

Supplementary Information

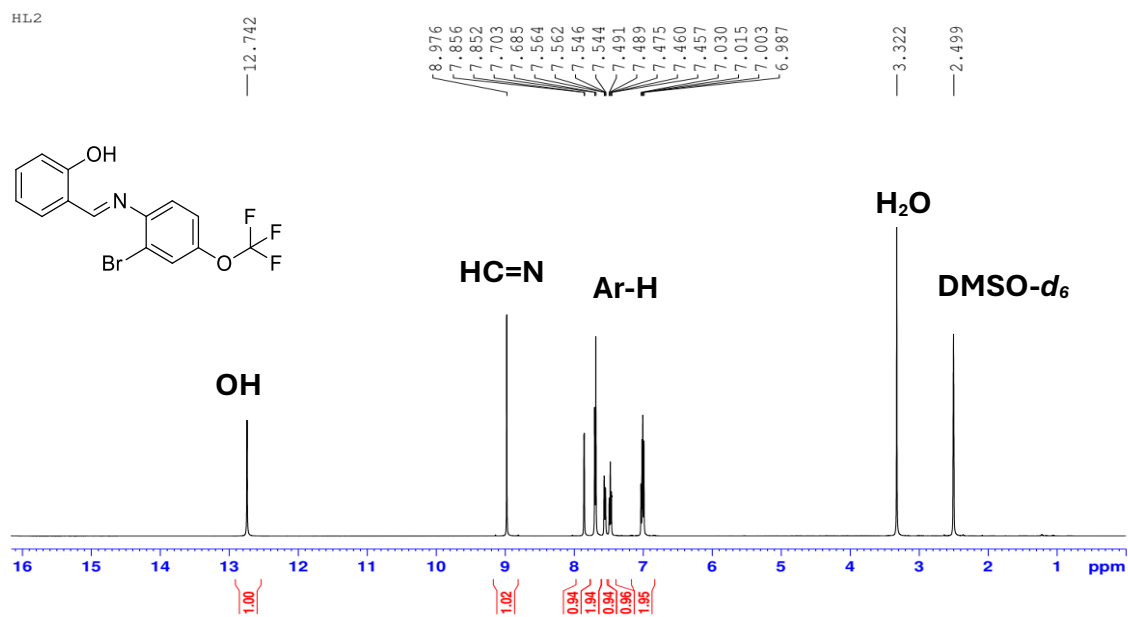


Figure S1: ¹H NMR spectrum of the **HL** recorded at 298 K using (500 MHz, DMSO-*d*₆)

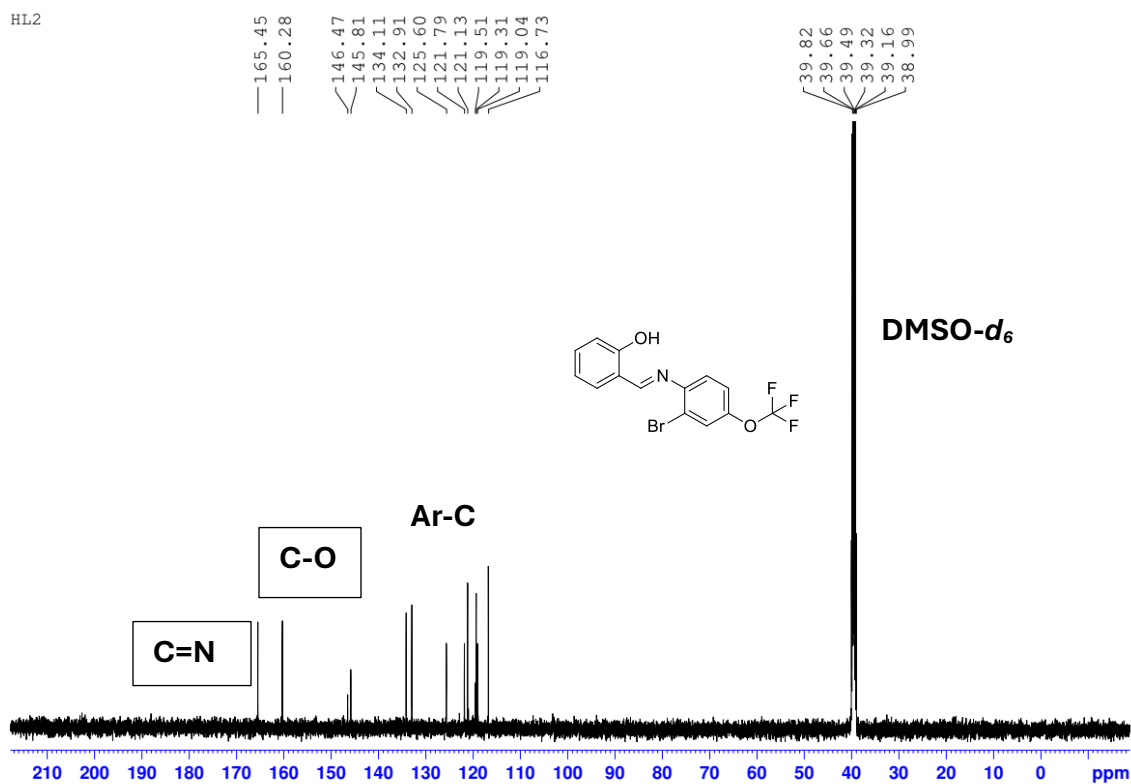


Figure S2: ¹³C NMR spectrum of the **HL** recorded at 298 K using (125 MHz, DMSO-*d*₆)

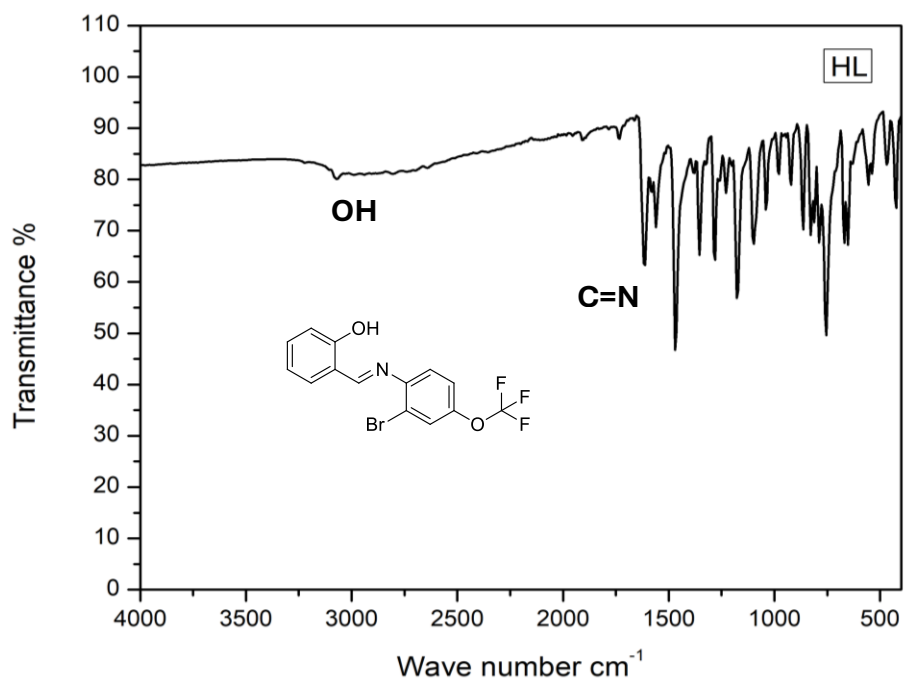


Figure S3: FTIR spectrum of **HL** recorded at solid state using ATR method at 298 K

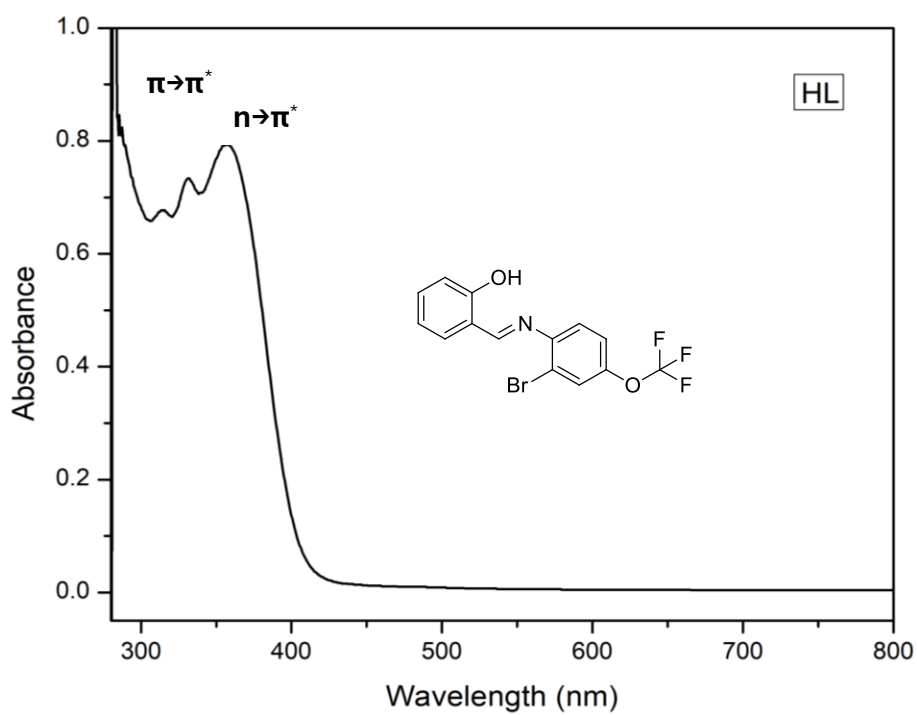


Figure S4: UV-Visible spectrum of **HL** recorded at 298 K in 10^{-3} M DMSO solution

Sample: H1
Size: 2.1430 mg
Method: Dual Ramp

DSC-TGA

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Operator: Meshack
Run Date: 06-Jun-2022 10:40
Instrument: SDT Q600 V20.9 Build 20

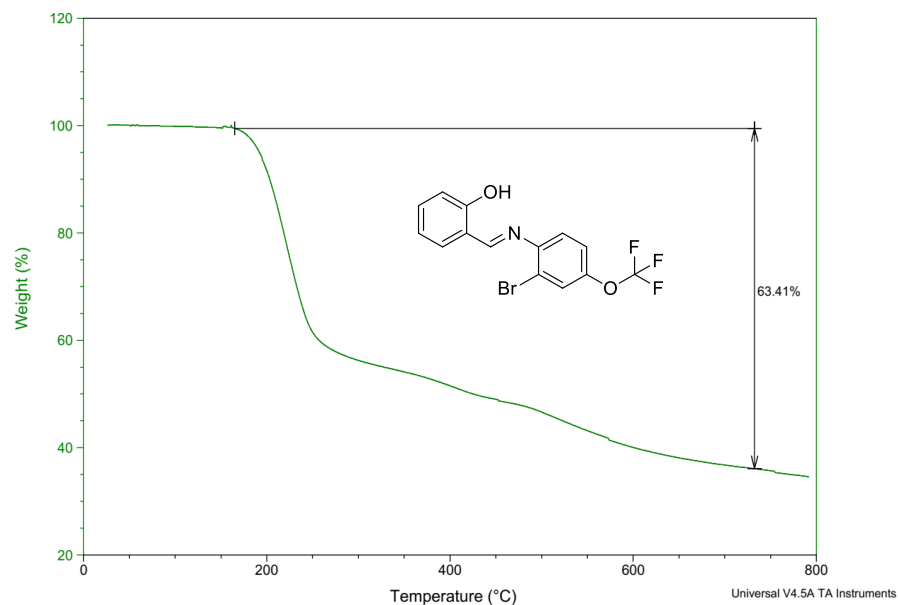


Figure S5: TGA thermogram of **HL** recorded under inert environment (N_2)

20230927_Muller_B8_p 31 (0.369)

LC-MS (Synapt) Facility

UP: Chemistry Dept.
1: TOF MS ES+
4.53e5

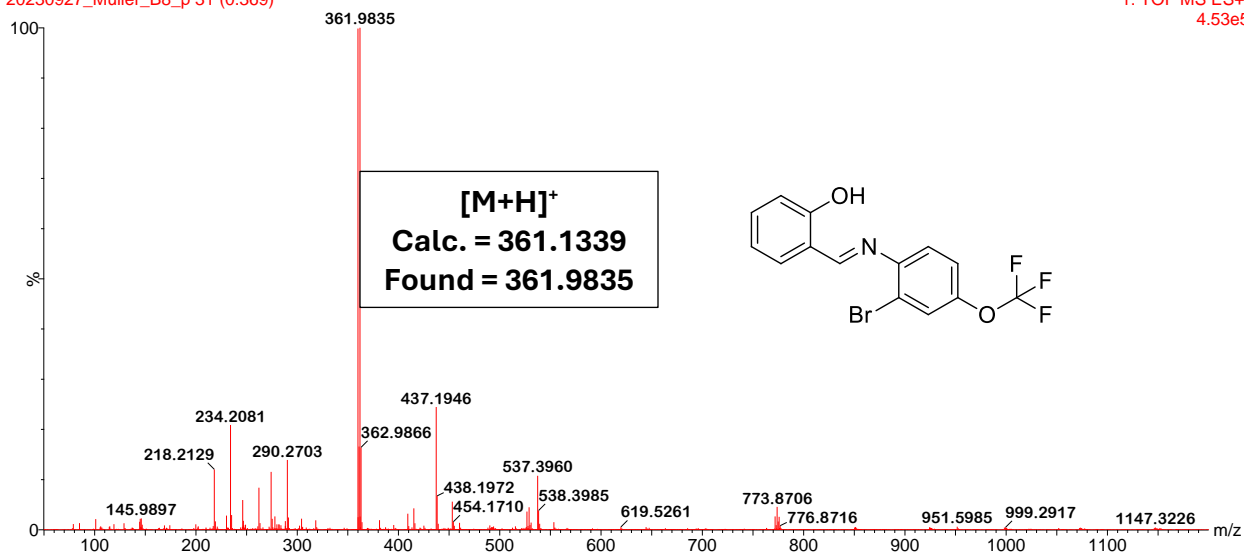


Figure S6: Mass spectrum of **HL** recorded in CH_3OH solution at 298 K using HRMS

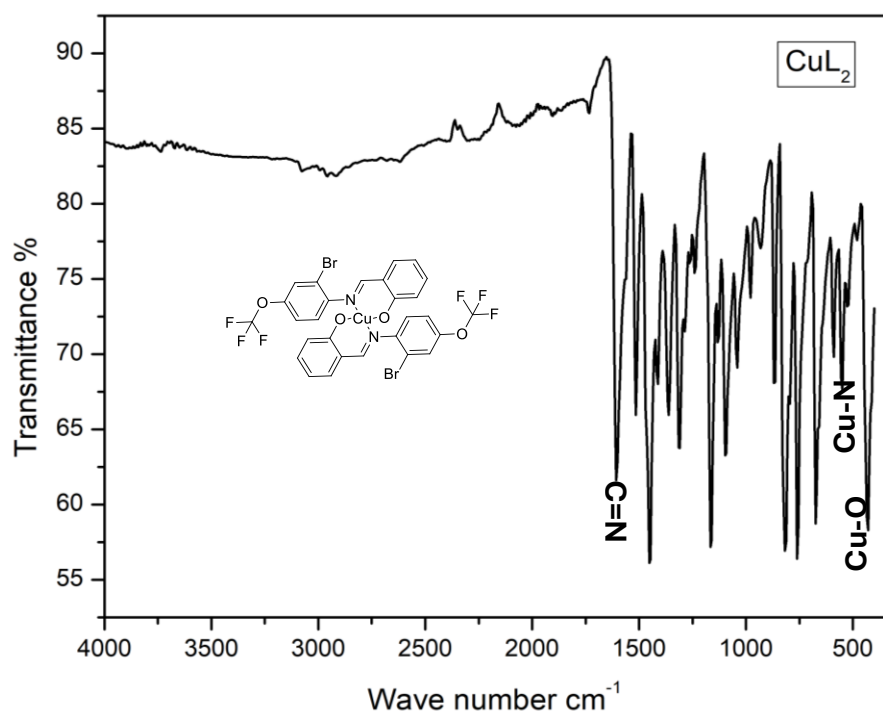


Figure S7: FTIR spectrum of CuL_2 recorded at solid state using ATR method at 298 K

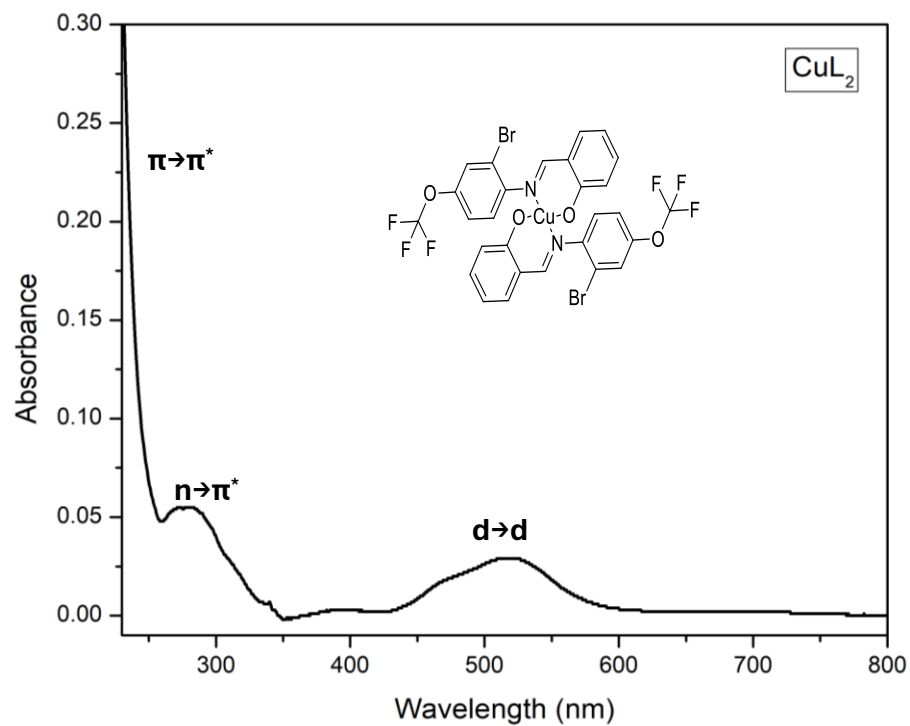


Figure S8: UV-Vis spectrum of the CuL_2 recorded at 298 K in 10^{-3} M DMSO solution

Sample: H5
Size: 1.5040 mg
Method: Ramp

DSC-TGA

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Operator: Meshack
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Instrument: SDT Q600 V20.9 Build 20

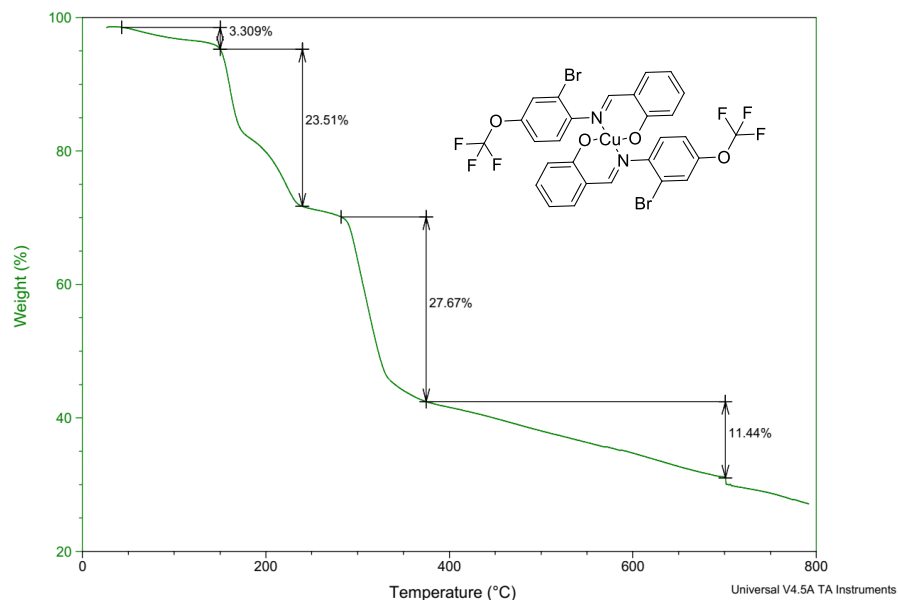


Figure S9: TGA thermograph of CuL_2 recorded under inert environment (N_2)

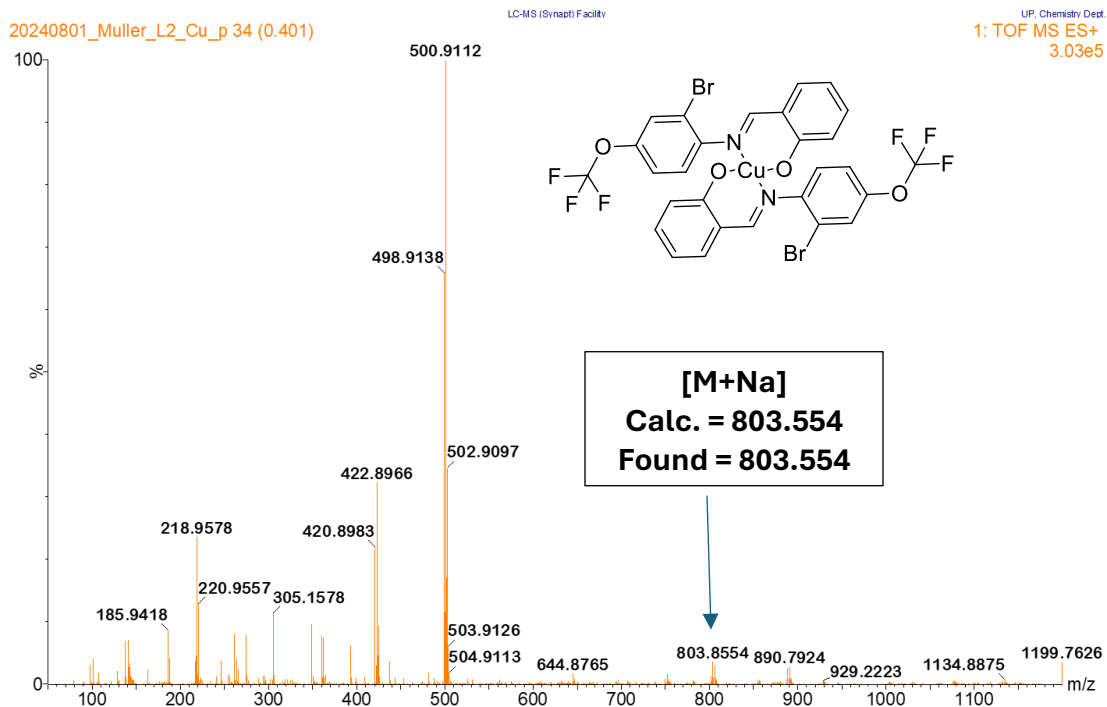
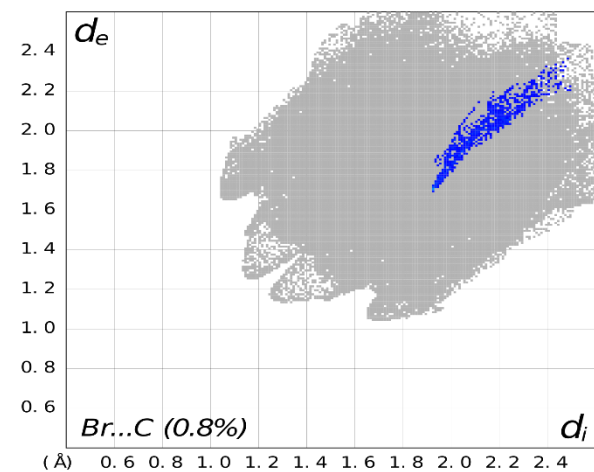
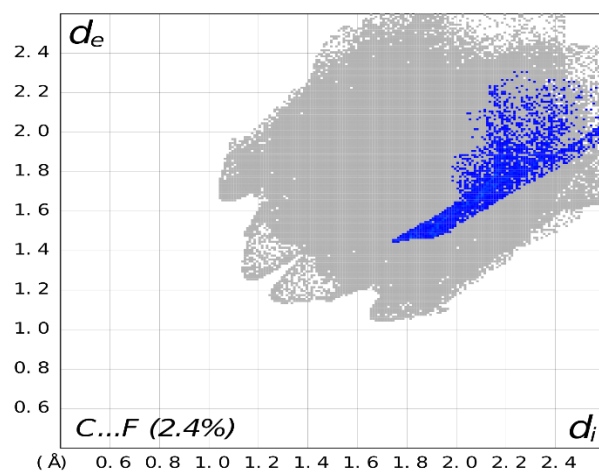
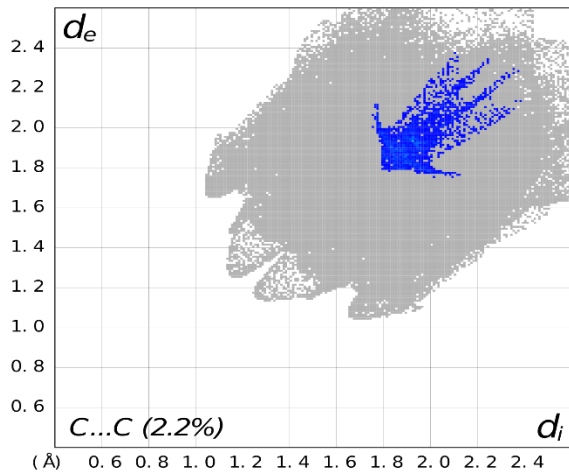
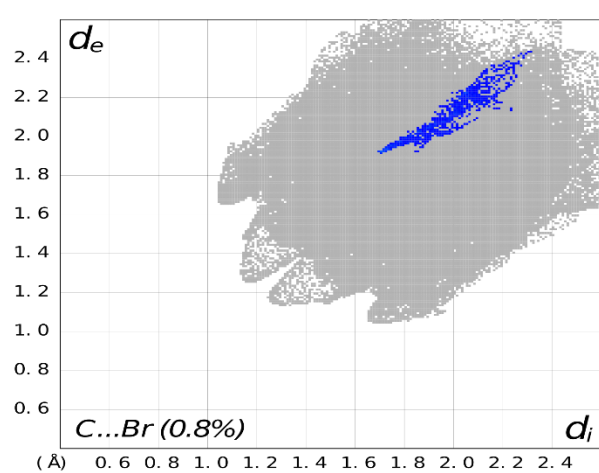
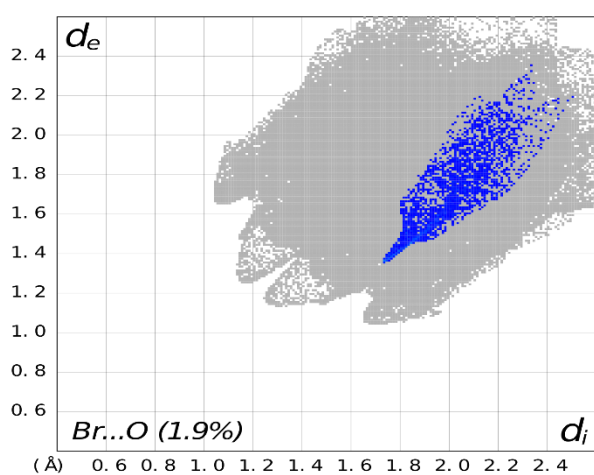
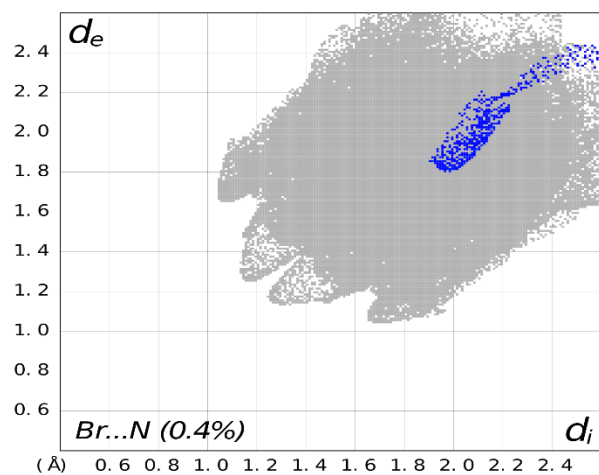


Figure S10: Mass spectrum of CuL_2 recorded in CH_3OH solution at 298 K using HRMS



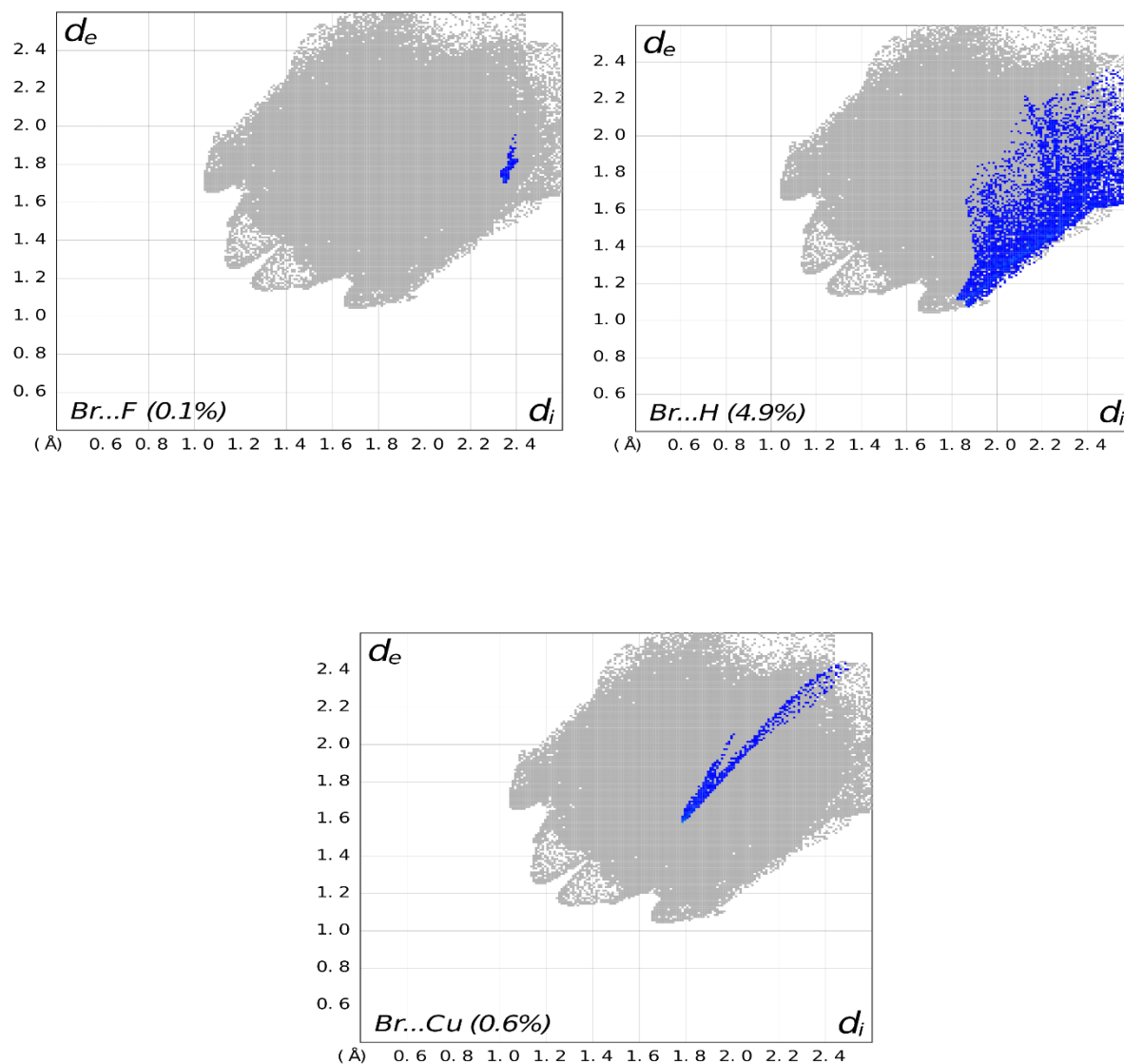


Figure S11: Two-dimensional fingerprint plots for atomic contributions during intermolecular interactions in **CuL₂** crystal lattice obtained at the B3LYP/6-31G(d,p) level of theory using Crystal Explorer 17.5 software.

Table S1: Crystal data and structure refinement for **CuL₂**

Identification code	CuL₂
Empirical formula	C ₂₈ H ₁₆ Br ₂ CuF ₆ N ₂ O ₄
Formula weight	781.79
Temperature/K	173.00
Crystal system	monoclinic
Space group	P2 ₁ /c

a/Å	26.7504(8)
b/Å	9.5297(3)
c/Å	11.1050(3)
α /°	90
β /°	94.9620(10)
γ /°	90
Volume/Å ³	2820.31(14)
Z	4
ρ_{calc} /cm ³	1.841
μ /mm ⁻¹	3.686
F(000)	1532.0
Crystal size/mm ³	0.236 × 0.105 × 0.069
Radiation	MoK α (λ = 0.71073)
2 Θ range for data collection/°	4.54 to 55.806
Index ranges	-30 ≤ h ≤ 35, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected	42523
Independent reflections	6749 [R _{int} = 0.0509, R _{sigma} = 0.0323]
Data/restraints/parameters	6749/0/388
Goodness-of-fit on F ²	1.035
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0343, wR ₂ = 0.0790
Final R indexes [all data]	R ₁ = 0.0445, wR ₂ = 0.0836
Largest diff. peak/hole / e Å ⁻³	1.86/-0.44

Table S2. Selected Bond parameters

Bond Distances	Length/Å
Br(1)–C(2)	1.891(3)
Br(2)–C(16)	1.894(3)
Cu(1)–O(1)	1.8891(19)
Cu(1)–O(2)	1.8832(19)
Cu(1)–N(1)	1.988(2)
Cu(1)–N(2)	1.993(2)

Bond Distances	Length/Å
O(1)–C(28)	1.302(3)
Bond angles	Angles
O(1)–Cu(1)–N(1)	91.57(9)
O(1)–Cu(1)–N(2)	93.22(9)
O(2)–Cu(1)–O(1)	156.38(9)
O(2)–Cu(1)–N(1)	93.17(9)
O(2)–Cu(1)–N(2)	89.58(9)
N(1)–Cu(1)–N(2)	161.46(9)

Table S3: Total interaction energies for **CuL₂** crystal lattice at the B3LYP/6-31G(d,p) basis set

Interaction Energies (kJ/mol)

R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, -y+1/2, z+1/2	10.38	B3LYP/DGDZVP	-2.3	-0.8	-14.8	11.6	-8.8
	2	x, y, z	9.53	B3LYP/DGDZVP	-17.3	-3.1	-42.7	39.3	-33.5
	2	x, -y+1/2, z+1/2	5.60	B3LYP/DGDZVP	-56.4	-7.9	-124.9	125.2	-96.9
	1	-x, -y, -z	13.89	B3LYP/DGDZVP	1.0	-0.4	-16.6	0.0	-13.8
	1	-x, -y, -z	14.09	B3LYP/DGDZVP	-3.2	-1.4	-18.5	0.0	-20.6
	2	-x, y+1/2, -z+1/2	14.58	B3LYP/DGDZVP	4.1	-0.8	-20.5	0.0	-14.1
	2	-x, y+1/2, -z+1/2	15.11	B3LYP/DGDZVP	-1.3	-0.4	-16.7	0.0	-16.2
	1	-x, -y, -z	14.41	B3LYP/DGDZVP	3.2	-0.4	-15.3	0.0	-10.3
	1	-x, -y, -z	17.01	B3LYP/DGDZVP	2.1	-0.3	-4.4	0.0	-1.9
	1	-x, -y, -z	14.60	B3LYP/DGDZVP	1.4	-0.1	-3.6	0.0	-1.7

Scale factors for benchmarked energy models

See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

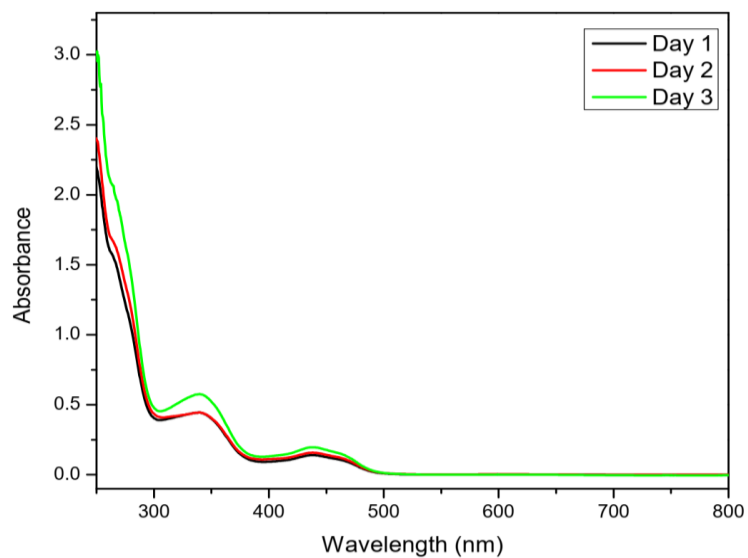


Figure S12. UV-Vis spectra of 30 μM solutions of CuL_2 recorded as a function of time in KH_2PO_4 buffer (50 mM pH 7.5). CuL_2 was present with a final concentration of 10% (v/v) DMSO.



Figure S13: Nematode infected okra roots that was used to obtain the nematode eggs.

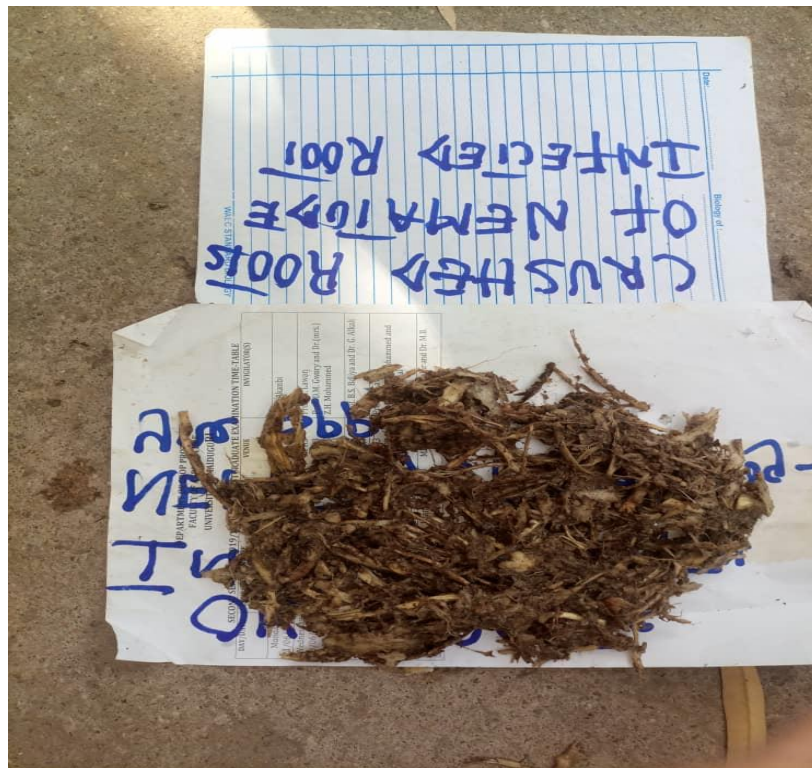


Figure S14: Crushed infected okra roots before egg extraction process.



Figure S15: The infected okra roots extracted with 200 mL of 0.5% NaOCI solution.



Figure S16: Extracted eggs before treatment with the compounds

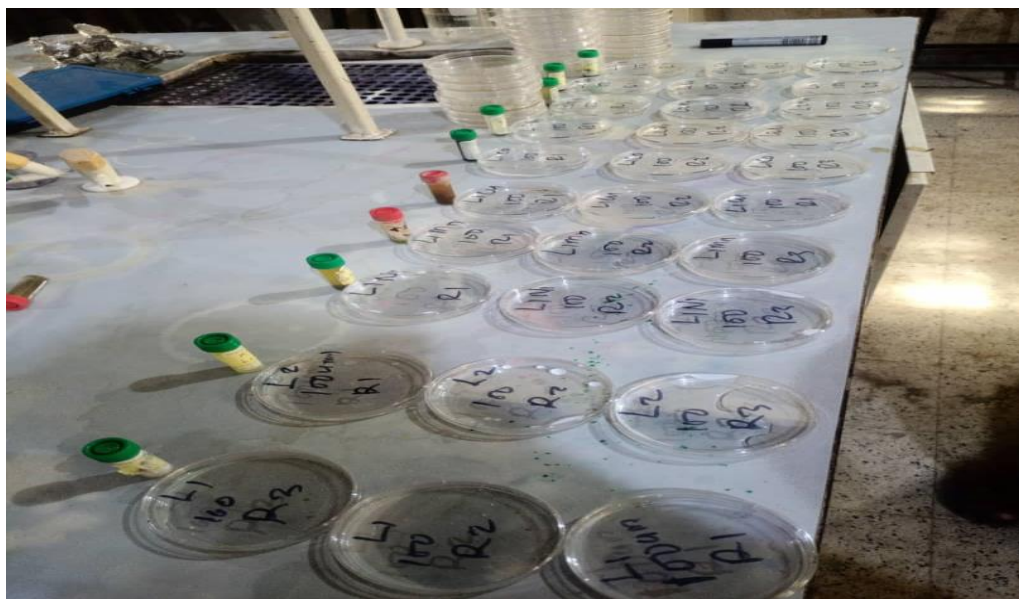


Figure S17: Extracted eggs after treatment with the compounds using concentrations of 100 μM



Figure S18: Micrograph of second stage juvenile (J2) before treatment with the compounds

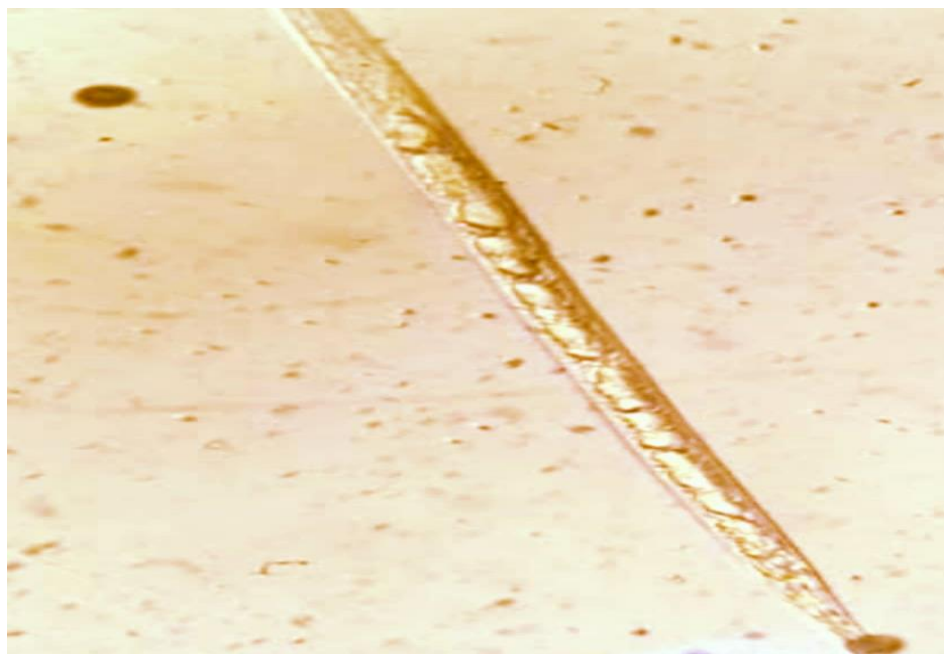


Figure S19: Micrograph of second stage juvenile (J2) after treatment with the compounds