Supporting Information

Development of an assay for colorimetric and fluorometric detection of H_2S

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Table S1. Comparison of activity parameters for different EDG and EWG used in this study

Chemosensor	Linker	Colorimetric detection	Fluorometric detection
N1	m-amino phenol (EDG)	Negligible	No
N2	p-anisidine (EDG)	No	No
N3	Aniline (EDG)	No	No
N4	m-nitro aniline (EWG)	Yellow to orange	No
N5	p-nitro aniline (EWG)	Yellow to purple	No
N6	1,8-napthalic anhydride + Hydrazine (EWG)	Colourless to Yellow	No
N7	3-amino-9-ethylcarbazole (EDG)	No	No
N8	1,8-napthalic anhydride + Ethylenediamine (EWG)	Negligible	Light blue fluorescence
N9	Picolyl amine (EWG)	Negligible	Cyan blue fluorescence
N10	Furfuryl amine (EWG)	No	Intense cyan blue fluorescence

^{1}H NMR of N1 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 15.39 (s, 1H), 9.25 (d, 1H), 8.04-8.02 (d, 1H, J=8), 7.81-7.79 (d, 1H, J=8), 7.69-7.67 (d, 1H, J=8), 7.54-7.50 (t, 1H), 7.34-7.32 (q, 2H), 7.07-7.05 (d, 1H, J=8), 6.99-6.97 (d,2H), 6.83-6.80 (1H,d). ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 159.36, 142.93, 136.57, 129.20, 127.87, 123.38, 122.96, 118.24, 110.57, 108.49, 50.74. HRMS (TOF MS): (m/z, %): for C17H13NO2+H^{+}: Found: m/z = 264.1002 (M+H^{+}).

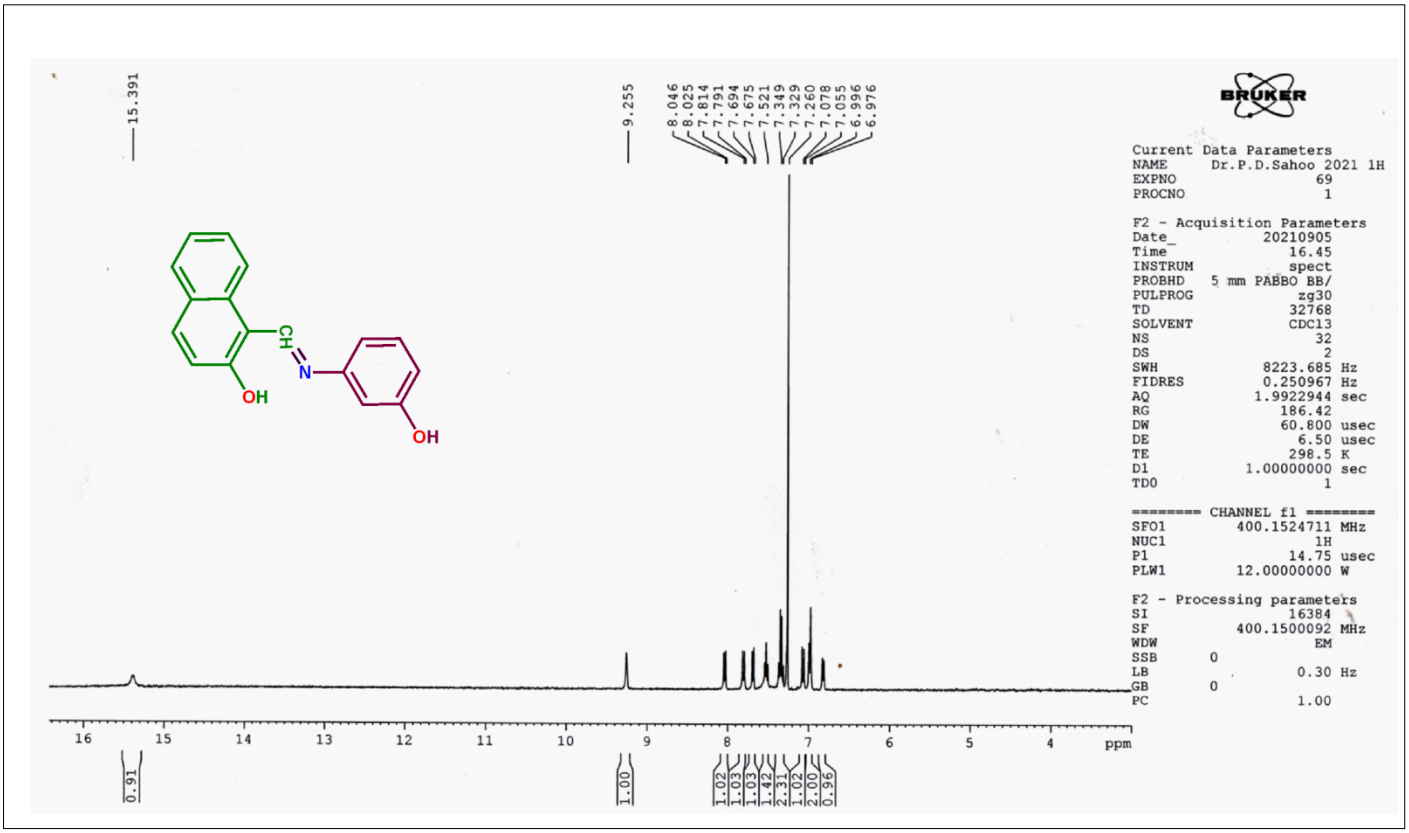


Figure S1.^{1}H NMR of **N1** in $CDCl_3$ (400 MHz).

^{13}C NMR of N1 in $CDCl_3$:

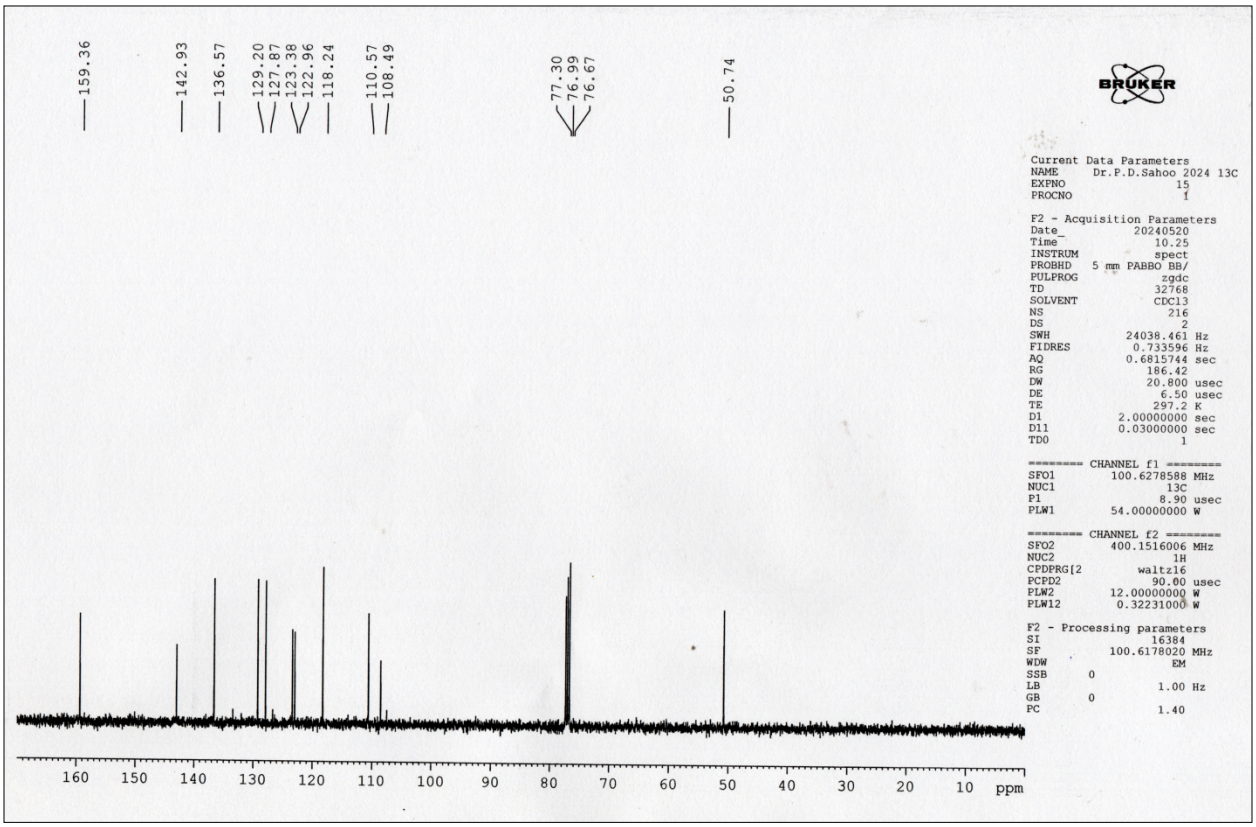


Figure S2. ^{13}C NMR of **N1** in $CDCl_3$ (100 MHz).

^{1}H NMR of N2 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 15.59 (s, 1H), 9.30 (s, 1H), 8.10-8.08 (d, 1H, J=8), 7.79-7.77 (d, 1H, J=12), 7.72-7.70 (d, 1H, J=8), 7.52-7.49 (t, 1H), 7.35-7.30 (d, 2H), 7.11-7.08 (d, 1H, J=8), 6.75-6.73 (1H,d), 6.66-6.63 (1H,d), 3.85 (3H,S). ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 169.24, 158.55, 153.73, 138.54, 136.01, 129.30, 127.88, 123.32, 122.00, 121.52, 118.81, 114.83, 55.55. HRMS (TOF MS): (m/z, %): C18H15NO2+H^{+}: Found: m/z = 278.1161 (M+H^{+}).

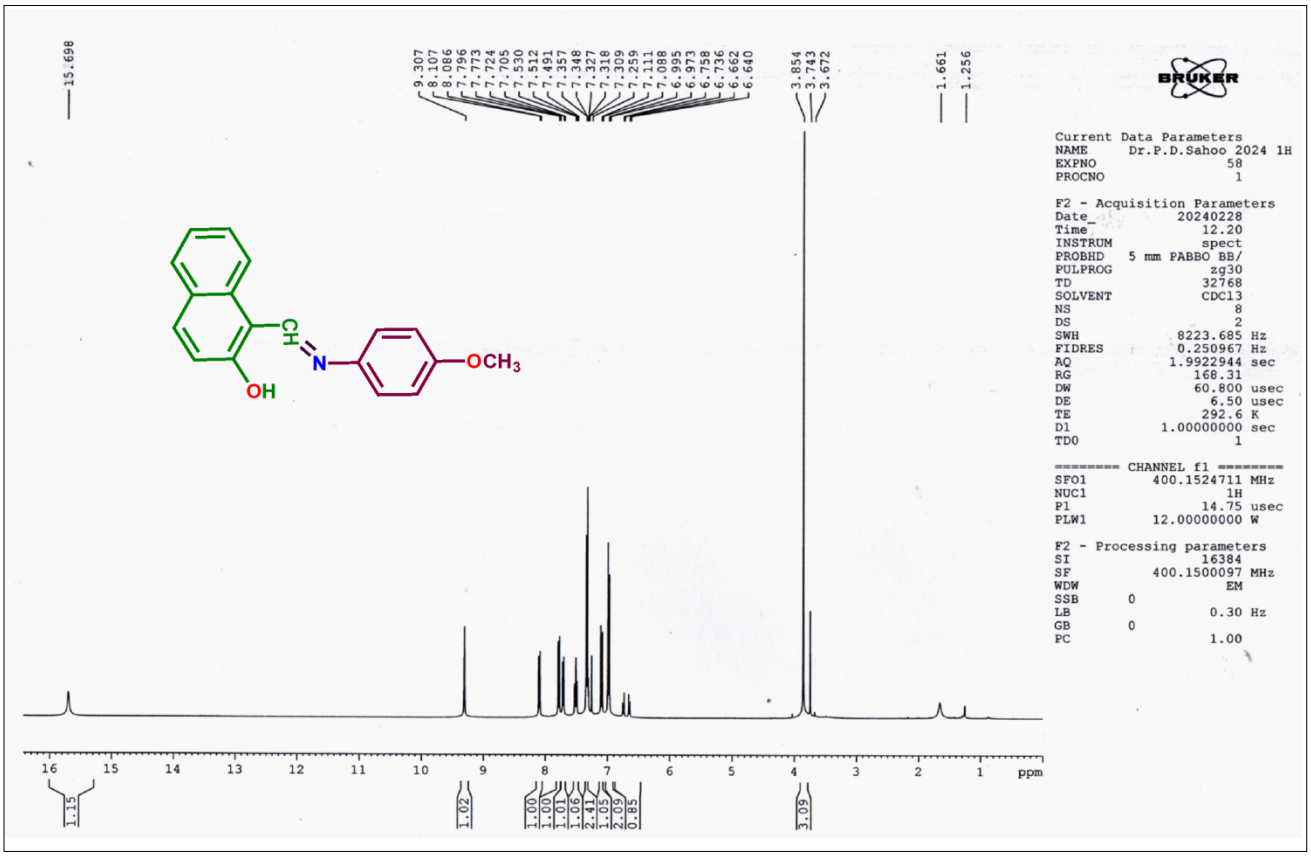


Figure S3. ^{1}H NMR of **N2** in $CDCl_3$ (400 MHz).

^{13}C NMR of N2 in $CDCl_3$:

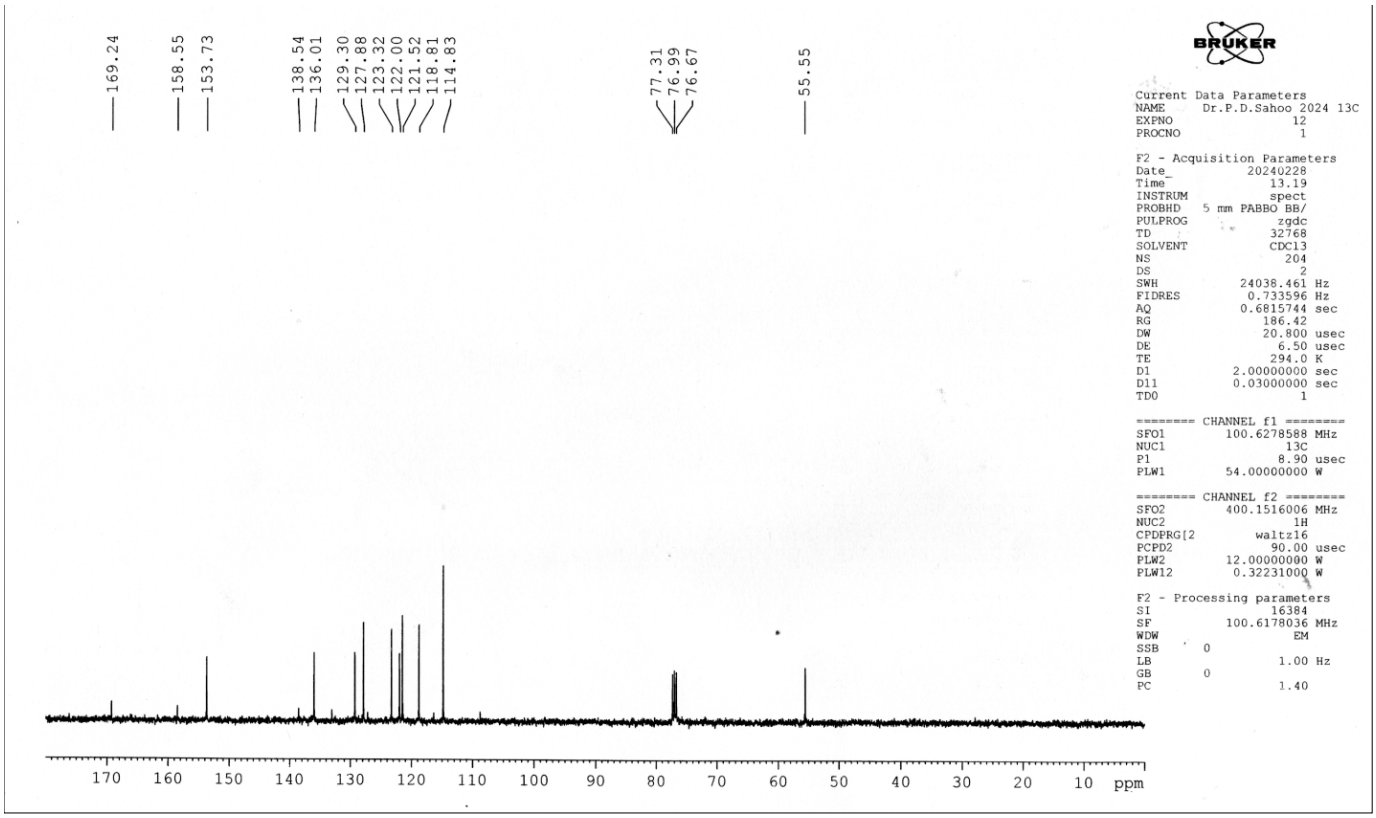


Figure S4. ^{13}C NMR of **N2** in $CDCl_3$ (100 MHz).

^{1}H NMR of N3 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 15.50 (s, 1H), 9.33-9.32 (d, 1H), 8.10-8.08 (d, 1H, J=8), 7.81-7.78 (d, 1H, J=12), 7.72-7.70 (d, 1H, J=8), 7.50-7.44 (m, 3H), 7.38-7.29 (m, 4H), 7.08-7.06 (d, 1H, J=8), ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 154.35, 136.87, 129.68, 128.10, 126.50,123.51, 122.49, 120.19, 118.76. HRMS (TOF MS): (m/z, %): for C17H13NO+H^{+}: Found: m/z = 248.1060 (M+H+).

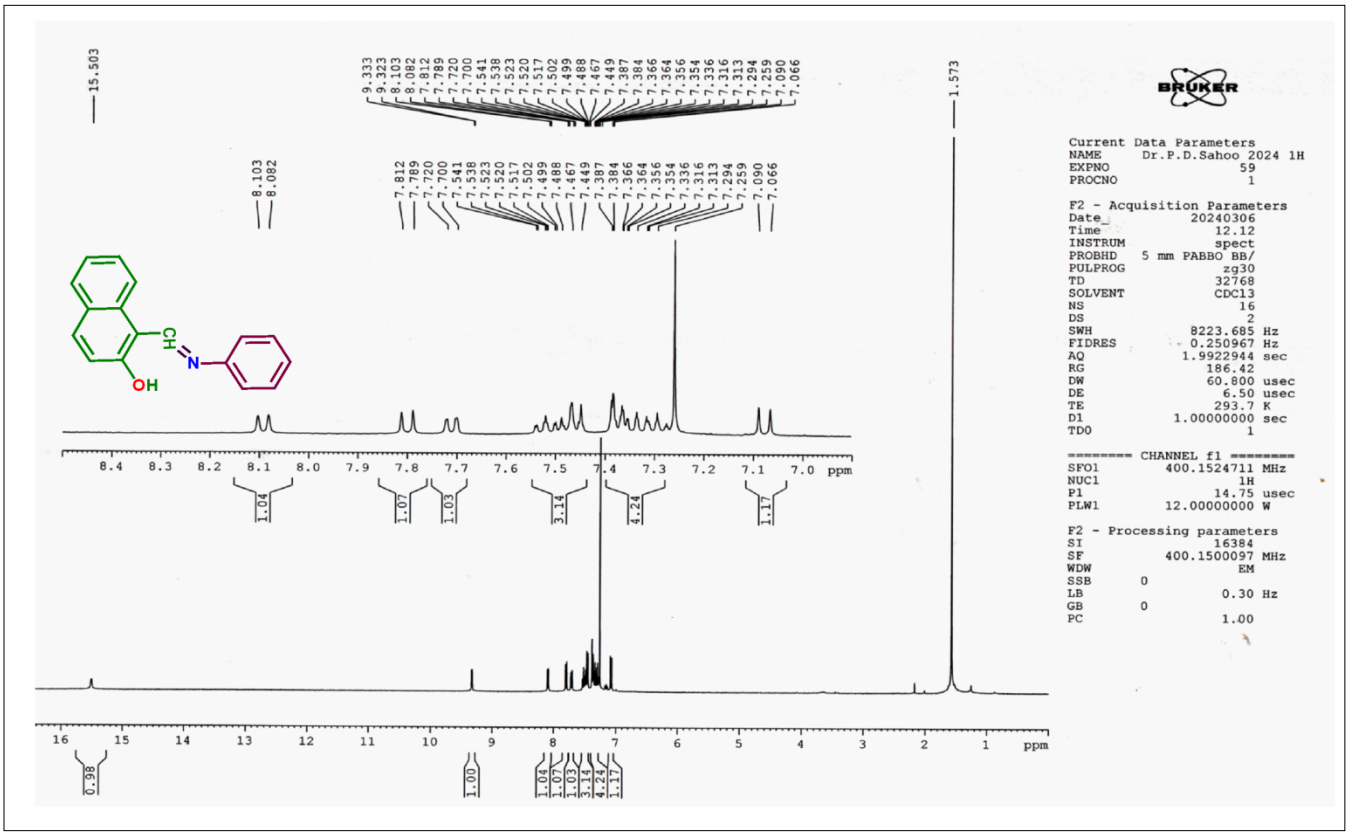


Figure S5. ^{1}H NMR of **N3** in $CDCl_3$(400 MHz).

^{13}C NMR of N3 in $CDCl_3$:

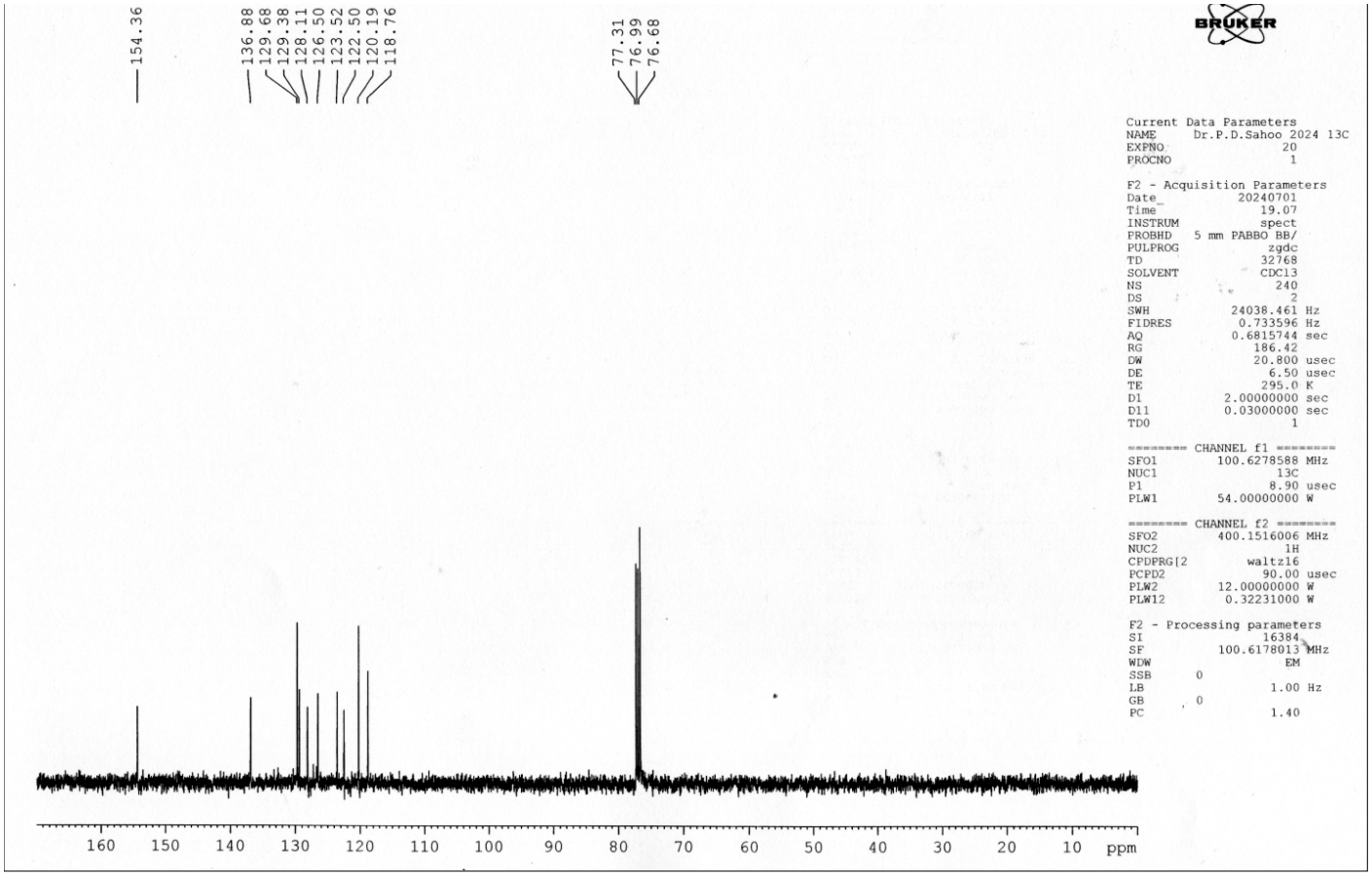


Figure S6. ^{13}C NMR of **N3** in $CDCl_3$ (100 MHz).

^{1}H NMR of N4 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 14.87 (s, 1H), 9.50 (s, 1H), 8.22-8.14 (m, 3H, J=8), 7.90-7.88 (d, 1H, J=8), 7.79-7.77 (d, 1H, J=8), 7.68-7.56 (m, 3H), 7.42-7.38 (t, 1H), 7.19-7.16 (d, 1H, J=12), ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 158.64, 136.87, 130.40, 129.48, 128.39, 127.58, 124.01, 120.96, 120.59, 119.15, 115.16. HRMS (TOF MS): (m/z, %): for C17H12N2O3+H^{+}:, Found: m/z = 293.0907 (M+H^{+}).

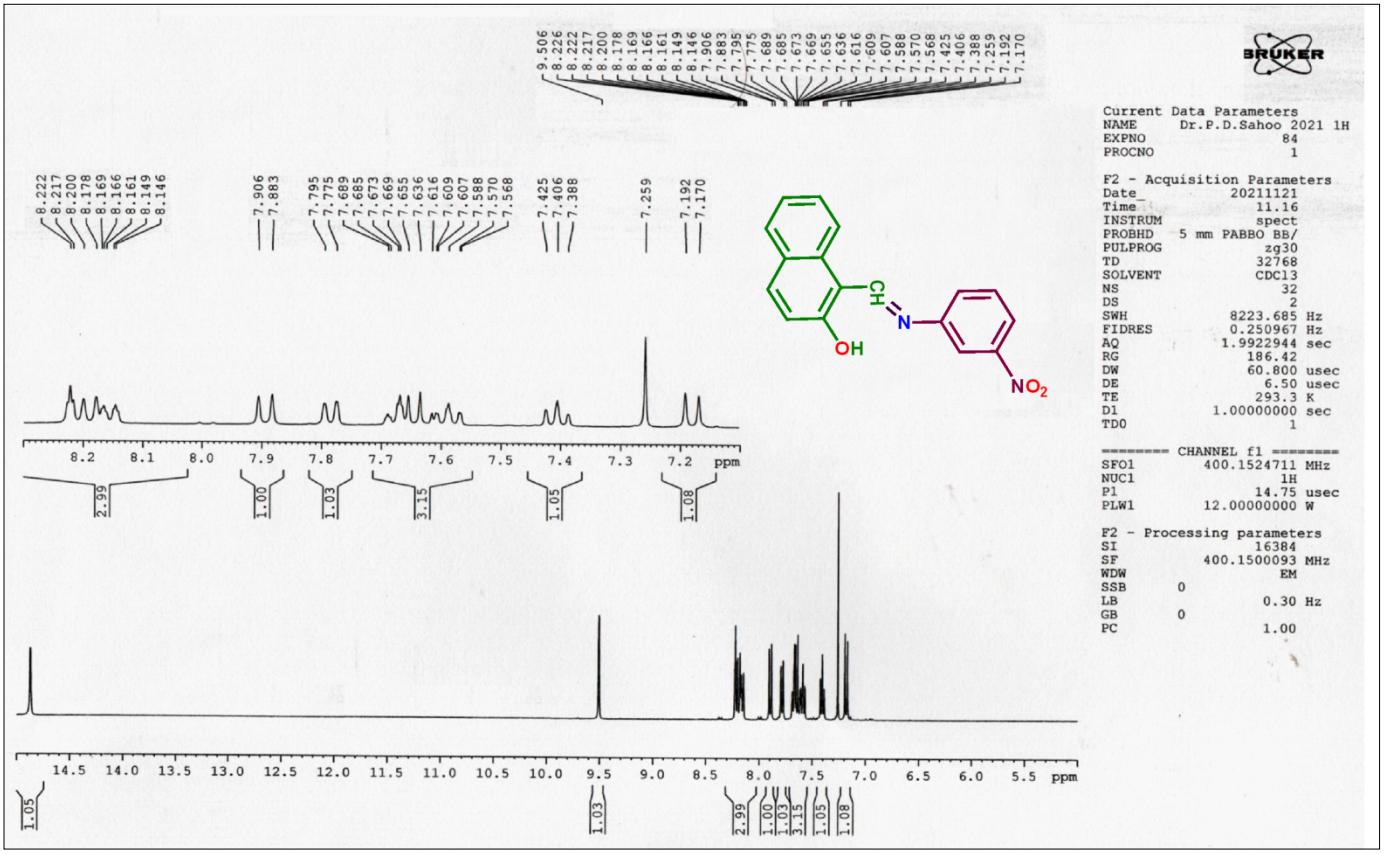


Figure S7. ^{1}H NMR of **N4** in $CDCl_3$(400 MHz).

^{13}C NMR of N4 in $CDCl_3$:

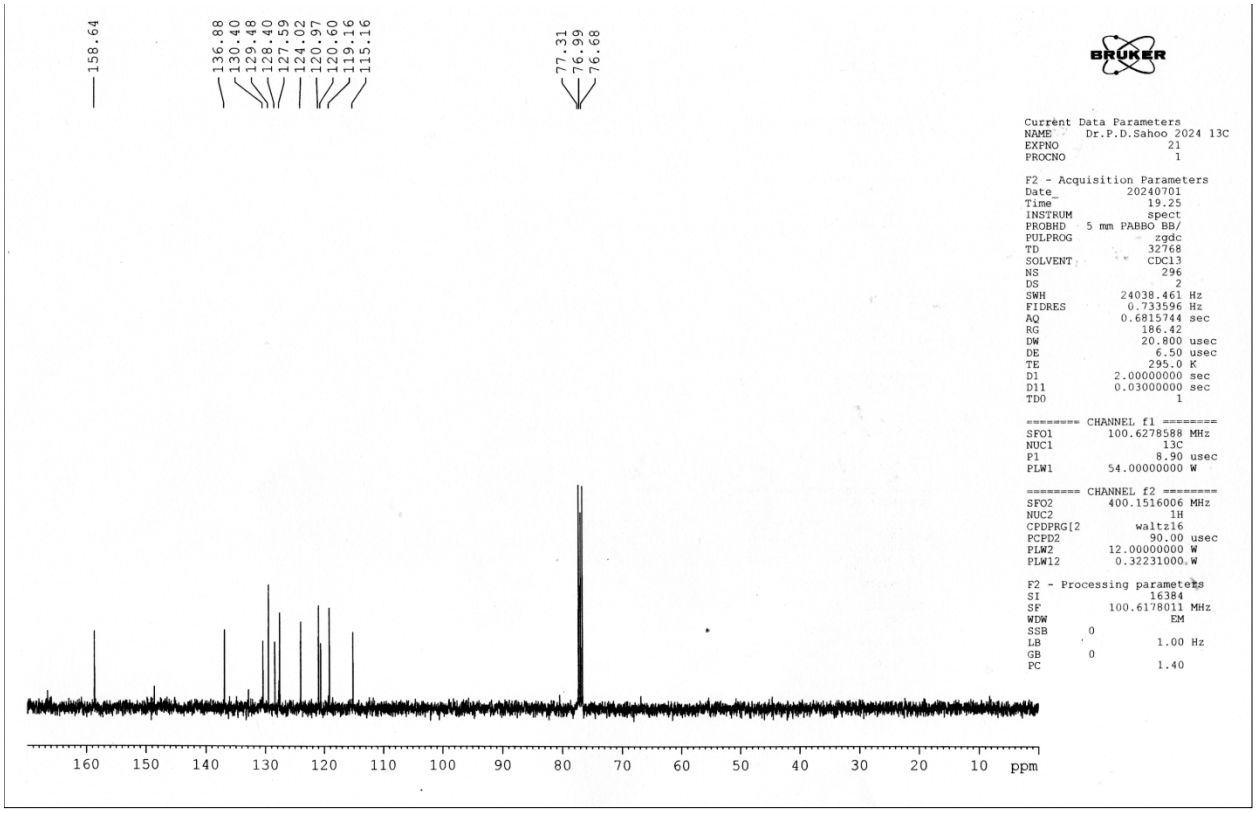


Figure S8. ^{13}C NMR of **N4** in $CDCl_3$ (100 MHz).

^{1}H NMR of N5 in DMSO-d_6

^{1}H NMR of N5 (400 MHz, DMSO-d_6): δ (ppm) = 15.26 (s, 1H), 9.68 (s, 1H), 8.55-8.52 (d, 1H, J = 12 Hz), 8.34-8.32 (d, 2H , J = 8 Hz), 7.99-7.97 (d, 1H, J = 8 Hz), 7.88-7.86 (d, 2H, J = 8 Hz), 7.81-7.79 (d, 1H, J = 8 Hz), 7.59-7.55 (t, 1H, J = 12 Hz), 7.40-7.36 (t, 1H, J = 12 Hz), 7.01-6.98 (t, 1H, J = 12 Hz), ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 156.51, 138.48, 129.19, 128.50, 126.88, 125.28, 124.11, 122.39, 121.21, 120.82, 110.61. HRMS (TOF MS): (m/z, %): for C17H12N2O3+H^{+}, Found: m/z = 293.0909 (M+H+).

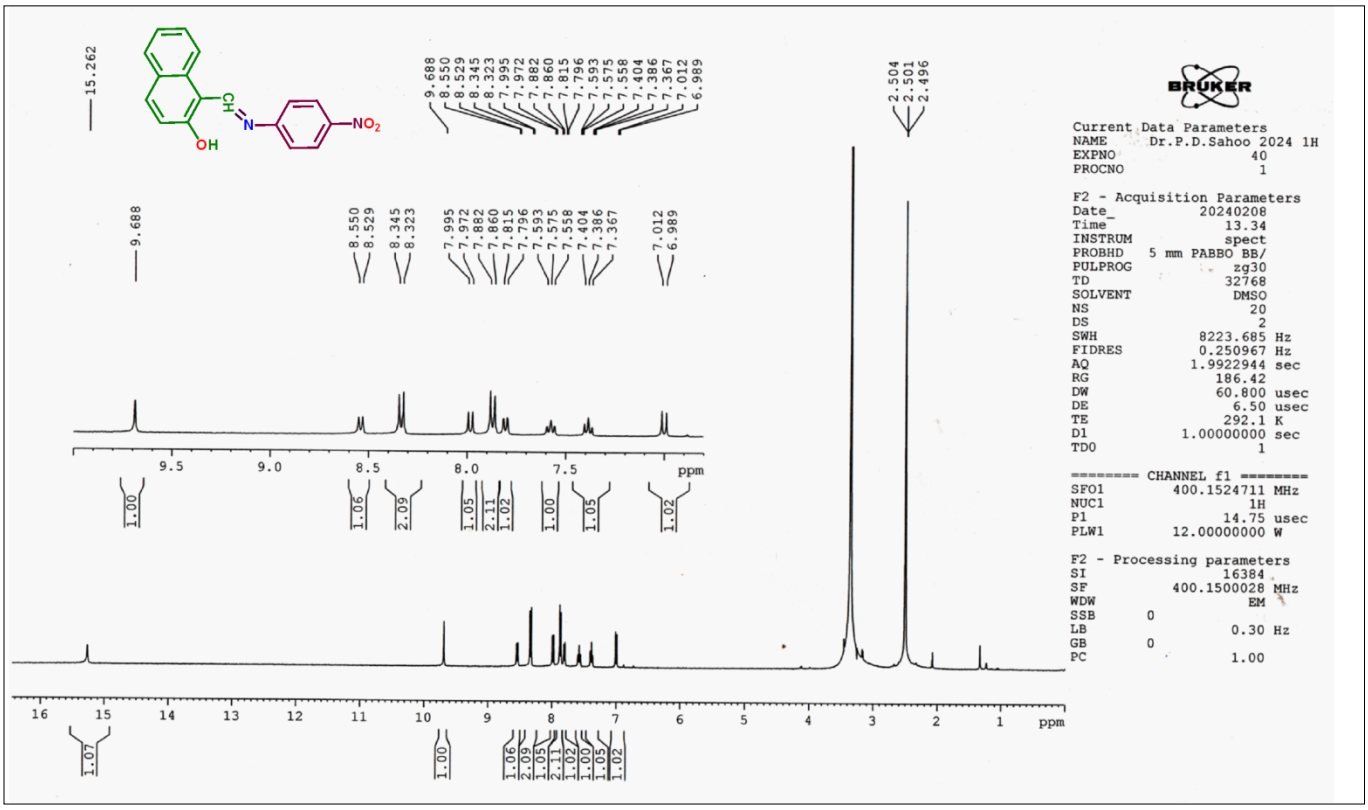


Figure S9. ^{1}H NMR of **N5** in DMSO-d_6 (400)

^{13}C NMR of N5 in DMSO-d_6:

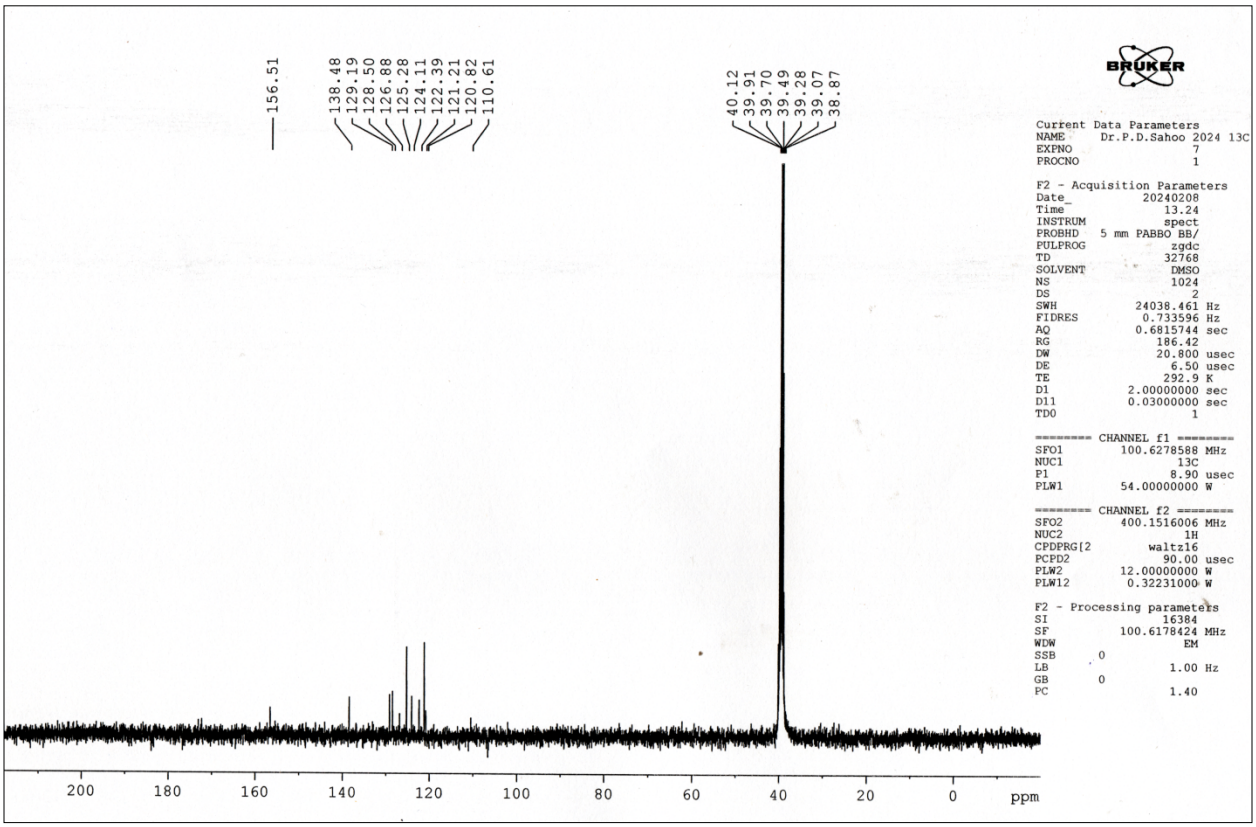


Figure S10. ^{13}C NMR of **N5** in DMSO-d_6 (100 MHz).

2. Selectivity

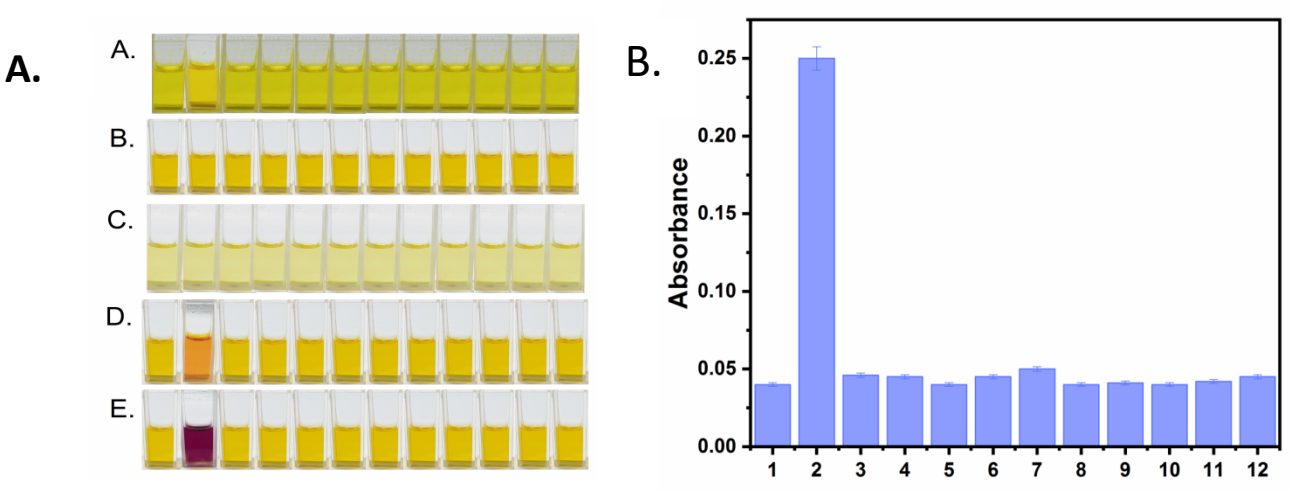


Figure S11. (A) colorimetric changes of (A) N1, (B) N2, (C) N3, (D) N4, (E) N5, in presence of 1) Blank, 2) H_2S, 3) SO_4^{2-} 4) CN^-, 5) SCN^{-1}, 6) F^-, 7) , ClO^-, 8) CN^-, 9) NO_3^-, 10) $H_2PO_4^-$, 11) CO, 12) cysteine,. (B) Absorbance spectra of **N5** in presence of different analytes at 544 nm in H_2O-CH_3CN (4:1, v/v) at neutral pH.

3. Fluorescence spectra of N1, N2, N3, N4 and N5

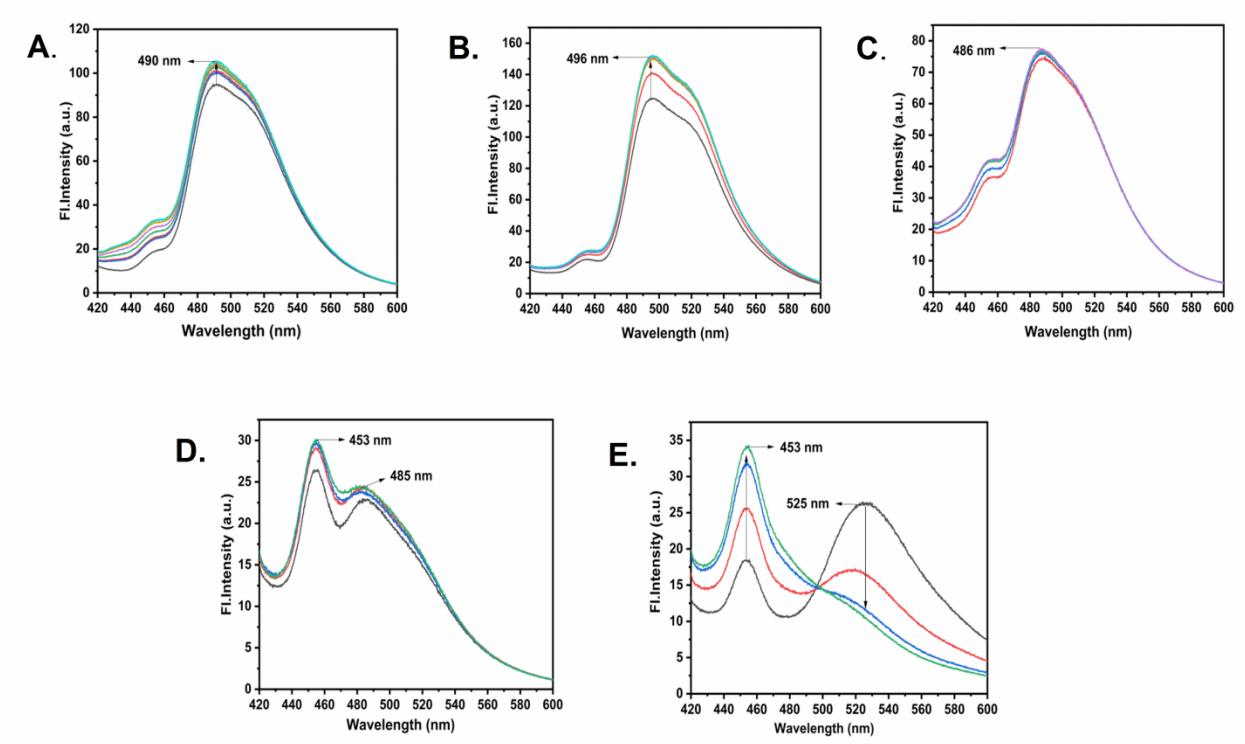


Figure S12. Fluorescence spectra of (A) N1, (B) N2, (C) N3, (D) N4, (E) N5 in presence of H_2S (upto 40 μM).

4. pH titration study:

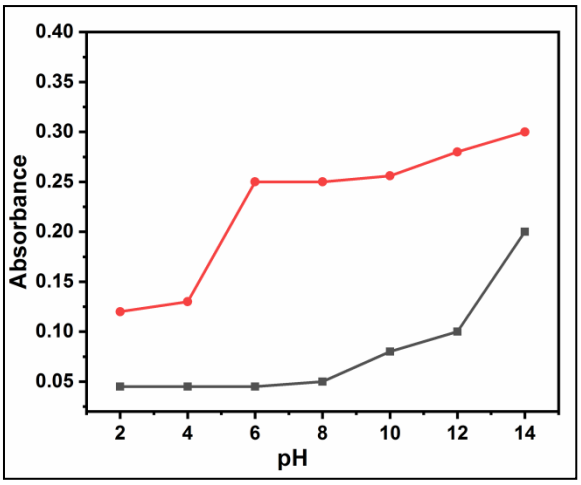


Figure S13. Effect of pH on the absorbance intensity of **N5** (10^{-5} M) in the absence of $\mathbf{H_2S}$ (black line) and in the presence of $\mathbf{H_2S}$ (10^{-4}M, red line).

5. Job' s plot

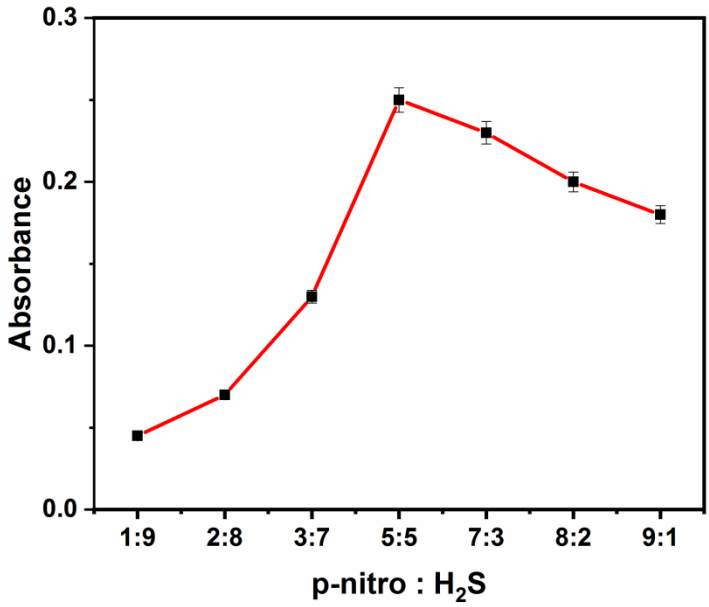


Figure S14. Job's plot of **N5** (10μM) with $\mathbf{H_2S}$ in DMSO-water (1:1, v/v), at neutral pH, by absorbance method, which indicate 1:1 stoichiometry for **N5** with $\mathbf{H_2S}$. Standard deviations are represented by error bar (n=3).

6. Calculation of limit of detection (LOD) of N5 with H_2S:

The detection limit of the chemosensor **N5** for **H_2S** was calculated on the basis of absorbance titration. To determine the standard deviation for the absorbance intensity, the absorbance intensity of four individual receptors without **H_2S** was measured by 10 times and the standard deviation of blank measurements was calculated.

The limit of detection (LOD) of **N5** for sensing **H_2S** was determined from the following equation[2-3]:

$$LOD = K \times SD/S$$

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank receptor solution; S is the slope of the calibration curve.

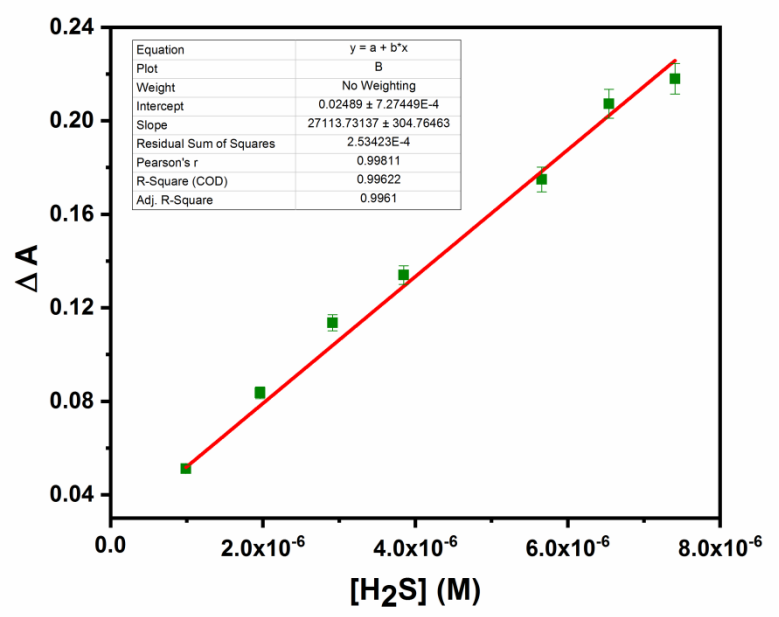


Figure S15. Linear fit curve of **N5** at 544 nm with respect to **H_2S** concentration

For **N5** with **H_2S:**

From the linear fit graph, we get slope = 27330.34743, and SD value is 0.0005890

Thus, using the above formula, we get the Limit of Detection = 6.51×10^{-8} M. Therefore **N5** can detect **H_2S** up to this very lower concentration by absorbance technique.

7. Calculation of limit of detection (LOD) of N4 with H_2S:

The detection limit of the chemosensor **N4** for **H_2S** was calculated on the basis of absorbance titration. To determine the standard deviation for the absorbance intensity, the absorbance intensity of four individual receptors without **H_2S** was measured by 10 times and the standard deviation of blank measurements was calculated.

The limit of detection (LOD) of **N4** for sensing **H_2S** was determined from the following equation[2-3]:

$$LOD = K \times SD/S$$

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank receptor solution; S is the slope of the calibration curve.

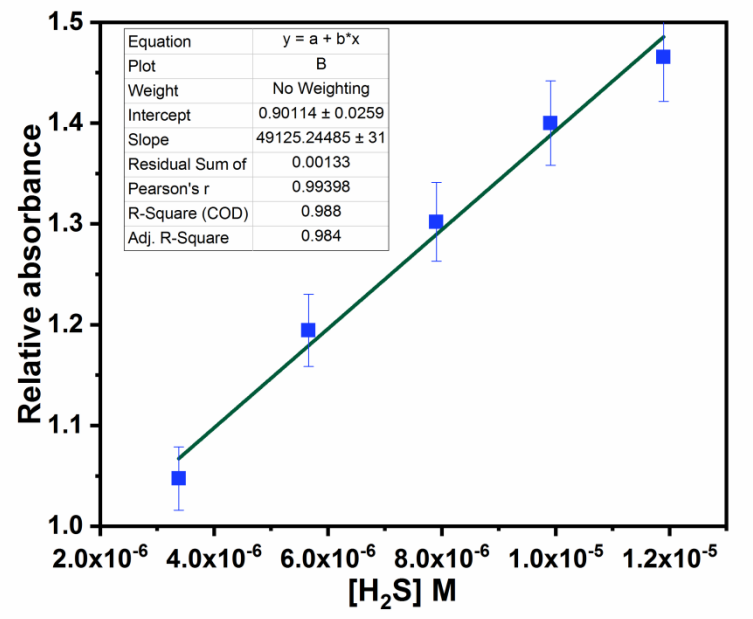


Figure S16. Linear fit curve of **N4** at 460 nm with respect to **H_2S** concentration

For **N4** with **H_2S:**

From the linear fit graph, we get slope = 49125.24485, and SD value is 0.0117969.

Thus, using the above formula, we get the Limit of Detection = 7.2×10^{-7} M. Therefore **N4** can detect **H_2S** up to this concentration by absorbance technique.

Table S2. Comparision Table

Sensors	Analytes	Detection medium	Sensitivity	Detection limits	Reference
2-hydroxy napthaldehyde conjugated 2,4-DNP (N5)	H_2S	DMSO:H2O (1:1) solution using 10 mM phosphate buffer at pH 7.0	High	65 nM	Present work
2,3-dihydroxybenzaldehyde and sulfanilamide	H_2S	DMSO: Bis–Tris buffer (4 : 6, 10 mM, pH 7.0)	High	30 µM	Anal. Methods, 2021, 13, 1332
Naminophthalimide and 8-hydroxyjulolidine-9-carboxaldehyde	Cu^{2+}, PO_4^{3-} and S^{2-}	____	Low	____	Ind. Eng. Chem. Res. 2017, 56, 30, 8399–8407
5-(azo-benzene)-salicylidene-aniline	H_2S	DMSO DMSO–phosphate-buffered saline (PBS) (4 :1, v/v, pH 7.4).	High	_____	Luminescence.2017 ,32(5),765-771
azo-dye based bis-Schiff base	S^{2-}	HEPES buffer (10 mL, pH 7.00).	High	16 µM	Anal. Methods, 2018,10, 2317-2326
2-aminoethyl piperazine and 4-chloro-7-nitrobenz-2-oxa-1,3-diazole	H_2S, Hg^{2+}	bis-tris buffer solution (10 mM, pH 7.0) to	Modarate	____	Dalton Trans., 2016,45, 5700-5712
Dabsyl based	H_2S, Hg^{2+}	HEPES-CH3CN buffer.	Modarate	28 mM	ChemistrySelect, 2016, 1(8):1533-1540
4-(piperidin-1-yl) naphthalene-1,2-dione	H_2S	CH3CN: HEPES buffer (50:50, v:v, pH-7.4)	High	0.77 µM	Org. Biomol. Chem., 2016,14, 570-576
2- hydroxy-1-napthylaldehyde	H_2S/HS^-	CH3CN:HEPES buffer solution	High	1.67 µM	New J. Chem., 2015,39, 5669-5675

8. Evaluation of the association constants for the formation of N5-H_2S complex:

By Absorbance Method:

Binding constant of the chemosensor **N5** was calculated through absorbance method by using the following equation:

$$1/ (A– A_0) = 1/K(A_{max}– A_0) [G] + 1/(A_{max}– A_0) \quad \text{……..(ii)}$$

Where A_0, A_{max}, and I represent the absorbance intensity of free **N5**, the maximum absorbance intensity observed in the presence of added **H_2S** at 544 nm, the absorbance intensity at a certain concentration of the **H_2S** respectively and [G] is the concentration of the guest **H_2S.**

Binding constant calculation graph (absorbance method):

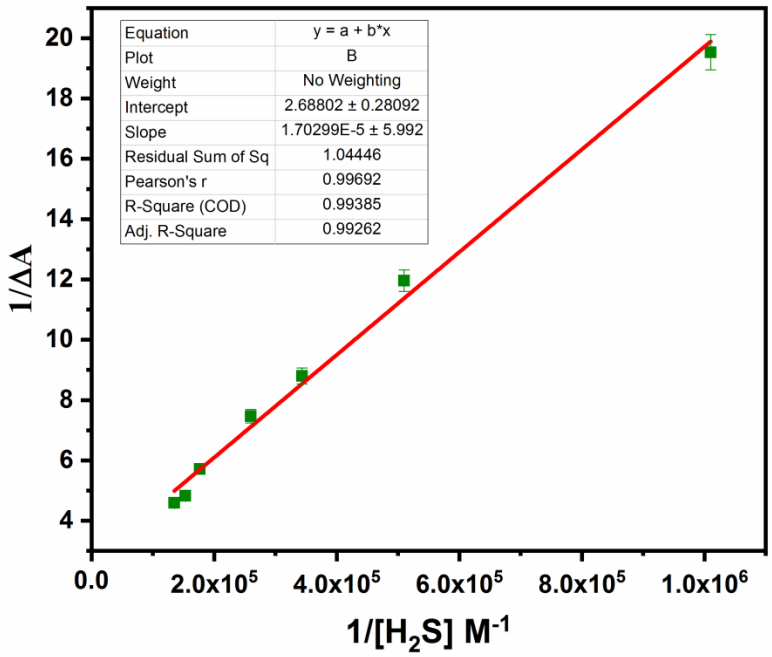


Figure S17. Linear regression analysis for the calculation of association constant value by absorbance titration method.

The association const. (K_a) of **N5** for sensing **H_2S** was determined from the equation:

K_a = intercept/slope. From the linear fit graph, we get intercept= 0.06348, slope = 1.52861×10^{-8}. Thus, we get, $\mathbf{K_a}$= (0.06348) / (1.52861×10^{-8}) = $\mathbf{4.15 \times 10^6\ M^{-1}}$.

9. DFT study

Table S3. Details of the geometry optimization in Gaussian 09 program

Details	N3	N3-H_2S
Calculation method	B3LYP	B3LYP
Basis set	aug ccpvdz	aug ccpvdz
E(CAM-B3LYP) (a.u.)	-785.727627	-785.730658
Charge, Multiplicity	0, 1	0, 1
Solvent (CPCM)	DMSO	DMSO

Details	N4	N4-H_2S
Calculation method	B3LYP	B3LYP
Basis set	aug ccpvdz	aug ccpvdz
E(CAM-B3LYP) (a.u.)	-990.270227	-990.271784
Charge, Multiplicity	0, 1	0, 1
Solvent (CPCM)	DMSO	DMSO

Details	N5	N5-H_2S
Calculation method	B3LYP	B3LYP
Basis set	aug ccpvdz	aug ccpvdz
E(CAM-B3LYP) (a.u.)	-990.272758	-990.275422
Charge, Multiplicity	0, 1	0, 1
Solvent (CPCM)	DMSO	DMSO

TDDFT- Calculations

Table S4. Selected electronic excitation energies (eV), oscillator strengths (f), main configurations of the low-lying excited states of CPLC. The data were calculated by TDDFT//B3LYP/ aug ccpvdz based on the optimized ground state geometries.

Molecules	Electronic Transition	Excitation Energy[a]	f[b]	Composition[c](%)
N3	$S_0 \rightarrow S_1$	3.1957 eV 387.98nm	0.5702	H → L (70.08%)
N3+H_2S	$S_0 \rightarrow S_1$	2.9007 ev 427.43 nm	0.5457	H → L (70.53%)
N4	$S_0 \rightarrow S_2$	3.1933 ev 388.26 nm	0.5303	H → L+1 (70.02%)
N4+H_2S	$S_0 \rightarrow S_2$	2.9388 ev 421.88 nm	0.4923	H → L+1 (70.37%)
N5	$S_0 \rightarrow S_1$	2.6019 ev 476.31 nm	0.5325	H → L (70.44%)
N5+H_2S	$S_0 \rightarrow S_1$	2.4749 ev 500.96 nm	0.6576	H → L (70.59%)

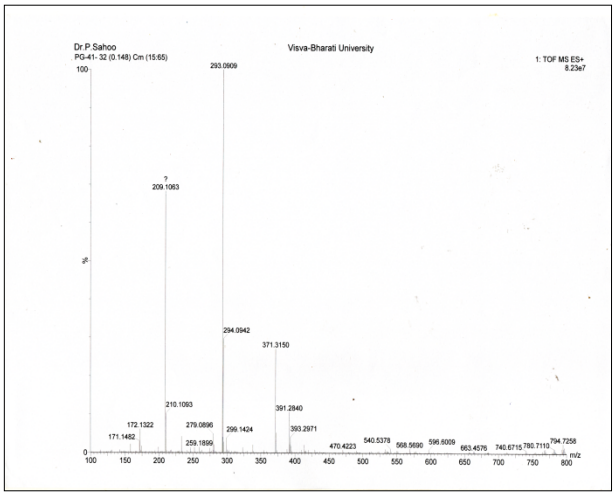
[a]Only selected excited states were considered. The numbers in parentheses are the excitation energy in wavelength. [b]Oscillator strength. [c]H stands for HOMO and L stands for LUMO.

Table S5. Energies of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO)

Species	**E_{HOMO} (a.u.)**	**E_{LUMO} (a.u.)**	**ΔE(a.u.)**	**ΔE(eV)**	**ΔE(kcal/mol)**
N3	-0.21877	-0.08439	0.13438	3.65	84.32
N3+H_2S	-0.21228	-0.09083	0.12145	3.30	76.21
N4	-0.22390	-0.08931	0.13459	3.66	84.45
N4+H_2S	-0.21804	-0.09457	0.12347	3.35	74.47
N5	-0.22579	-0.11646	0.10933	2.97	68.80
N5+H_2S	-0.22121	-0.11811	0.10316	2.80	64.73

10. HRMS

A.



B.

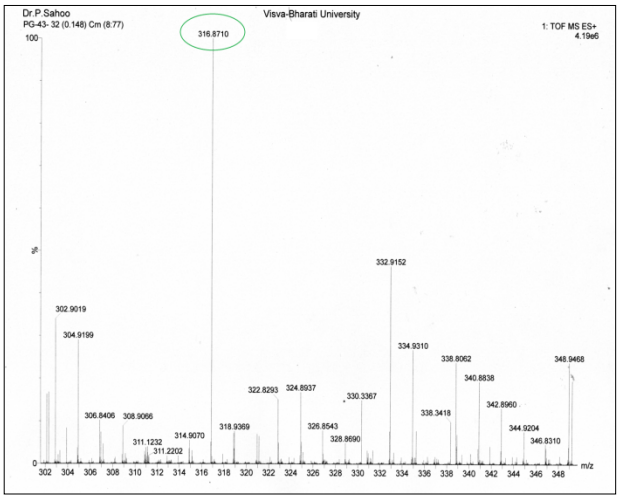


Figure S18. HRMS spectra; The experimental mass (A): N5 is 293.0909 ($C_{17}H_{12}N_2O_3$) and (B): N5+H_2S complex is 316.8710 ($C_{17}H_{12}N_2O_3$+ Na).

11. ^{1}H NMR of N6 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 12.46 (s, 1H), 9.78 (s, 1H), 8.56-8.58 (d, 2H, J=8), 8.55-8.52 (d, 3H, J=12), 8.12-8.10 (1H,d), 7.96-7.92 (d, 3H), 7.64-7.59 (t, 1H), 7.47-7.43 (t, 1H), 7.33-7.31 (d, 1H, J=8). ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 170.11, 160.64, 160.48, 135.77, 134.81, 132.21, 131.46, 131.25, 129.04, 128.47, 127.85, 127.43, 126.94, 124.03, 122.38, 122.01, 118.81, 108.06. ESI MS: (m/z, %): for C23H14N2O3+H$^+$: Found: m/z = 367.10 (M+H$^+$).

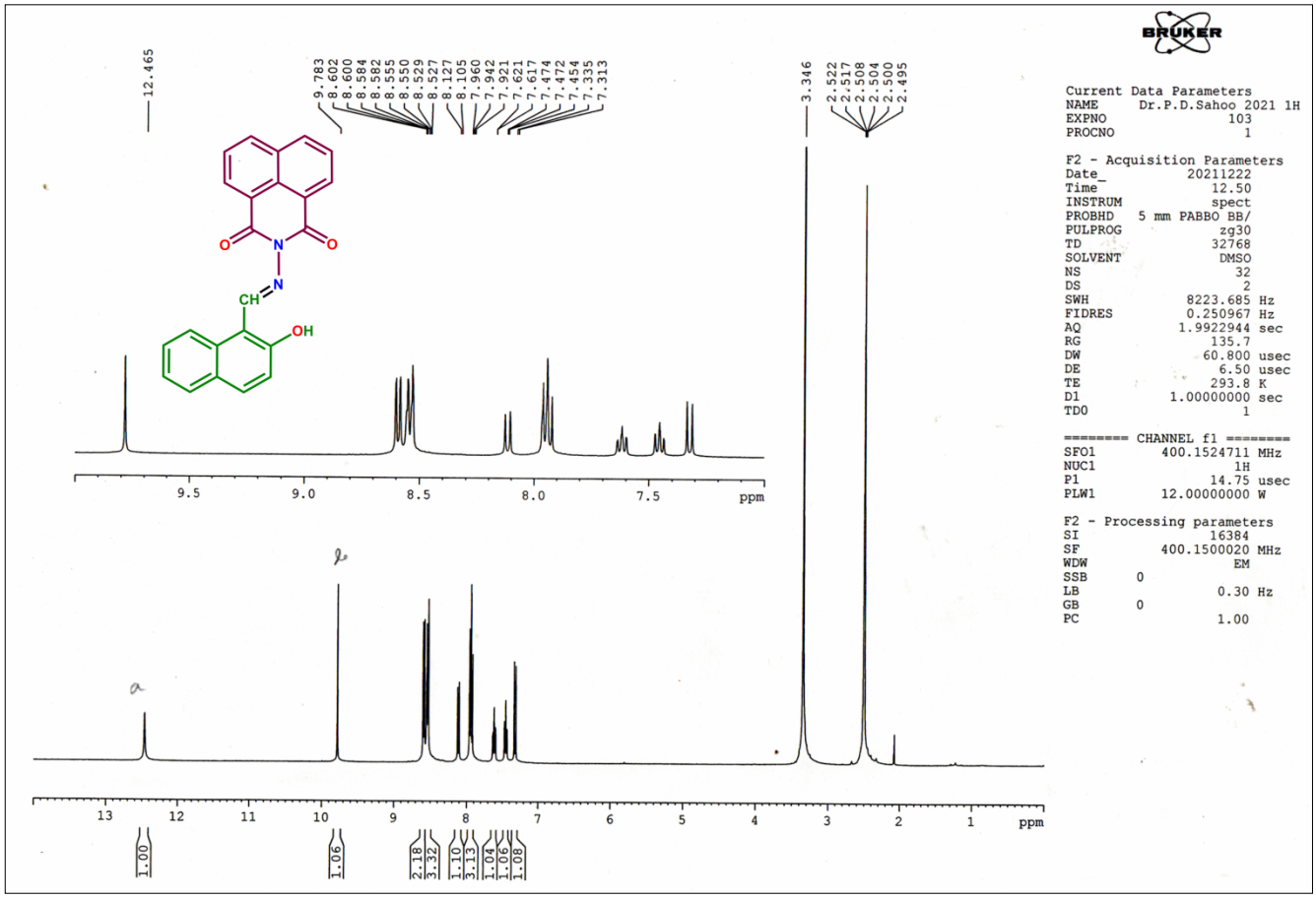


Figure S19. ^{1}H NMR of **N6** in $CDCl_3$ (400 MHz).

^{13}C NMR of N6 in DMSO-d_6:

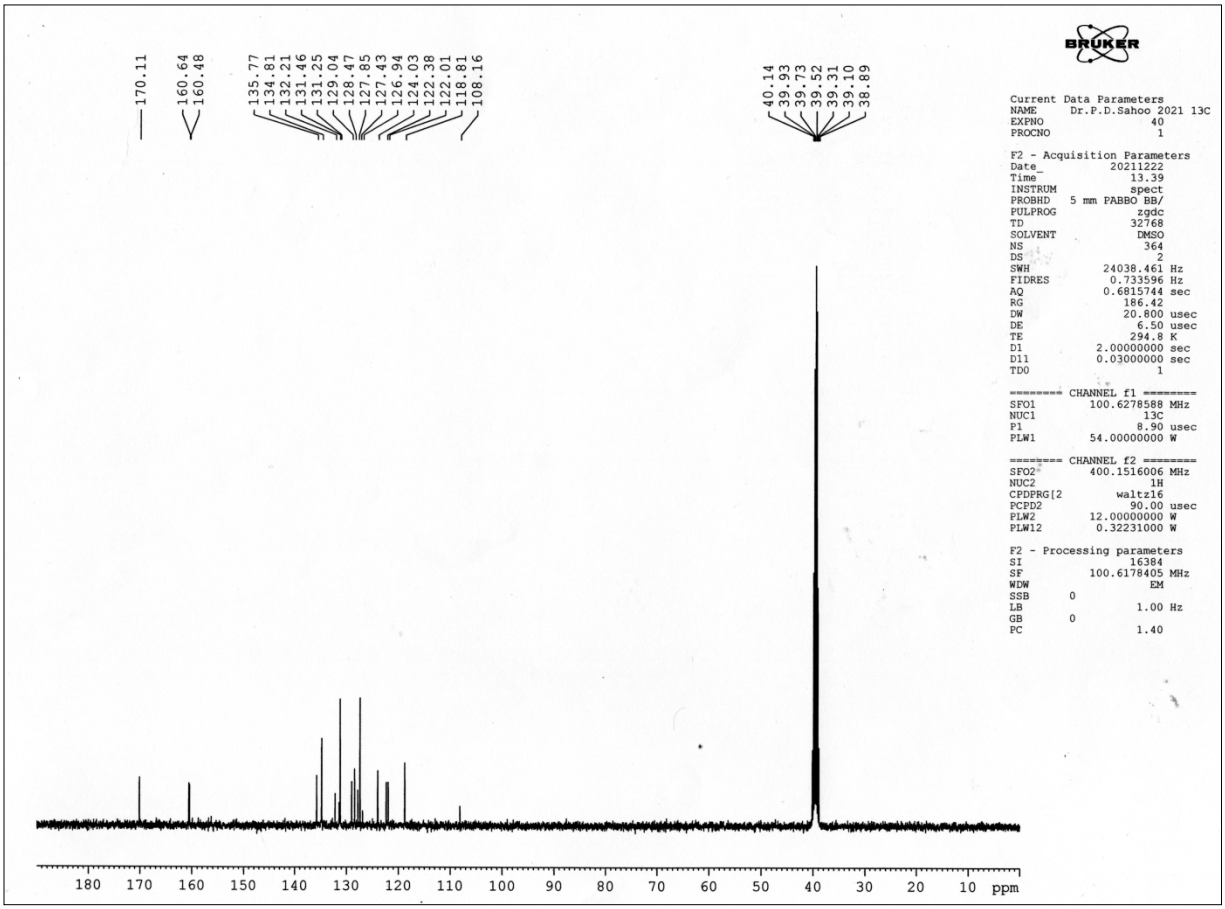


Figure S20. ^{13}C NMR of **N6** in DMSO-d_6 (100 MHz).

^{1}H NMR of N7 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 16.37 (s, 1H), 9.84 (s, 1H), 8.57–8.59 (d, 2H, J = 8 Hz), 8.26–8.28 (d, 1H, J = 8 Hz), 7.90–7.92 (d, 1H, J = 8 Hz), 7.77–7.82 (t, 2H, J = 20 Hz), 7.71–7.73 (d, 1H, J = 8 Hz), 7.62–7.64 (t, 1H, J = 8 Hz), 7.55–7.57 (t, 1H, J = 8 Hz), 7.47–7.51 (t, 1H, J = 16 Hz), 7.34–7.37 (t, 1H, J = 12 Hz), 7.23–7.26 (t, 1H, J = 12 Hz), 7.04–7.06 (d, 1H, J = 8 HZ), 4.47–4.49 (q, 2H, J = 8 Hz), 1.31–1.34 (t, 3H, J = 12 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 169.46, 153.90, 140.30, 138.46, 135.94, 133.15, 129.04, 127.93, 126.67, 126.32, 123.28, 123.02, 122.26, 122.11, 120.92, 120.36, 119.55, 119.05, 112.08, 109.98, 109.52, 108.67, 37.19, 13.83. HRMS (TOF MS): (m/z, %): Calcd. for C25H20N2O: 364.1576. Found: m/z = 365.1283 (M + H^{+}).

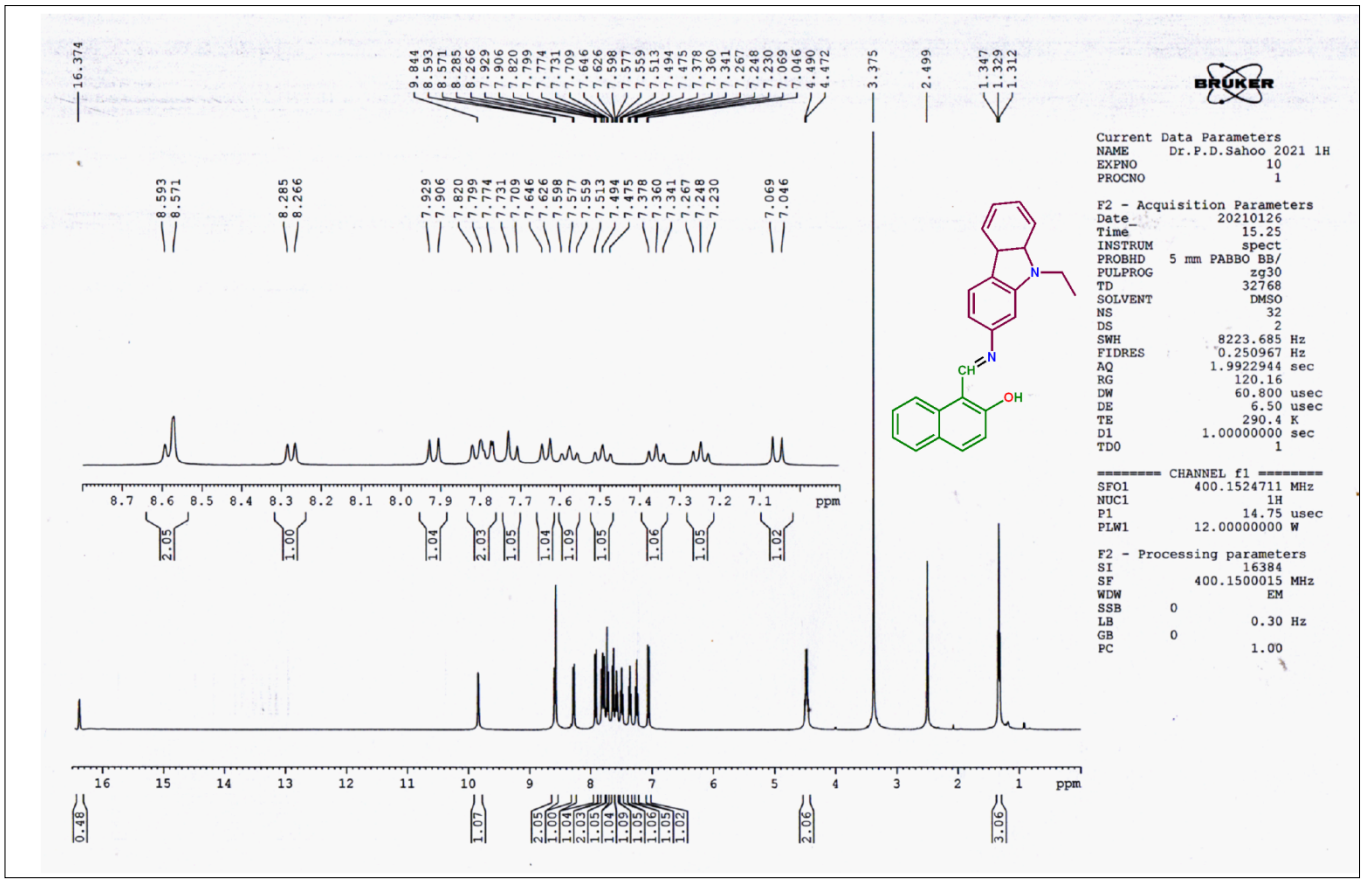


Figure S21. ^{1}H NMR of **N7** in $CDCl_3$ (400 MHz).

^{13}C NMR of N7 in DMSO-d_6:

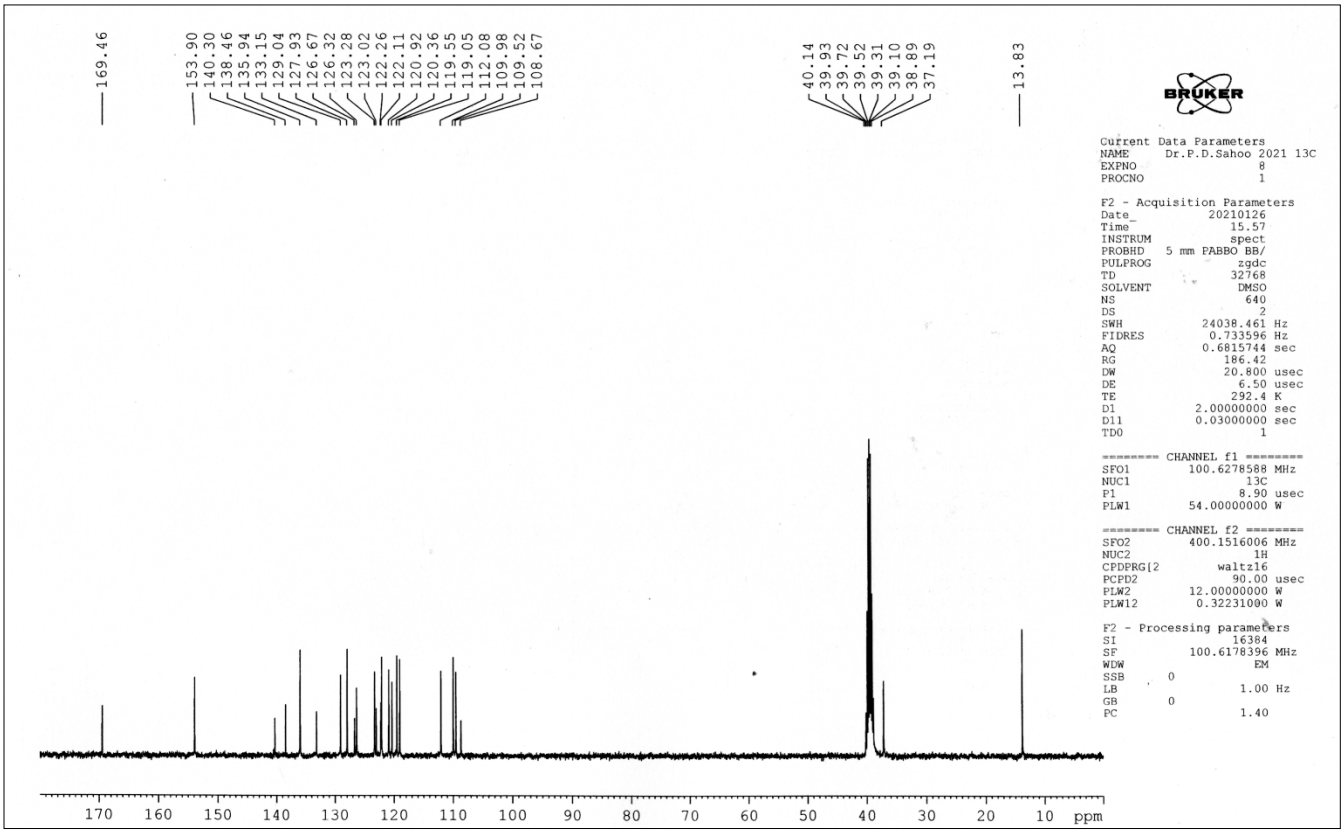


Figure S22. ^{13}C NMR of **N7** in DMSO-d_6 (100 MHz).

12. Fluorescence spectra of N6 and N7

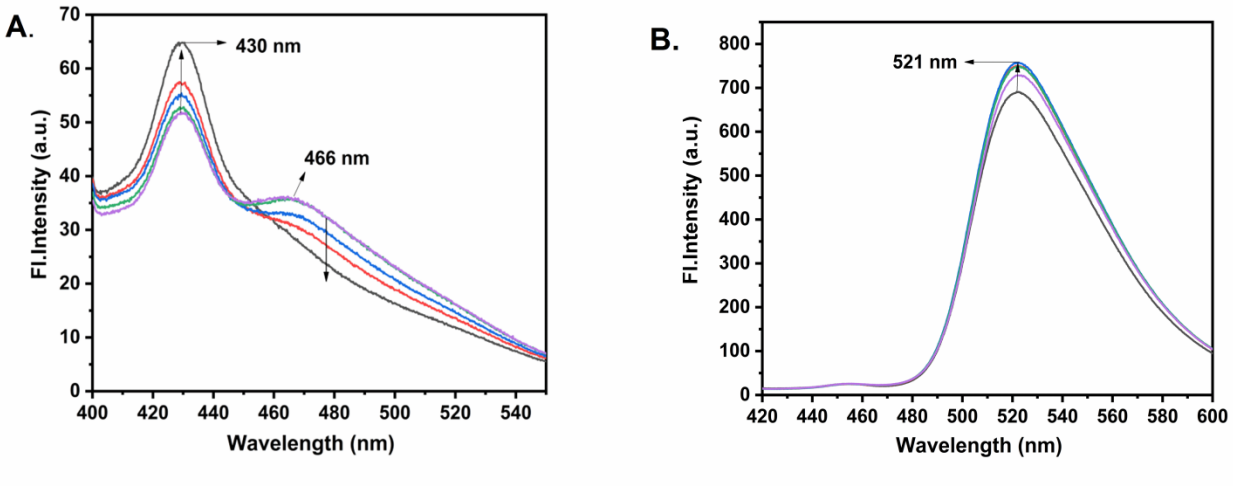


Figure S23. Fluorescence spectra of (A) N6 and (B) N7 in presence of H_2S (upto 40 μM).

^{1}H NMR ofN8 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 14.04 (s, 1H), 9.09-9.11 (d, 1H, J=8), 8.47-8.49 (d, 2H, J=8), 8.43-8.45 (d, 2H, J=8), 7.94-7.96 (d, 1H, J=8), 7.83-7.87 (t, 2H, J=16), 7.67-7.70 (d, 1H, J=12), 7.59-7.60 (d, 1H, J=4), 7.30-7.34 (t, 1H, J=16), 7.13-7.17 (t, 1H, J=16), 6.68-6.70 (d, 1H, J=8), 4.41-4.44 (t, 2H, J=12), 3.98-4.02 (q, 2H, J=16).^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 175.63, 163.53, 159.92, 136.72, 134.36, 134.03, 131.29, 130.78, 128.75, 127.70, 127.44, 127.18, 125.31, 124.82, 122.17, 122.00, 118.57, 106.12 and 49.68. HRMS (TOF MS): (m/z, %): Calcd. for C25H19N2O3+H^{+}: 395.1390, Found: m/z = 395.1412 (M+H^{+}).

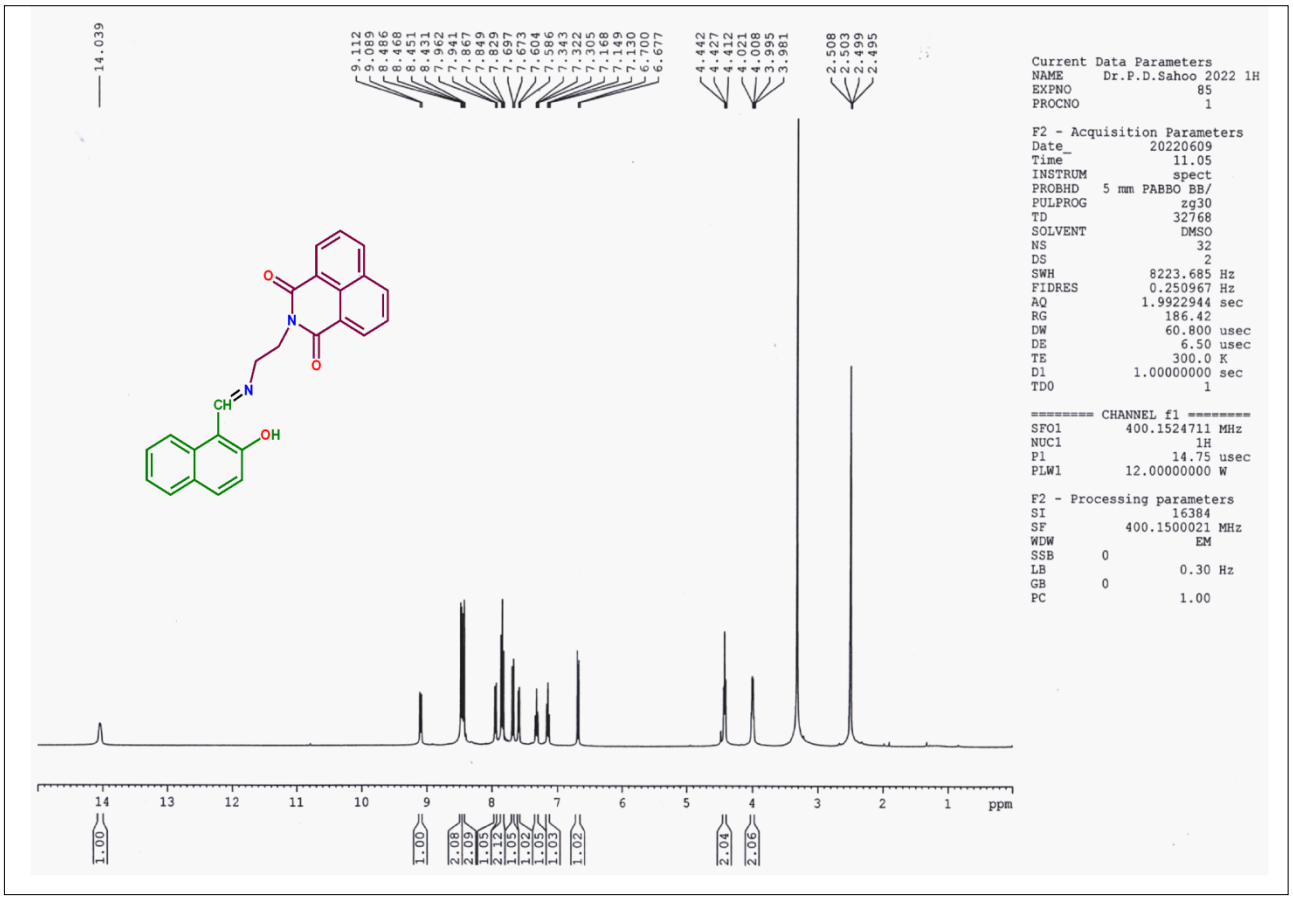


Figure S24. ^{1}H NMR of **N8** in $CDCl_3$ (400 MHz).

^{13}C NMR of N8 in DMSO-d_6:

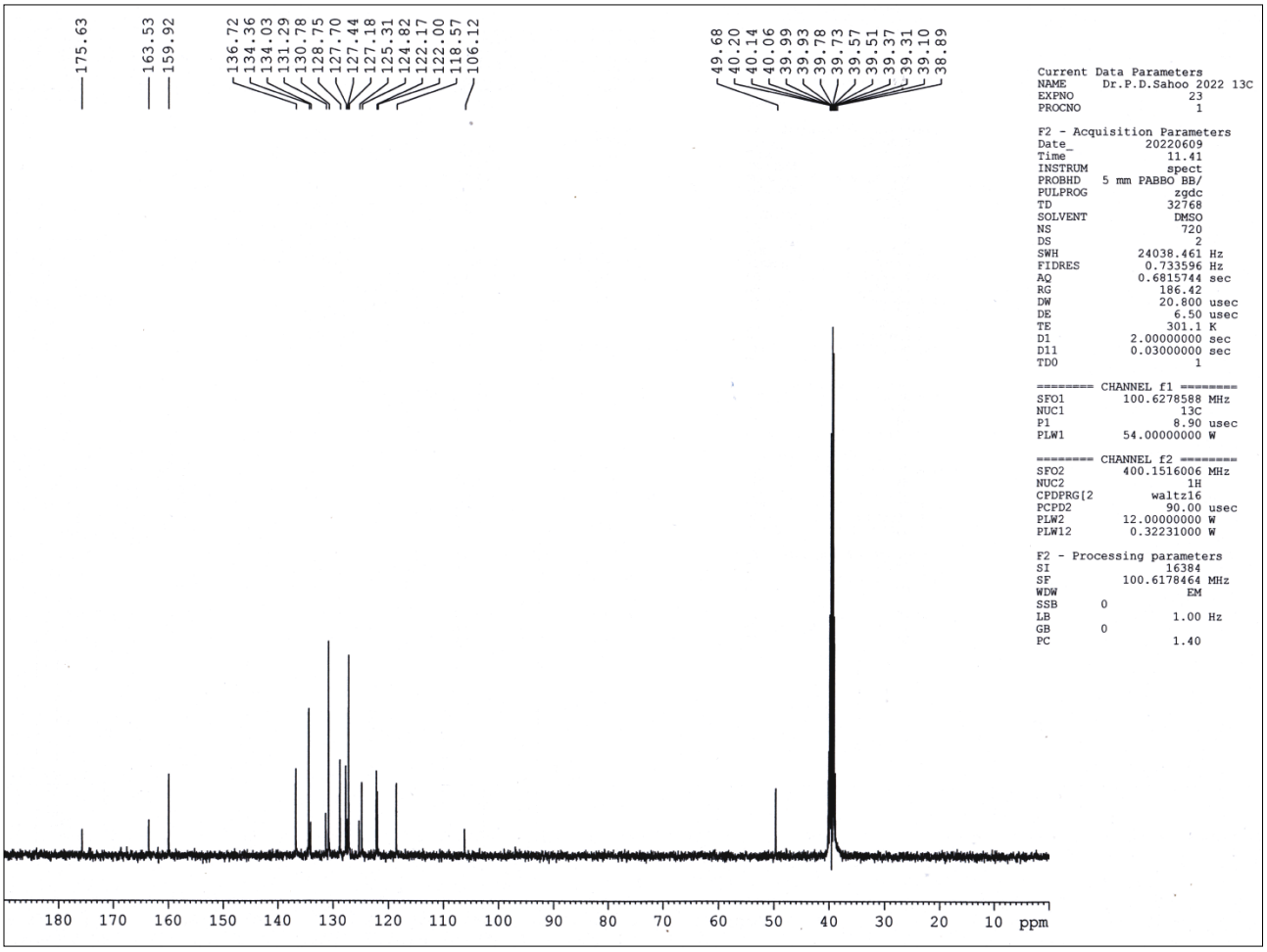


Figure S25. ^{13}C NMR of **N8** in DMSO-d_6 (100 MHz).

^{1}H NMR of N9 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 14.32 (s, 1H), 9.28–9.30 (d, 1H, J = 8 Hz), 8.58–8.59 (d, 1H, J = 8 Hz), 8.09–8.11 (d, 1H, J = 8 Hz), 7.80–7.84 (dd, 1H, J = 16 Hz), 7.73– 7.75 (d, 1H, J = 8 Hz), 7.63–7.65 (d, 1H, J = 8 Hz), 7.42–7.46 (dd, 2H, J = 16 Hz), 7.32–7.35 (d, 1H, J = 12 Hz), 7.18–7.22 (dd, 1H, J = 16 Hz), 6.73–6.75 (d, 1H, J = 8 Hz), 4.99–5.00 (s, 2H, J = 4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 176.86, 159.89, 156.71, 149.45, 137.22, 134.27, 128.94, 127.98, 125.37, 125.25, 122.85, 122.35, 121.93, 118.57, 106.11, 56.18. HRMS (TOF MS): (m/z, %): calcd for C17H14N2O: 262.1106. Found: m/z = 263.1183 (M + H^+).

Figure S26. ^{1}H NMR of **N9** in $CDCl_3$ (400 MHz).

^{13}C NMR of N9 in DMSO-d_6:

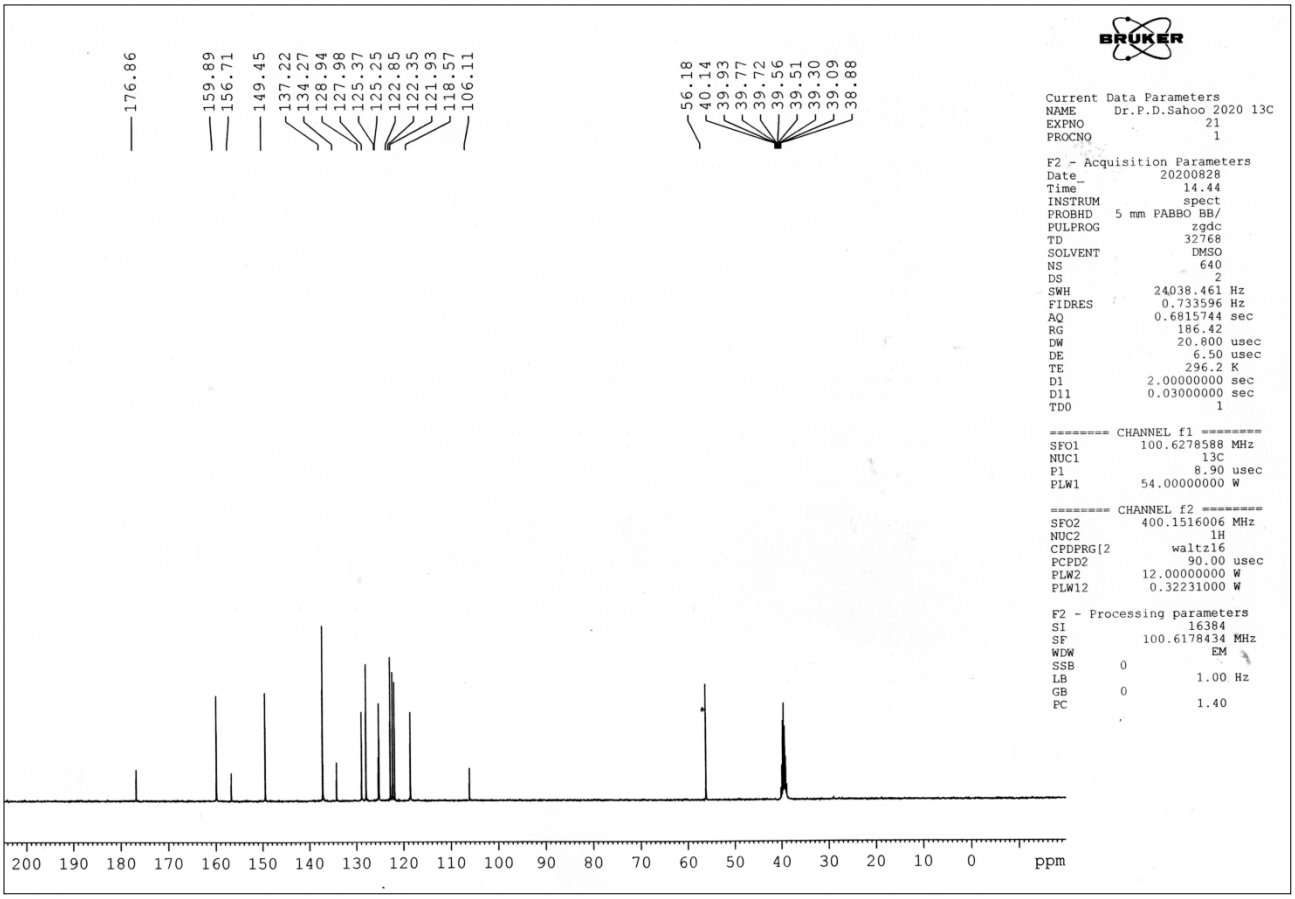


Figure S27. ^{13}C NMR of **N9** in DMSO-d_6 (100 MHz).

^{1}H NMR of N10 in DMSO-d_6:

^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) = 14.31 (s, 1H); 9.31-9.28 (d, 1H, J= 12 Hz); 8.12-8.10 (d, 1H, J = 8 Hz); 7.78-7.76 (d, 1H, J = 8 Hz); 7.68-7.67 (q, 2H); 7.49-7.45 (m, 1H); 7.25-7.22 (t, 1H, J= 12 Hz); 6.79-6.76 (d, 1H, J =12 Hz); 6.47-6.46 (d, 2H); 4.90-4.89 (d, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) = 172.63, 159.36, 142.93, 136.57, 133.28, 129.20, 127.87, 126.57, 123.38, 122.96, 118.24, 110.57, 108.49, 107.57, 50. 74. C16H13NO2: ESI-MS: 274.25 (M + H^{+})

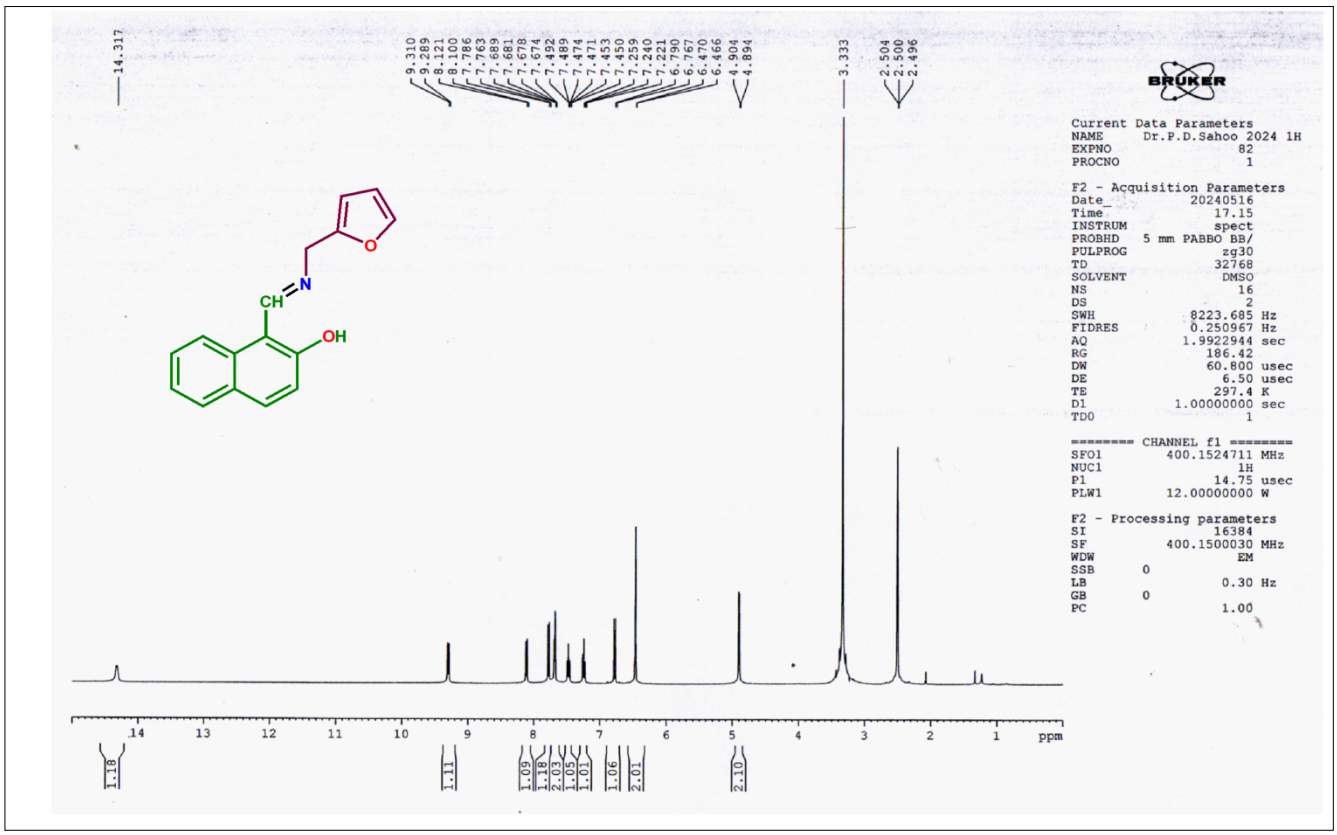


Figure S28. ^{1}H NMR of **N10** in $CDCl_3$ (400 MHz).

^{13}C NMR of N10 in DMSO-d_6:

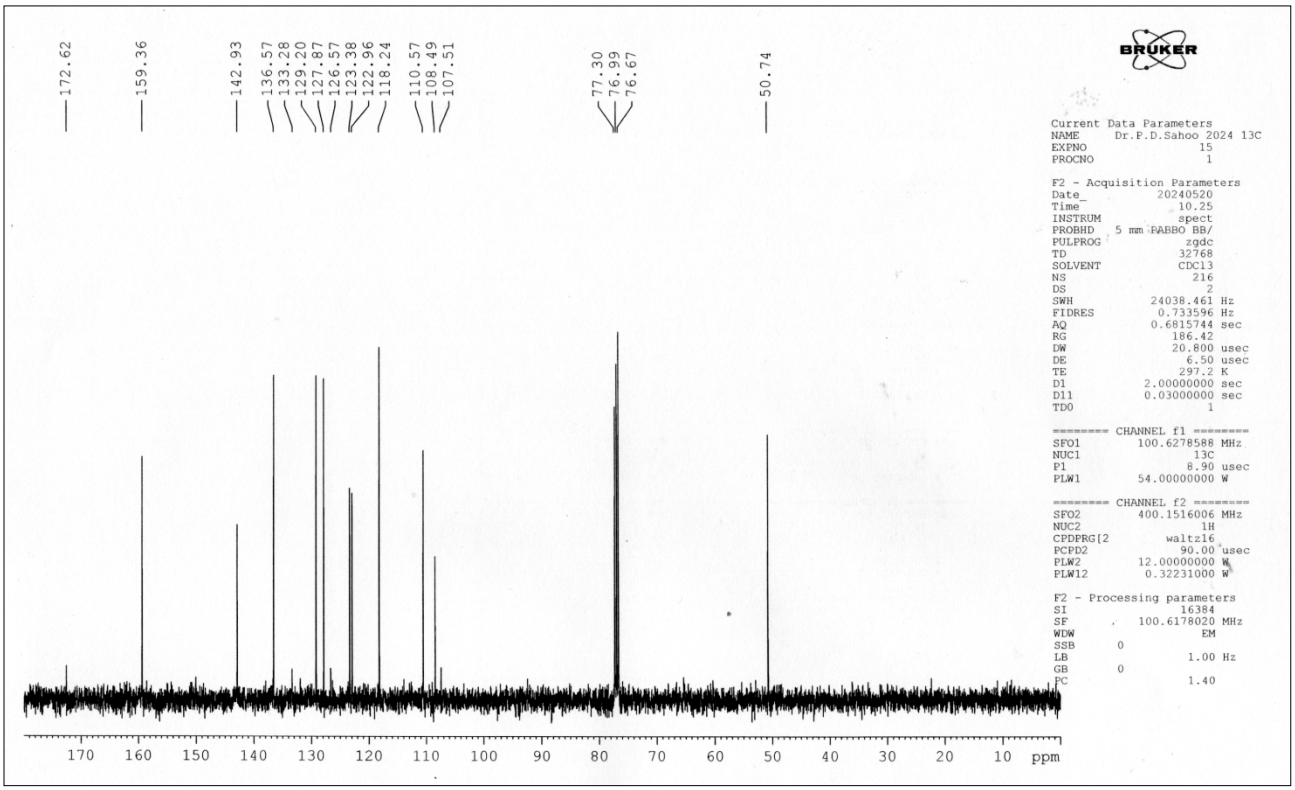


Figure S29. ^{13}C NMR of **N10** in DMSO-d_6 (100 MHz).

13. NMR tritration of N10

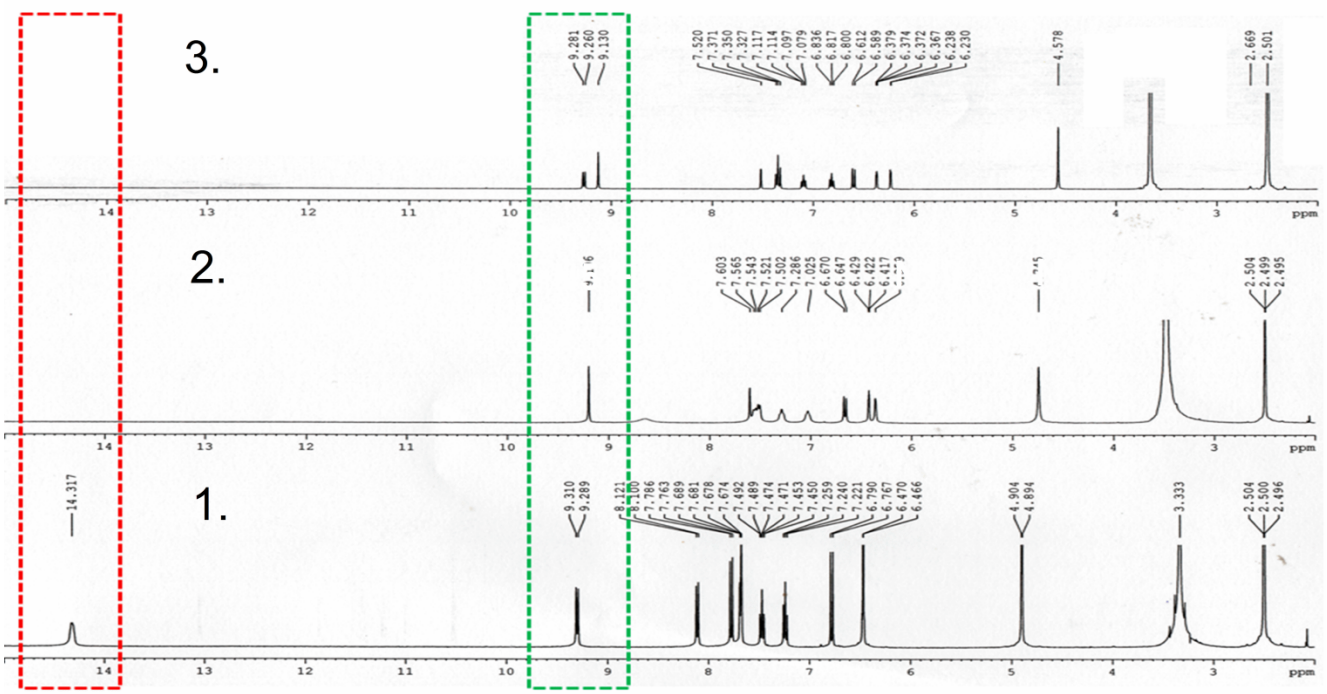


Figure S30. ^{1}H NMR titration [400 MHz] of N10 in DMSO-d_6 at 25 °C and the corresponding changes after the addition of Na_2S in D_2O from (1) only N10, (2) N10 + 1.5 equivalent, (2) N10 + 2 equivalent of Na_2S.

12. Top view of energy optimized geometry:

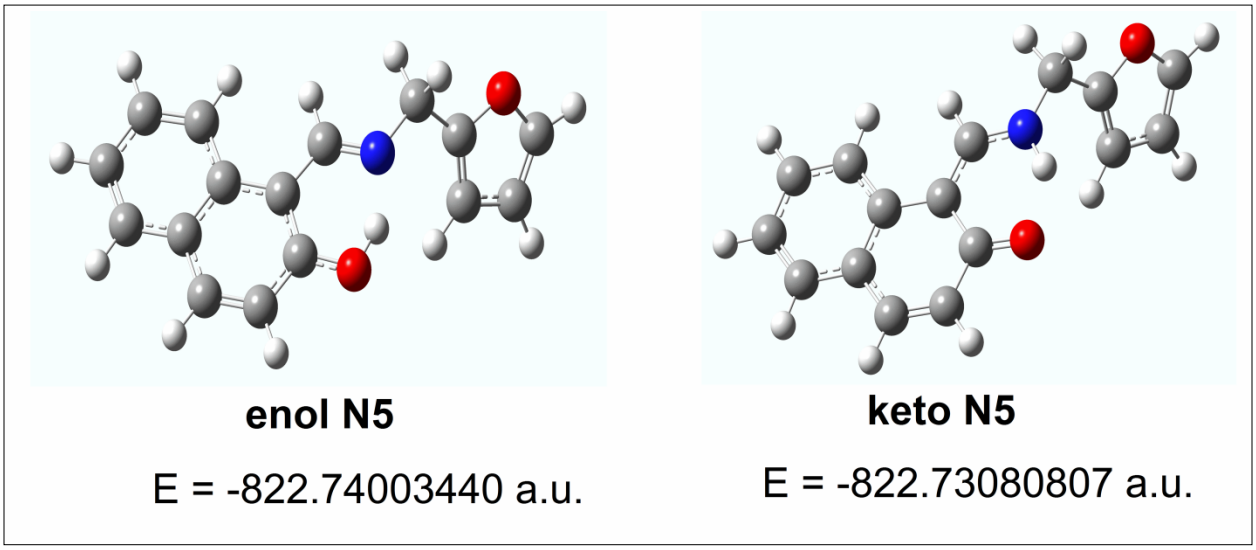


Figure S31. Optimized structures of enol-N10 and keto-N10 moiety with their corresponding energies.

13. Calculation of limit of detection (LOD) of N10 with H_2S:

The detection limit of the chemosensor **N10** for **H_2S** was calculated on the basis of fluorescence titration. To determine the standard deviation for the fluorescence intensity, the fluorescence intensity of four individual receptors without **H_2S** was measured by 10 times and the standard deviation of blank measurements was calculated.

The limit of detection (LOD) of **N10** for sensing **H_2S** was determined from the following equation[2-3]:

$$LOD = K \times SD/S$$

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank receptor solution; S is the slope of the calibration curve.

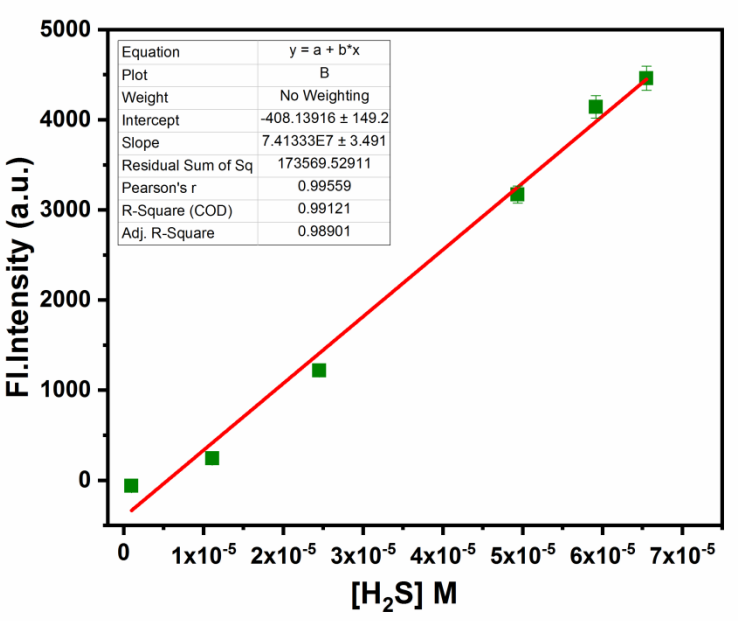


Figure S32. Linear fit curve of **N10** at 461 nm with respect to **H_2S** concentration

For **N10** with **H_2S:**

From the linear fit graph, we get slope = 7.41333×10^7, and SD value is 0.46724.

Thus, using the above formula, we get the Limit of Detection = 0.18×10^{-7} M. Therefore **N10** can detect **H_2S** up to this concentration by fluorescence technique.