

Supplementary Information

Design, structural and theoretical characterizations of novel Schiff base compounds: Enzymes inhibitory potential using *in vitro* and *in silico* methods

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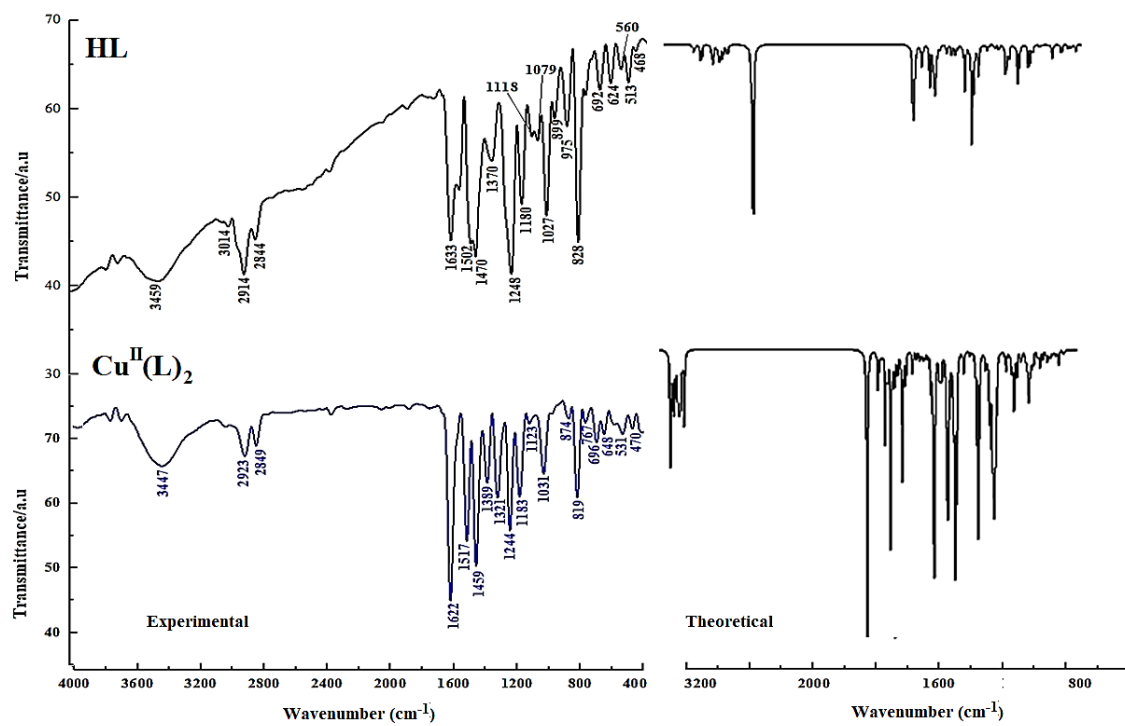


Fig. S1 — Infrared experimental and theoretical spectra of HL and its copper complex (Cu^{II}(L))

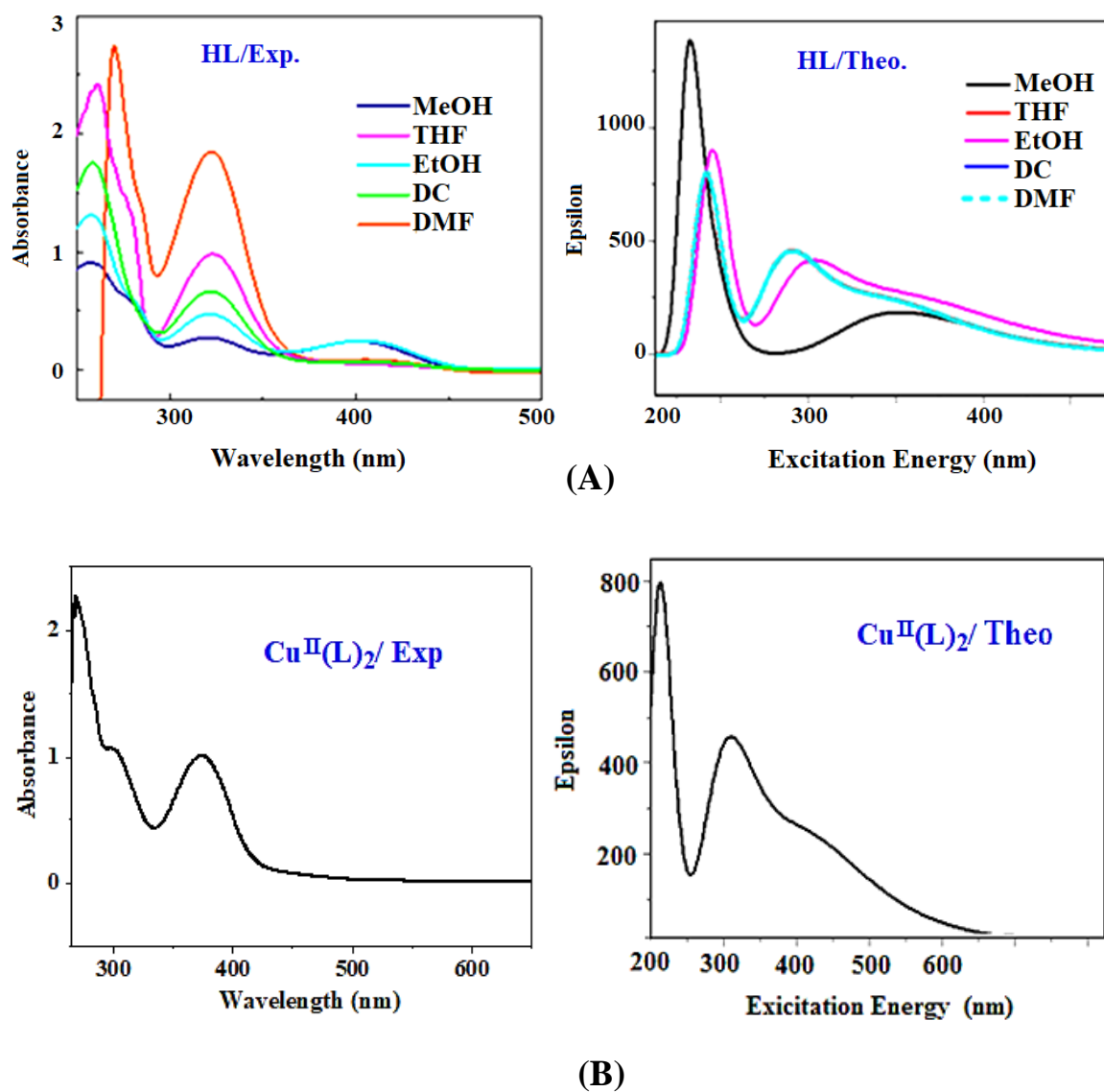


Fig. S2 —UV-visible experimental and theoretical absorption spectra of (A) HL ($1.0 \cdot 10^{-5}$ M) in different solvents and (B) $\text{Cu}^{\text{II}}(\text{L})_2$ in DMF selected medium

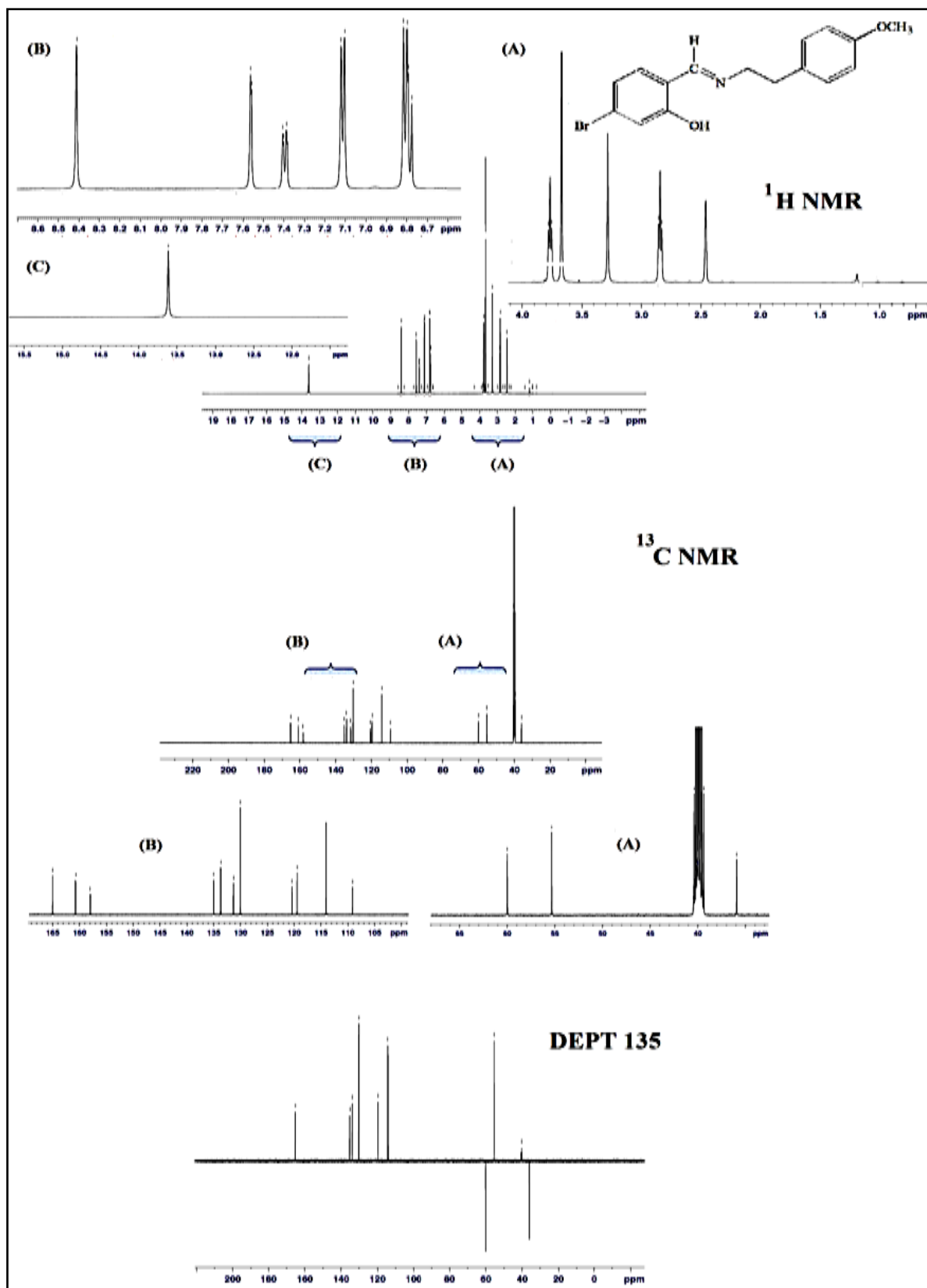


Fig. S3 — ¹H-, ¹³C-, and DEPT 135-NMR spectra of the Schiff base ligand (HL)

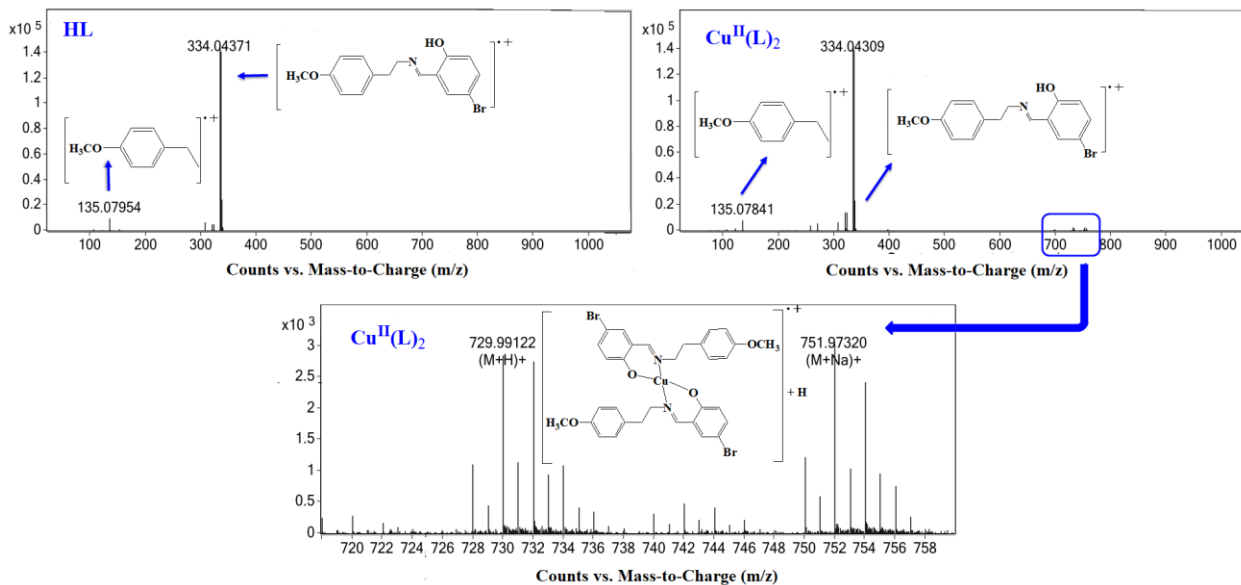


Fig. S4 — Mass spectra of HL and its copper complex ($\text{Cu}^{\text{II}}(\text{L})_2$)

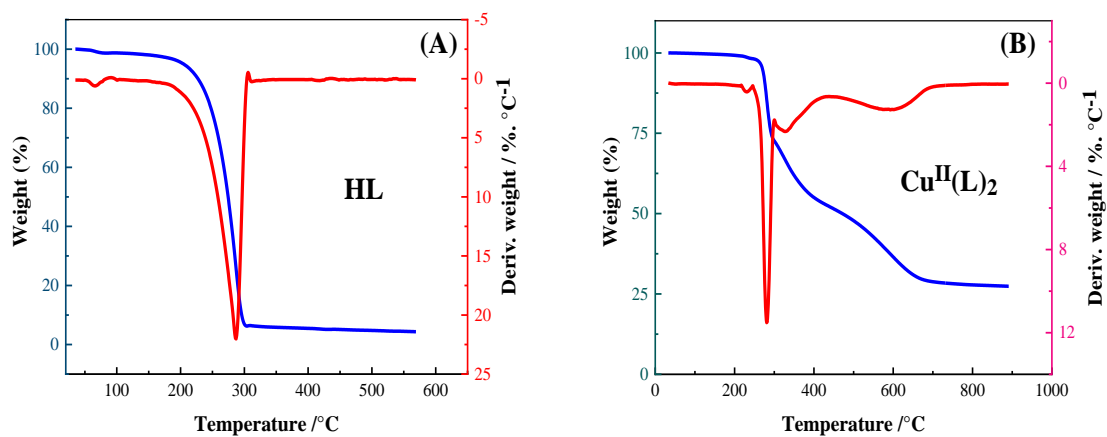
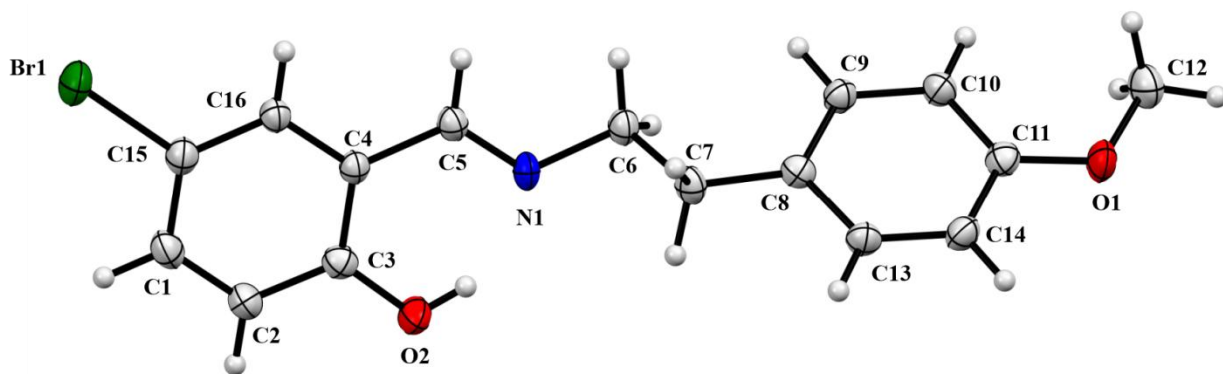
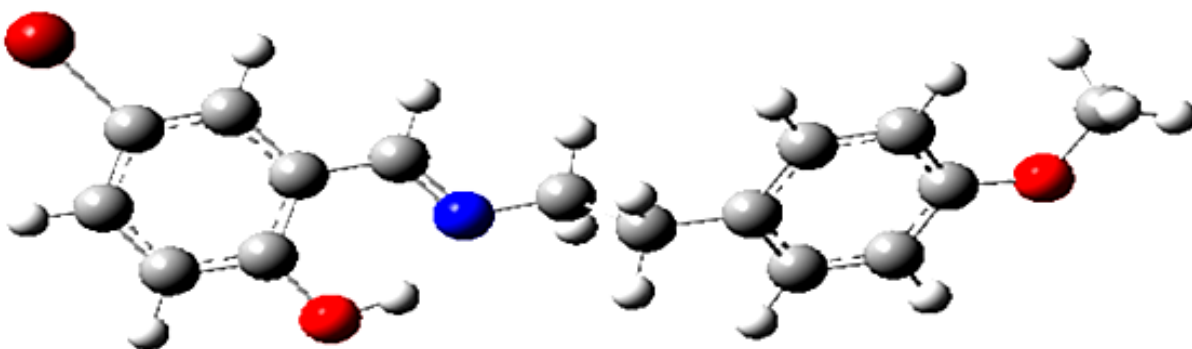


Fig. S5 — TG and DTG thermograms of HL (A) and (B) its copper complex ($\text{Cu}^{\text{II}}(\text{L})_2$)



(A)



(B)

Fig. S6 — The experimental (A), optimized geometric structure (B) for HL ligand at B3LYP/6-6-31G(d,p) level

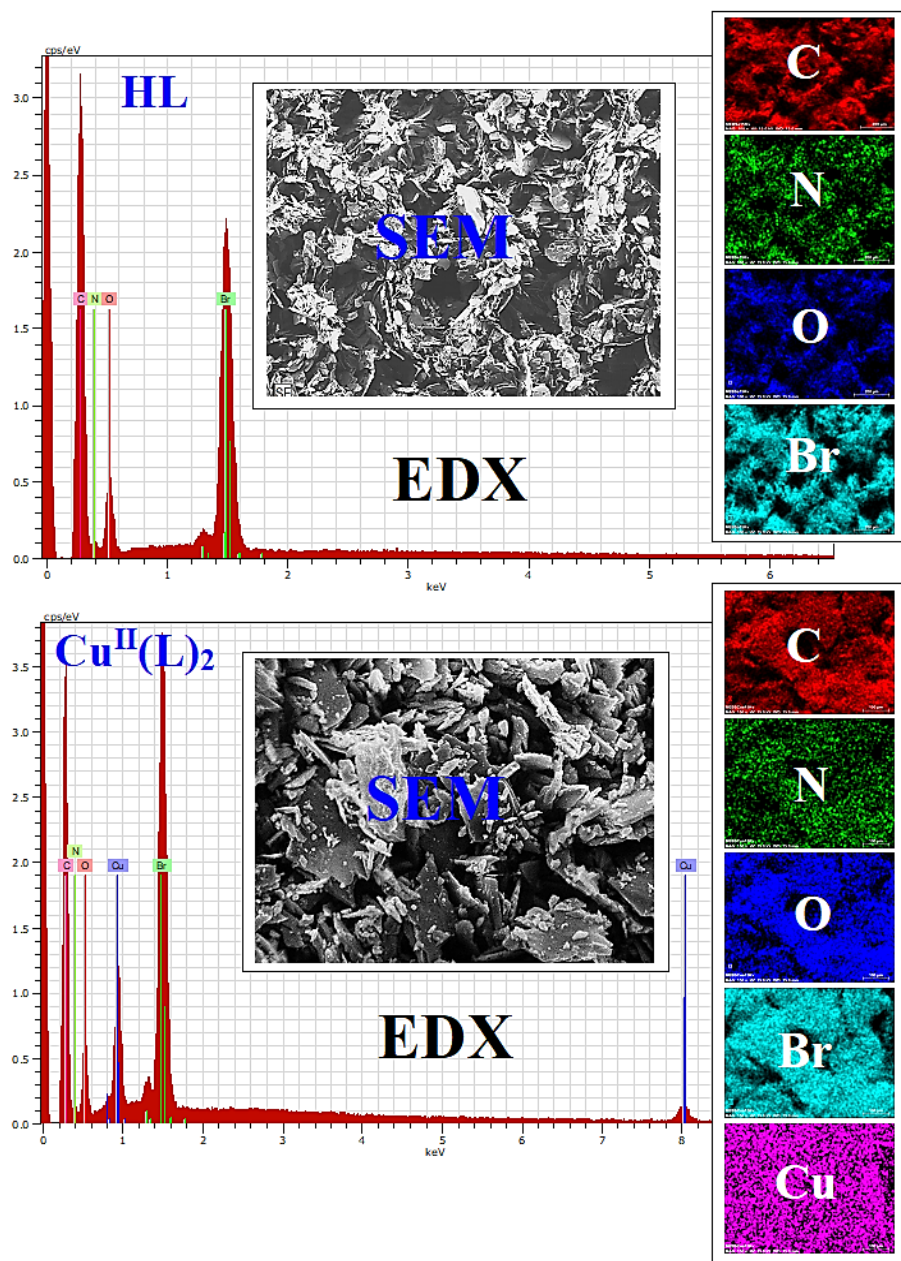


Fig. S7 — SEM images and EDX spectra of HL and Cu^{II}(L)₂

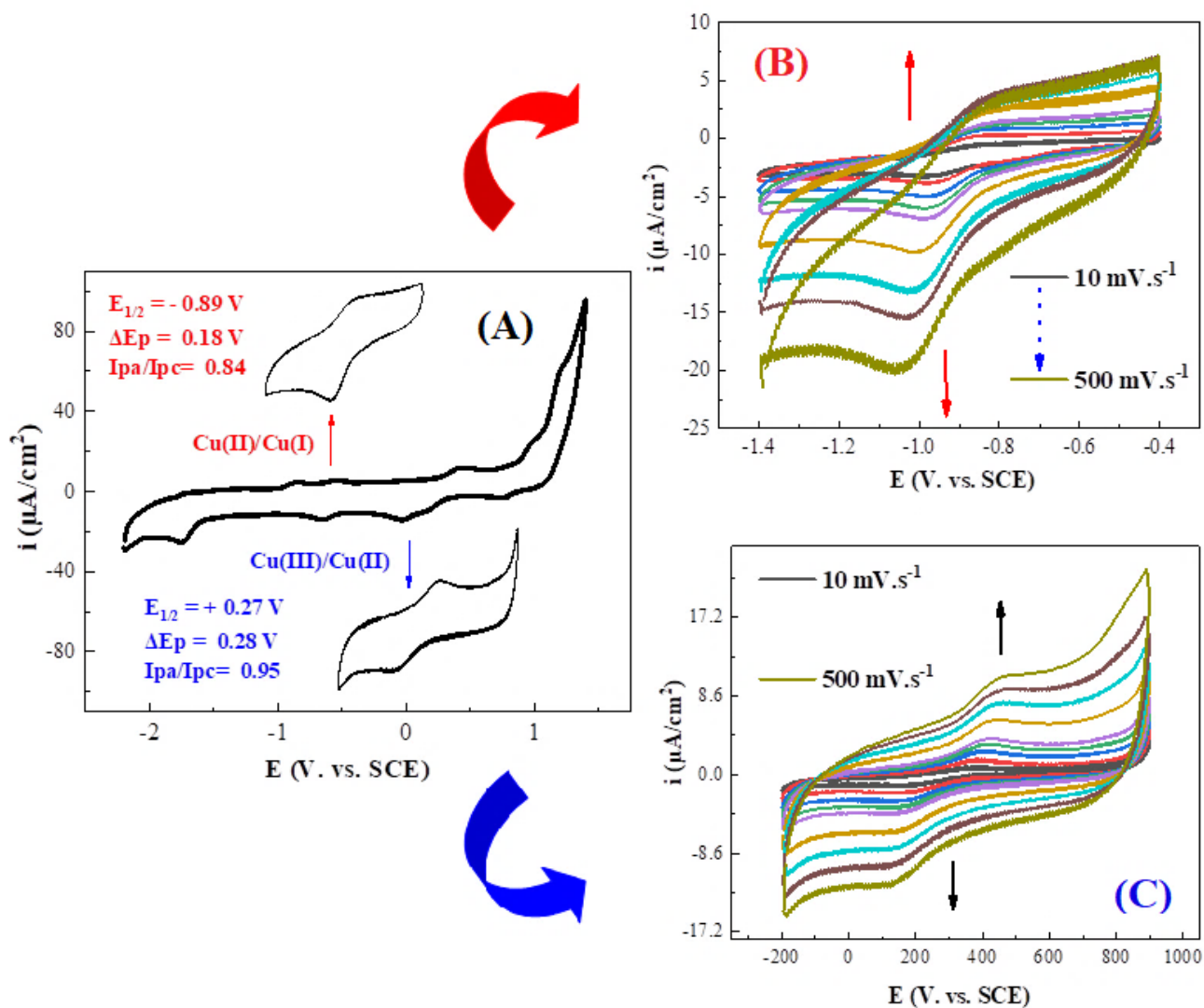


Fig. S8 — Cyclic voltammograms of 10^{-3} M solution of $\text{Cu}^{\text{II}}(\text{L})_2$ complex in DMSO solution 10^{-1} M of TBAP: (A) at 100 Mv/s between +1.5 and -2.2 V/SCE; (B) Cu(II)/Cu(I) redox system at various scan rates between -0.4 and -1.4 V/SCE and (C) Cu(III)/Cu(II) redox system at various scan rates between -0.2 and +0.9 V/SCE

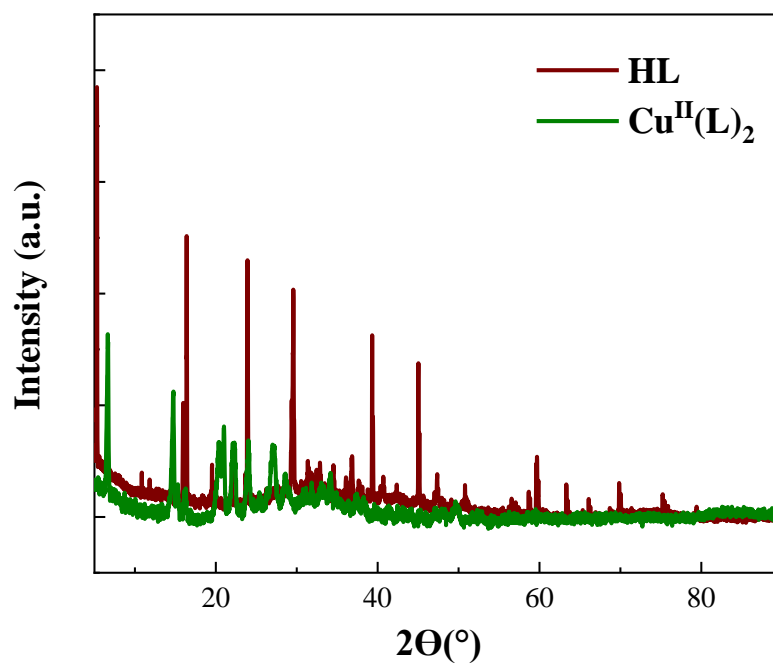


Fig. S9 — Powder XRD graphs for HL and $\text{Cu}^{\text{II}}(\text{L})_2$ complex

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Samples		Absorption band assignments							
		$\nu(\text{OH})$	$\nu(\text{C-H})$	$\nu(\text{C=N})$	$\nu(\text{C-O})$	$\nu(\text{C=C})$	$\nu(\text{C-Br})$	$\nu(\text{M-N})$	$\nu(\text{M-O})$
HL	Experimental Frequencies (cm^{-1})	3459	2914	1633	1370	1502	828	-	-
	Theoretical Frequencies (cm^{-1})	3249	2999	1634	1370	1515	828	-	-
$\text{Cu}^{\text{II}}(\text{L})_2$	Experimental Frequencies (cm^{-1})	3447	2923	1622	1389	1517	819	470	698
	Theoretical Frequencies (cm^{-1})	3379	3059	1626	1374	1518	819	464	701

HL				Cu ^{II} (L) ₂		
	Experimental	Calculated		Experimental	Calculated	
	λ (nm)	λ (nm)	f_{os}	λ (nm)	λ (nm)	f_{os}
MeOH	321	328.91	0.00046			
	257	241.15	0.0326			
EtOH	322	358.17	0.0109			
	258	268.2	0.0198			
DC	322	358.17	0.0109			
	258	268.2	0.0198			
THF	323	353.7	0.0097			
	261	262.26	0.0223			
DMF	322	357.77	0.0198	381	448	0.0058
	270	230.73	0.0197	322	342	0.0119
				270	223	0.0168

\mathcal{E} = molar absorption coefficient ($\times 10^6, \text{dm}^3 \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$), f_{os} = oscillator strength

HL		Cu ^{II} (L) ₂			
Atom	Charge	Atom	Charge	Atom	Charge
C1	-0.136867	C1	-0.072103	C49	-0.346179
C2	-0.129591	C2	-0.176983	C50	-0.323653
C3	0.262189	C3	0.270973	C51	-0.182801
C4	-0.144653	C4	-0.012772	O52	-0.540403
C5	-0.145912	C5	-0.085730	O53	-0.644694
C6	0.055095	C6	-0.149833	Br54	0.124269
H7	0.124607	H7	0.118412	N55	-0.455683
H8	0.135413	H8	0.138668	C56	0.058989
H9	0.129925	H9	0.173890	H57	0.152551
C10	-0.091934	C10	-0.074690	H58	0.165281
C11	-0.094453	C11	-0.140441	H59	0.148606
C12	0.155412	C12	0.244360	H60	0.326674
C13	0.144783	C13	0.106192	H61	0.246182
C14	-0.144916	C14	-0.154518	H62	0.213661
C15	-0.315074	C15	-0.323123	H63	0.168822
H16	0.152060	H16	0.142048	H64	0.134269
H17	0.148152	H17	0.159693	Cu65	0.624911
H18	0.152536	H18	0.138960	O66	-0.505679
O19	-0.573720	O19	-0.652937	C67	-0.185261
H20	0.374275	C20	-0.267243	H68	0.150478
C21	-0.324673	C21	-0.269619	H69	0.152029
C22	0.280514	C22	0.047722	H70	0.170724
C23	-0.011344	N23	-0.358512		
N24	-0.265577	H24	0.240190		
H25	0.240134	H25	0.240456		
H26	0.248372	H26	0.183294		
H27	0.183482	H27	0.152385		
H28	0.139429	H28	0.125061		
H29	0.115258	Br29	0.131874		
Br30	0.157258	C30	0.280737		
O31	-0.548725	C31	-0.120044		
C32	-0.177276	C32	-0.134270		

H33	0.156849	C33	0.018356		
H34	0.146217	C34	-0.143064		
H35	0.145211	C35	-0.140513		
H36	0.128760	H36	0.148500		
		H37	0.177995		
		H38	0.131154		
		H39	0.136473		
		C40	0.115419		
		C41	-0.157276		
		C42	-0.319629		
		C43	-0.073394		
		C44	-0.136746		
		C45	0.262993		
		H46	0.137505		
		H47	0.142682		
		H48	0.144357		

Element	Weight /%				Atomic /%		Error /%	
	HL		Cu ^{II} (L) ₂		HL	Cu ^{II} (L) ₂	HL	Cu ^{II} (L) ₂
	Unnormalized concentration in weight	Normalized concentration in weight	Unnormalized concentration in weight	Normalized concentration in weight				
C-6	60.41	59.74	52.93	52.21	77.94	77.33	7.0	6.3
N-7	6.31	6.24	4.27	4.21	6.99	5.34	1.2	0.9
O-8	10.85	10.72	8.03	7.92	10.50	8.81	1.5	1.2
Br-35	23.56	23.30	26.07	25.71	4.57	5.72	1.1	1.2
Cu-29	-	-	10.08	9.95	-	2.78	-	0.4