Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Material

Novel fluorescent probes based on rhodamine for naked-eye detection of Fe^{3+} and application of imaging in living cells

Meipan Yang, Wenfei Meng, Na Su, Xiaojing Liu, Ming Zhang, Bingqin Yang*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry, Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an 710069, PR China

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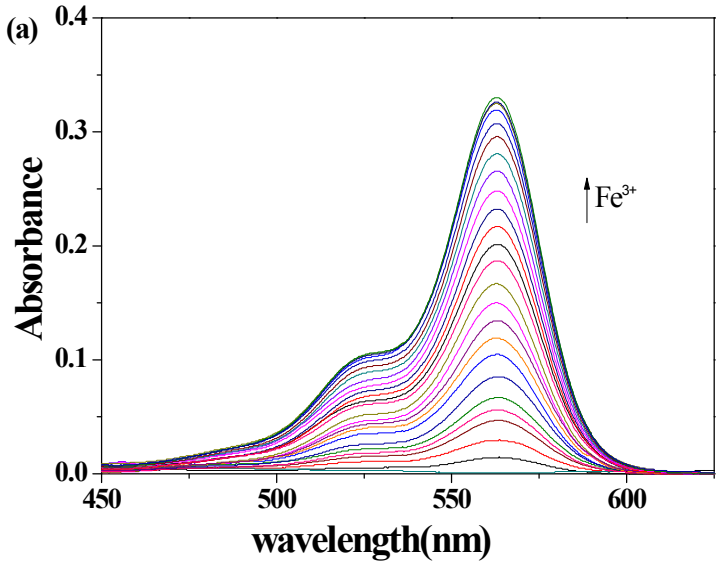
Table S1 X-ray table of compound **L1**.

Compound	**L1**
Formula	$C_{35}H_{37}N_3O_2S$
Formula weight	563.74
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
space group	P2(1)/c
Volume ($Å^3$)	3035.2(9)
Z	4
Unit cell dimensions /(Å, °)	a = 8.7284(15) α= 90 b =17.138(3) β= 90.986(4) c = 20.293(4) γ= 90
Calculated density (Mg/m^3)	1.234
Absorption coefficient (mm^{-1})	0.143
F(000)	1200
Crystal size (mm^3)	0.37 x 0.29 x 0.14
Theta range for data collection (°)	2.01 - 25.05
Limiting indices	-10<=h<=9 -16<=k<=20 -24<=l<=24
Reflections collected / unique	14870 / 5365 [*R*(int) = 0.0844]
Completeness to θ = 25.10	99.7 %
Max. and min. transmission	0.9800 and 0.9498
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5365 / 4 /397
Goodness-of-fit on F^2	1.028
Final R indices [I>2σ (I)]	R1 = 0.0804, wR2 = 0.1809
R indices (all data)	R1 = 0.1756, wR2 = 0.2260
Largest diff. peak and hole/(e. $Å^{-3}$)	0.373 and -0.335
CCDC	1029970

Table S2 X-ray table of compound **L2**.

Compound	**L2**
Formula	$C_{37}H_{39}N_3O_2S$
Formula weight	589.21
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
space group	P2(1)2(1)2(1)
Volume ($Å^3$)	3199.7(5)
Z	4
Unit cell dimensions /(Å, °)	a = 9.0224(8) α= 90 b =11.6701 (10) β= 90 c = 30.389 (3) γ= 90
Calculated density (Mg/m^3)	1.224
Absorption coefficient (mm^{-1})	0.138
F(000)	1256
Crystal size (mm^3)	0.36x 0.31 x 0.23
Theta range for data collection (°)	1.87 - 25.10
Limiting indices	-9<=h<=10 -11<=k<=13 -33<=l<=36
Reflections collected / unique	16148 / 5709 [*R*(int) = 0.0486]
Completeness to θ = 25.10	99.9 %
Max. and min. transmission	0.9684 and 0.9521
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5709 / 5 /414
Goodness-of-fit on F^2	1.063
Final R indices [I>2σ (I)]	R1 = 0.0580, wR2 = 0.1180
R indices (all data)	R1 = 0.0722, wR2 = 0.1245
Largest diff. peak and hole/(e. $Å^{-3}$)	0.178 and -0.150
CCDC	1029971



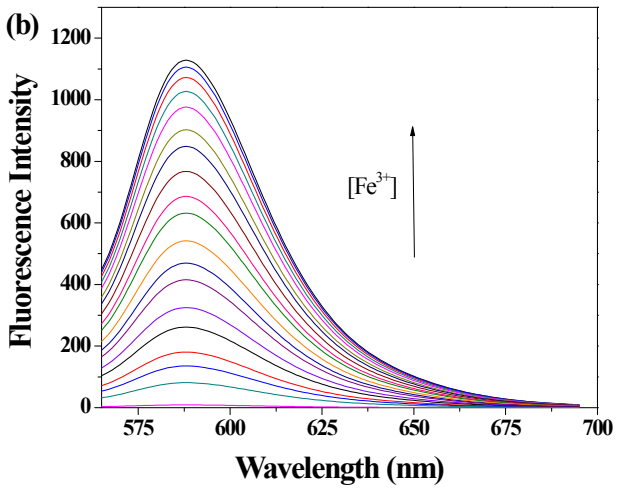


Fig. S1 Absorbance (a) and fluorescence (b) titration spectra of **L2** (20 μM) in methanol-water (1:1, v/v) upon addition of Fe^{3+} (λ_{ex}=550 nm).

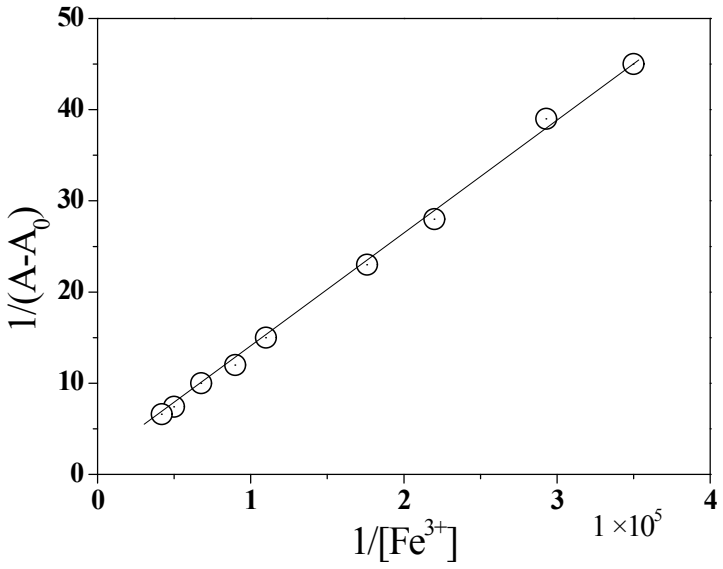


Fig. S2 Benesi-Hildebrand plot of **L1** using 1:1 stoichiometry for association between **L1** and Fe^{3+}.

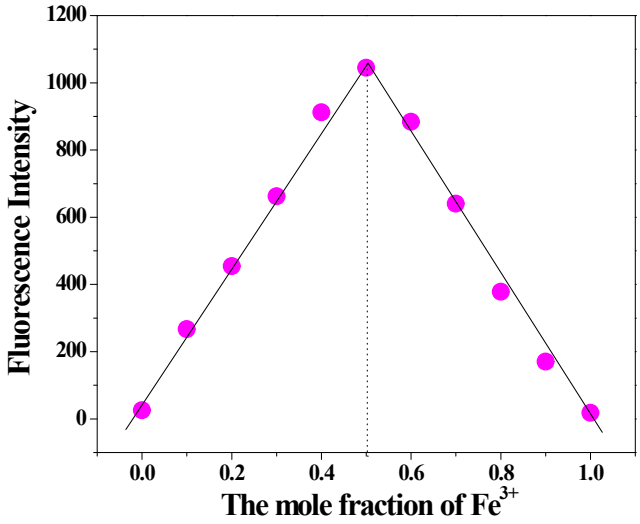


Fig. S3 The Job's plot of probe **L2** and Fe^{3+} (the total concentration was 20 μM).

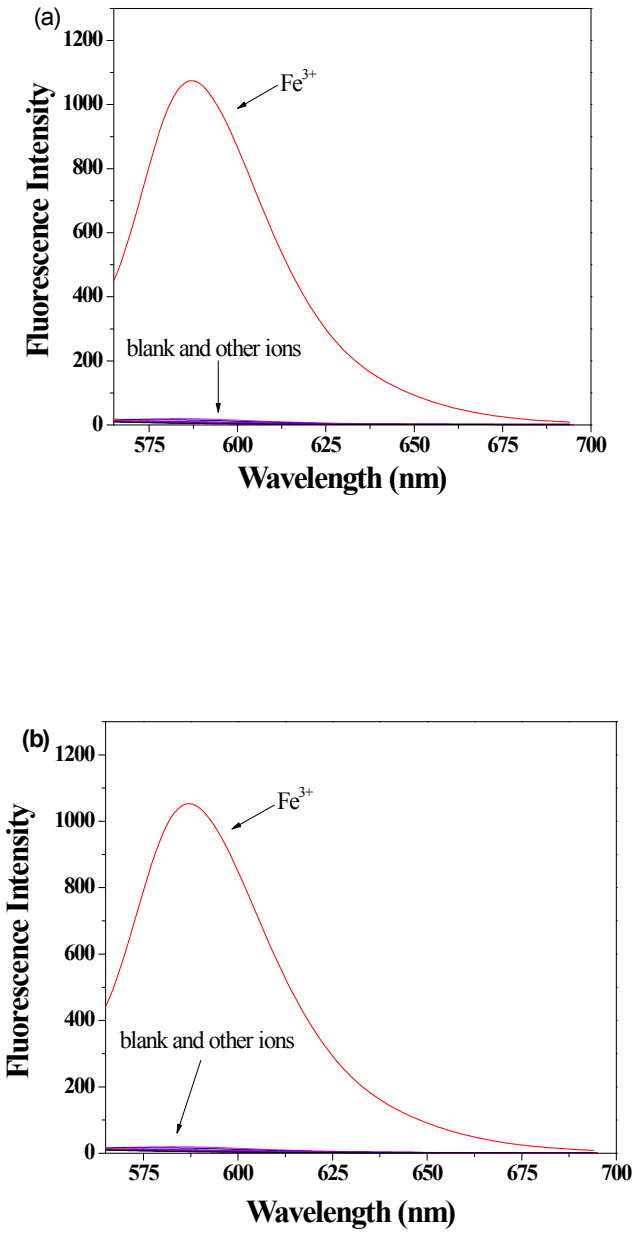


Fig. S4 Fluorescence spectra of **L1** (a) and **L2** (b) upon addition of different metal ions in methanol-water (1/1, v/v) solution.

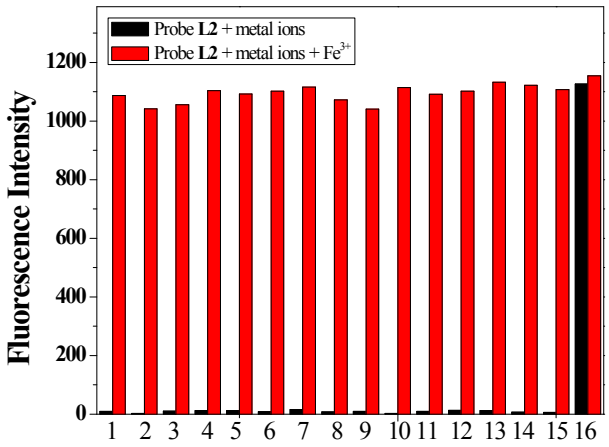


Fig. S5 Fluorescence intensity changes of **L2** (20 μM) upon the addition of various metal ions (20 μM) in and without the presence of Fe^{3+} (20 μM). The black bars represent the fluorescence response of **L2** and competing ions: 1, blank; 2 K^{+}; 3, Ca^{2+}; 4, Cd^{2+}; 5, Mg^{2+}; 6, Co^{2+}; 7, Mn^{2+}; 8, Cu^{2+}; 9, Al^{3+}; 10, Zn^{2+}; 11, Ni^{2+}; 12, Fe^{2+}; 13, Hg^{2+}; 14, Cr^{3+}; 15, Na^{+}; 16, Fe^{3+}. The red bars represent the subsequent addition of 20 μM Fe^{3+} to the above solutions. λ_{ex} = 550 nm.

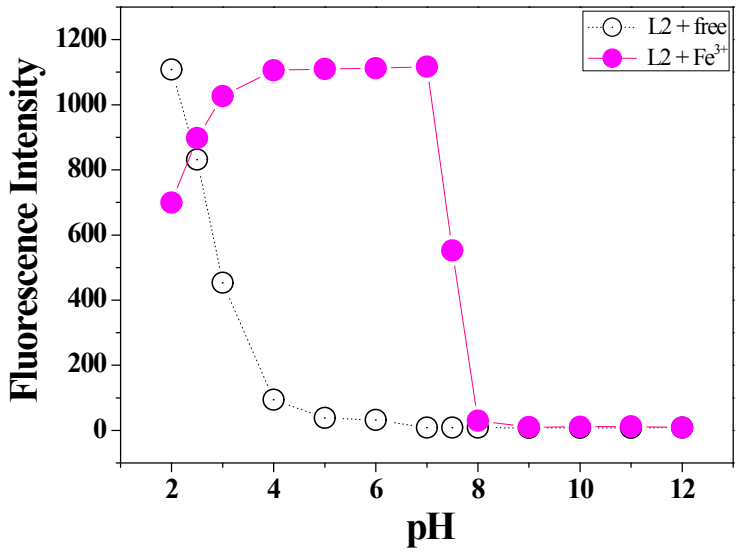


Fig. S6 Effect of pH on fluorescence intensity of **L2** in the absence and presence of Fe^{3+}.

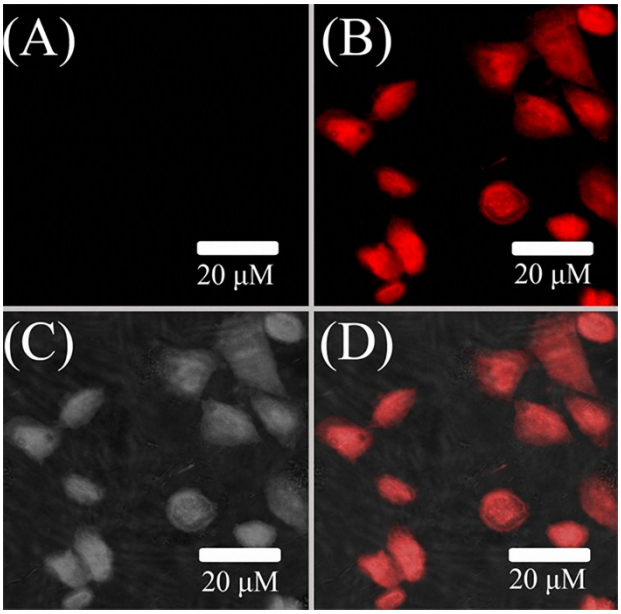


Fig. S7 Confocal fluorescence and bright-field images of HepG2 cells (scale bar = 20 μM). (A) Cells incubated with 20 μM **L2** for 60 min. (B) and then further incubated with 20 μM Fe^{3+} for 90 min. (C) Bright-field image of cells shown in panel, confirming their viability. (D) The overlay image of (B) and (C).

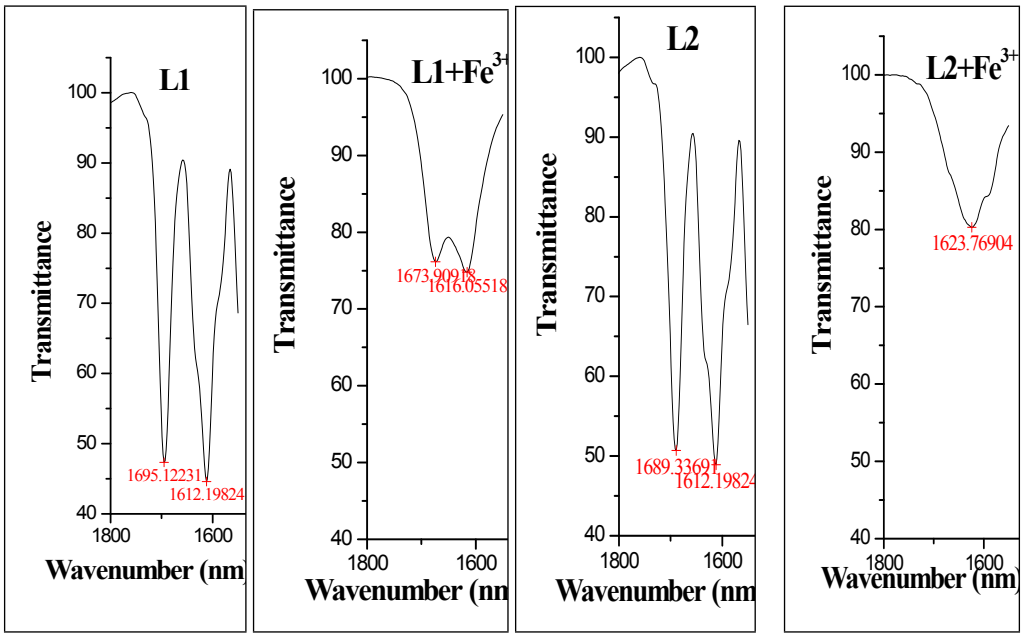


Fig. S8 IR spectra of **L1**, **L1** + Fe^{3+}, **L2**, **L2** + Fe^{3+}.

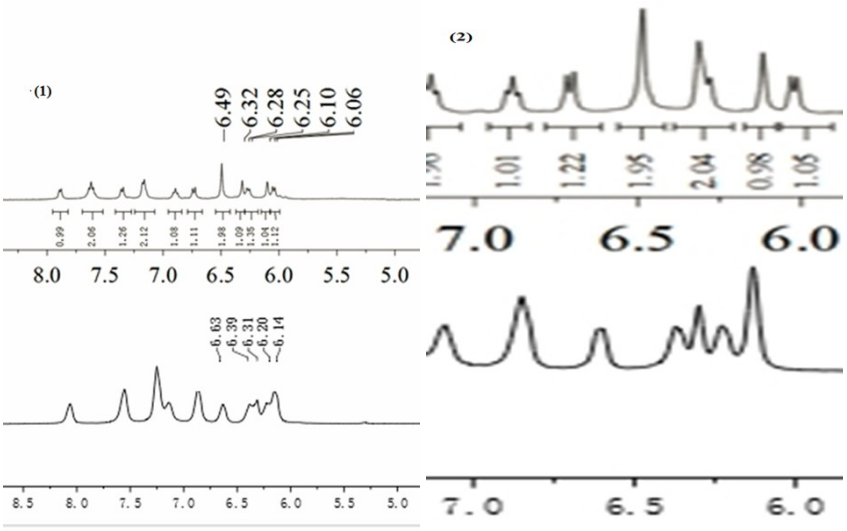


Fig. S9 ^{1}H NMR spectrum changes of **L1** (1) and **L2** (2) after addition of Fe^{3+}.

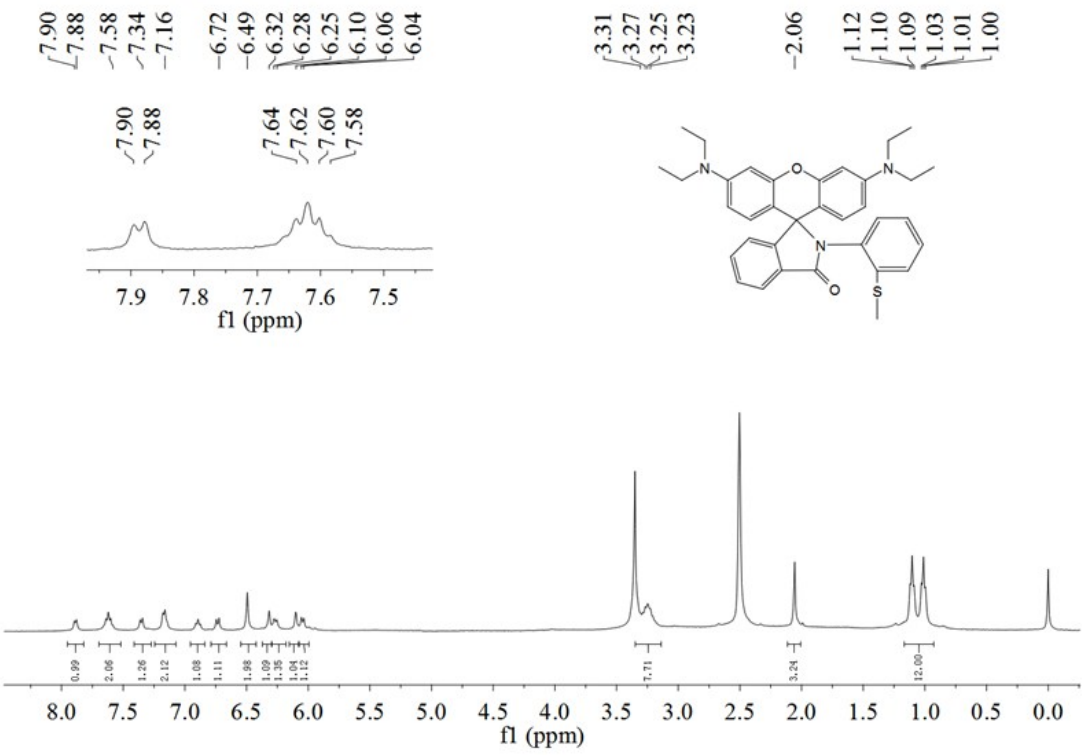


Fig. S10 ^{1}H NMR spectrum of **L1** in DMSO-d_6

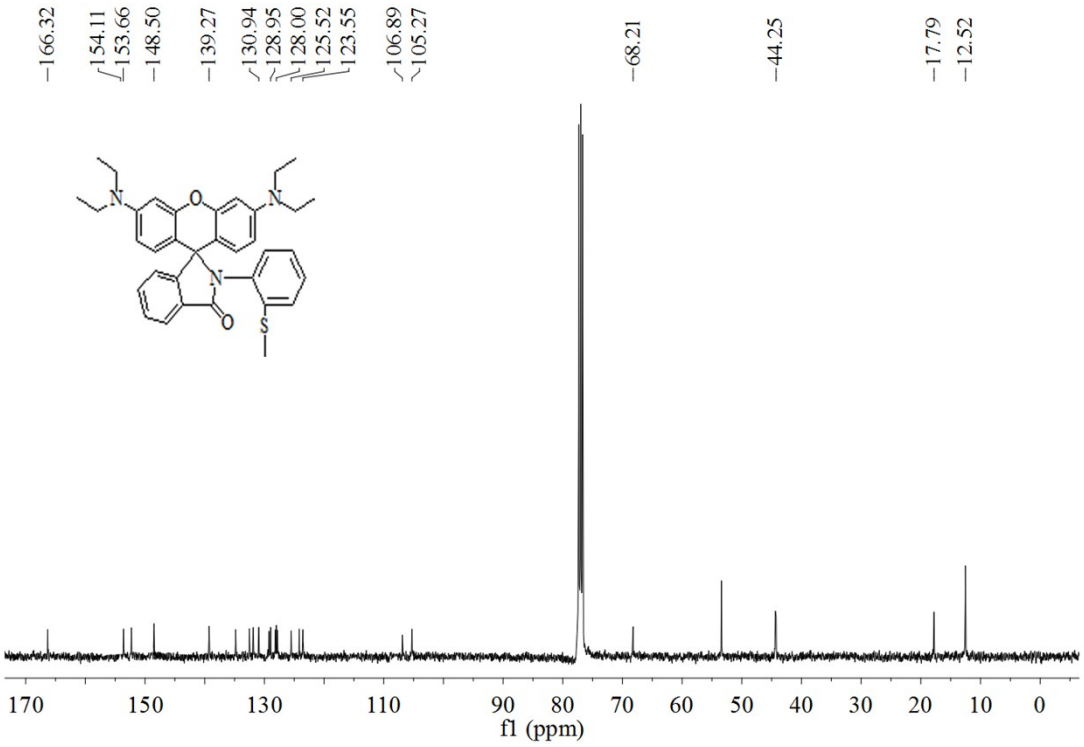


Fig. S11 ^{13}C NMR spectrum of **L1** in $CDCl_3$.

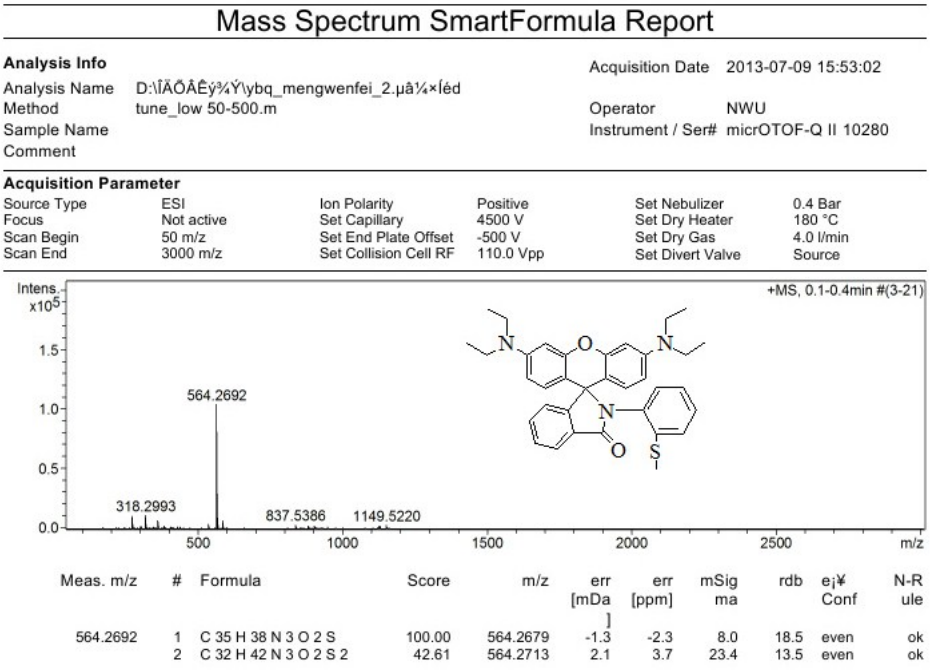


Fig. S12 Mass spectrum of **L1**.

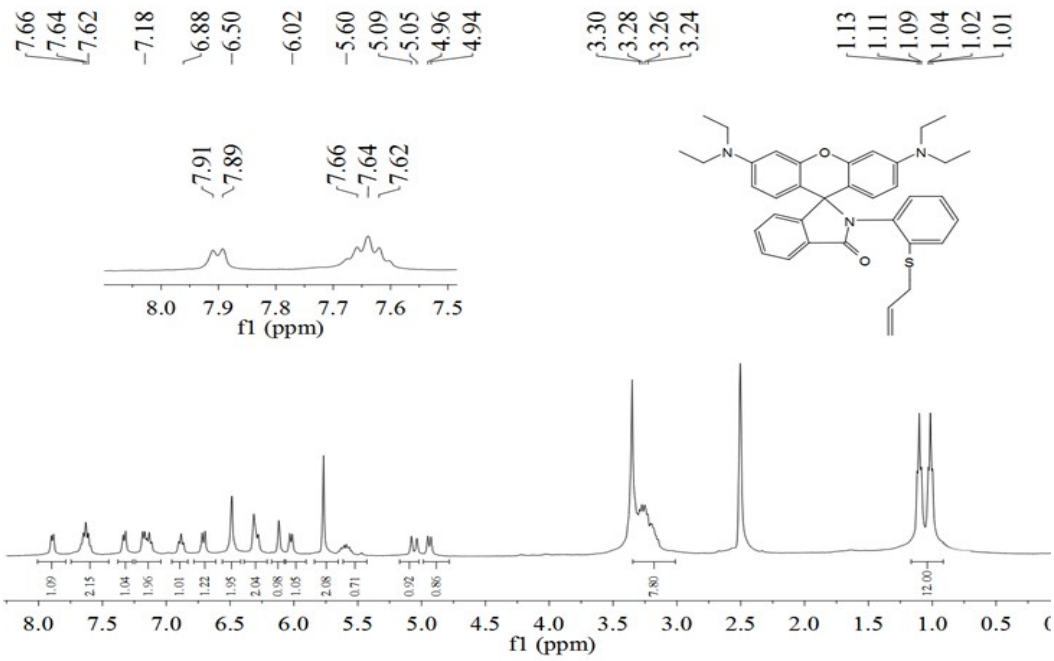


Fig. S13 ^{1}H NMR spectrum of **L2** in DMSO-d_6

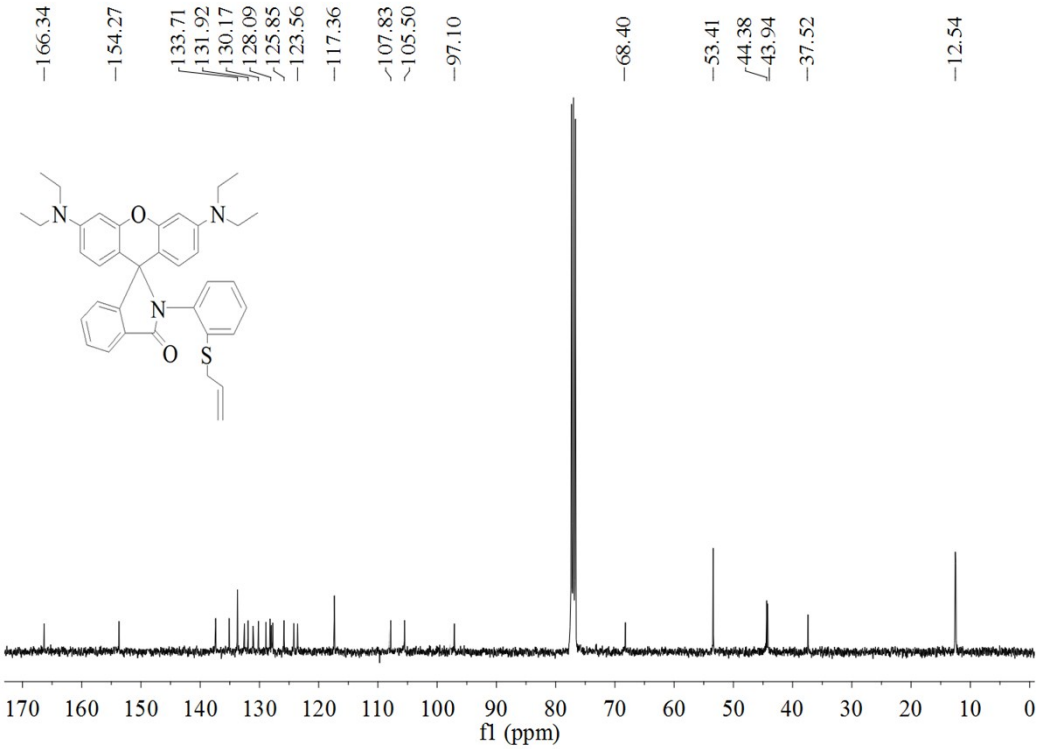
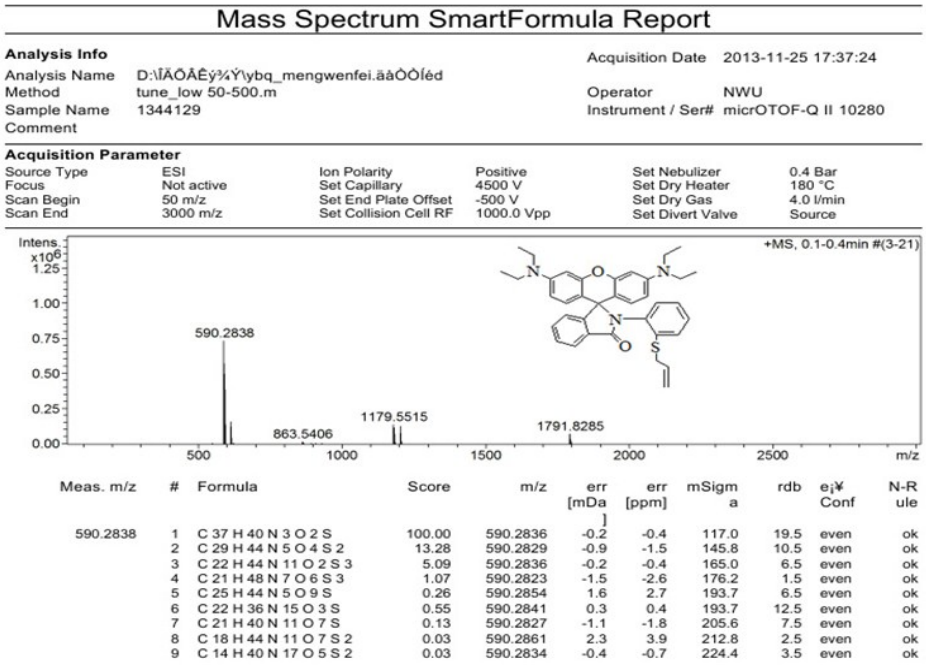


Fig. S14 ^{13}C NMR spectrum of **L2** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¡¥Conf	N-Rule
590.2838	1	C 37 H 40 N 3 O 2 S	100.00	590.2836	-0.2	-0.4	117.0	19.5	even	ok
	2	C 29 H 44 N 5 O 4 S 2	13.28	590.2829	-0.9	-1.5	145.8	10.5	even	ok
	3	C 22 H 44 N 11 O 2 S 3	5.09	590.2836	-0.2	-0.4	165.0	6.5	even	ok
	4	C 21 H 48 N 7 O 6 S 3	1.07	590.2823	-1.5	-2.6	176.2	1.5	even	ok
	5	C 25 H 44 N 5 O 9 S	0.26	590.2854	1.6	2.7	193.7	6.5	even	ok
	6	C 22 H 36 N 15 O 3 S	0.55	590.2841	0.3	0.4	193.7	12.5	even	ok
	7	C 21 H 40 N 11 O 7 S	0.13	590.2827	-1.1	-1.8	205.6	7.5	even	ok
	8	C 18 H 44 N 11 O 7 S 2	0.03	590.2861	2.3	3.9	212.8	2.5	even	ok
	9	C 14 H 40 N 17 O 5 S 2	0.03	590.2834	-0.4	-0.7	224.4	3.5	even	ok

Fig. S15 Mass spectrum of **L2**.