Rational design and bioimaging application of water-solubility Fe^{3+} fluorescent probe

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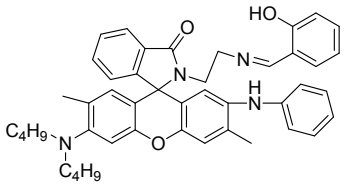
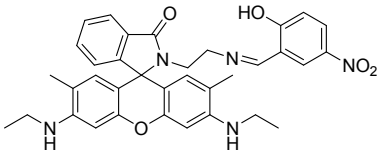
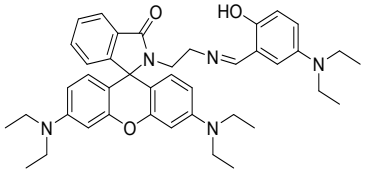
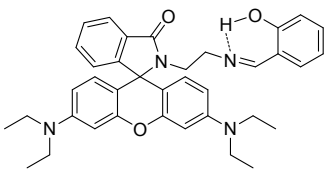
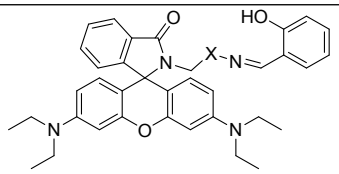
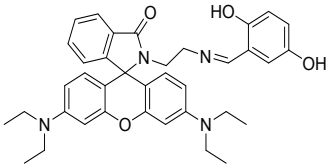
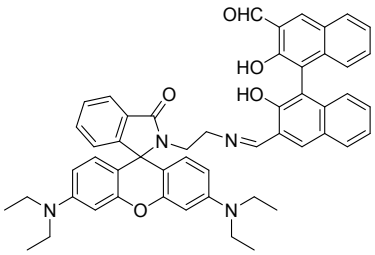
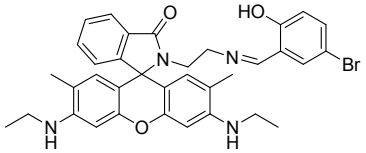
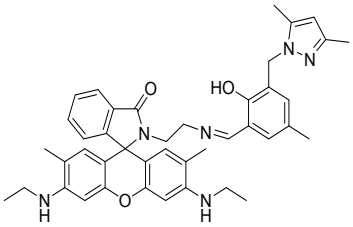
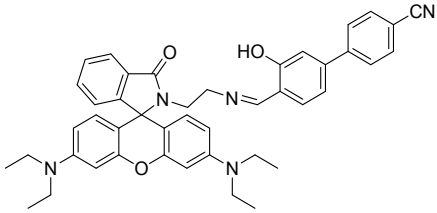
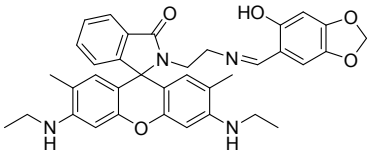
1. Supplementary Spectra and chart

Table S1: Comparison of fluorescent probes for Fe (III) ions with similar structures.

Probes	Medium	Limit of detection (μM)	Reference
	CH_3CN	-	Molecular Crystals and Liquid Crystals, 2009, 504(1): 155-163.
	H_2O/CH_3CN (95 : 5, v/v)	-	Chemical Communications, 2010, 46(9): 1407-1409.
	CH_3OH/HEPES buffer (1:1, v/v)	-	RSC Advances, 2013, 3(24): 9189-9192.
	EtOH	-	Inorganic Chemistry Communications, 2013, 35 : 255-259.

	CH_3CN/H_2O (1:1, v/v)	2.0×10^{-2}	Sensors and Actuators B-chemical, 2012,174 : 231-236.
	$MeOH/H_2O$ (1:1, v/v)	1.9×10^{-2}	Sensors and Actuators B: Chemical, 2016, 223: 101-113.
	THF/H_2O (v/v, 3/7)	1.83×10^{-1}	Sensors and Actuators B: Chemical, 2016, 224: 592-599.
	H_2O/methanol = 3:7 (v/v)	4.04×10^{-3}	Sensors and Actuators B: Chemical, 2017, 246: 518-534.
	methanol/H_2O (1:1, v/v)	2.9×10^{-1}	New Journal of Chemistry, 2017, 41(16): 8359-8369.
	MeOH/HEPES buffer(1:1, v/v)	8.7×10^{-2}	Dalton Transactions, 2018, 47(10): 3378-3387.
	CH_3OH/H_2O (1:9, v/v)	3×10^{-2}	Anal. Methods, 2019, 11, 794-799

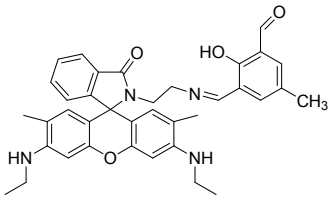
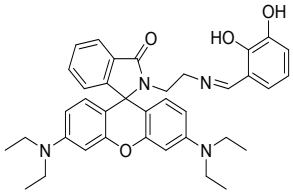
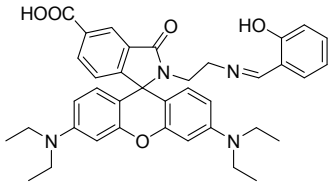
	MeOH /water (9:1, v/v)	1.4×10^{-2}	Dalton Transactions, 2019,48: 17594–17604.
	CH_3CN and HEPES solution (1:1, v:v)	8.1×10^{-3}	Journal of fluorescence, 2019, 29(5): 1221-1226.
	water	5.2	This work

Table S2: Photophysical properties on the **T1** and **T2**

	λ_{abs} (nm)	λ_{em} (nm)	$\triangle\lambda$ (nm)	Ɛ (M^{-1} cm^{-1})	Φ [a]	Φ [b]
T1	563	590	27	6.5×10^3	0.01	0.47
T2	565	587	22	1.3×10^3	0.05	0.12

a: only probe (10 μM)

b: probe (10 μM) + Fe^{3+} (40 μM)

* Φ was relevant to rhodamine B, Φ = 0.69 in MeOH

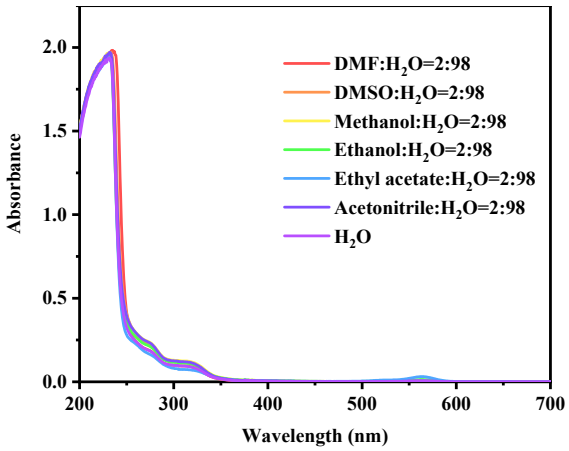


Figure S1. UV-vis absorption spectra of **T1** (10 μM) in different solvents.

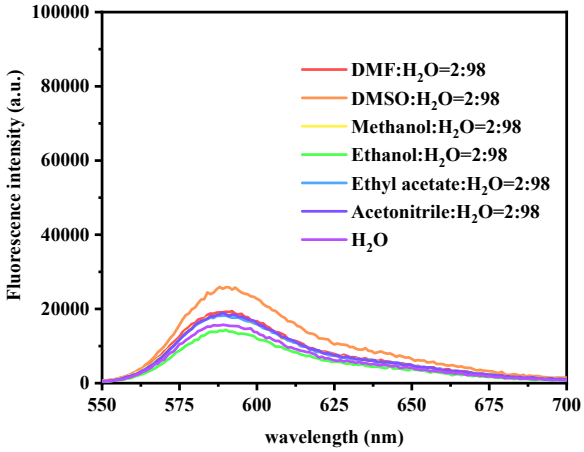


Figure S2. Fluorescence emission spectra of **T1** (10 μM) in different solvents.

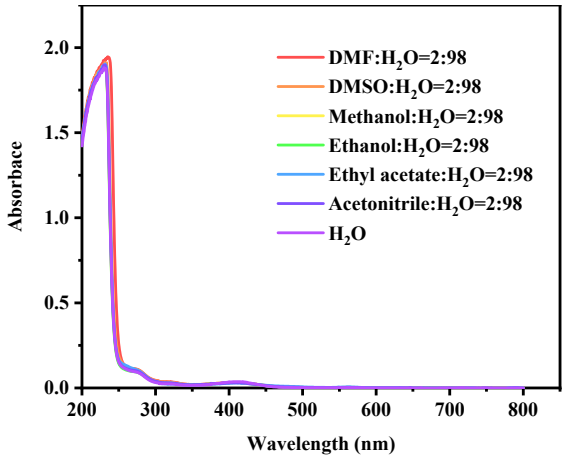


Figure S3. The UV-vis absorption spectra of **T2** (10 μM) in different solvents.

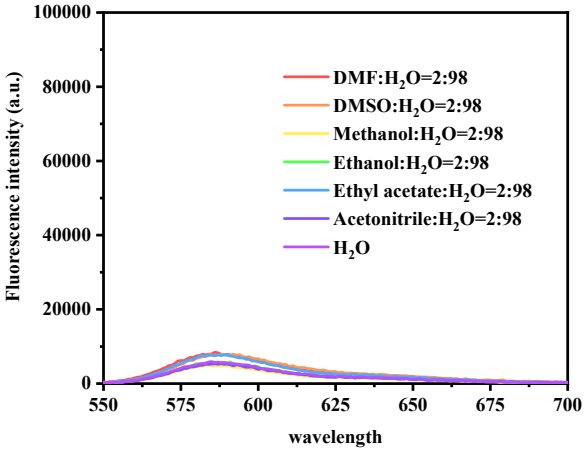


Figure S4. Fluorescence emission spectra of **T2** (10 μM) in different solvents.

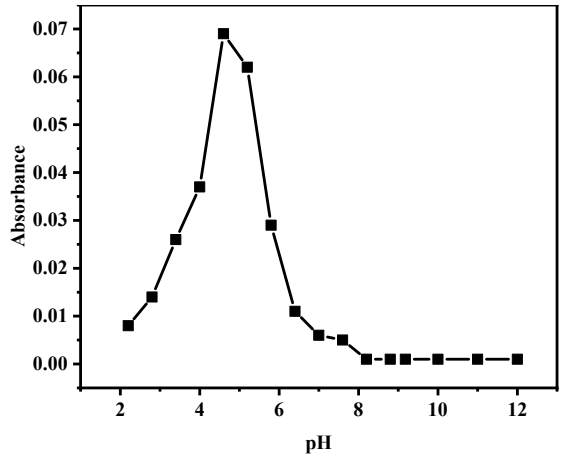


Figure S5. UV-vis absorption changes of **T1** (10 μM) at 570 nm at various pH values (pH 2 to 12).

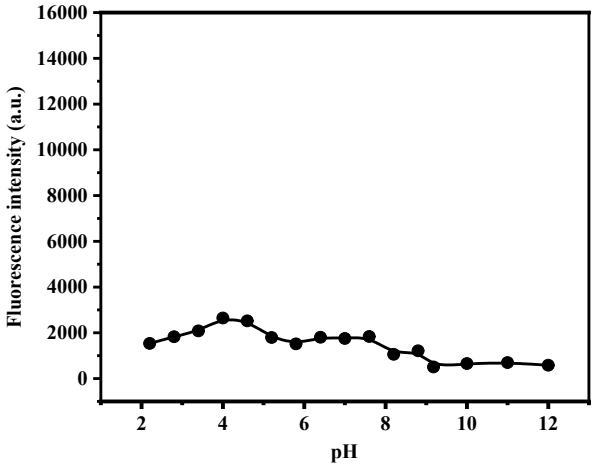


Figure S6. Emission changes of **T1** (10 μM, λex = 570 nm) at 590 nm at various pH values (pH 2 to 12).

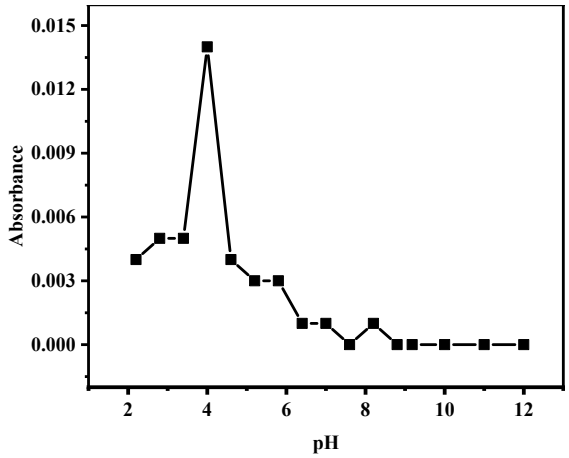


Figure S7. UV-vis absorption changes of **T2** (10 μM) at 570 nm at various pH values (pH 2 to 12).

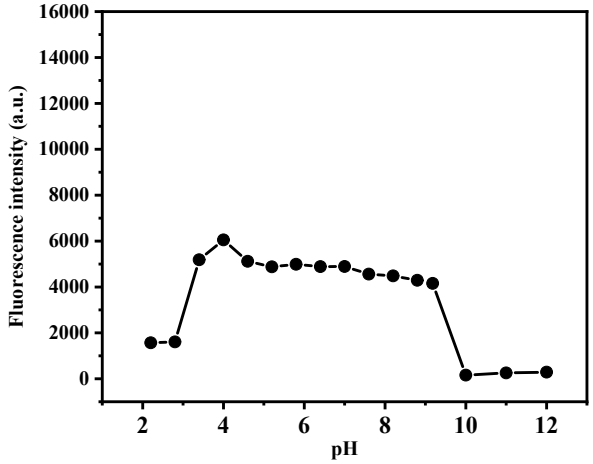


Figure S8. Emission changes of **T2** (10 μM, λex = 570 nm) at 590 nm at various pH values (pH 2 to 12).

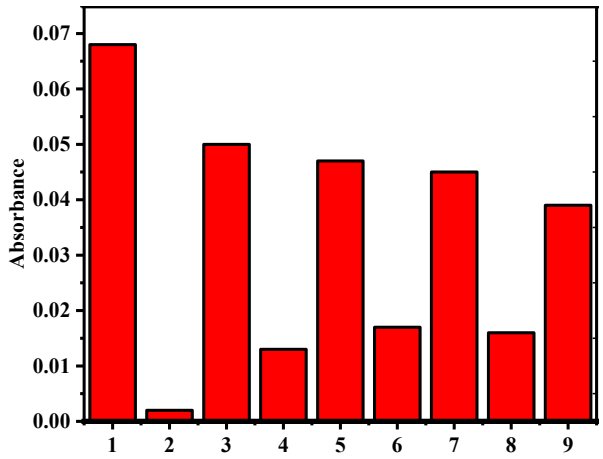


Figure S9. UV-vis absorbance at 560 nm of **T1** (10 μM) in water (pH=7.4) solution with the alternate adding of Fe^{3+} (20 μM) and EDTA (20 μM).

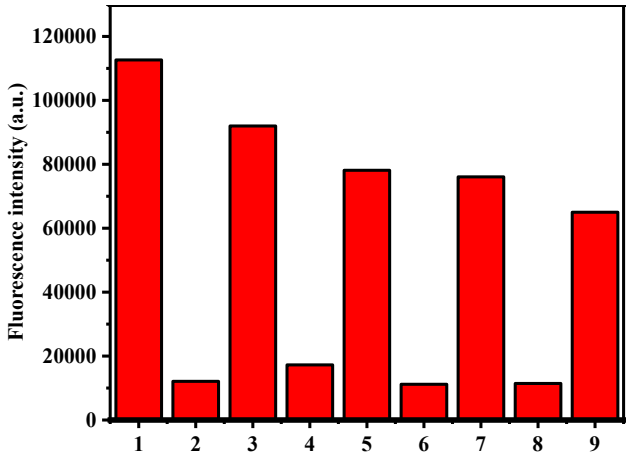


Figure S10. Fluorescence emission intensity at 590 nm of **T1** (10 μM) in water (pH=7.4) solution with the alternate adding of Fe^{3+} (20 μM) and EDTA (20 μM).

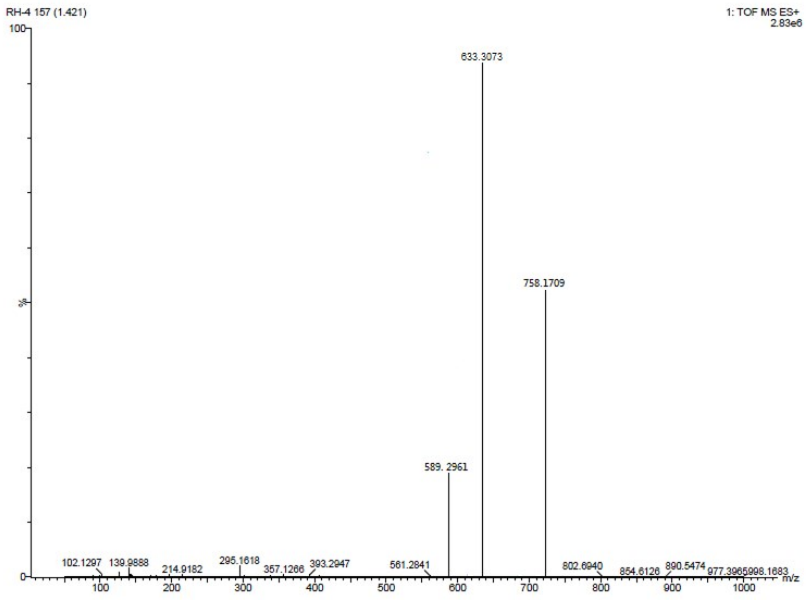


Figure S11. ESI-MS of **T1**-Fe^{3+} complex. ESI-mass: m/z = 633.3073 [**T1**+1], m/z = 758.1709 [**T1**+ Fe^{3+}+2Cl^{-})]$^{+}$.

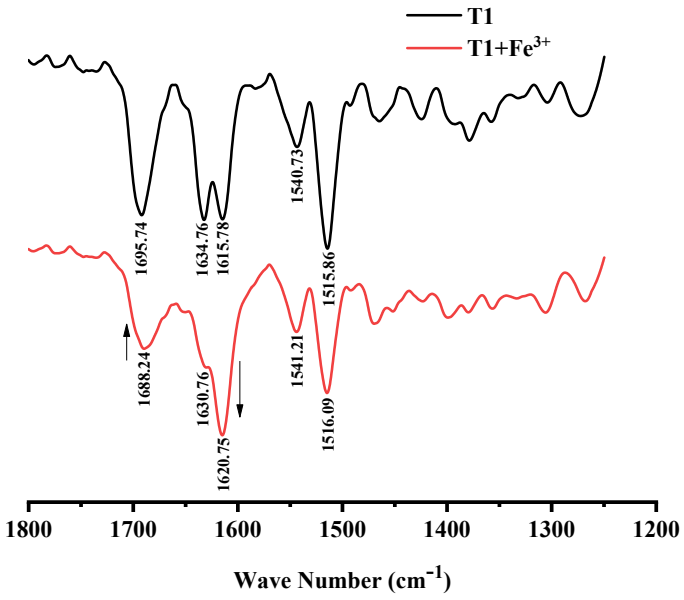


Figure S12. IR spectra of **T1** (2 mM) alone and upon addition of 1 mM Fe^{3+} ions. Upward arrow shows the decrement in the intensity of spitolactam ring 'C=O' and downward arrow shows the increment in the intensity of metal bound ring opened 'C-O'.

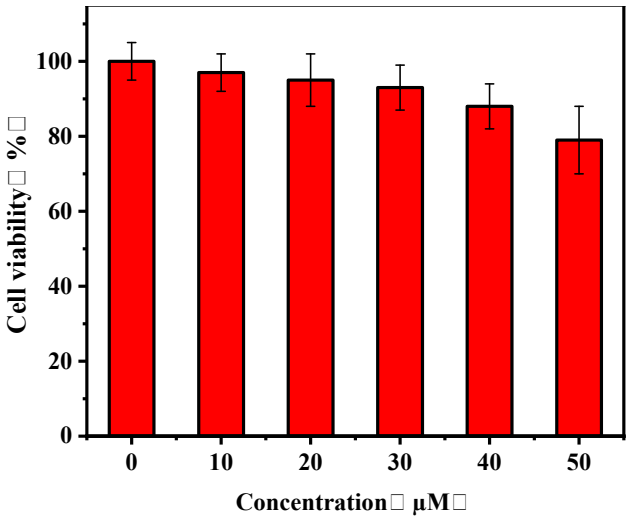


Fig. S13 Cell viability of HeLa cells treated with different concentrations of **T1** (0-50 μM) for 24 h.

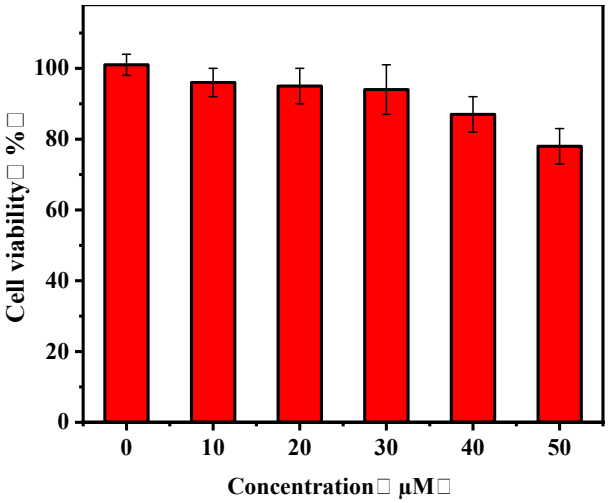


Fig. S14 Cell viability of HeLa cells treated with different concentrations of **T2** (0-50 μM) for 24 h.

2. ^{1}H NMR, ^{13}C NMR and MS charts

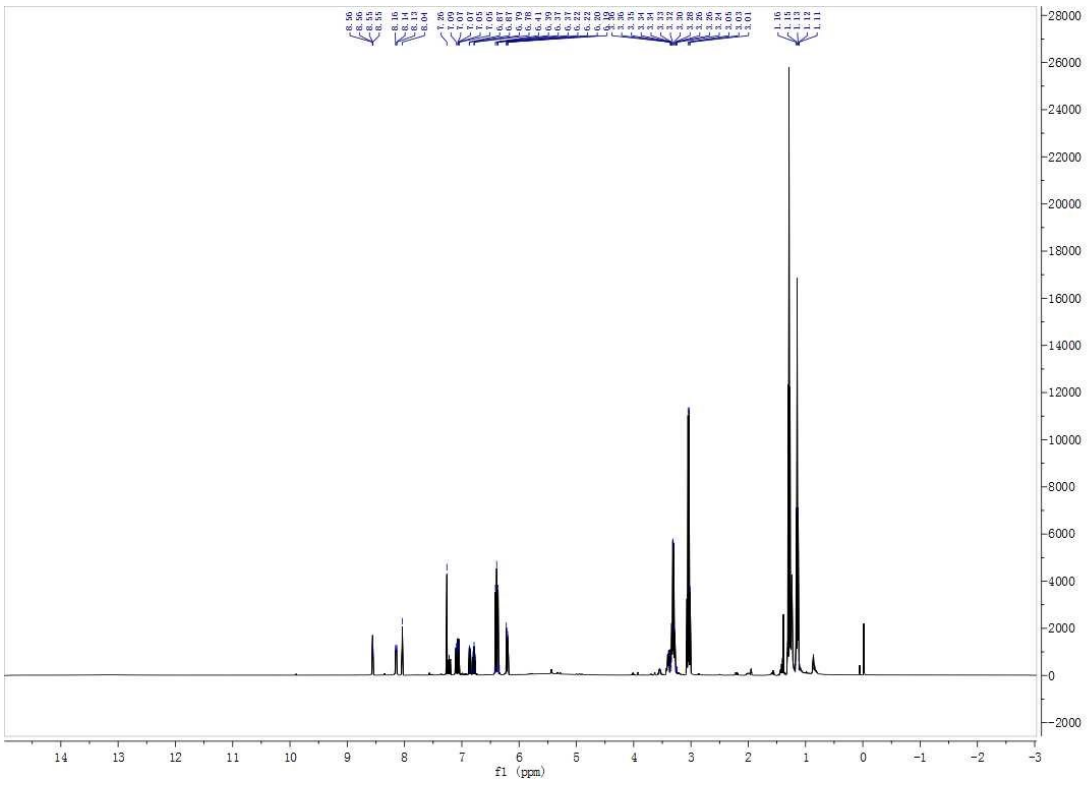


Figure S15. ^{1}H NMR of **T1** in $CDCl_3$ (δ = 7.26).

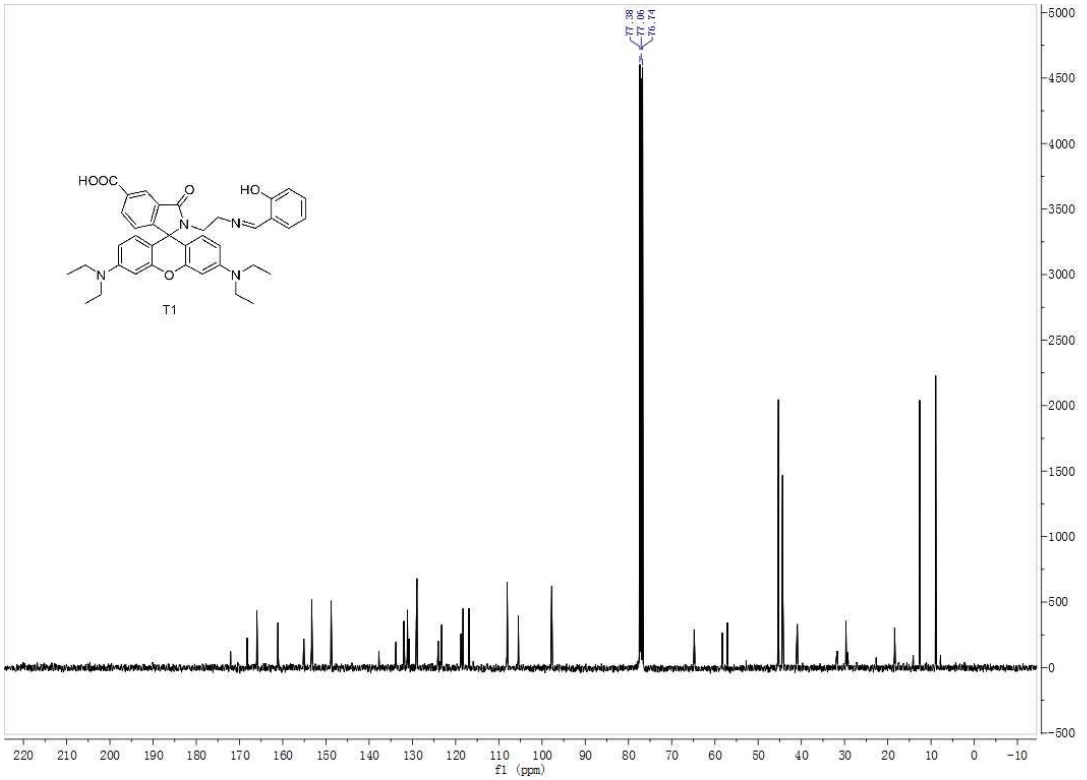


Figure S16. ^{13}C NMR spectra of **T1** in $CDCl_3$ (δ = 77.23).

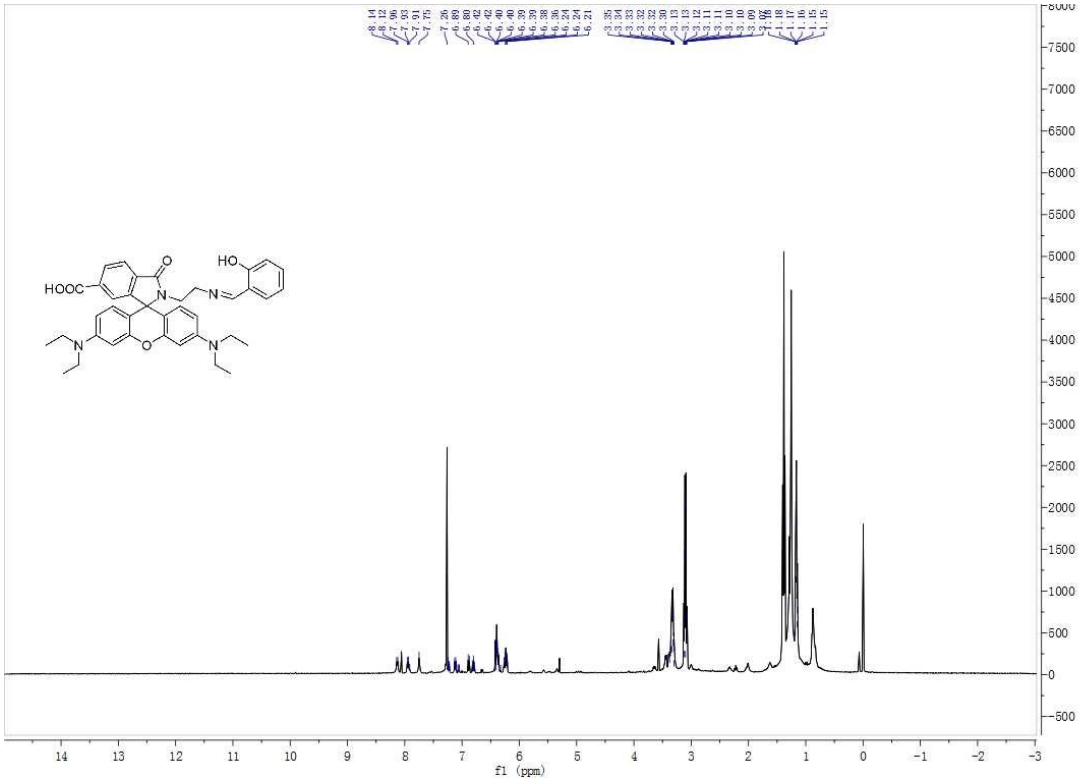


Figure S17. ^{1}H NMR of **T2** in $CDCl_3$ (δ = 7.26).

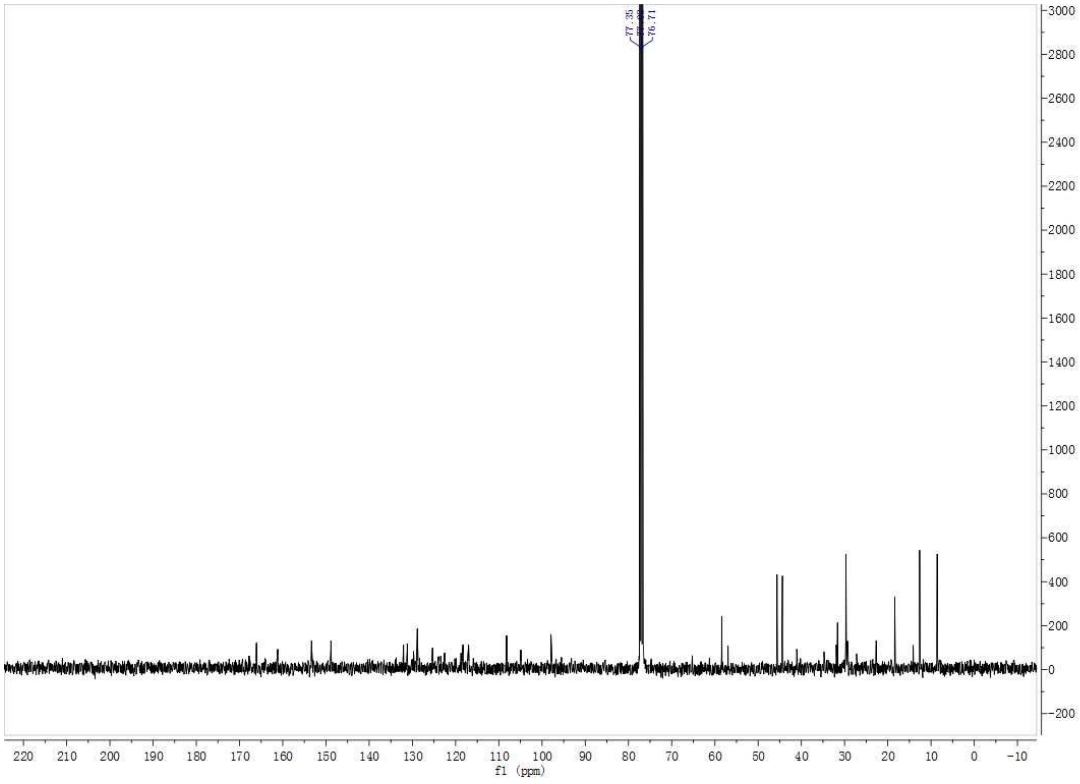


Figure S18. ^{13}C NMR spectra of **T2** in $CDCl_3$ (δ = 77.23).

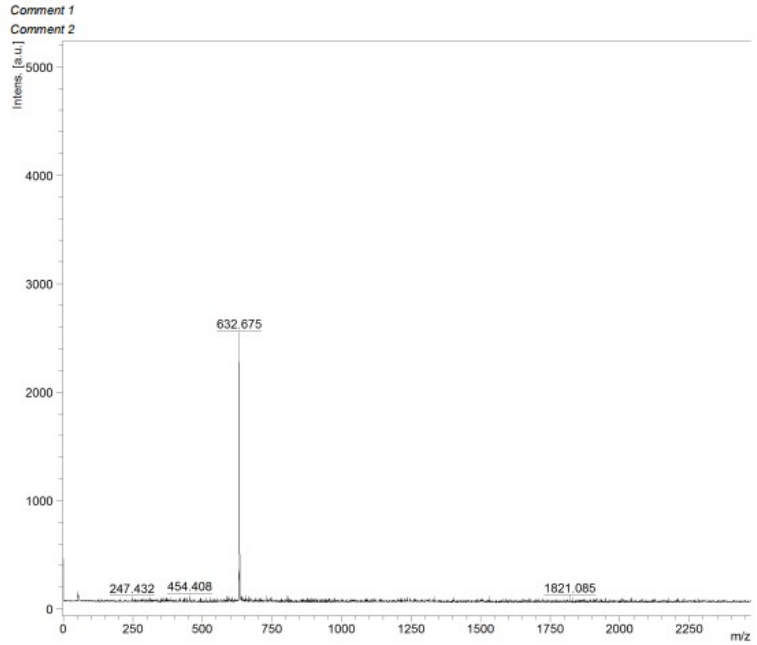


Figure S19. MS spectra of **T1**.

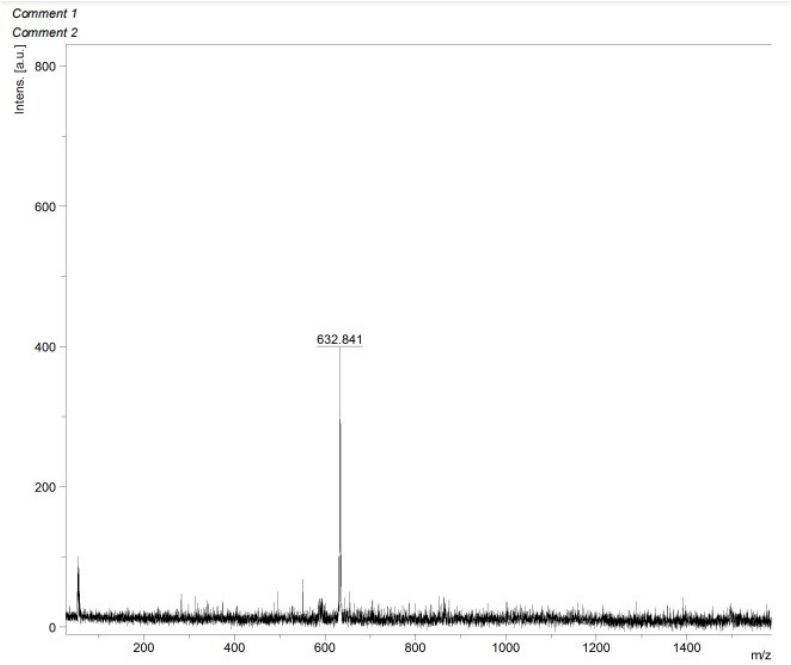


Figure S20. MS spectra of **T2**.