

Electronic Supplementary Information

Fluorescent In-based MOFs showing “turn on” luminescence to thiols and acting as a ratiometric fluorescence thermomete

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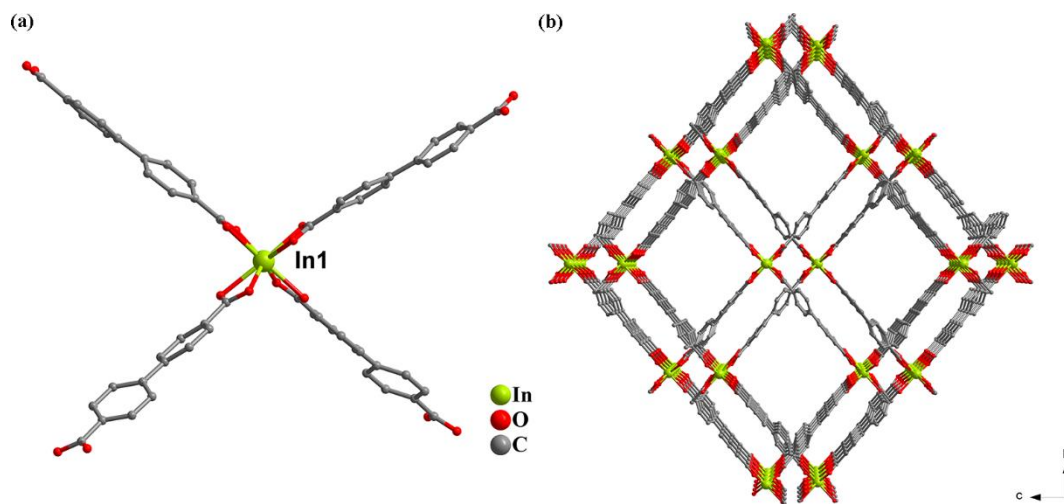
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Table S1 Crystallographic data and structural refinement details for compound **2**.

Empirical formula	C _{91.5} H _{83.5} Cl ₂ In ₃ N _{5.5} O _{27.5}
Formula weight	2115.49
Crystal system	orthorhombic
Space group	<i>P</i> 222 ₁
<i>a</i> /Å	9.3390(2)
<i>b</i> /Å	15.6217(5)
<i>c</i> /Å	33.6709(19)
<i>V</i> /Å ³	4912.3(3)
<i>Z</i>	2
λ	0.71073
<i>T</i> /K	295(2)
ρ_{calcd} /g cm ⁻³	1.430
μ /mm ⁻¹	0.829
<i>F</i> (000)	2144
Independent refls.	9353
No. of parameters	431
^a <i>R</i> ₁ (<i>I</i> > 2 σ (<i>I</i>))	0.0632
^b <i>wR</i> (<i>F</i> ₂) (<i>I</i> > 2 σ (<i>I</i>))	0.1565
Flack parameter	0.13(5)

$${}^a R_1 = \frac{\sum \|F_o\| - |F_c|}{\sum \|F_o\|}, \quad {}^b wR_2 = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right]^{1/2}$$

**Fig. S1** Coordination environments of In³⁺ ion in compound **1** and the 3D framework according to the literature.¹

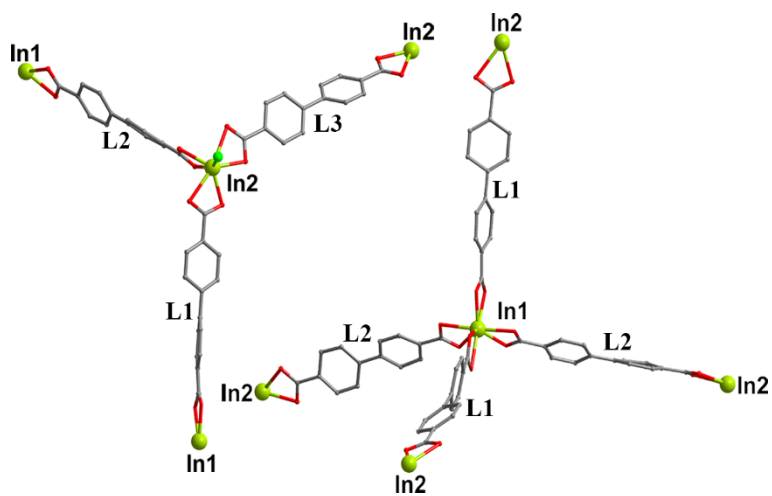


Fig. S2 (b) Coordination environments of the unique In³⁺ ions in compound **2**.

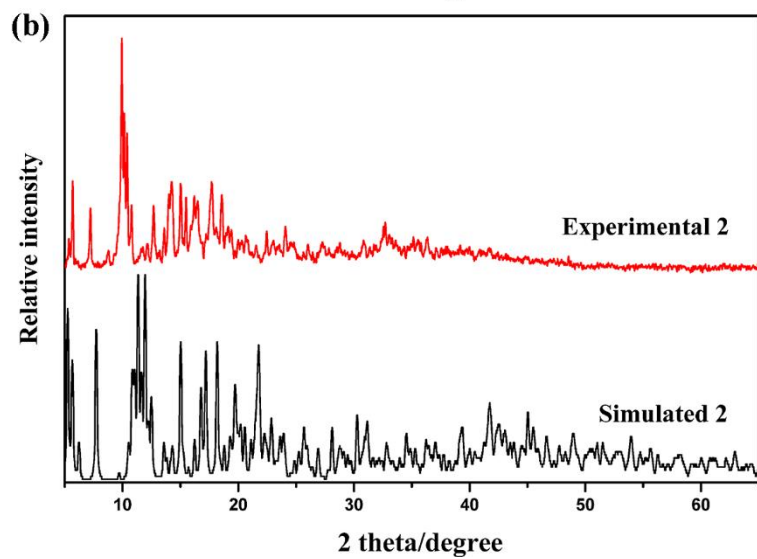
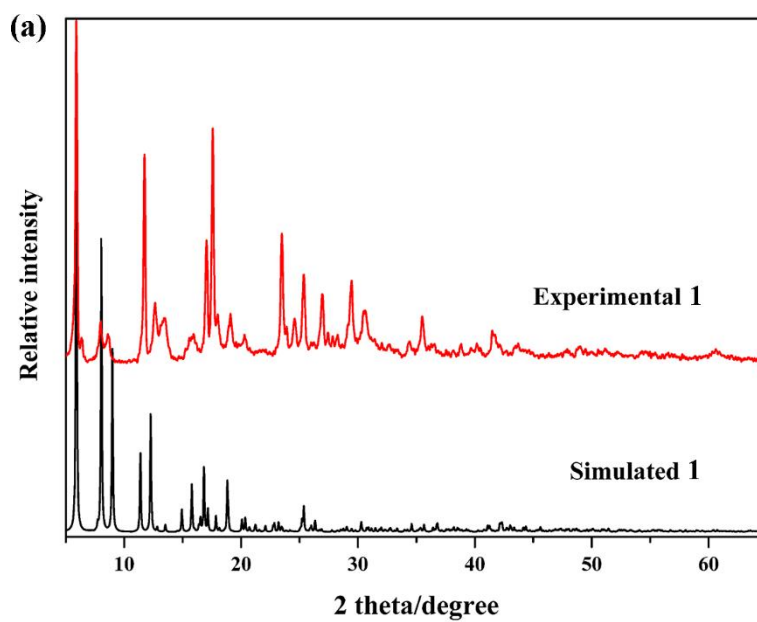


Fig. S3 PXRD patterns of the title compounds and the simulated ones from single-crystal X-ray structures.

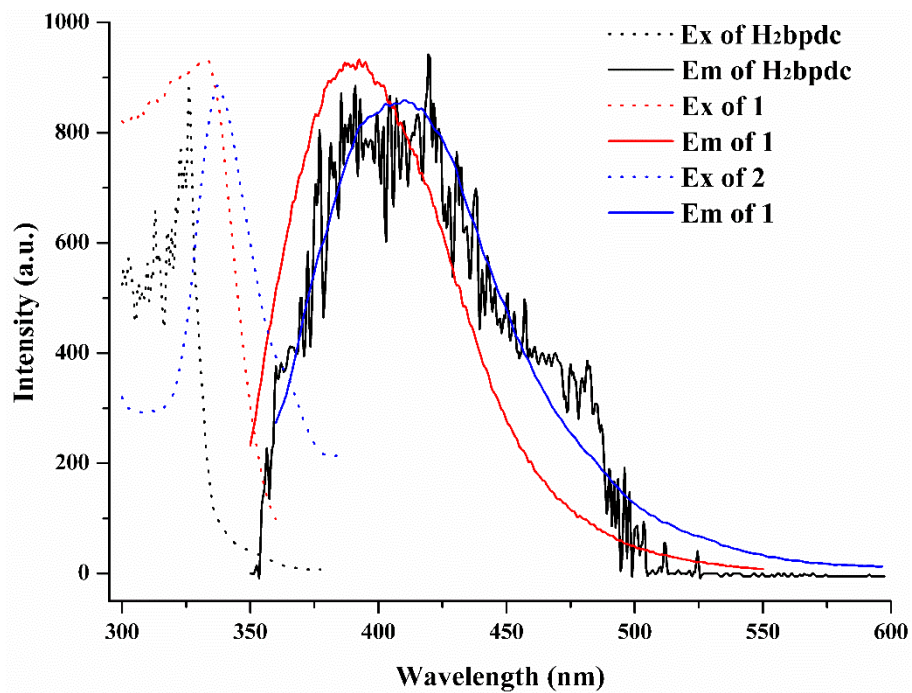


Fig. S4 Solid state FL spectra for bpdc ligand and compounds **1** and **2**.

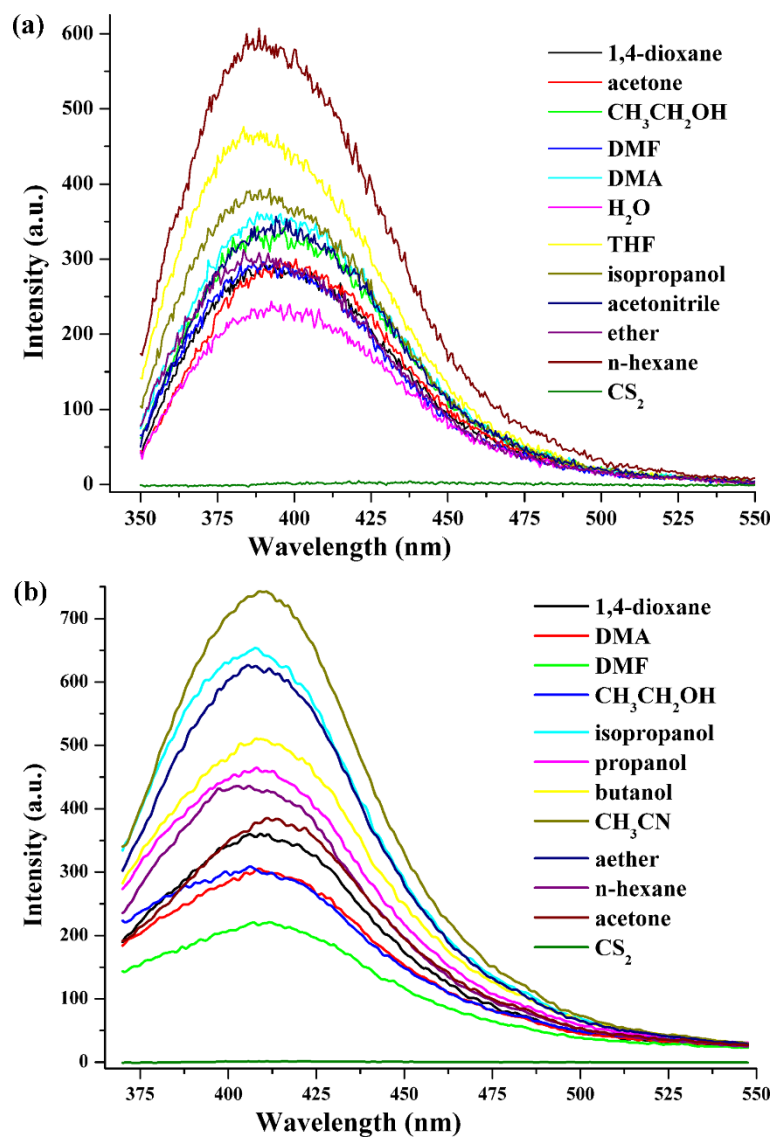


Fig. S5 Emission spectra of 1 (a) and 2 (b) dispersed in different solvents.

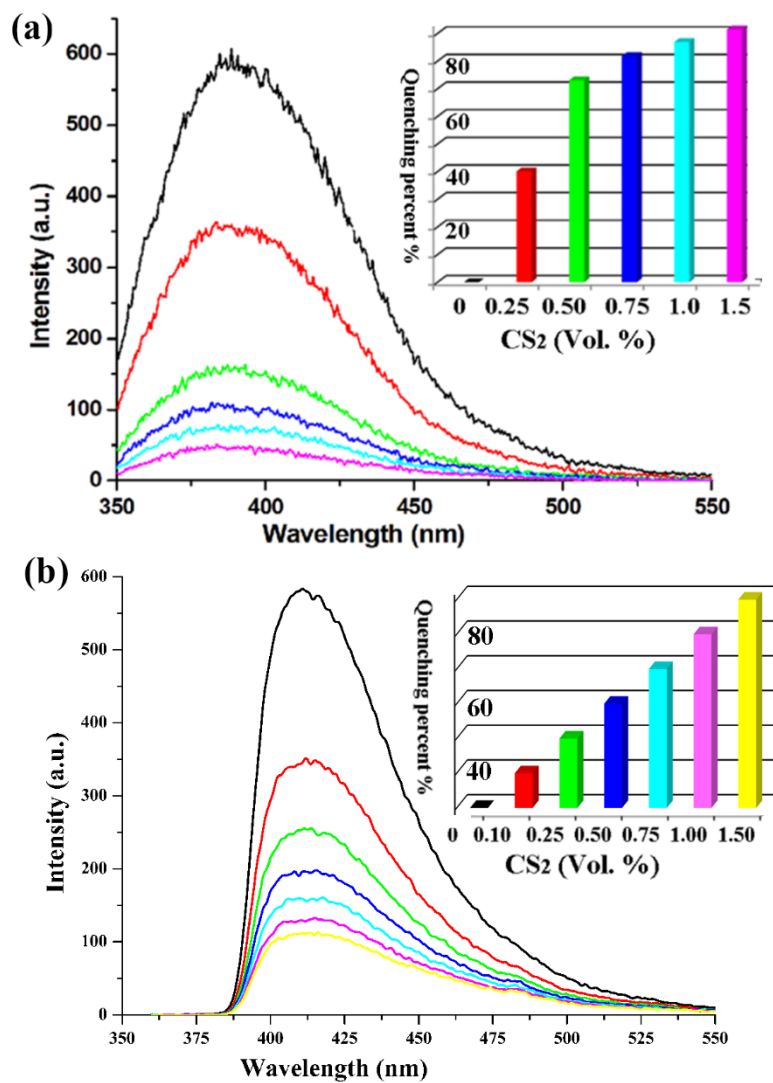


Fig. S6 Emission spectra of **1** (a) and **2** (b) upon addition of various amounts of CS₂.

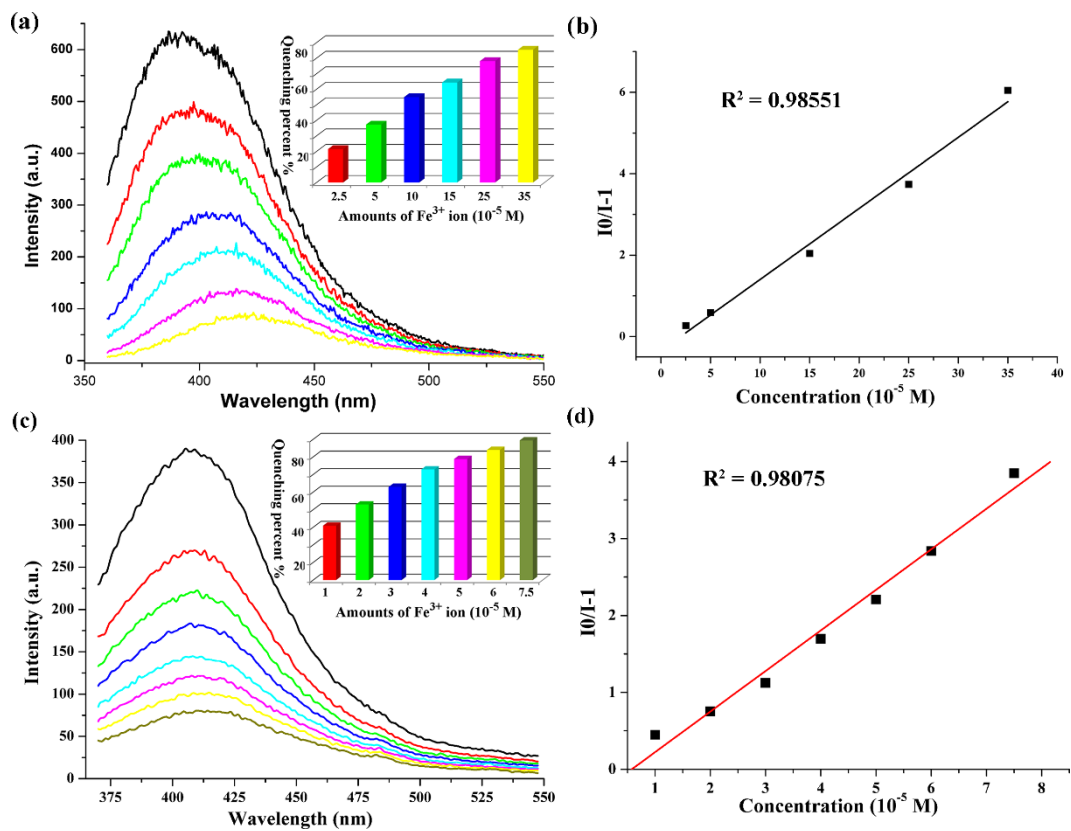


Fig. S7 Emission spectra of **1** (a) and **2** (c) with various contents of Fe³⁺, and the corresponding SV plots of **1** (b) and **2** (d).

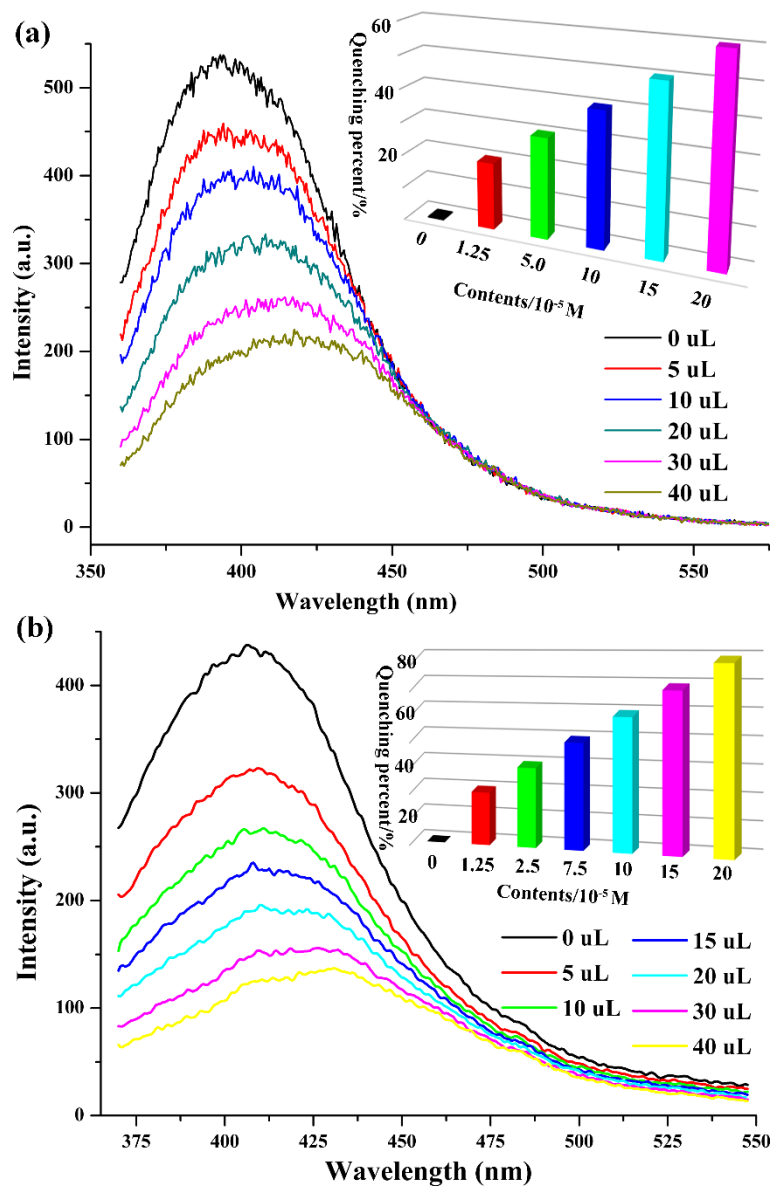


Fig. S8 (a) Fluorescence spectra of 1 (a) and 2 (b) with various contents of TNP.

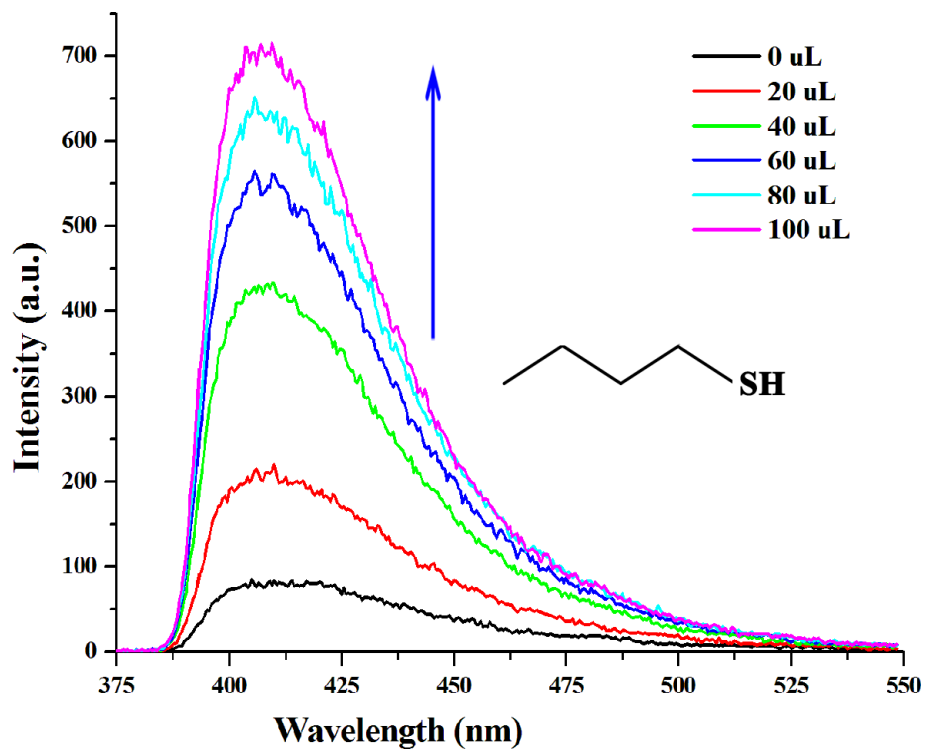


Fig. S9 Emission spectra of **2** with various contents of 10^{-2} M 1-butane-1-thiol.

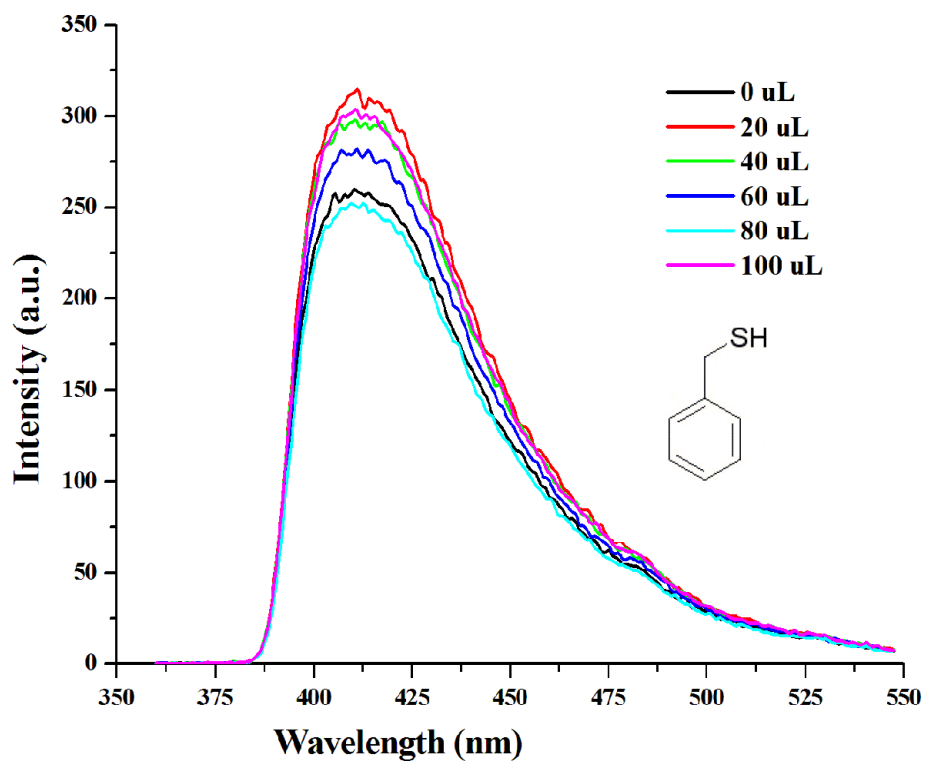


Fig. S10 Emission spectra of **2** with various contents of benzyl mercaptane.

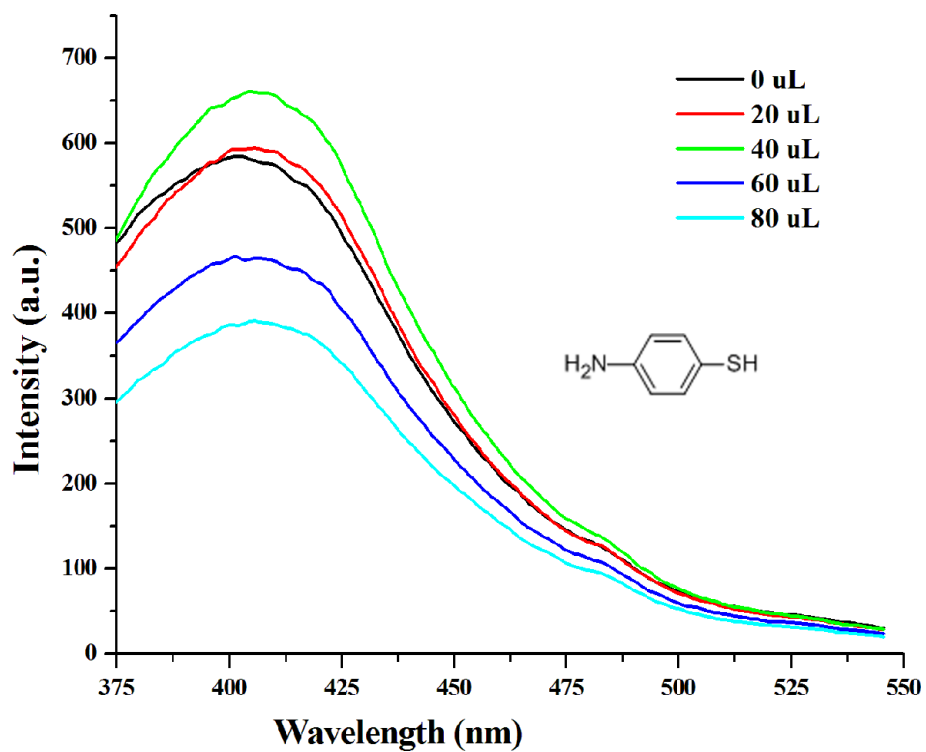


Fig. S11 Emission spectra of 2 with various contents of 4-aminophenol.

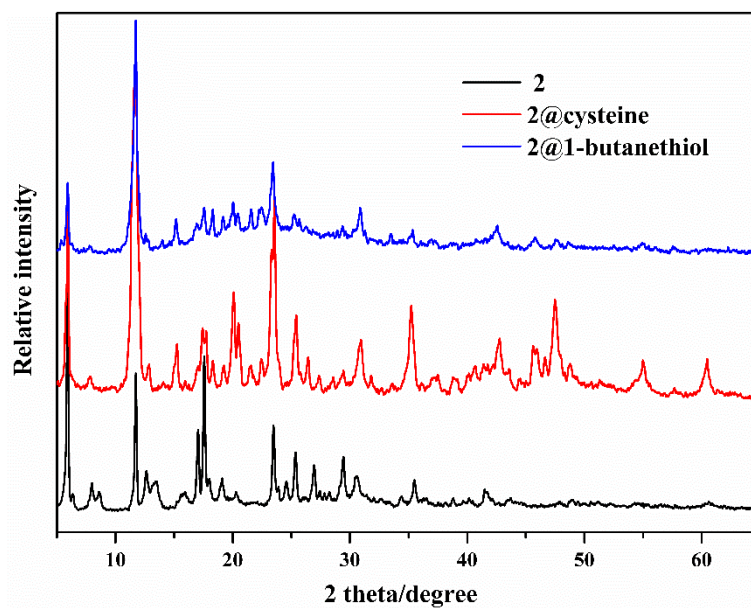


Fig. S12 PXRD patterns of 2 and the samples immersed in 10^{-2} M ethanol solution of thiols for 24h.

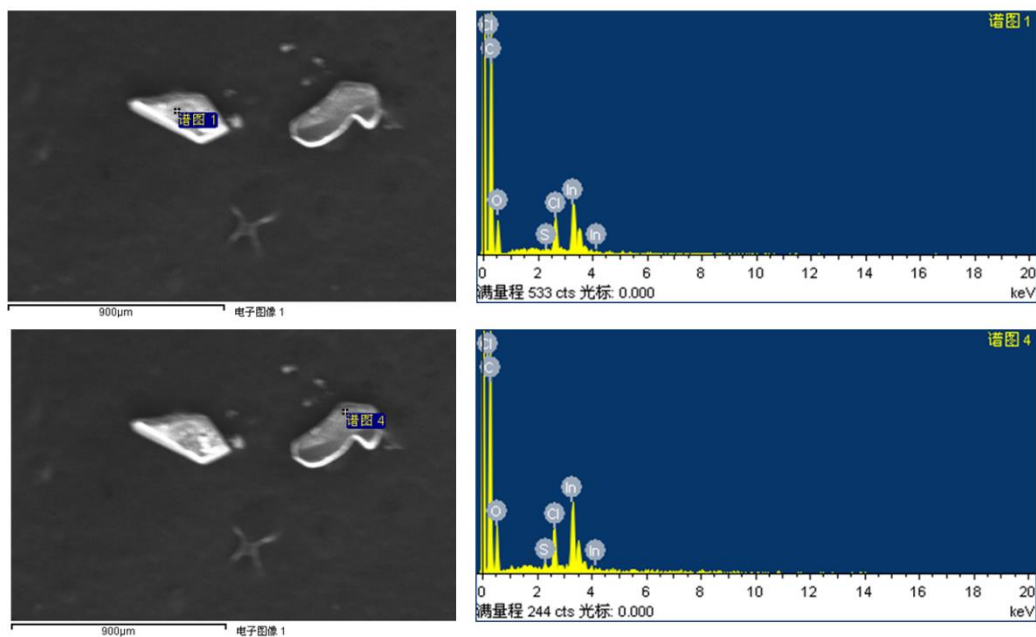


Fig. S13 EDS spectra of solid state sample of **2** treated with cysteine (up) and 1-butanethiol (down) respectively.

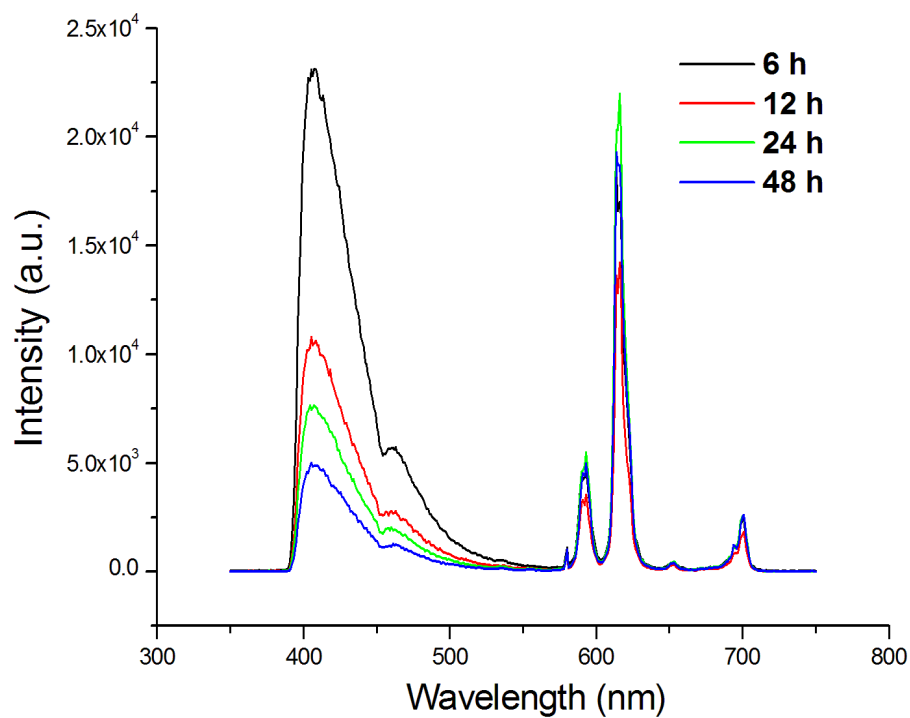


Fig. S14 Emission spectra of **2** treated with 10^{-2} M ethanol solution of Eu^{3+} at different times.

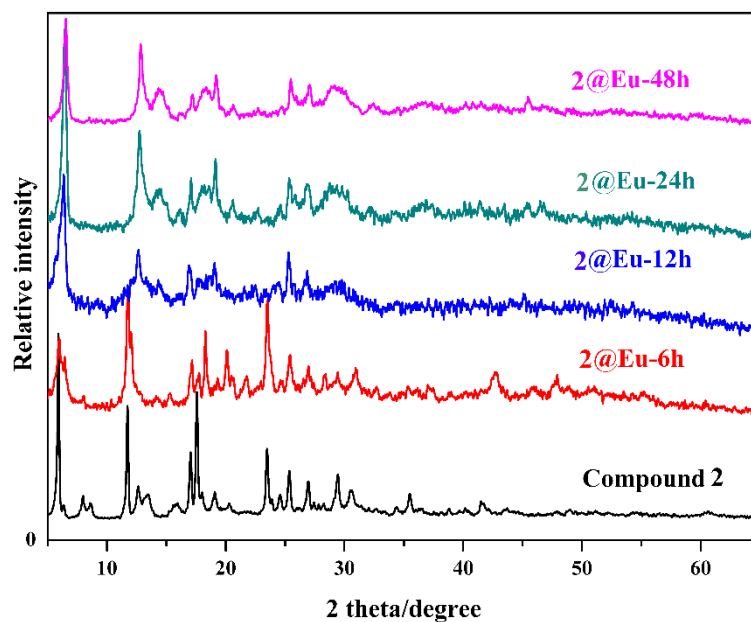


Fig. S15 PXR D patterns of **2** treated with 10^{-2} M ethanol solution of Eu^{3+} at different times.

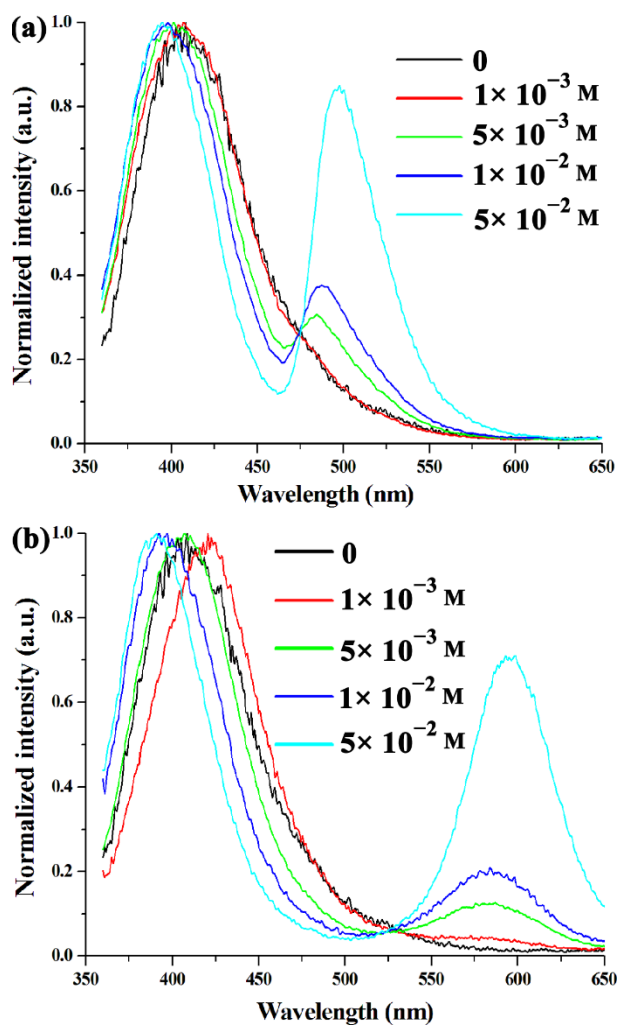


Fig. S16 Emission spectra of **2** treated with ethanol solution of different contents of AF (a) and DSM (b) for 12 h.

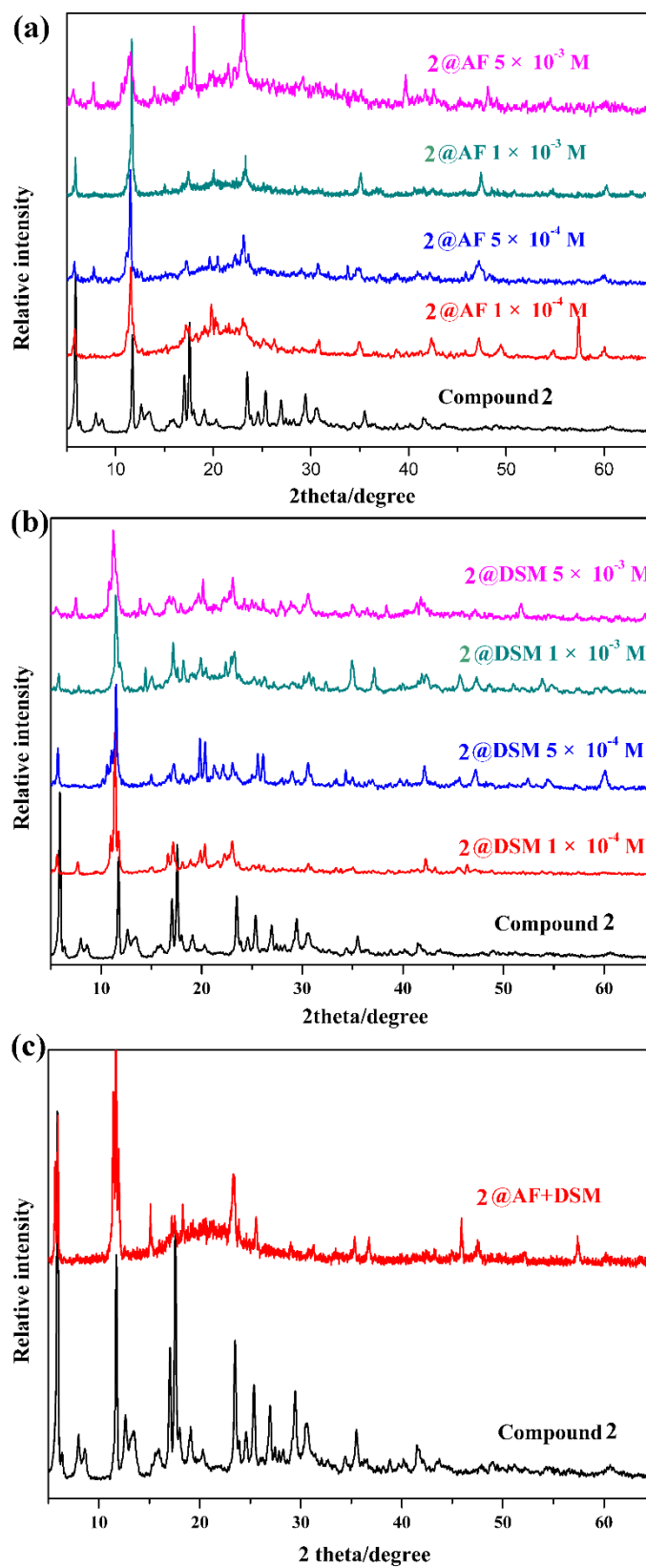


Fig. S17 PXR D patterns of **2** treated with 10^{-2} M ethanol solution of AF (a), DSM (b) with different concentrations and **2** treated with 10^{-2} M ethanol solution of both AF and DSM (c), respectively.

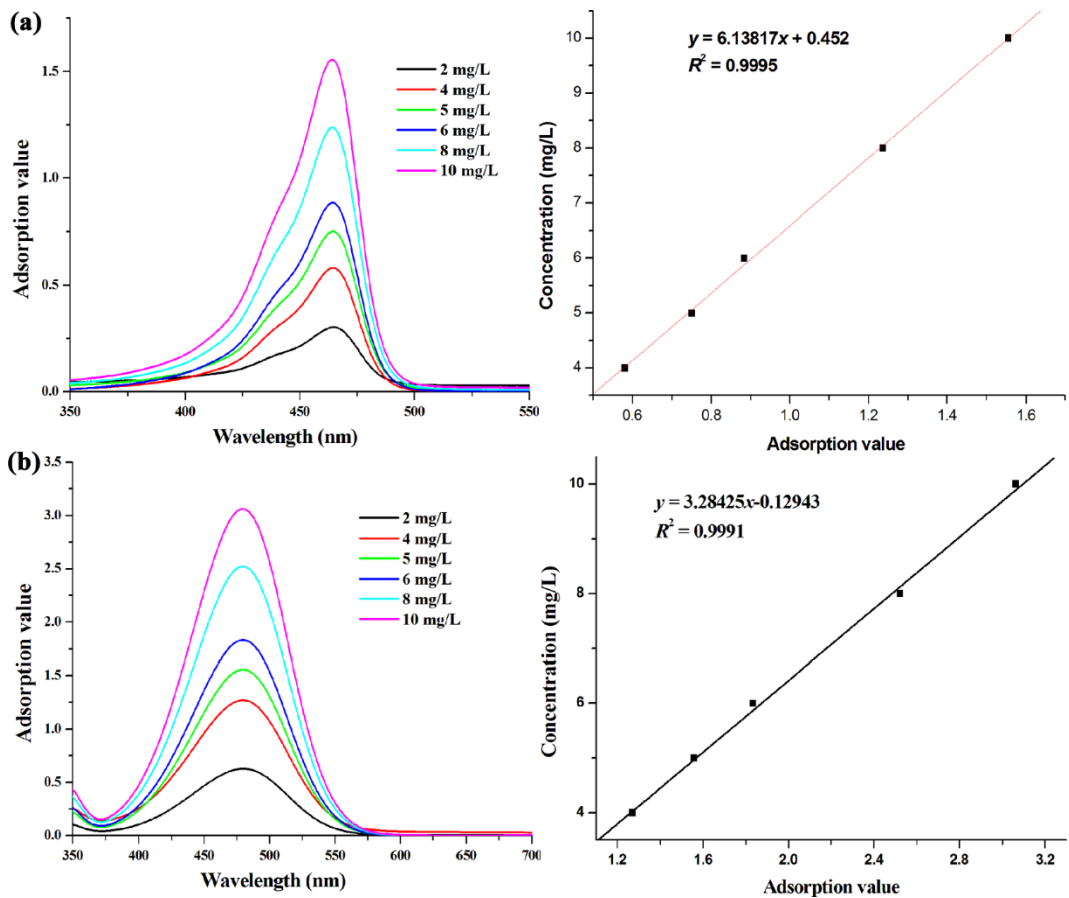


Fig. S18 Adsorption spectra of ethanol solution of dyes for the determination of AF (a) and DSM (b) contents in 2.