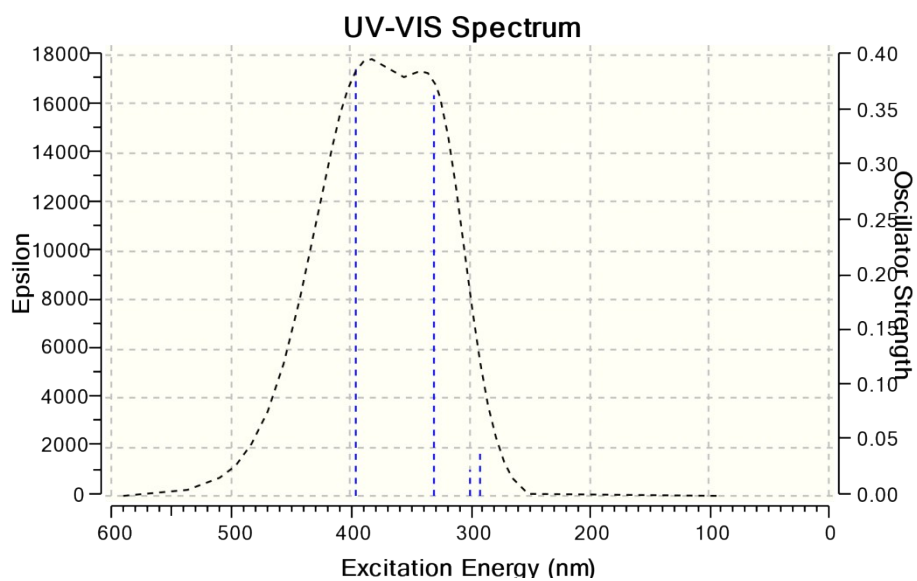


Figure S4 : Simulated spectrum of ligand L.

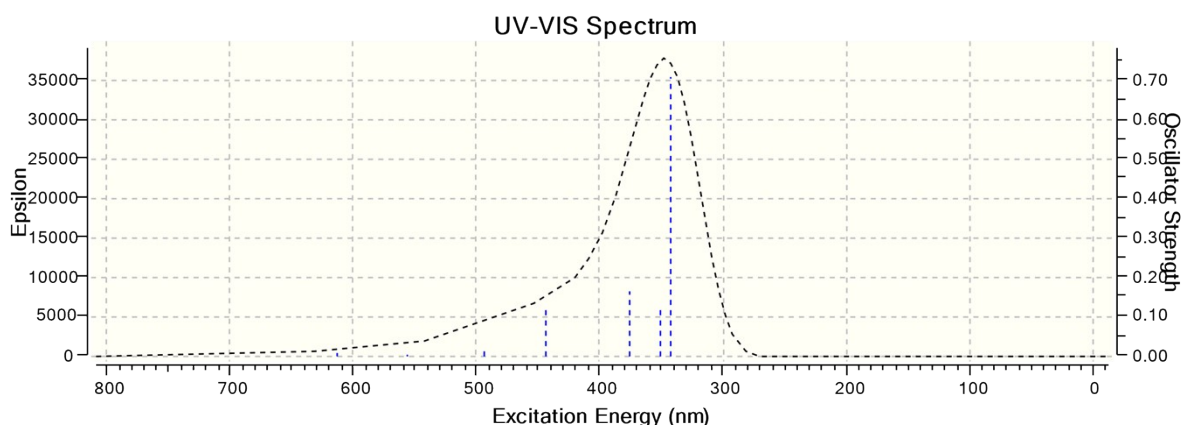


Figure S5: Simulated spectrum of the L-Cu²⁺ complex.

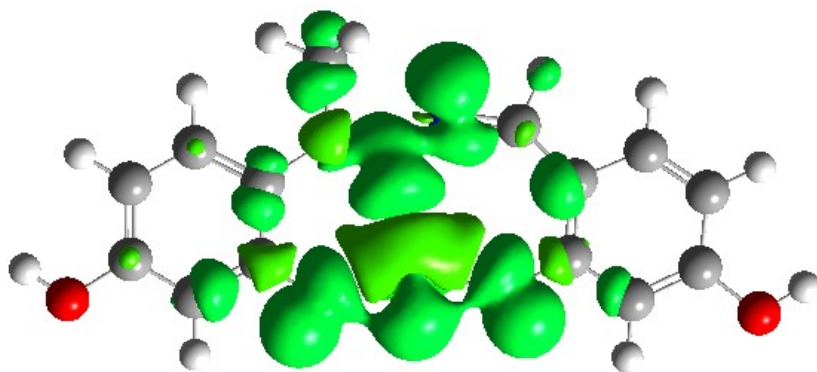


Figure S6: Mulliken spin-density distribution.

Table S1. Crystal data and structure refinement for ligand	
Identification code	L
Empirical formula	C ₁₅ H ₁₄ N ₂ O ₄
Temperature/K	293(2)
Crystal system	triclinic
Space group	P -1
a/Å	6.8450(7)
b/Å	7.2531(8)
c/Å	15.6037(17)
α/°	95.832(3)
β/°	98.967(3)
γ/°	108.964(3)
Volume/Å ³	714.00(13)
Z	14
ρ _{calc} /cm ³	1.415
μ/mm ⁻¹	0.108
F(000)	320.0
Radiation	Mo/K _α (λ = 0.71073)
2θ range for data collection/°	3.0431 to 27.8734
Index ranges	-8 ≤ h ≤ 8, -8 ≤ k ≤ 8, -18 ≤ l ≤ 19
No of Reflections measured	2676
Independent reflections	2171
Goodness-of-fit on F ²	1.089
R [F ² > 2σ (F ²)], wR(all data)	0.0746, 0.1762

Table S1. Crystal data and structure refinement for ligand.

Excitation	Spin Multiplicity	Transition	Weight (%)	Excitation Energy	Wavelength (nm)	Oscillator Strength

				(eV)		(f)
1	¹ A''	HOMO-1→LUMO	49	3.07	404	0.0008
2	¹ A'	HOMO→LUMO	48	3.14	395	0.3934
3	¹ A'	HOMO-2→LUMO	47	3.75	331	0.3633
4	¹ A'	HOMO-3→LUMO	34	4.12	301	0.0233
5	¹ A'	HOMO→LUMO+1	30	4.25	292	0.0397
6	¹ A''	HOMO-1→LUMO+1	42	4.47	277	0.0002

Table S2: Excitation energies and oscillator strengths of ligand **L**.

Excitation	Spin Multiplicity	Transition	Weight (%)	Excitation Energy (eV)	Wavelength (nm)	Oscillator Strength (f)
4	² A'	β HOMO-3→LUMO	33	2.02	613	0.0073
5	⁴ A'	β HOMO→LUMO+1	48	2.07	599	0.0006
		α HOMO→LUMO	42			
6	² A'	β HOMO-3→LUMO	22	2.23	556	0.0027
8	² A'	β HOMO-10→LUMO	39	2.51	494	0.0233
10	² A'	α HOMO→LUMO	18	2.79	444	0.1206
11	⁴ A'	α HOMO-2→LUMO		2.83	438	0.0010

Table S3: Excitation energies and oscillator strengths for the complex

S.No	Limit of Detection (LOD; nM)
1	42.091
2	42.10

3	42.087
Average	42.0927

Table S4: Showing the trials of calculated detection limits.

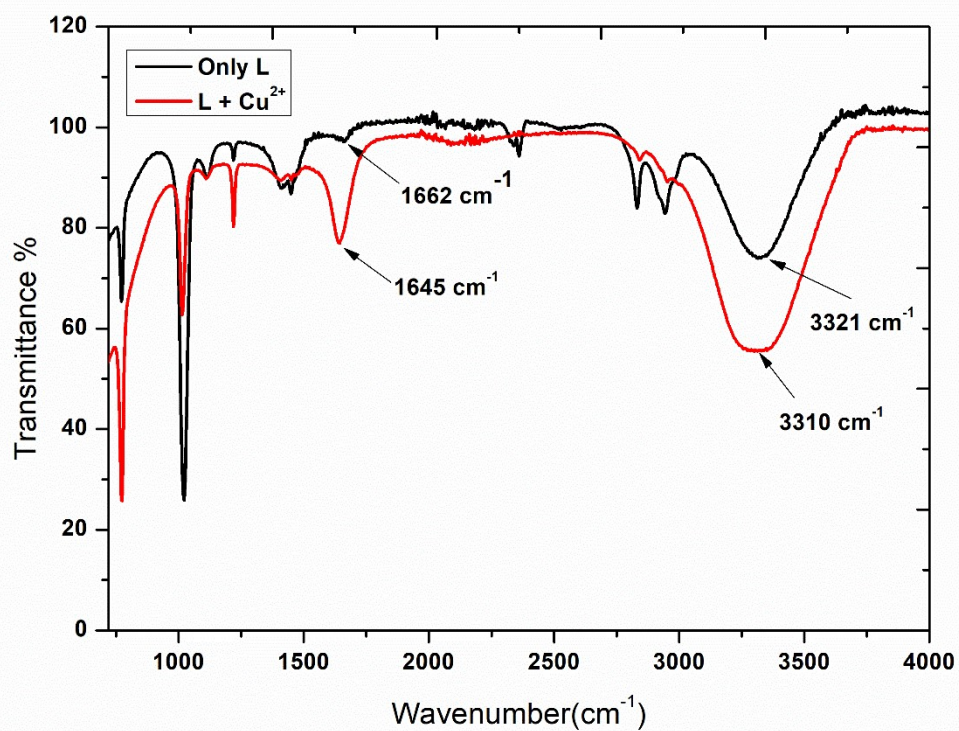


Figure S7. IR Spectrum of ligand L & L-Cu²⁺