

Supporting Information

A bifunctional fluorescent probe for sensing of Al^{3+} and H_2S

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Fig. S1. ^1H NMR ($\text{DMSO}-d_6$, 600 MHz) spectrum of **L**.

Fig. S2. ESI-MS spectrum of **L**.

Fig. S3. The dihedral angle of **L**

Fig. S4. Competition experiment of **L** toward Al^{3+} in the presence of 5 equiv. of other metal ions in $\text{MeOH}/\text{H}_2\text{O}$ (9/1, v/v, $\text{pH}=7.4$).

Fig. S5. Fluorescence intensity at 477 nm of **L** (10 μM) at various pH values in $\text{MeOH}/\text{H}_2\text{O}$ (9/1, v/v) medium in the absence and presence of Al^{3+} (5 equiv).

Fig. S6. ^1H NMR ($\text{DMSO}-d_6$, 600 MHz) spectra of **L** with Al^{3+} .

Fig. S7. Job's plot of **L**- Al^{3+} system in $\text{Me}/\text{H}_2\text{O}$ (9/1, V/V, $\text{pH}=7.4$) medium.

Fig. S8. Benesi-Hildebrand plot of **L**- Al^{3+} system in $\text{MeOH}/\text{H}_2\text{O}$ (9/1, v/v, $\text{pH}=7.4$) medium.

Fig. S9. Competition experiment of **L** toward H_2S in the presence of 5 equiv. of other anions in $\text{EtOH}/\text{H}_2\text{O}$ (7/3, v/v, $\text{pH}=7.4$).

Fig. S10. Fluorescence intensity at 495 nm of **L** (10 μM) at various pH values in $\text{EtOH}/\text{H}_2\text{O}$ (9/1, v/v) medium in the absence and presence of H_2S (5 equiv).

Fig. S11. ^1H NMR ($\text{DMSO}-d_6$, 600 MHz) spectra of **L** with H_2S .

Fig. S12. Job's plot of **L**- H_2S system in $\text{EtOH}/\text{H}_2\text{O}$ (7/3, V/V, $\text{pH}=7.4$) medium.

Fig. S13. Benesi-Hildebrand plot of **L**- H_2S system in $\text{EtOH}/\text{H}_2\text{O}$ (7/3, v/v, $\text{pH}=7.4$) medium.

Table S1 Summary of crystal data and structure refinement parameters for **L**

Table S2 Selected bond lengths ($\text{\AA}$) and angles ($^\circ$) for **L**.

Table S3 Determination of Al^{3+} in water samples from different water sources by

standard-addition method (n =3).

Table S4 Determination of H₂S in water samples from different water sources by standard-addition method (n =3).

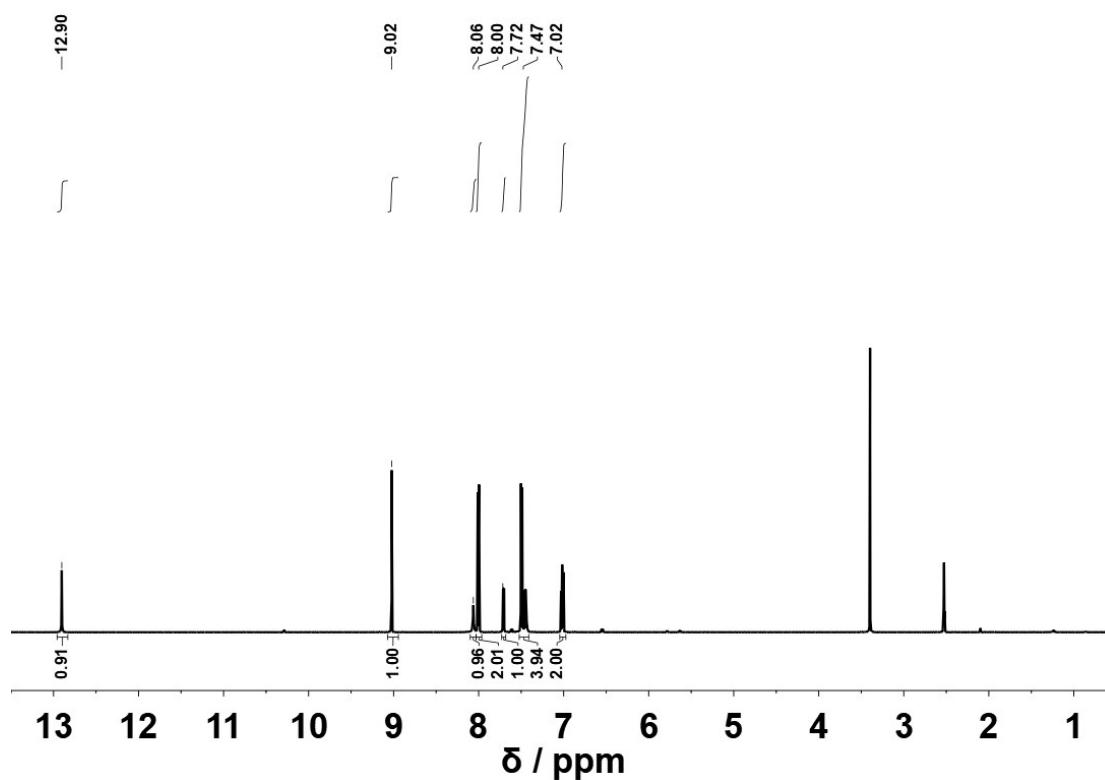


Fig. S1. ^1H NMR ($\text{DMSO}-d_6$, 600 MHz) spectrum of **L**.

Sample Name	6	Position	P1-A2	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	6.d	ACQ Method	0103.m	Comment		Acquired Time	7/23/2020 8:51:32 PM

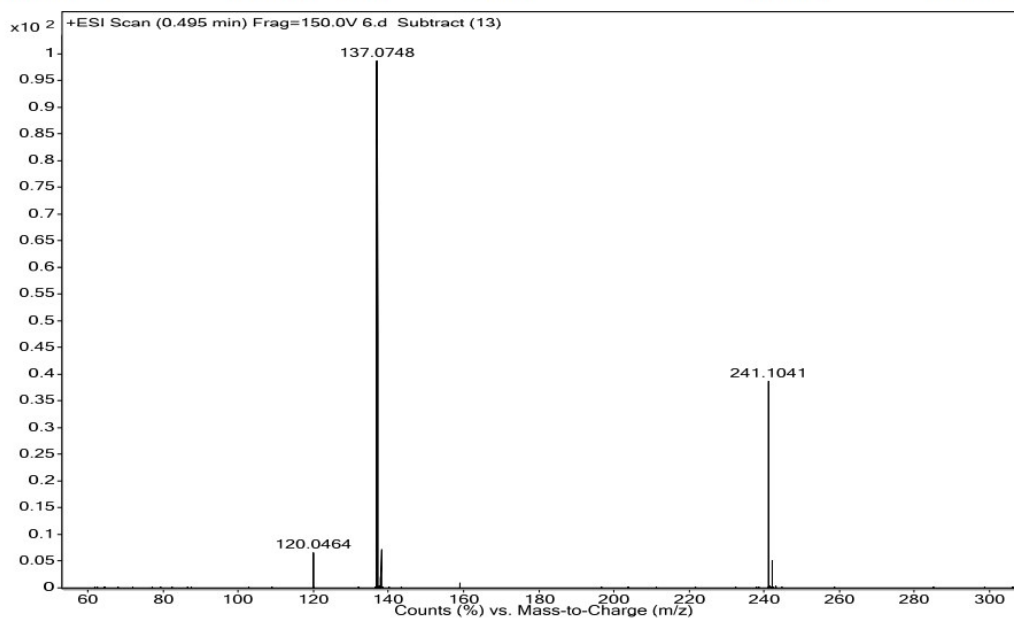


Fig. S2. The ESI-MS spectrum of compound **L**.

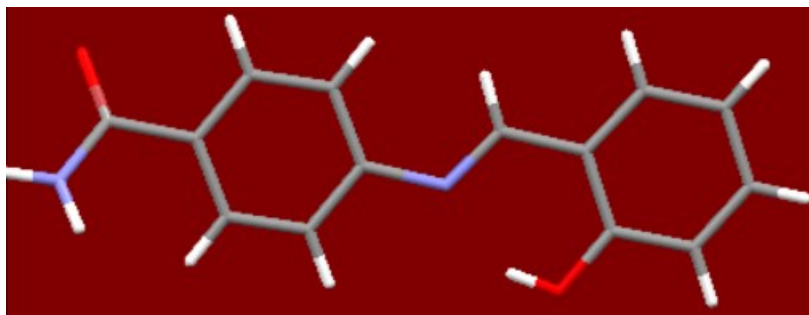


Fig. S3. The dihedral angle of **L**.

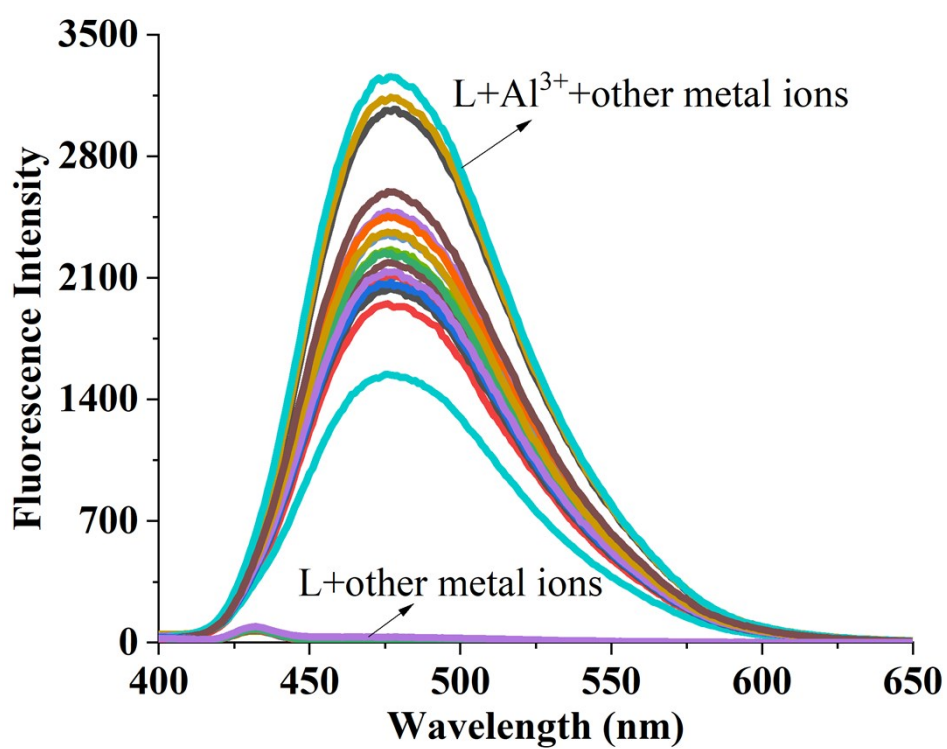


Fig. S4. Competition experiment of **L** toward Al^{3+} in the presence of 5 equiv. of other metal ions in MeOH/H₂O (9/1, v/v, pH=7.4), $\lambda_{\text{ex}} = 380 \text{ nm}$.

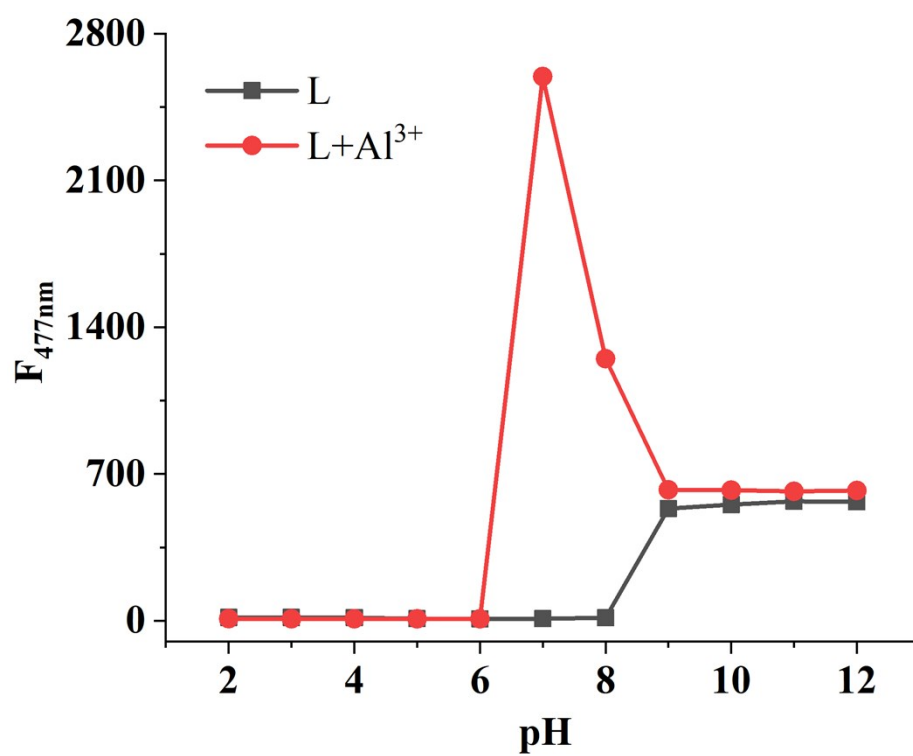
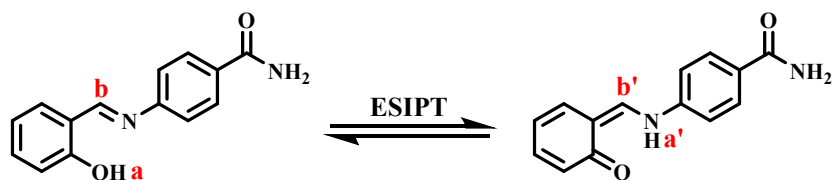


Fig. S5. Fluorescence intensity at 477 nm of **L** (10 μM) at various pH values in MeOH/H₂O (9/1, v/v) medium in the absence and presence of Al³⁺ (5 equiv).



L + 1 equiv. Al^{3+}



L + 0.5 equiv. Al^{3+}



L

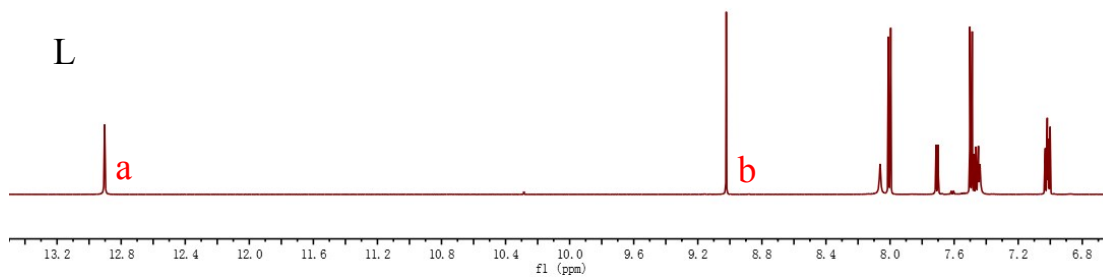


Fig. S6. ^1H NMR ($\text{DMSO}-d_6$, 600 MHz) spectra of **L** with Al^{3+} .

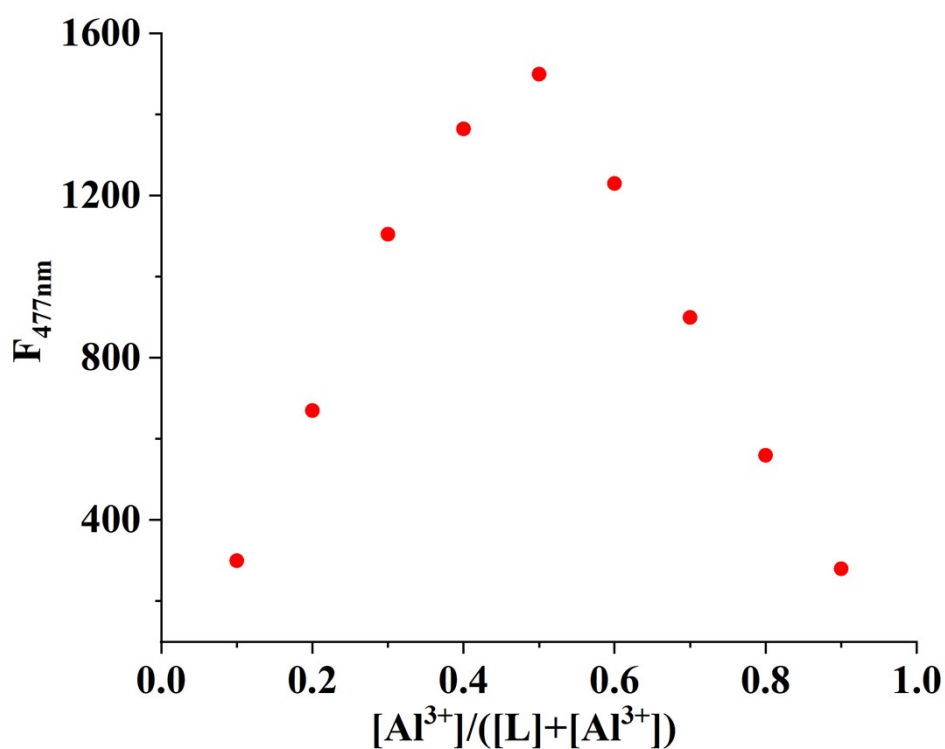


Fig. S7. Job's plot of L- Al^{3+} system in MeOH/ H_2O (9/1, V/V, pH=7.4) medium.

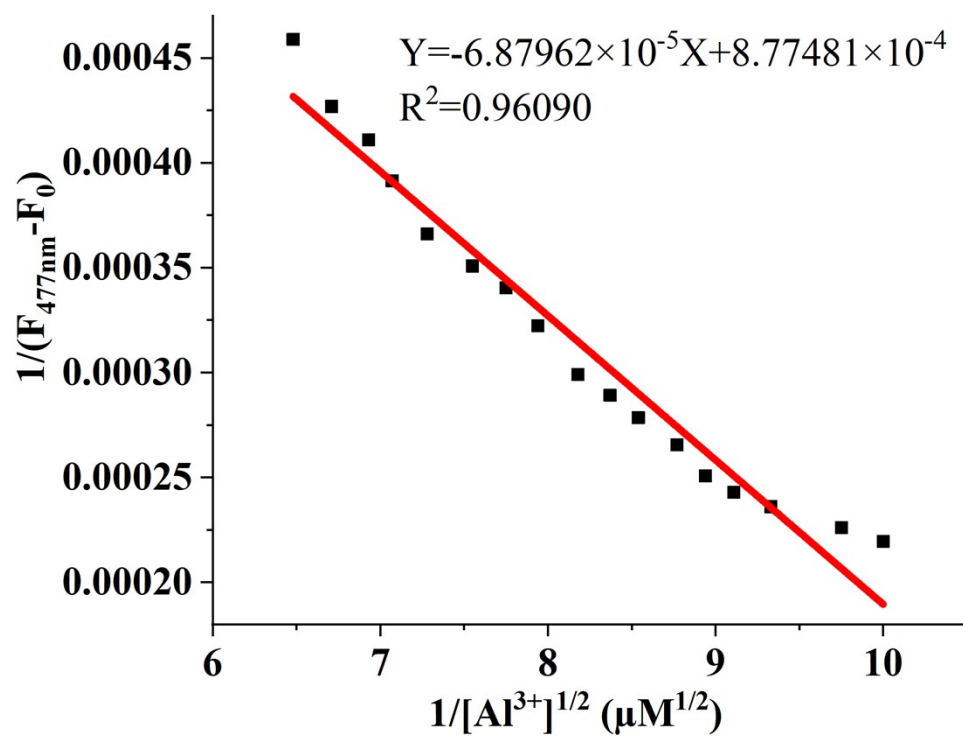


Fig. S8. Benesi-Hildebrand plot of L- Al^{3+} system in MeOH/ H_2O (9/1, v/v, pH=7.4) medium.

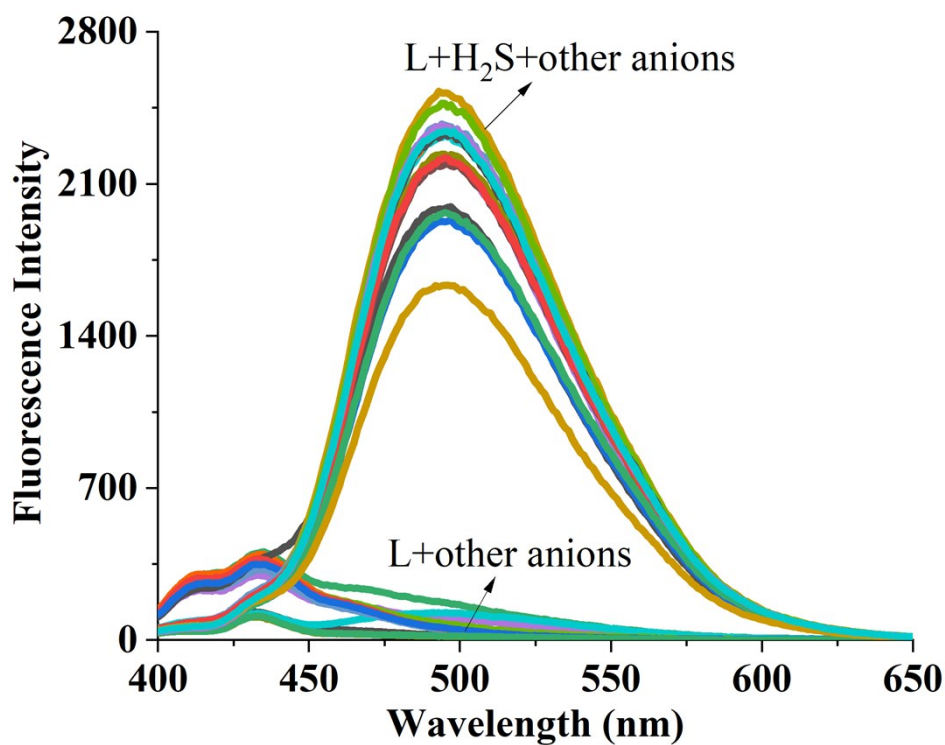


Fig. S9. Competition experiment of L toward H₂S in the presence of 5 equiv. of other anions in EtOH/H₂O (7/3, v/v, pH=7.4).

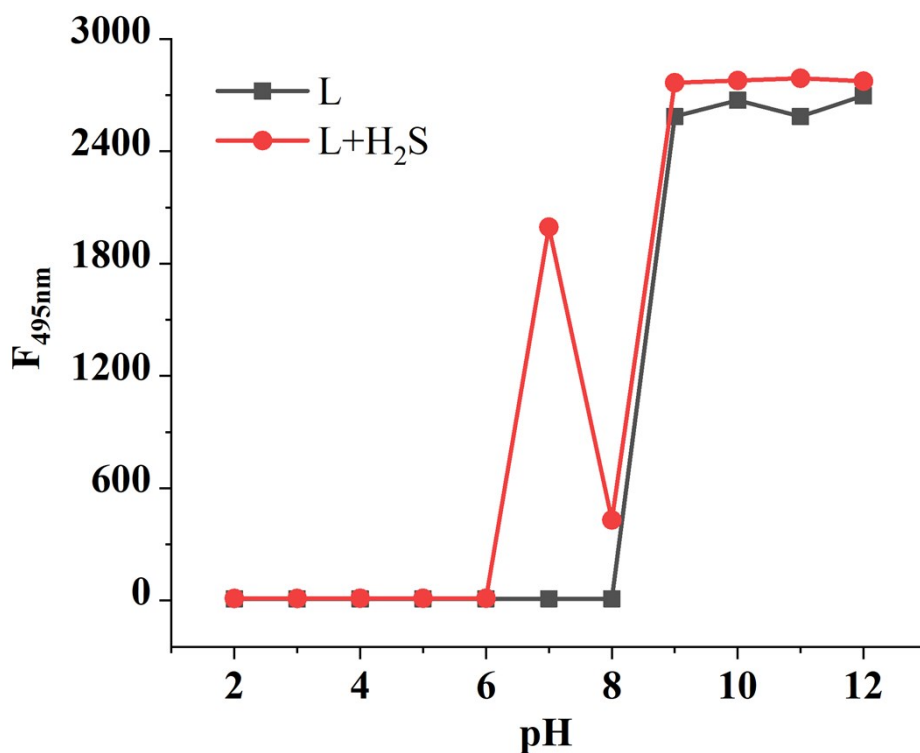
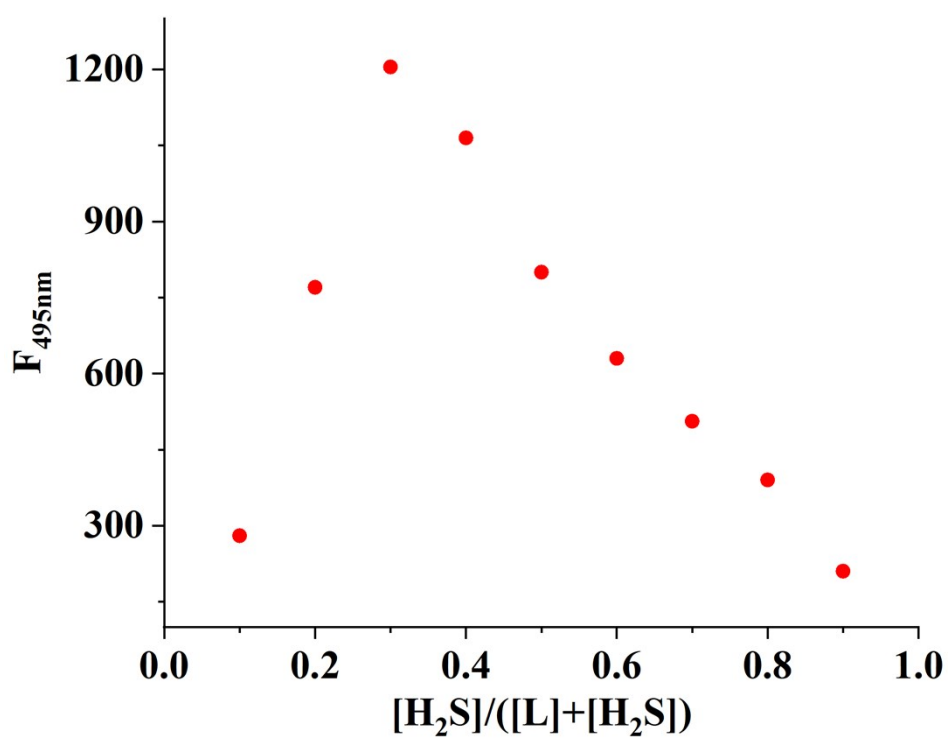
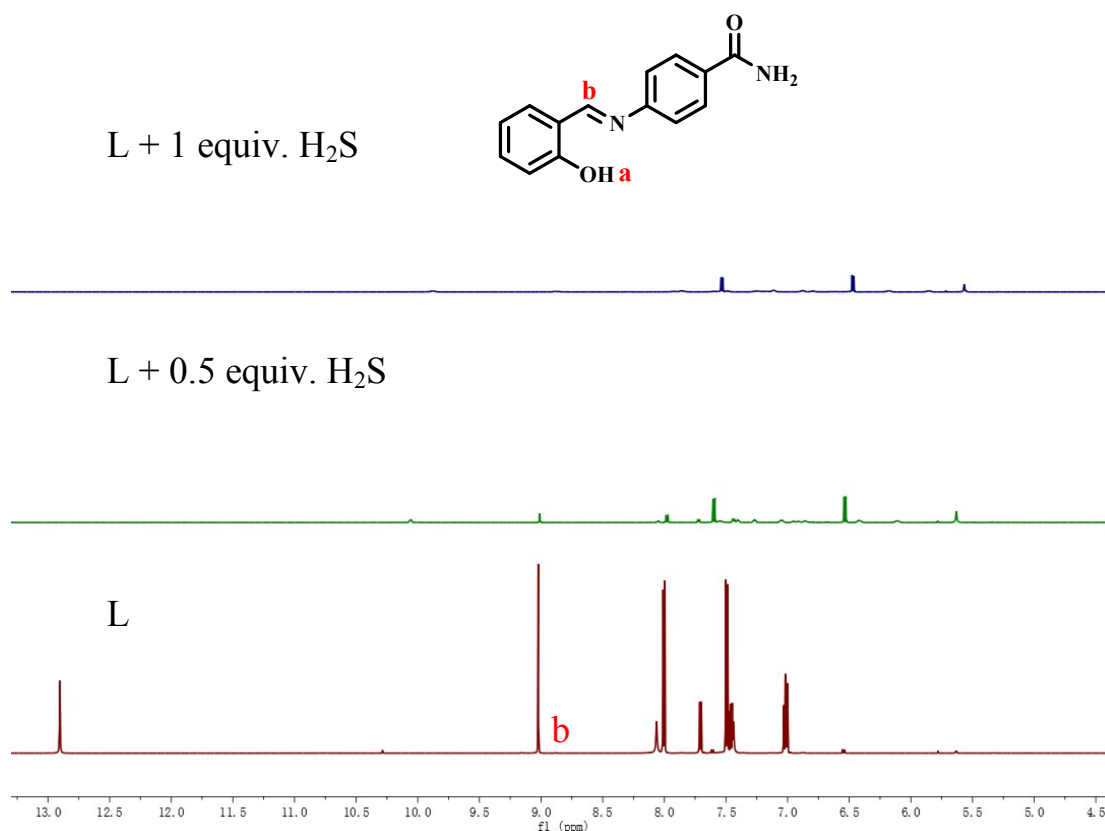


Fig. S10. Fluorescence intensity at 495 nm of L (10 μ M) at various pH values in EtOH/H₂O (7/3, v/v) medium in the absence and presence of H₂S (5 equiv).



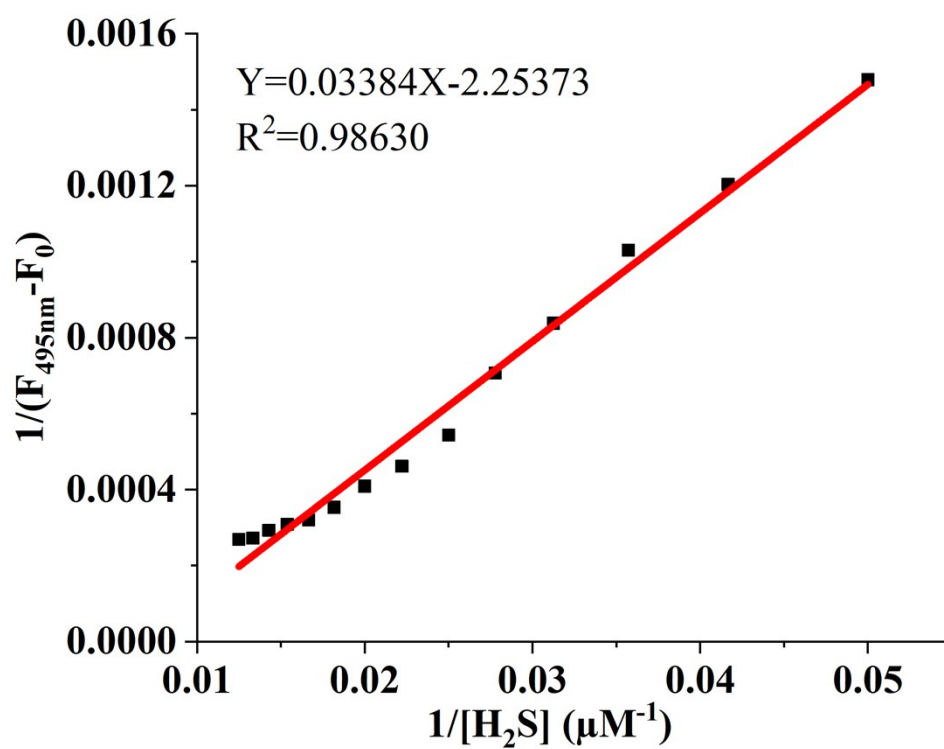


Fig. S13. Benesi-Hildebrand plot of L-H₂S system in EtOH/H₂O (7/3, v/v, pH=7.4) medium.

Table S1 Summary of crystal data and structure refinement parameters for **L**

Crystal data	
Empirical formula	C ₁₄ H ₁₂ N ₂ O ₂
Formula weight	240.26
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.0646 (4), 5.1677 (5), 43.549 (4)
β (°)	92.595 (4)
<i>V</i> (Å ³)	1138.61 (18)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.096
Crystal size (mm)	0.19 × 0.15 × 0.12
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.29, -0.27

Table S2 Selected bond lengths (Å) and angles (°) for **L**.

Bond lengths (Å)		bond angles (°)	
O1—C14	1.2462 (18)	C7—N1—C8	121.93 (14)
O2—C1	1.346 (2)	O2—C1—C2	119.40 (15)
N1—C7	1.278 (2)	C2—C1—C6	119.51 (15)
N2—C14	1.3338 (19)	C5—C6—C1	118.23 (15)
C1—C2	1.393 (2)	C5—C6—C7	120.40 (15)
C1—C6	1.397 (2)	N1—C7—C6	121.90 (15)
C5—C6	1.397 (2)	C10—C9—C8	120.84 (15)
C8—C9	1.388 (2)	C9—C10—C11	120.24 (15)
C10—C11	1.392 (2)	O1—C14—N2	122.34 (12)
C11—C12	1.390 (2)	N2—C14—C11	117.30 (13)

Table S3 Determination of Al^{3+} in water samples from different water sources by standard-addition method (n =3).

Water samples studied	Amount of standard Al^{3+} added (μM)	Total Al^{3+} found (n=3) (μM)	Recovery of Al^{3+} (n=3) added (%)	RSD (%)	Relative error (%)
Tap water	3.0	3.02	100.67	1.20	1.75
	3.5	3.48	99.43	0.65	-1.18
	4.0	4.03	100.75	2.57	0.86
	4.5	4.48	99.56	1.36	-1.62
	5.0	4.97	99.40	1.56	-2.16
	5.5	5.56	101.09	0.78	0.69
Lake water	3.0	3.01	100.33	1.72	1.06
	3.5	3.53	100.86	2.00	3.18
	4.0	3.95	98.75	1.56	-0.59
	4.5	4.54	100.89	1.25	1.76
	5.0	4.89	97.80	0.26	-2.35
	5.5	5.60	101.82	0.38	2.16

Table S4 Determination of H₂S in water samples from different water sources by standard-addition method (n =3).

Water samples studied	Amount of standard H ₂ S added (μM)	Total H ₂ S found (n=3) (μM)	Recovery of H ₂ S (n=3) added (%)	RSD (%)	Relative error (%)
Tap water	6.0	5.96	103.80	2.20	2.75
	6.5	6.48	95.70	0.50	-2.18
	7.0	6.95	102.87	3.57	0.63
	7.5	7.42	98.90	1.50	-1.82
	8.0	7.91	97.36	2.56	-3.12
	8.5	8.53	97.17	0.30	-0.78
Lake water	6.0	6.04	101.80	1.60	2.07
	6.5	6.51	103.30	3.00	3.28
	7.0	6.92	95.67	1.16	-2.59
	7.5	7.52	104.35	3.75	1.62
	8.0	8.05	102.60	0.16	2.68
	8.5	8.46	95.60	0.29	-2.66