

Electronic Supplementary Information

For the Manuscript Entitled

Detection of sulfide ion and gaseous H₂S using a series of pyridine-2,6-dicarboxamide based scaffolds

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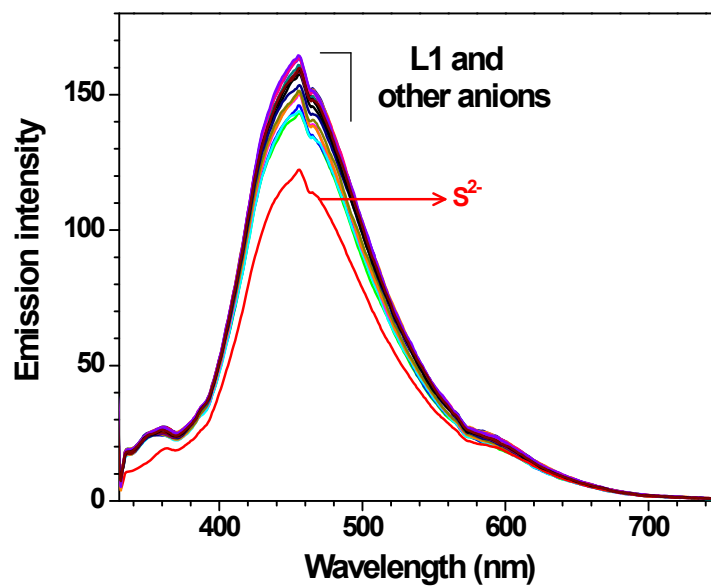


Figure S1. Change in emission intensity of chemosensor L1 (10 μM) in presence of different anions (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

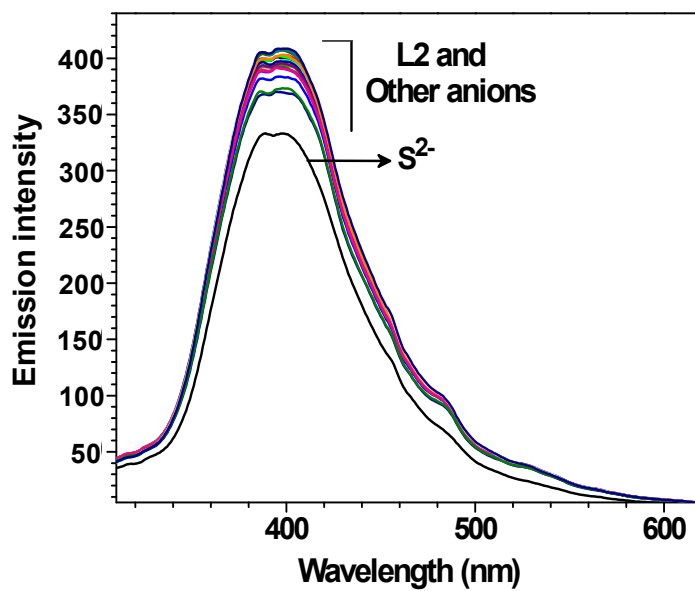


Figure S2. Change in emission intensity of chemosensor L2 (10 μM) in presence of different anions (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

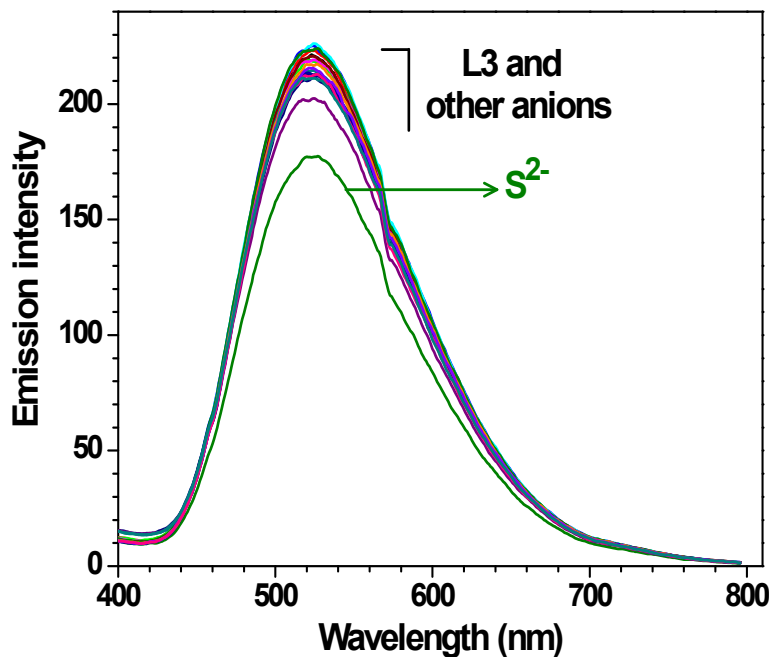


Figure S3. Change in emission intensity of chemosensor L3 (10 μM) in presence of different anions (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

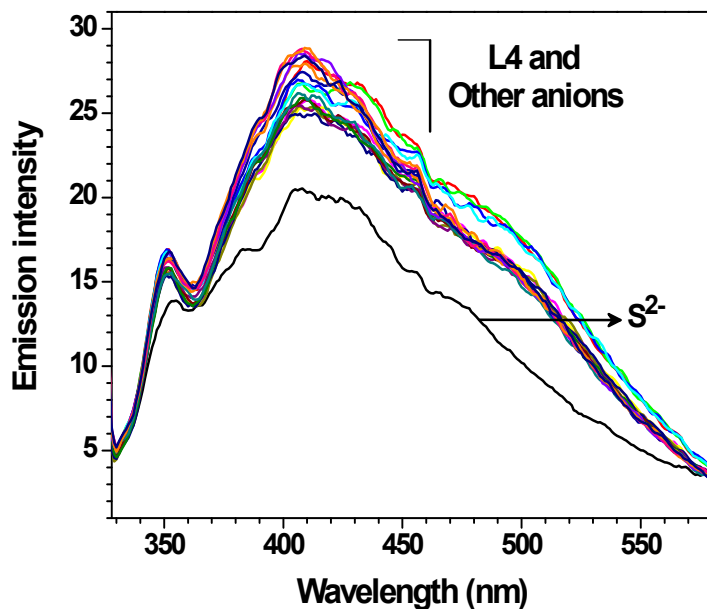


Figure S4. Change in emission intensity of chemosensor L4 (10 μM) in presence of different anions (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

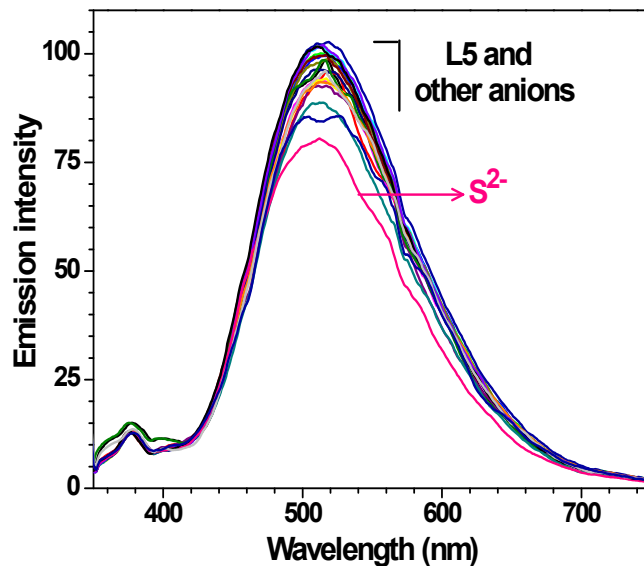


Figure S5. Change in emission intensity of chemosensor L5 (10 μM) in presence of different anions (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

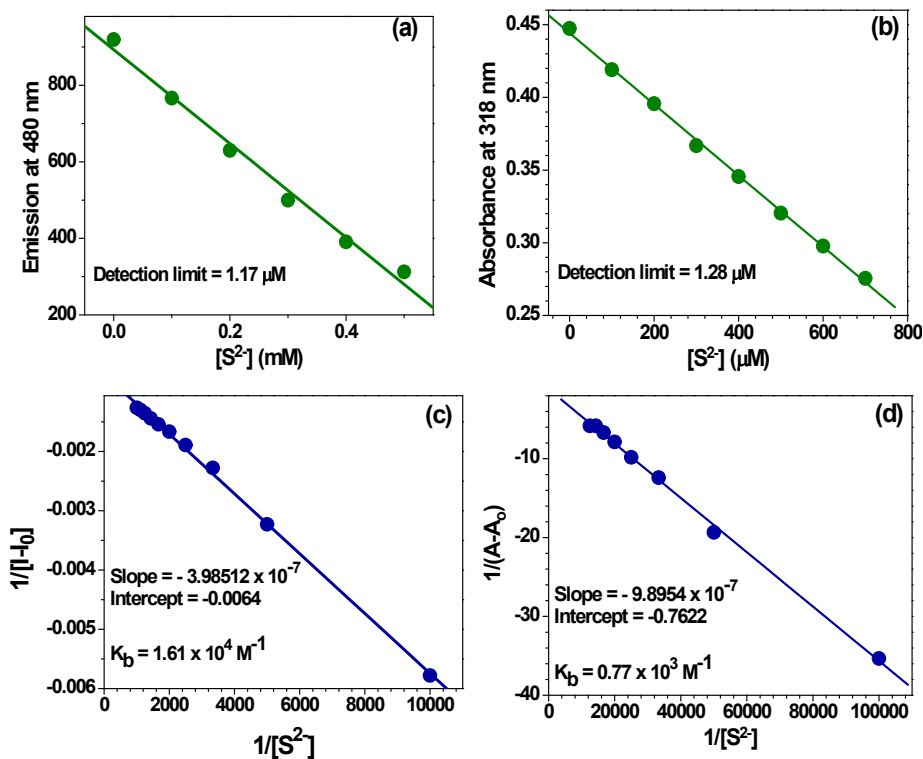


Figure S6. Determination of detection limit for S^{2-} ion by chemosensor L6 using (a) fluorescence spectral titration and (b) UV-visible spectral titration. Benesi-Hildebrand plots for the detection of S^{2-} ion by chemosensor L6 using (c) fluorescence spectral titration and (d) UV-visible spectral titration.

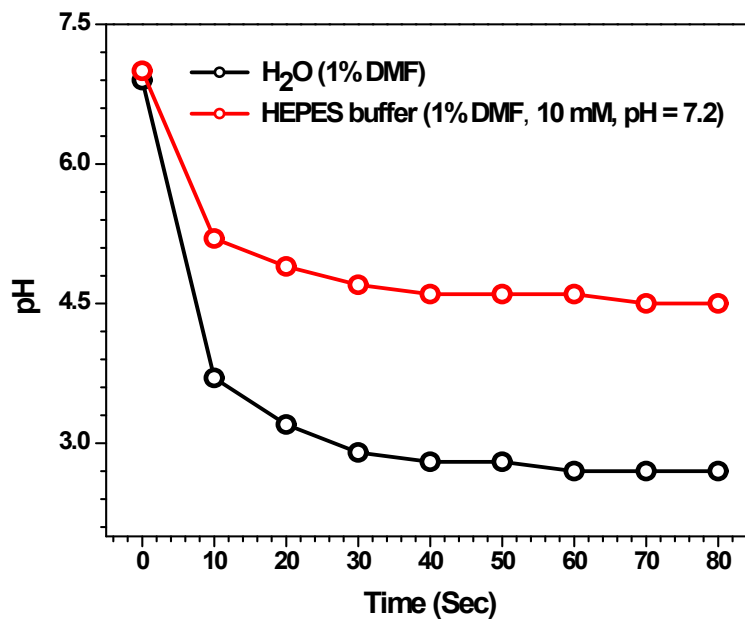


Figure S7. Effect of purging H₂S gas to a solution of chemosensor L6 as a function of time either in water (containing 1% DMF) or in HEPES buffer (1% DMF; 10 mM; pH = 7.2).

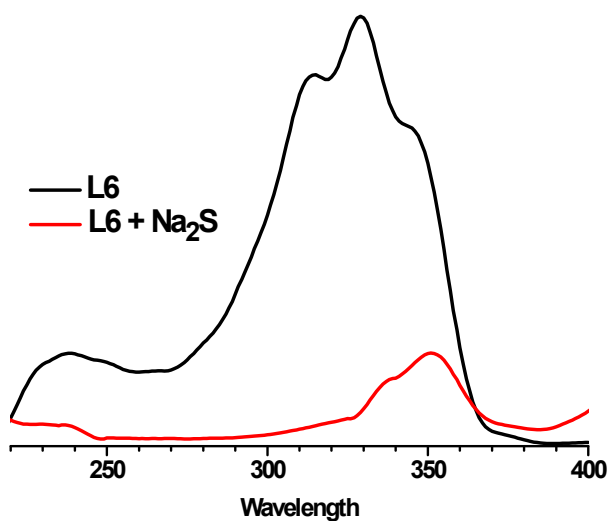


Figure S8. Excitation spectra of chemosensor L6 in absence and in presence of Na₂S in aqueous medium ($\lambda_{em} = 480$ nm).

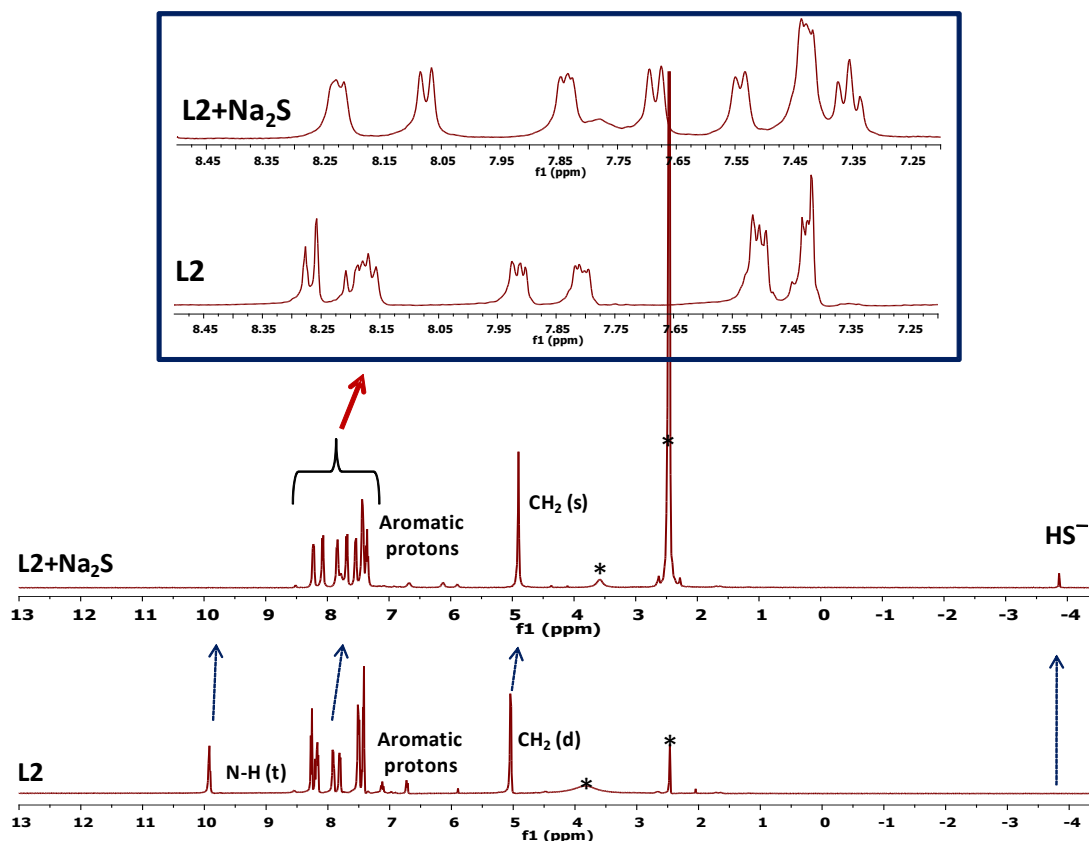


Figure S9. ^1H NMR spectrum of L2 (2.5 mM, DMSO-d_6) in absence and presence of Na_2S (2.0 equiv.). * represents the residual solvent and/or adventitious water peaks.

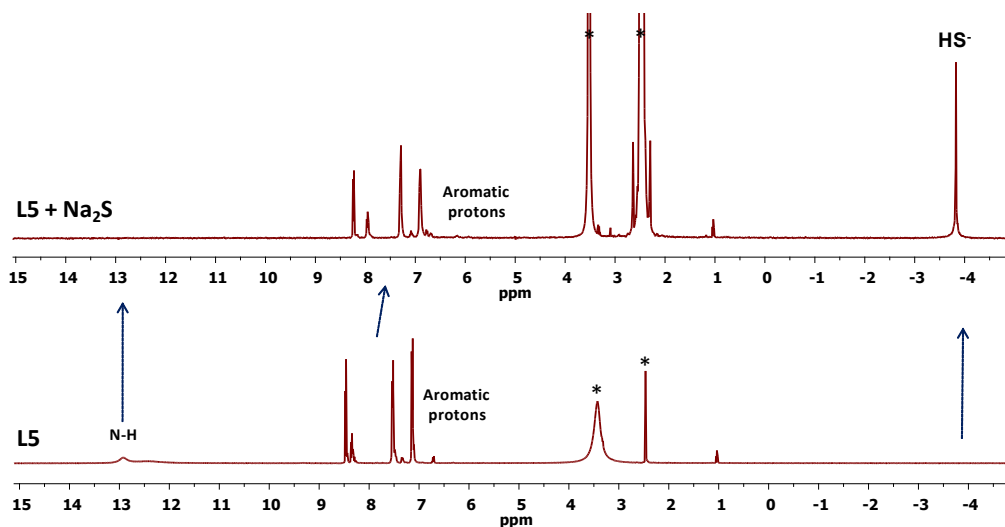


Figure S10. ^1H NMR spectrum of L5 (2.5 mM, DMSO-d_6) in absence and presence of Na_2S (2.0 equiv.). * represents the residual solvent and/or adventitious water peaks.

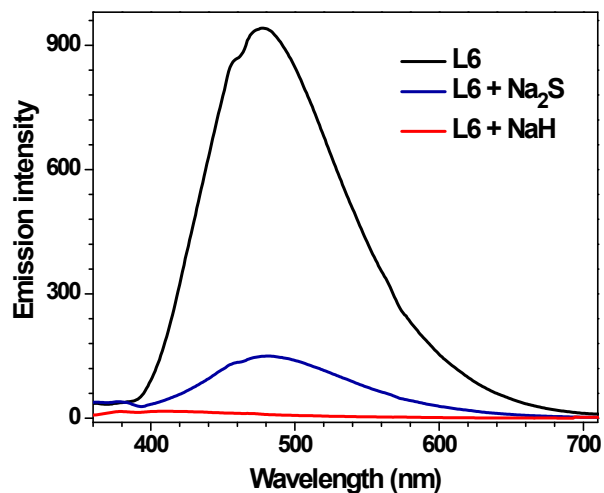


Figure S11. Emission spectra of L6 (10 μM) in absence and in presence of Na₂S (1 mM) and NaH (2.2 equivalent) in water.

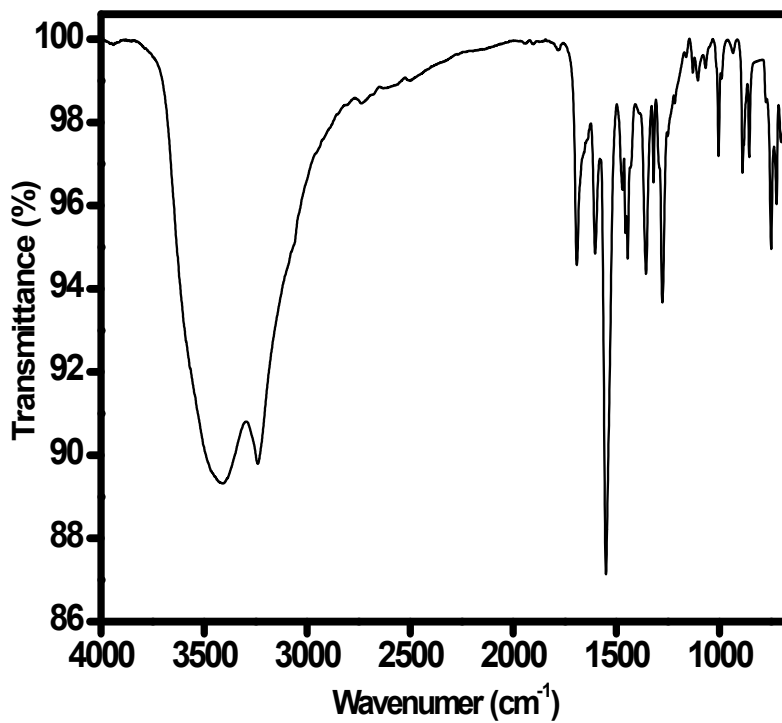


Figure S12. FTIR spectrum of chemosensor L7.

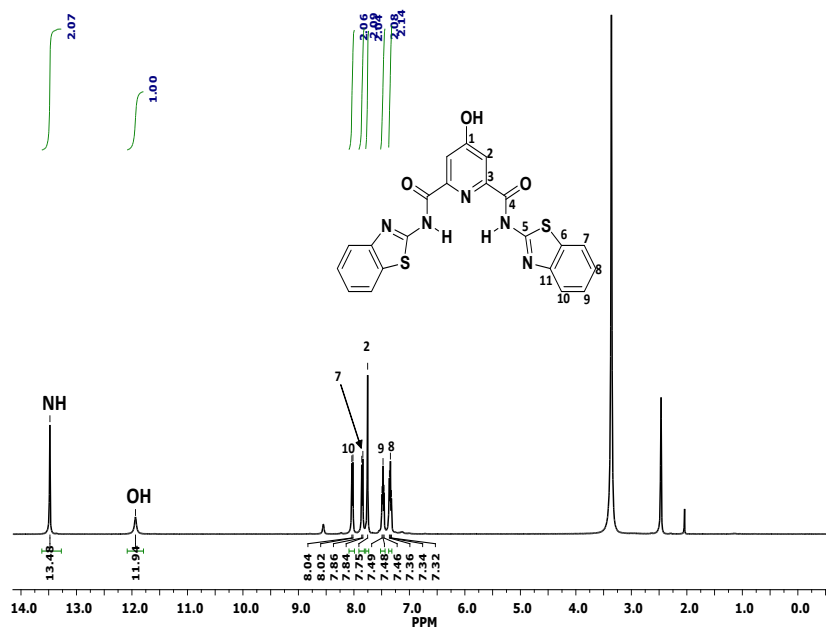


Figure S13. ^1H NMR spectrum of chemosensor L7 in DMSO-d_6 .

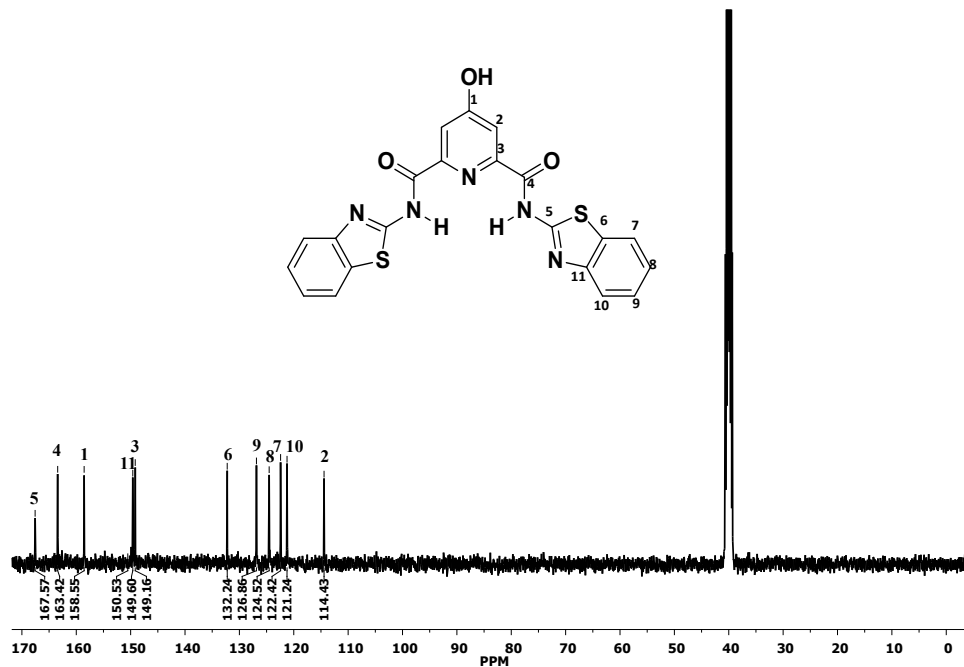


Figure S14. ^{13}C NMR spectrum of chemosensor L7 in DMSO-d_6 .

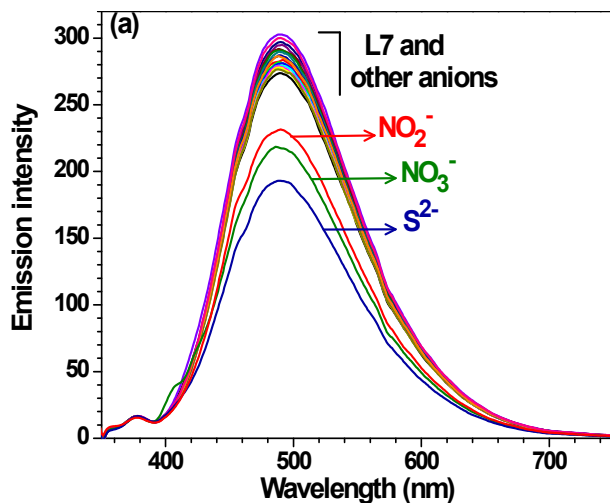


Figure S15. Change in the emission intensity of chemosensor L7 (10 μM) in presence of different anions (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

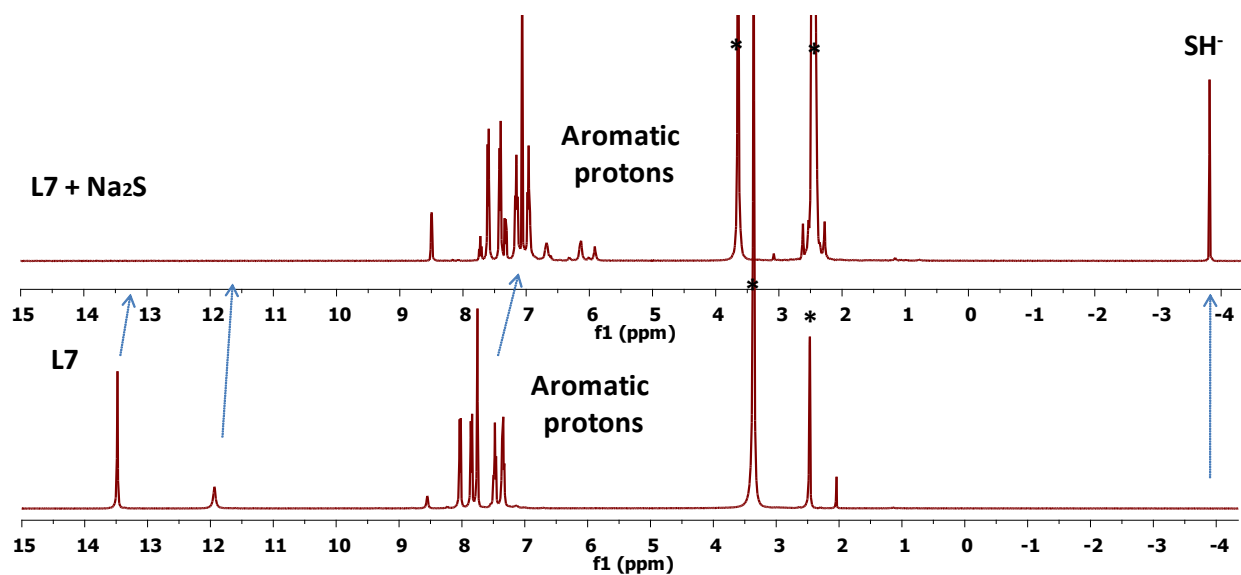


Figure S16. ^1H NMR spectrum of L7 (2.5 mM, DMSO-d_6) in absence and in presence of Na_2S (2.0 equiv.). * represents the residual solvent and/or adventitious water peaks.

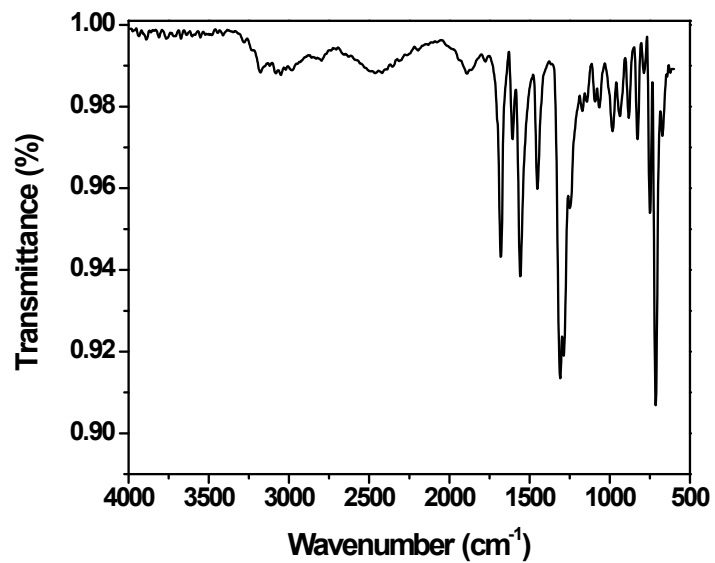


Figure S17. FTIR spectrum of chemosensor L8.

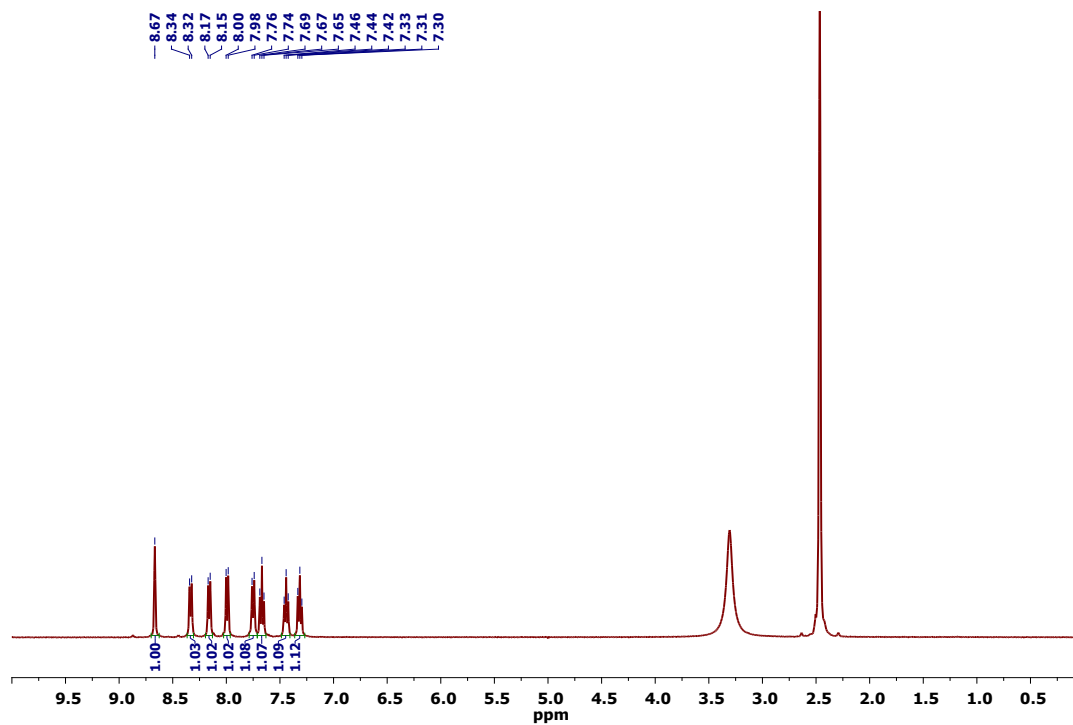


Figure S18. ¹H NMR spectrum of chemosensor L8 in DMSO-d₆.

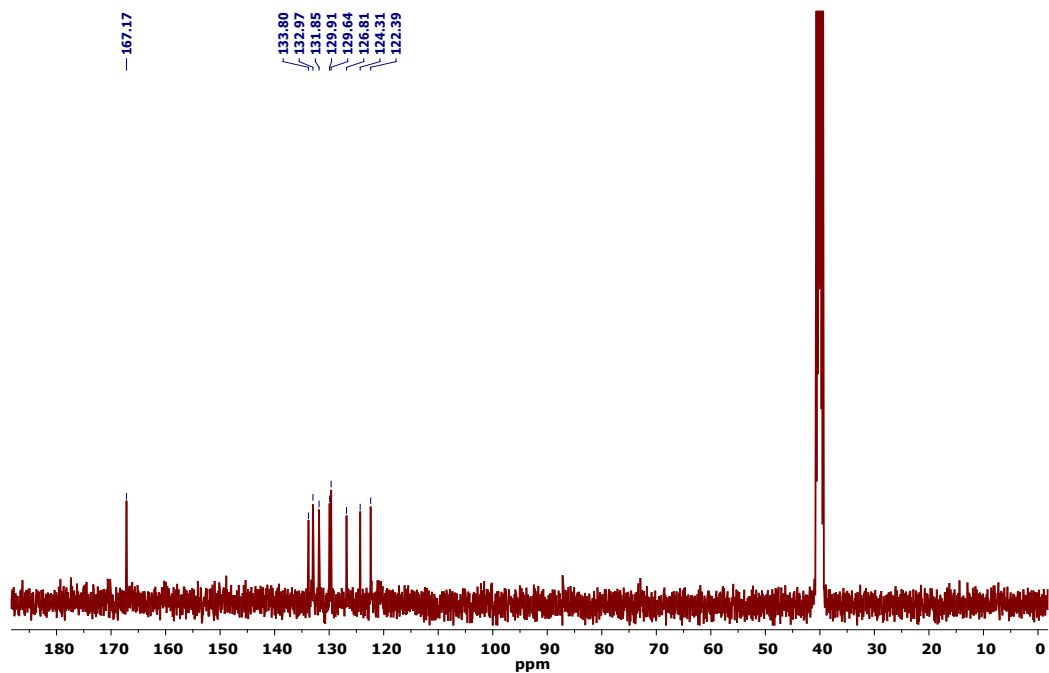


Figure S19. ^{13}C NMR spectrum of chemosensor L8 in DMSO-d_6 .

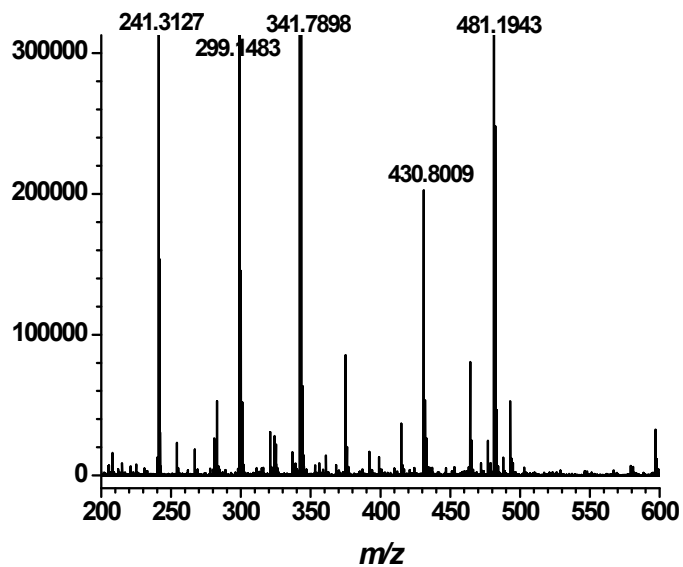


Figure S20. ESI^+ mass spectrum of chemosensor L8 in DMF.

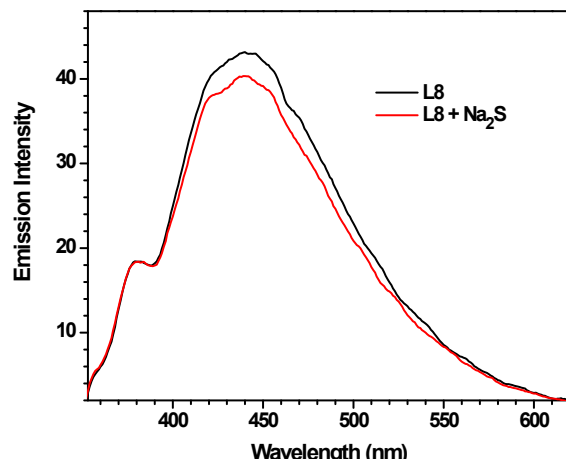


Figure S21. Change in the emission intensity of chemosensor L8 (10 μM) in absence and in presence of S^{2-} ion (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

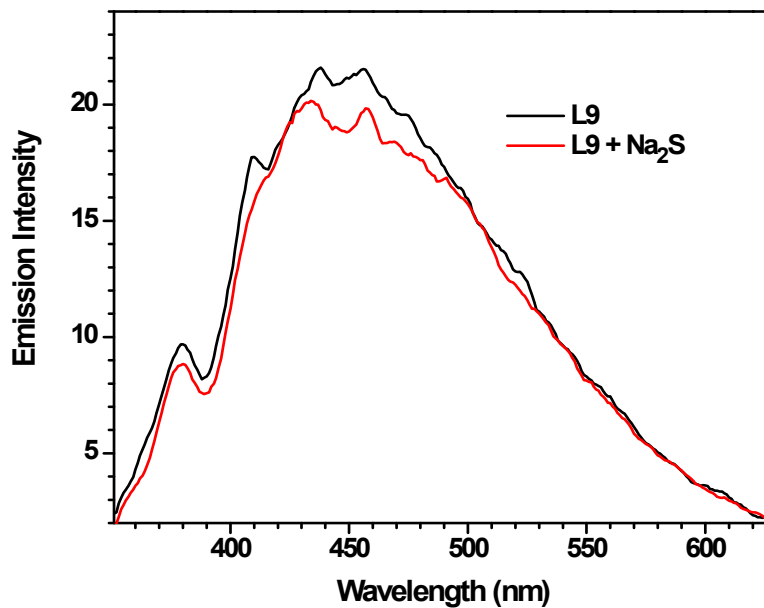


Figure S22. Change in the emission intensity of chemosensor L9 (10 μM) in absence and in presence of S^{2-} ion (1mM) in HEPES buffer (10 mM, pH = 7.2) containing 1% DMF.

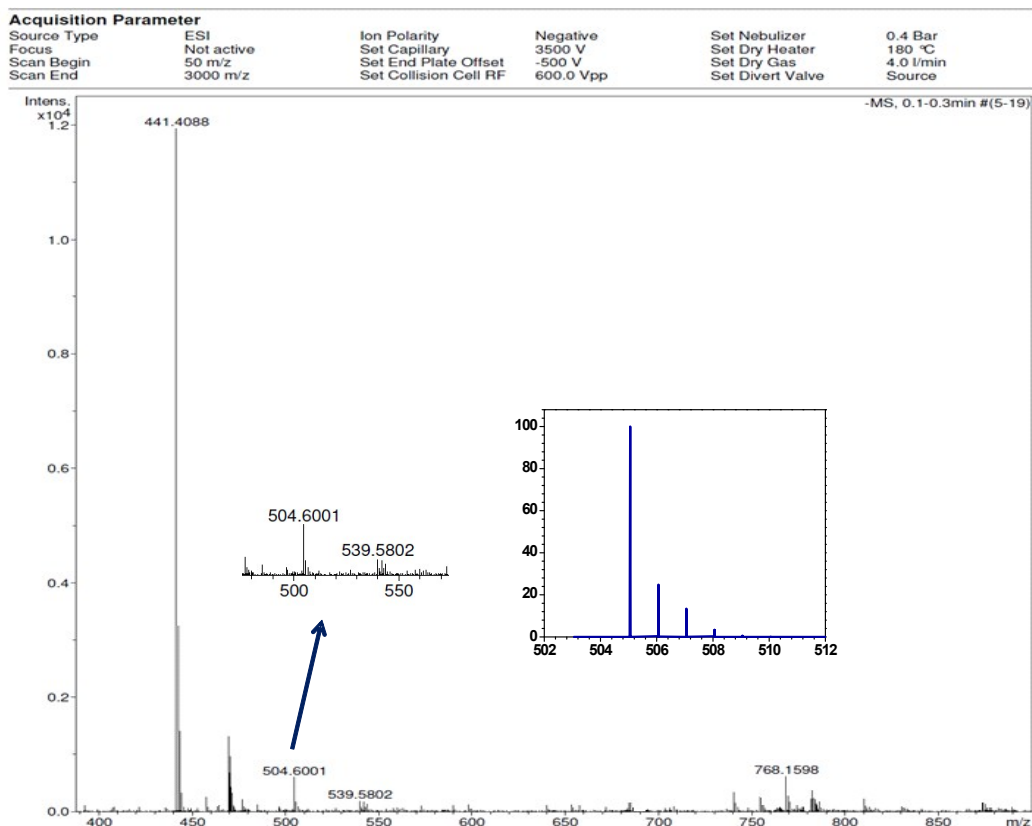


Figure S23. Negative mode ESI-MS spectrum of [L6-S] recorded in CH_3CN and its simulated pattern.

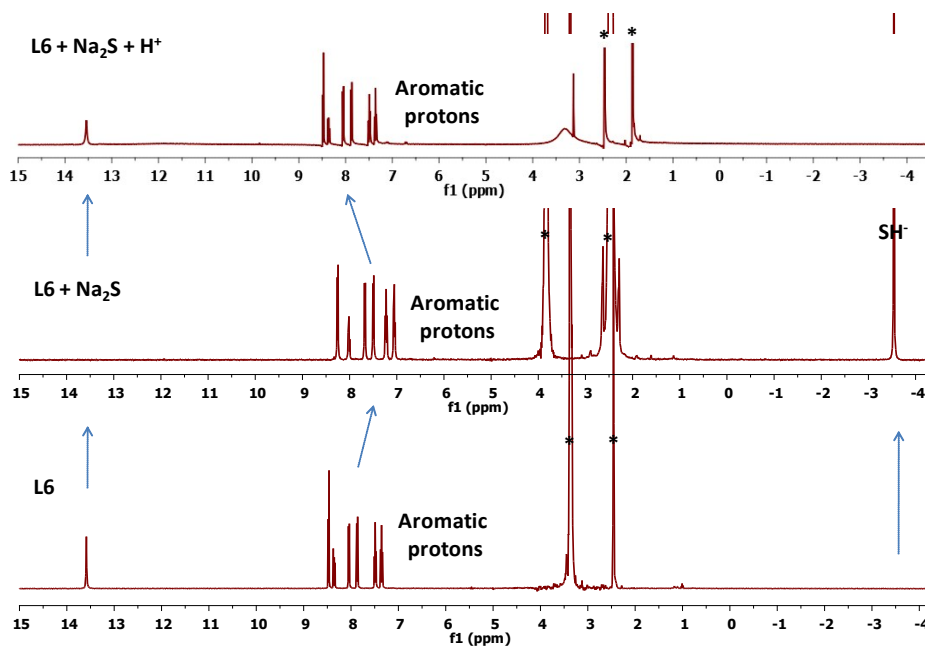


Figure S24. ^1H NMR spectrum of chemosensor L6 (2.5 mM, DMSO-d_6); L6 + Na_2S (2.0 equiv.) and L6 + Na_2S + CH_3COOH . * represents the residual solvent and water peaks.

Table S1. Fluorescence lifetime parameters for chemosensor L6, L6 + Na₂S and L6 + H₂S in HEPES buffer (pH = 7.2, 10 mM) ($\lambda_{\text{ex}} = 280$ nm and $\lambda_{\text{em}} = 480$ nm).

	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	B_1	B_2	B_3	A	Average Lifetime τ_{av} (ns)
L6	3.9023	0.9061	12.9051	0.03786	0.05351	0.01201	3.8088	7.43
L6 + Na₂S	3.1609	0.6943	16.1626	0.01657	0.11595	0.00256	1.34347	5.12
L6 + H₂S	3.1429	0.5158	14.6731	0.01701	0.13946	0.00289	3.21791	4.94

Table S2. Crystallographic data collection and structure solution parameters for L6·DMF.

Formula	C ₂₄ H ₂₀ N ₆ O ₃ S ₂
Fw	504.58
T(K)	298(2)
Crystal System	monoclinic
Space Group	<i>C2/c</i>
<i>a</i> (Å)	21.6495(7)
<i>b</i> (Å)	7.3556(3)
<i>c</i> (Å)	30.0659(9)
α (°)	90
β (°)	103.501(3)
γ (°)	90
<i>V</i> (Å ³)	4655.5(3)
<i>Z</i>	8
<i>d</i> (Mg/m ³)	1.440
<i>F</i> (000)	2096
Goodness-of-fit on <i>F</i> ²	1.068
<i>R</i> ₁ , <i>wR</i> ₂ [I > 2(I)]	0.0433, 0.1032
<i>R</i> ₁ , <i>wR</i> ₂ [all data]	0.0537, 0.1093
CCDC No.	1835393