Support Information

A curcumin-based AIEE-active fluorescent probe for Cu^{2+} detection in aqueous solution

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1. NMR Spectra

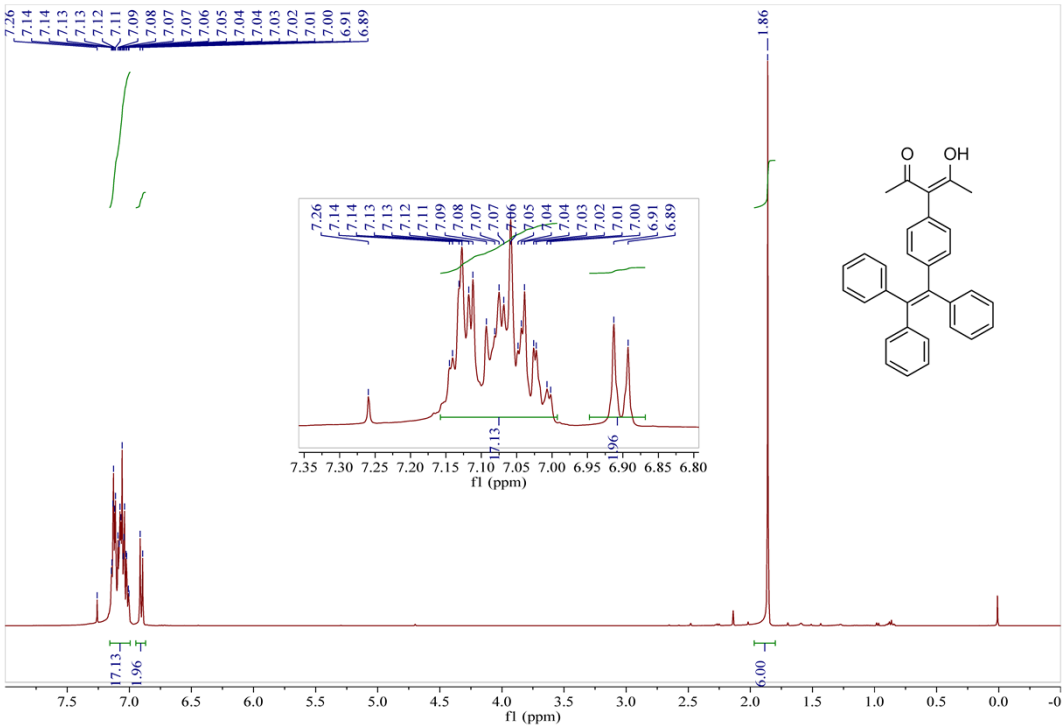


Fig. S1 ^{1}H NMR spectrum of compound **1** conducted in chloroform-*d*.

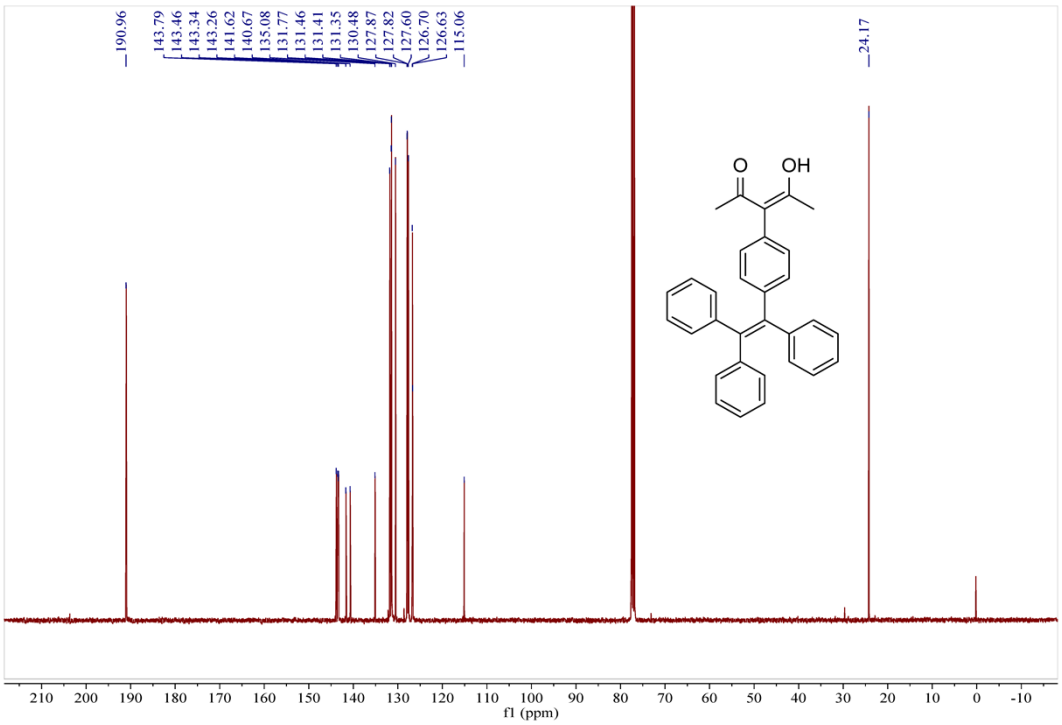


Fig. S2 ^{13}C NMR spectrum of compound **1** conducted in chloroform-*d*.

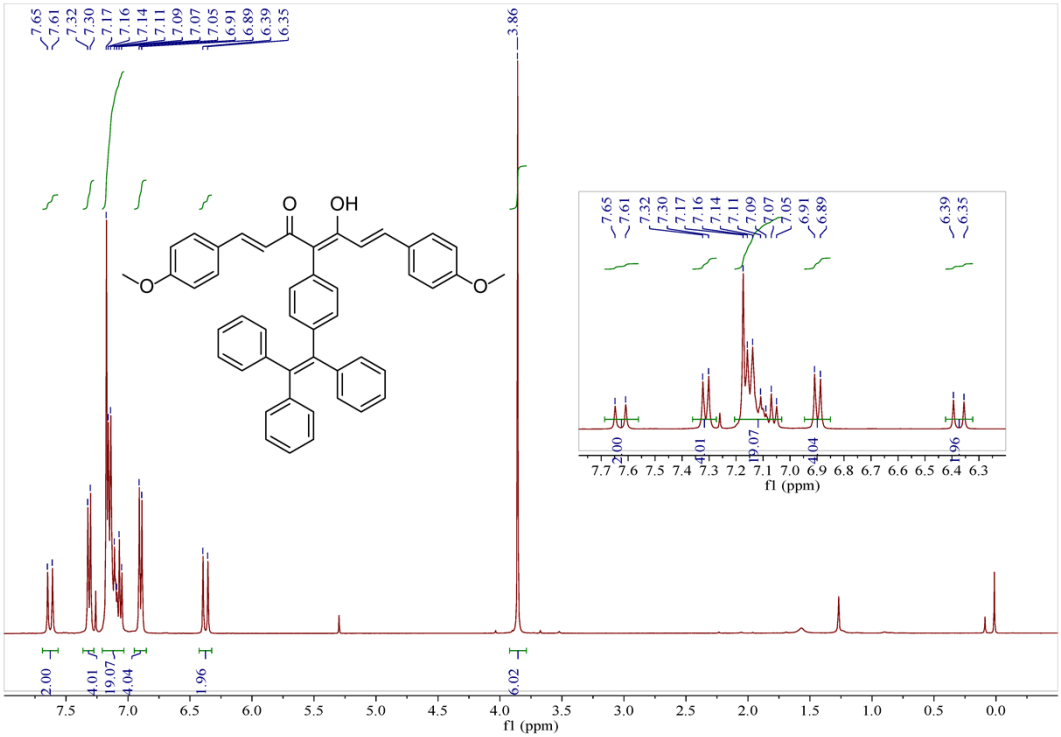


Fig. S3 ^{1}H NMR spectrum of compound **L1** conducted in chloroform-*d*.

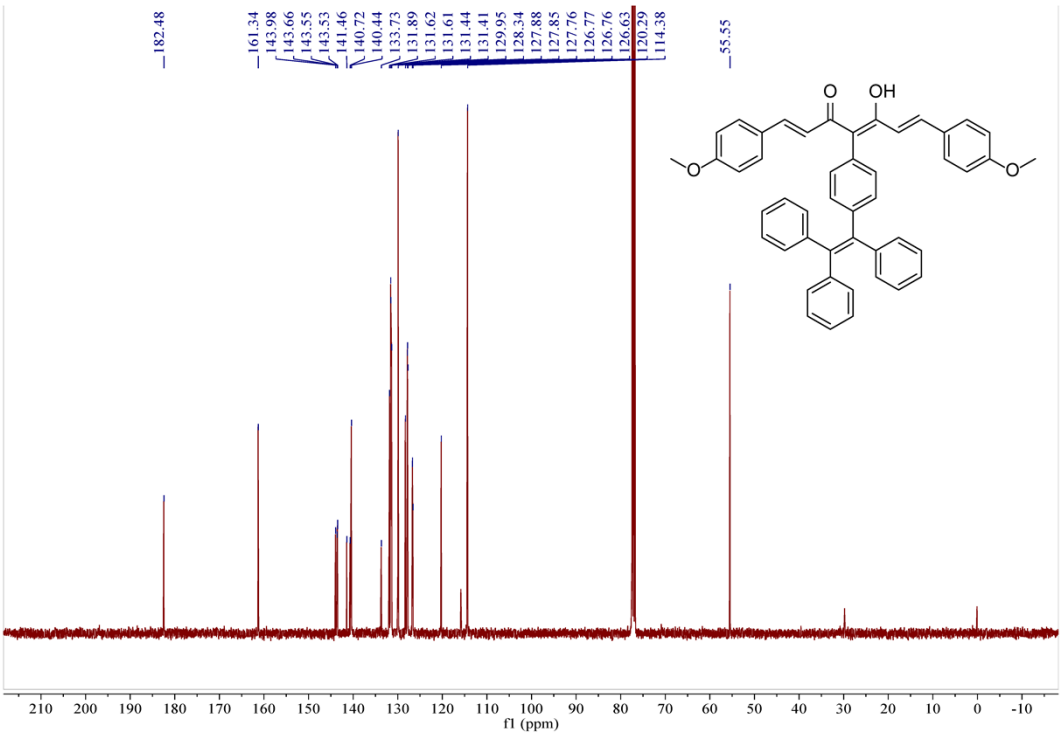


Fig. S4 ^{13}C NMR spectrum of compound **L1** conducted in chloroform-*d*.

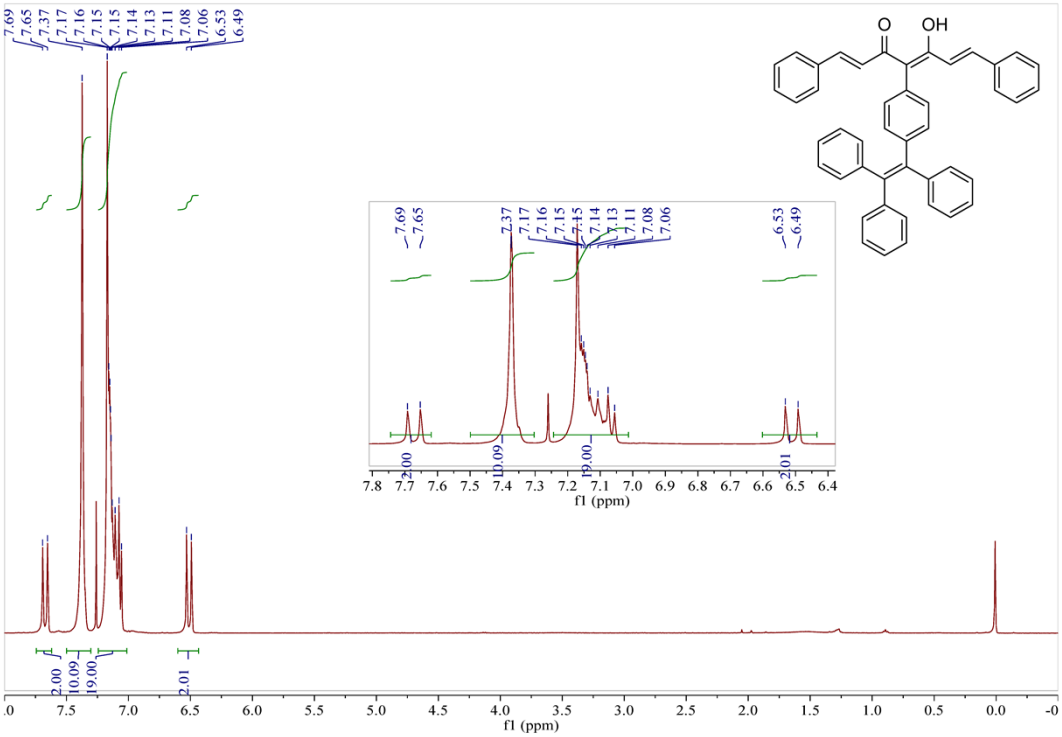


Fig. S5 ^{1}H NMR spectrum of compound **L2** conducted in chloroform-*d*.

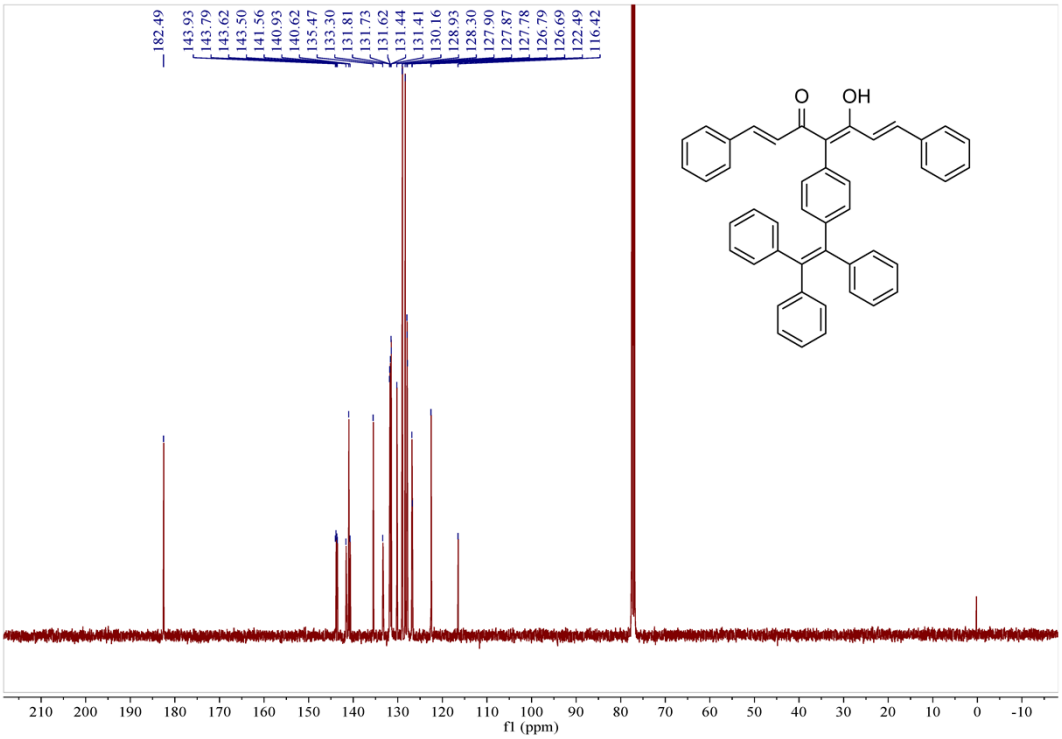


Fig. S6 ^{13}C NMR spectrum of compound **L2** conducted in chloroform-*d*.

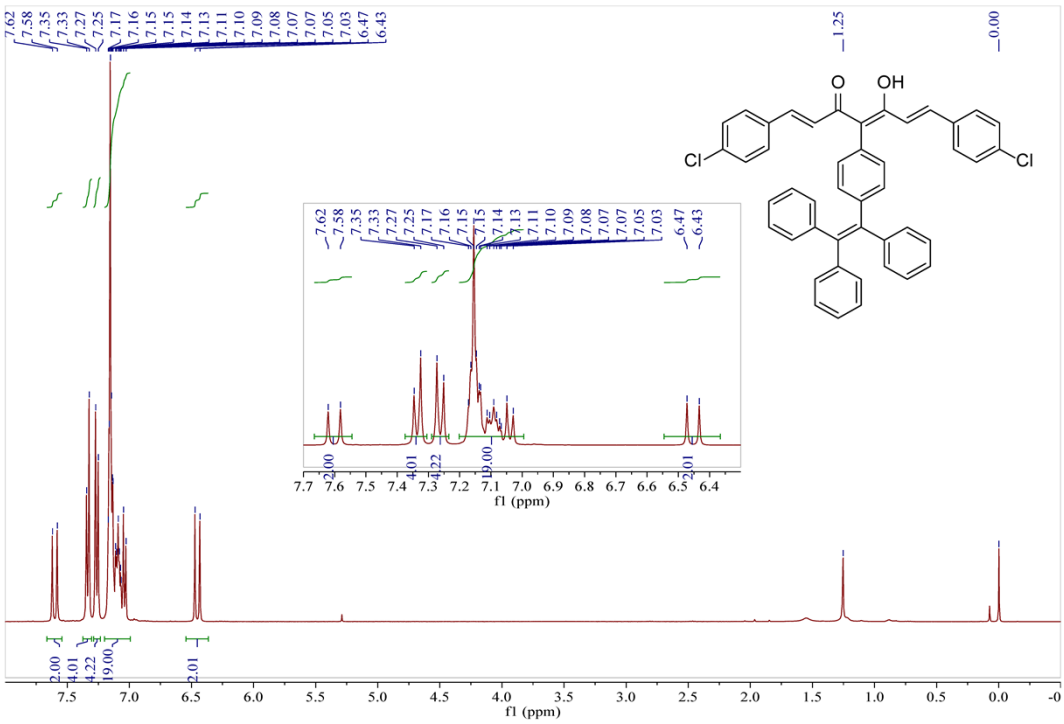


Fig. S7 ^{1}H NMR spectrum of compound **L3** conducted in chloroform-*d*.

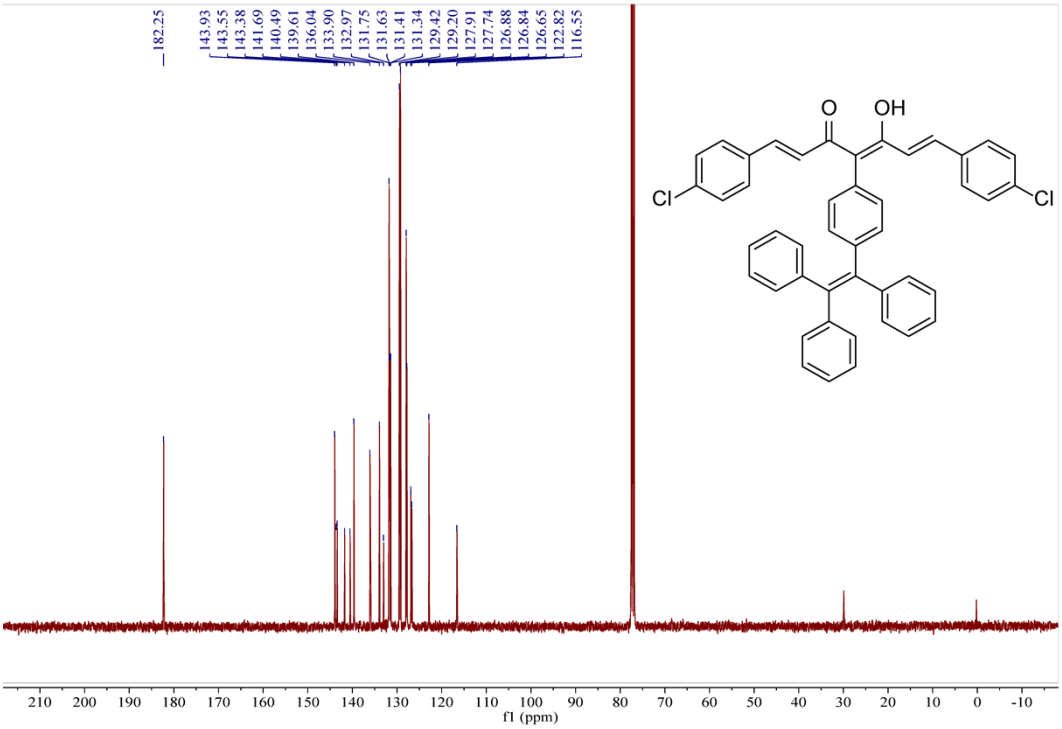


Fig. S8 ^{13}C NMR spectrum of compound **L3** conducted in chloroform-*d*.

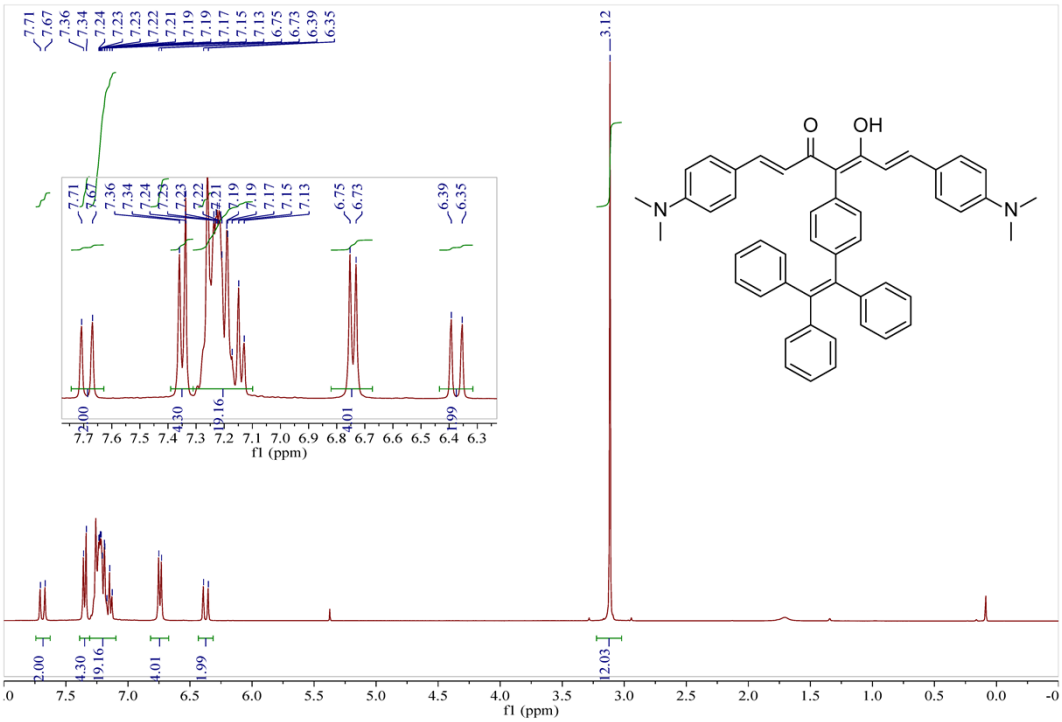


Fig. S9 ^{1}H NMR spectrum of compound **L4** conducted in chloroform-*d*.

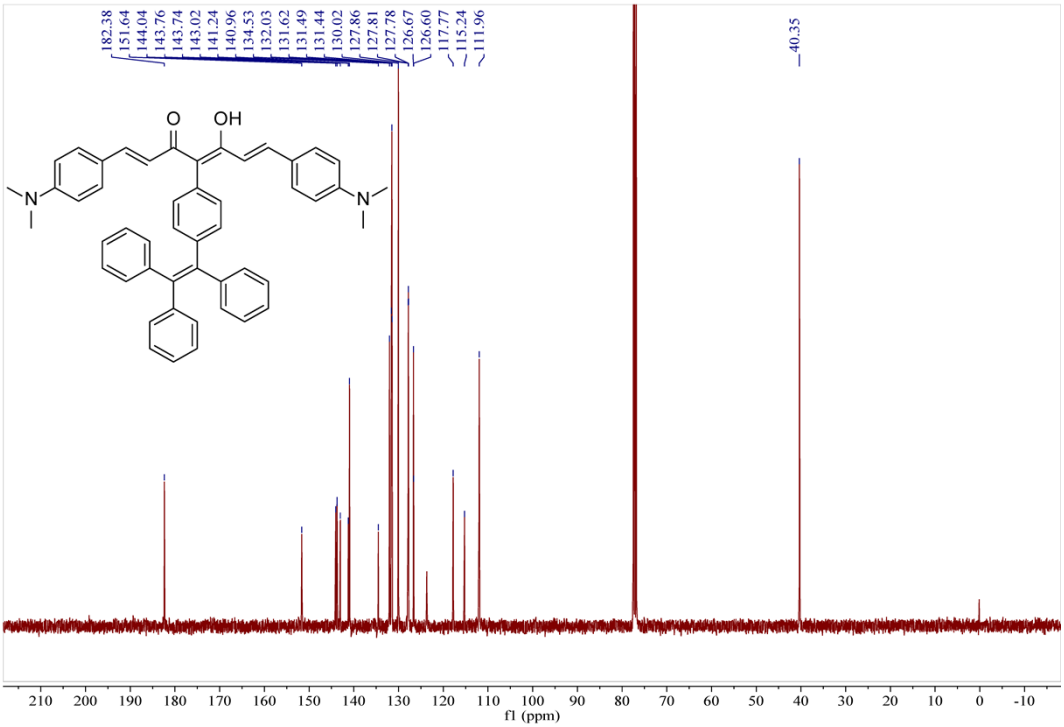


Fig. S10 ^{13}C NMR spectrum of compound **L4** conducted in chloroform-*d*.

2. HRMS Spectra

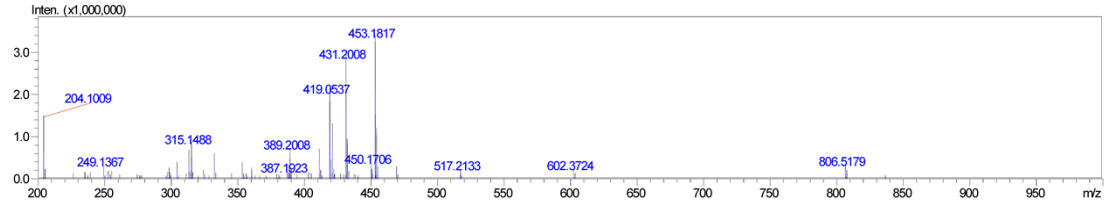


Fig. S11 HRMS spectrum of compound **1**.

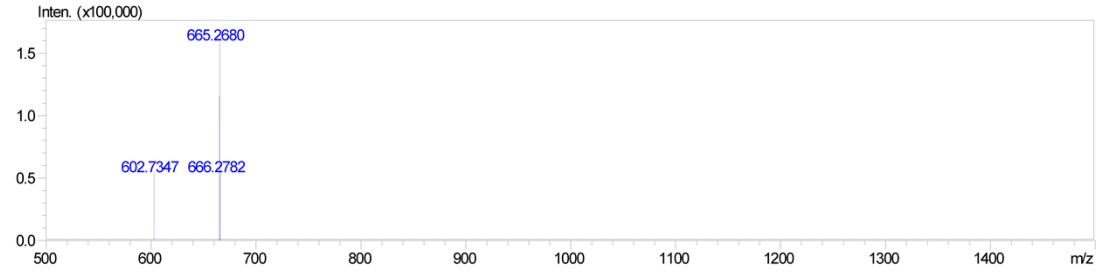


Fig. S12 HRMS spectrum of compound **L1**.

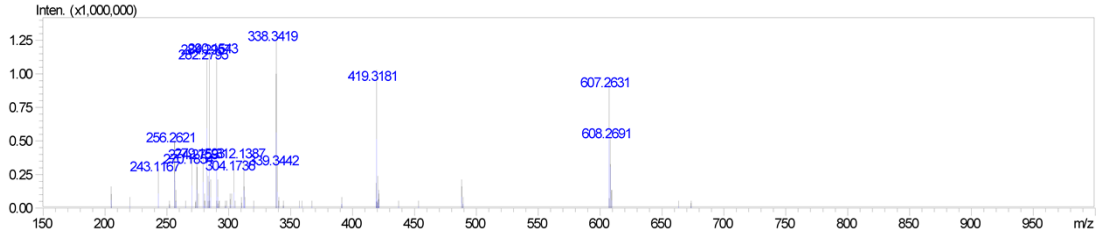


Fig. S13 HRMS spectrum of compound **L2**.

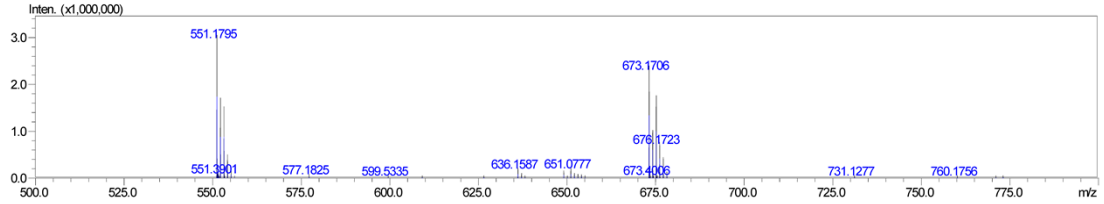


Fig. S14 HRMS spectrum of compound **L3**.

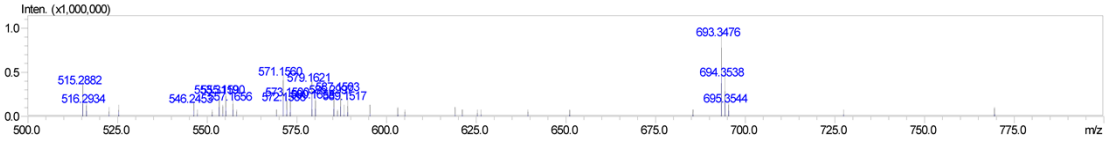


Fig. S15 HRMS spectrum of compound **L4**.

Fig. S16 HRMS spectrum of complex **[2L1+Cu^{2+}]**.

3. Crystal photo of L1

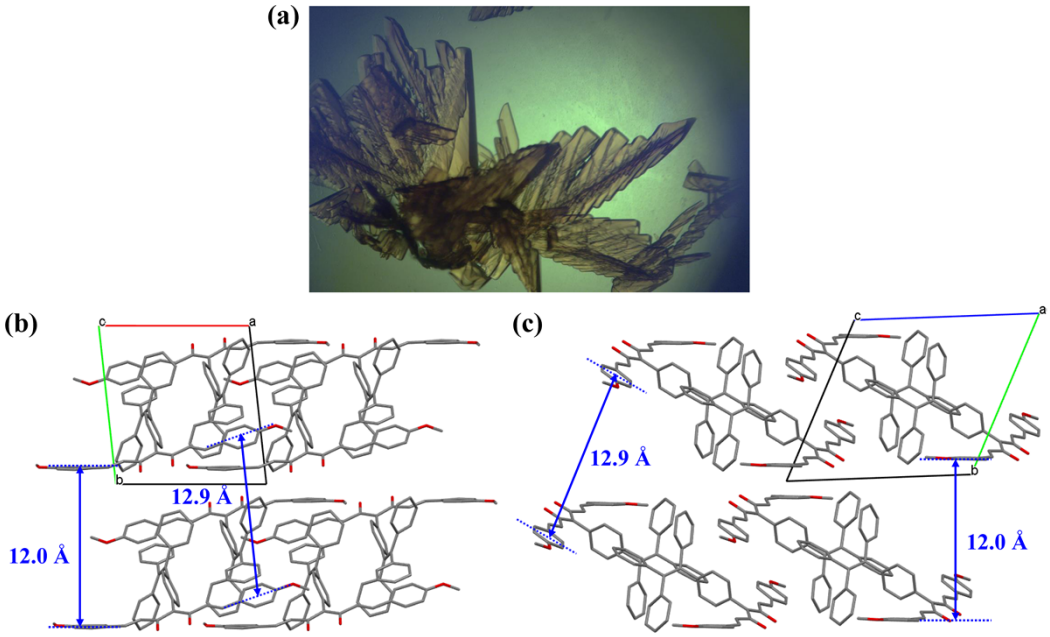


Fig. S17 (a) Crystal photograph of **L1**; (b) and (c) Different views of the extended-crystal structure viewed from c-axis (the hydrogen atoms are hided for clarity). The hydrogen atoms are marked in white, carbon atoms in gray, and oxygen atoms in red.

4. X-ray crystallography Analysis

Table S1 Summary of crystal data of **L1**.

Parameter	**L1**
Empirical formula	$C_{47}H_{38}O_4$
Formula weight	666.77
Temperature/K	150.0
Crystal system	triclinic
Space group	*P*-1
a/Å	11.3529 (9)
b/Å	13.0942 (11)
c/Å	13.9528 (12)
α/°	63.486 (5)
β/°	77.327 (6)
γ/°	78.923 (6)
Volume/Å^3	1800.2 (3)
Z	2
ρ_{calc}g/cm^3	1.230
μ/mm^{-1}	0.607
F(000)	704.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.164 to 144.646

Index ranges	$-14 \le h \le 14, -16 \le k \le 16, -17 \le l \le 17$
Reflections collected	20467
Independent reflections	7034 [R_{int} = 0.0365, R_{sigma} = 0.0456]
Data/restraints/parameters	7034/0/463
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0770, wR_2 = 0.2143
Final R indexes [all data]	R_1 = 0.0876, wR_2 = 0.2316
Largest diff. peak/hole / e $Å^{-3}$	0.40/-0.19

5. Cu^{2+} response of L1

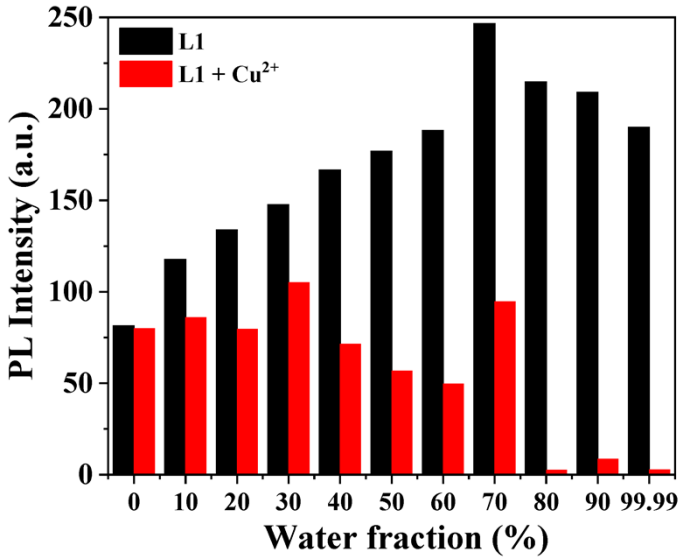


Fig. S18 The fluorescence intensity of **L1** at 525 nm before and after adding Cu^{2+} in THF/water mixtures. The concentrations of **L1** and Cu^{2+} are 1×10^{-5} mol L^{-1}.

6. Particle size of L1

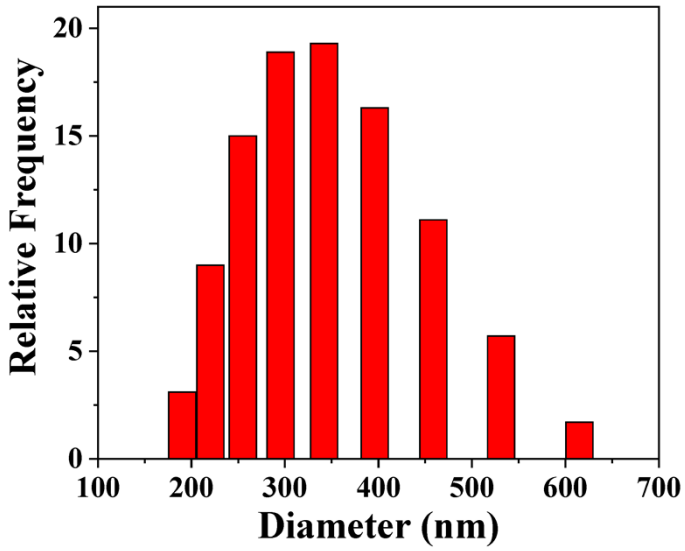


Fig. S19 Particle size distribution of **L1** in the solution (1×10^{-5} mol L^{-1}, V_{water}/V_{THF} = 4/1)

7. Fluorescence lifetime

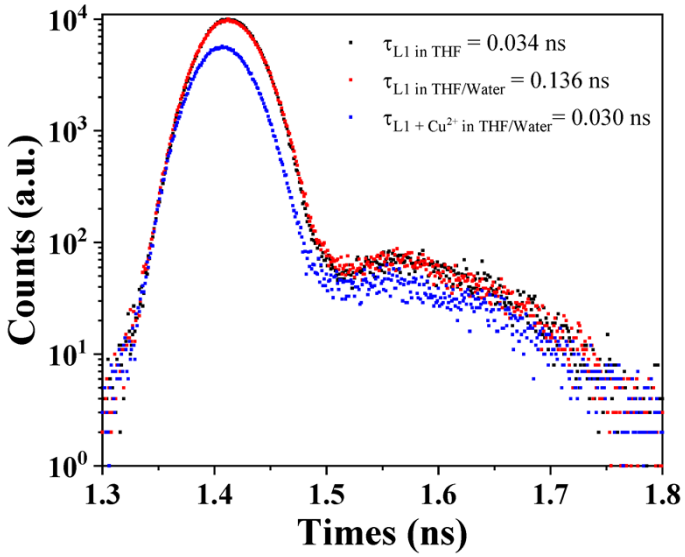


Fig. S20 Fluorescence lifetimes of **L1** in THF, **L1** and **L1**+Cu^{2+} in the solution (V_{water}/V_{THF} = 4/1). The concentrations of **L1** and Cu^{2+} are 1 × 10^{-5} mol L^{-1}.

8. Effect of pH

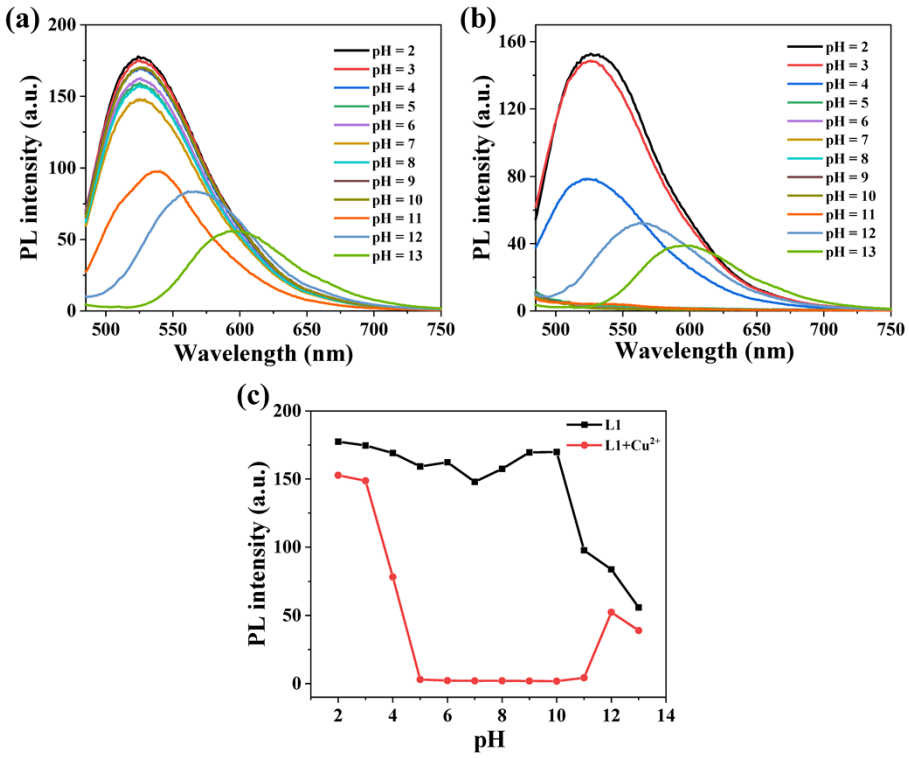


Fig. S21 Fluorescence spectra of (a) **L1** and (b) **L1**+Cu^{2+} in solutions (V_{water}/V_{THF} = 4/1) with different pH values; (c) The fluorescence intensity of **L1** and **L1**+Cu^{2+} as a function of pH values. The concentrations of L1 and Cu^{2+} are 1 × 10^{-5} mol L^{-1}. λ_{ex} = 467 nm.

9. Job′s Plot

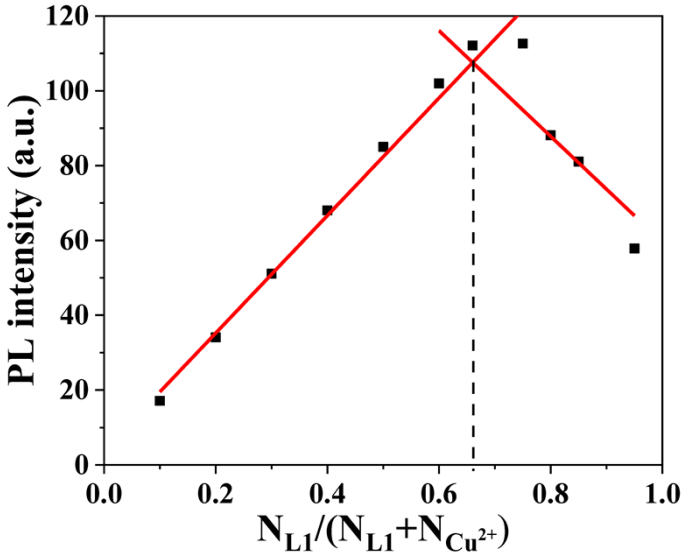


Fig. S22 Job′s Plot for determining the stoichiometry of **L1** and Cu^{2+} in the solution (V_{water}/V_{THF} = 4/1). The emission intensity at 525 nm was plotted against the mole fraction of **L1** at an invariant total concentration of 1×10^{-5} mol L^{-1}.

10. Benesi-Hildebrand plot

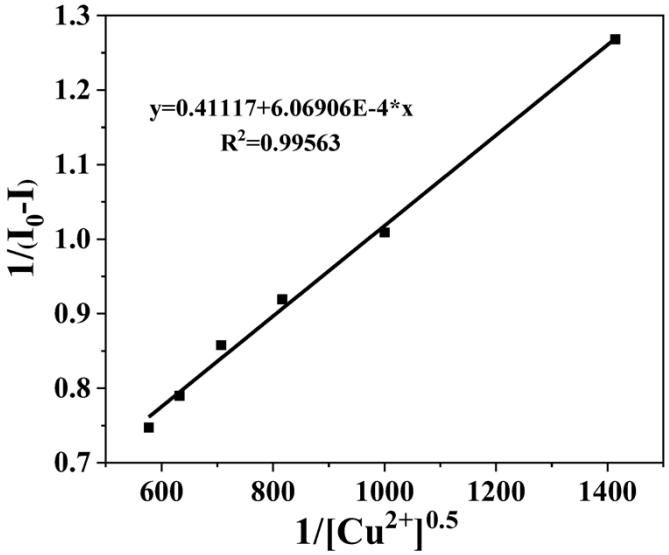


Fig. S23 Benesi–Hildebrand plot of fluorescence intensity response of the **L1** toward Cu^{2+}.

11. Detection limit

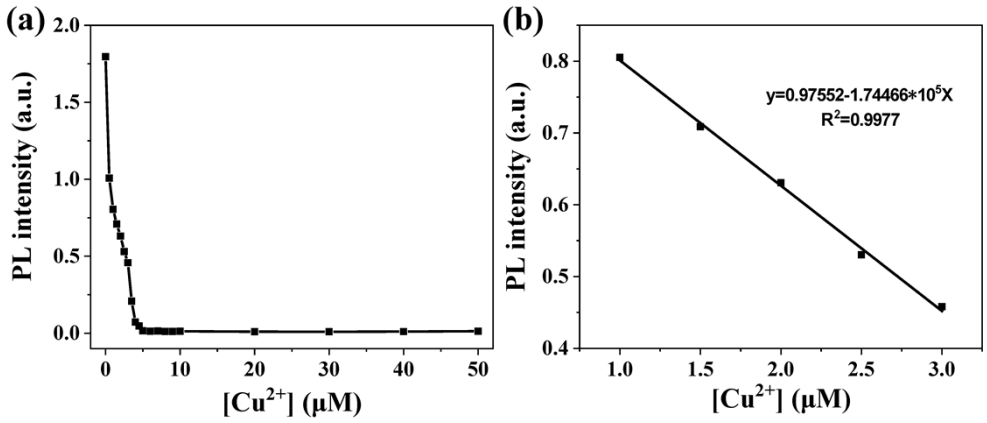
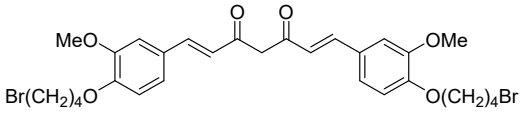
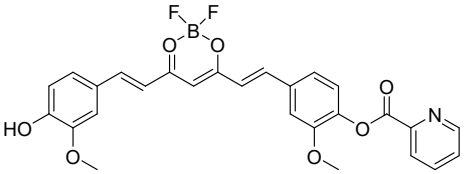
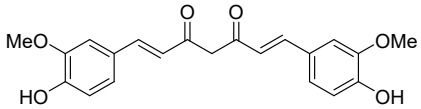
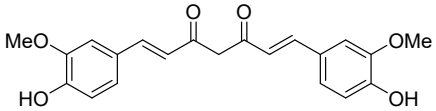
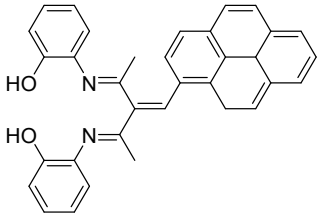
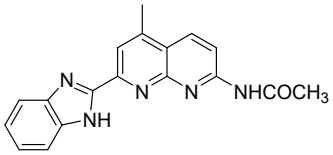
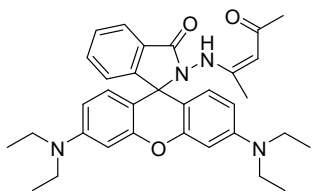
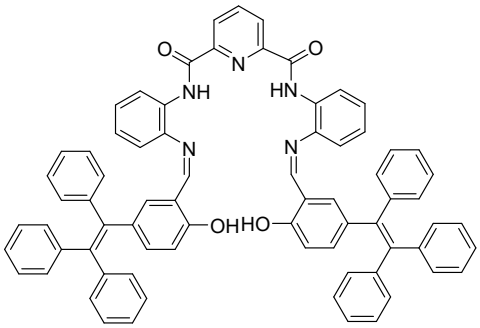
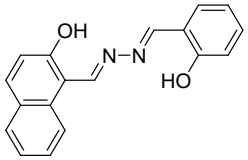
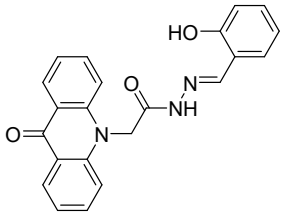
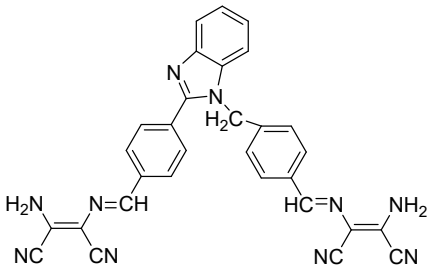
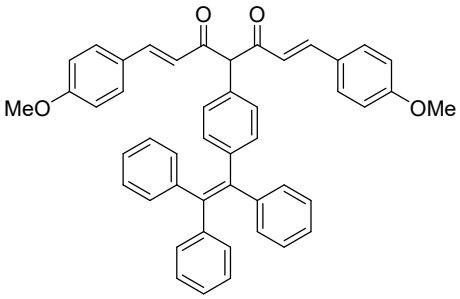


Fig. S24 (a) The fluorescence intensity of **L1** (1×10^{-5} mol L^{-1} in V_{water}/V_{THF} = 4/1) at 525 nm as a function of the addition of Cu^{2+} (0–50 μM). (b) Linear fitting of the emission data upon addition of Cu^{2+}.

Table S2 Comparison of the reported DL values of Cu^{2+} probes

Chemical structural formula	Solvent system	DL	Ref.
	PBS:CH_3CN (8:2, V/V)	2.54 μM	1
	TBS:DMSO (6:4, V/V)	120 nM	2
	BR buffer	0.07 μg mL^{-1}	3
	acetate buffer	1.431 ng mL^{-1}	4
	CH_3CN:HEPES (7:3, V/V)	1.21 μM	5
	HEPES:C_2H_5OH (3:1, V/V)	7.09 μM	6

	EtOH:water (9:1, V/V)	2.0 μM	7
	THF:Tris (4:1, V/V)	236 nM	8
	PBS	200 nM	9
	DMSO:Water (4:1, V/V)	800 nM	10
	CH_3CN:Tris (1:1, V/V)	490 nM	11
	Water:THF (8: 2, V/V)	149 nM	This work

12. Fluorescence intensity of Cu^{2+} indicator paper

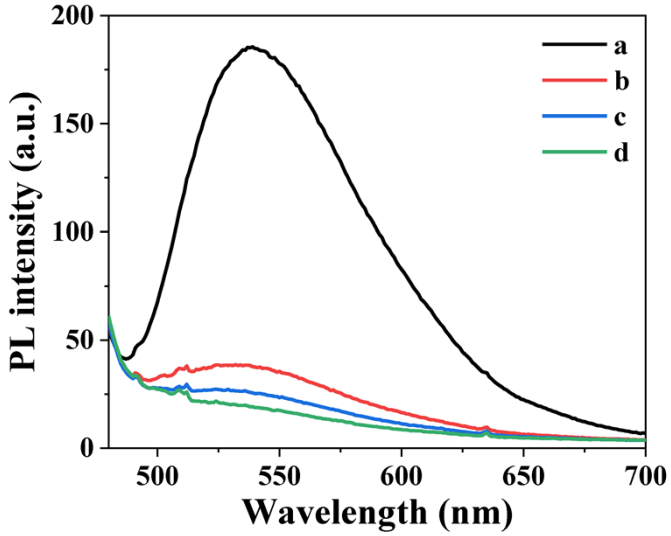


Fig. S25 Fluorescence intensities of dried **L1** indicator papers after soaking in Cu^{2+} solutions with different concentrations for 10 s: (a) Cu^{2+}-free, (b) 0.01 mM, (c) 0.1 mM, and (d) 1 mM.

Referemces

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