

Electronic Supporting Information

Molecular Trafficking Based on Latch Circuit

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- S23** ^{13}C NMR Spectrum of **3**.

General experimental procedures:

All reagents were purchased from Aldrich and were used without further purification. AR grade THF was used for analytical studies. The fluorescence spectra were recorded with Shimadzu RF 5301 PC spectrofluorimeter. ¹H and ¹³C NMR spectra were recorded with JEOL-FT NMR-AL 300 spectrometer using CDCl₃ or CD₃CN as the solvent and TMS as internal standards. Data are reported as follows: chemical shifts in ppm (δ), multiplicity (s = singlet, d = doublet, br. = broad singlet, m = multiplet), coupling constants J [Hz], integration and interpretation. Silica gel 60 (60–120 mesh) was used for column chromatography. Perchlorates salts of all the metal ions and tertabutyl ammonium salts of all the anions were used for analytical studies. Universal buffer was prepared in millipore water (50 ml of a solution 0.1M in citric acid, (21. 01 g/1); 0.1 M in KH₂PO₄, (13.61 g/1); 0.1M in sodium tetraborate, (19.07 g/1); 0.1 M Tris, (12 .11 g/1); 0.1 M KCl, (7 .46 g/1); to which is added x ml 0.4M HCl or 0.4M NaOH, followed by dilution to 200 ml).

Synthesis of 3.

Dansyl chloride **2** (82.2 mg, 0.31 mmol) was added drop wise to the stirred solution of diamine **1** (100 mg, 0.12 mmol) and Et₃N (61 mg, 0.6 mmol) in 50ml dry dichloromethane. The reaction was stirred at room temperature for 6h. After the completion of reaction, the reaction mixture was washed with water. The organic layer was separated, dried over anhydrous sodium sulphate and distilled under reduced pressure to give a crude residue. The pure compound **3** was obtained in 44% yield after column Chromatography on silica gel (ethyl acetate); mp, 190°C; IR ν_{max} (KBr pellet, cm⁻¹) 3310 cm⁻¹ (N-H stretching); ¹H NMR (300 MHz, CDCl₃): δ = 0.86 -1.08 (m, 6H, CH₃), 0.92 (s, 18H, C(CH₃)₃), 1.14 (s, 9H, C(CH₃)₃), 1.28 (s, 9H, C(CH₃)₃), 1.23 - 1.43 (m, 4H, CH₂), 2.86 (s, 6H, NCH₃), 3.38 (d, J =18, 2H, Ar-CH₂-Ar), 3.46 - 3.53 (4H, m, NCH₂), 3.56-3.61(4H, m, Ar-CH₂-Ar), 3.66 - 3.74 (8H, m, OCH₂), 3.90 (d, J =18, 2H, Ar-CH₂-Ar), 6.49 (2H, d, J = 2.4 Hz, Ar-H), 6.63 (2H, d, J = 2.1 Hz , Ar-H), 6.96 (2H, s, Ar-H), 7.06 (2H, s, Ar-H), 7.17 (d, J = 9 Hz, 4H, Ar-H), 7.43-7.58 (m, 4H, Ar-H), 8.20- 8.25 (m, 2H, Ar-H), 8.37-8.54 (m, 2H, ArH); ¹³C NMR(300 MHz, CDCl₃): δ 10.75 [CH₃], δ 24.06 [CH₂], δ 30.95 [CH₃], δ 31.52 [CH₃], δ 31.73 [C], δ 32.0 [C], δ 33.81 [CH₂], δ 34.18 [CH₂], δ 38.19 [CH₂], 124.70 [Ar-C], δ 125.0 [Ar-C], δ 125.19 [Ar-C], δ 125.28 [Ar-C], δ 125.68 [Ar-C], δ 126.43 [Ar-C], δ 126.83 [Ar-C] , δ 127.85 [Ar-C], δ 128.91 [Ar-C], δ 130.02 [Ar-C], δ 131.34 [Ar-C], δ 131.87 [Ar-C], δ 132.41 [Ar-C], δ 133.29 [Ar-C], δ 135.90 [Ar-C], δ 143.54 [Ar-C], δ 153.66 [Ar-C]; FAB-MS: *m/z* 1282 (M-2)⁺; Anal cal. for C₇₈H₁₀N₄S₂O₈; C, 72.84 %; H, 7.78 %; N, 4.35% , Found: C, 72.20%; H, 7.75 %; N, 4.57%.

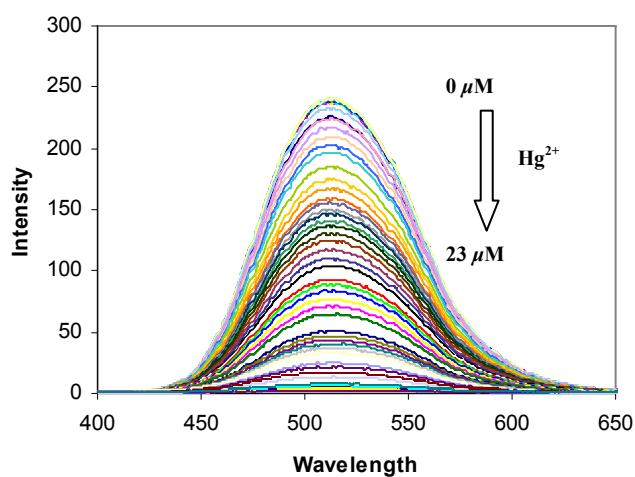


Figure S1. Fluorescence spectra of **3** (1 μM) in response to the presence of Hg^{2+} ions (23 μM) in THF:H₂O (9:1, v/v) buffered with universal buffer; pH = 7.0; $\lambda = 338$ nm.

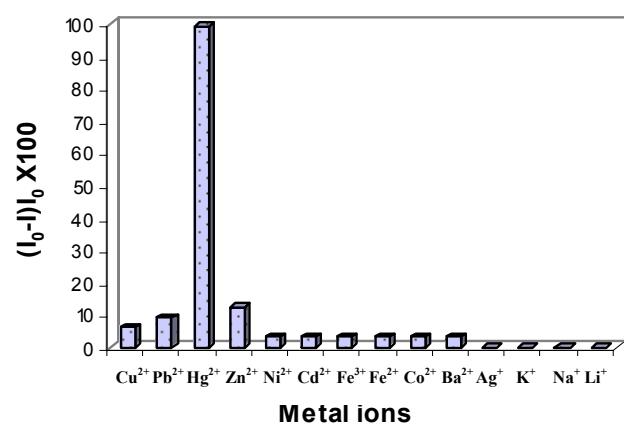


Figure S2. Fluorescence intensity changes $[(I_0 - I)/I_0 \times 100]$ of **3** (1 μ M) in THF:H₂O (9:1, v/v) upon addition of 23 μ M of various metal perchlorates. The excitation wavelength was 338 nm. I_0 is the fluorescence intensity at 515 nm of free host and I is the fluorescence intensity after adding metal ions.

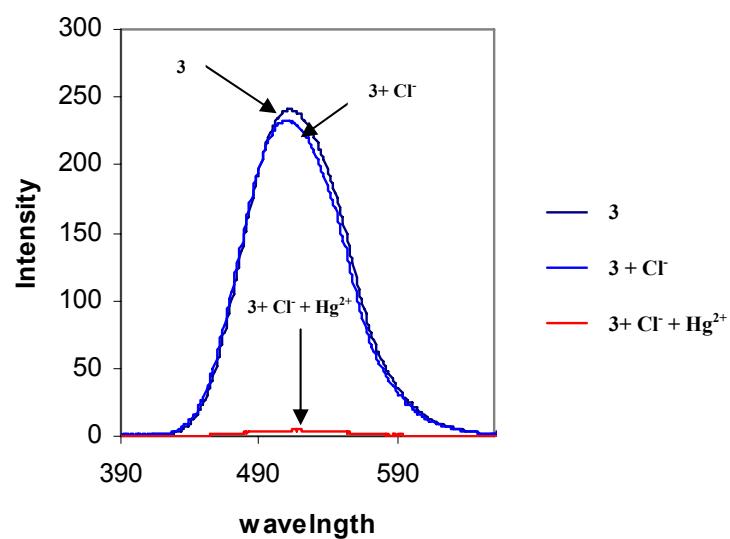


Figure S3. Fluorescence emission spectra of (a) **3**; (c) **3+ Cl⁻** (b) **3+ Cl⁻ + Hg²⁺** in THF:H₂O (9:1,v/v) buffered with Universal Buffer, pH = 7 ; λ = 338 nm.

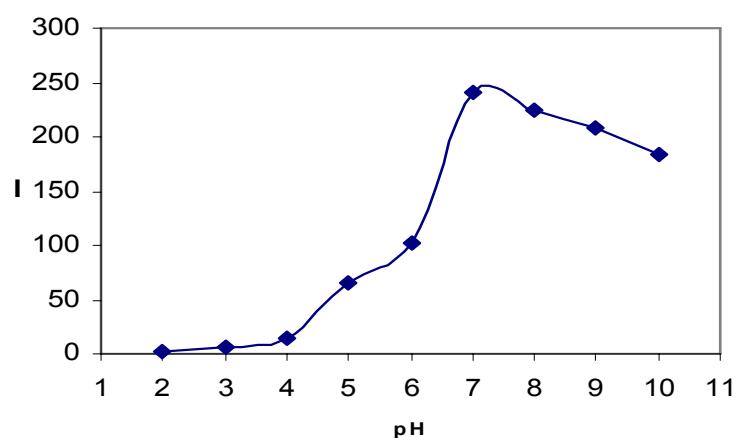


Figure S4. Fluorescence Intensity plot of **3** at different pH in THF: H₂O (9:1).

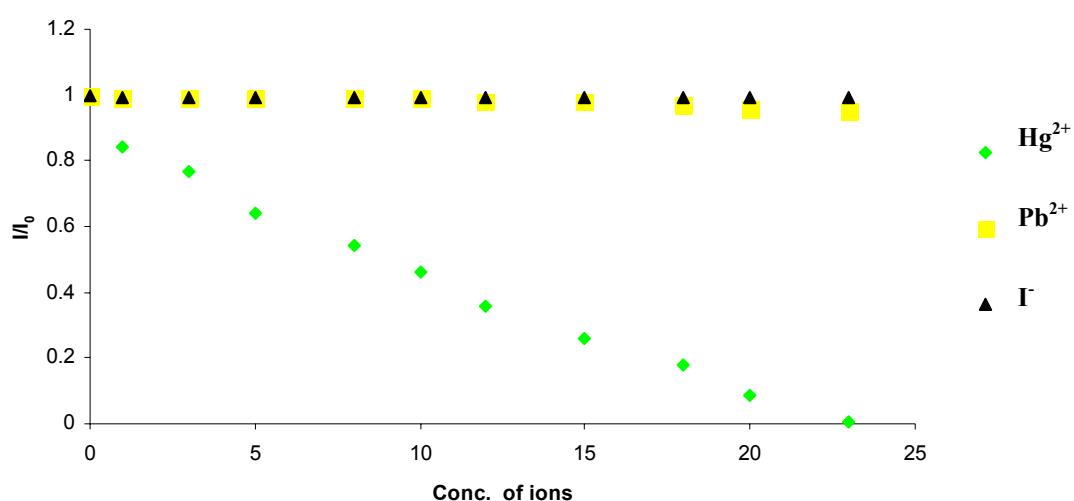


Figure S5. Titration plot of **3** with Hg^{2+} , Pb^{2+} and I^- . Normalized fluorescence intensity of **3** vs ion conc.

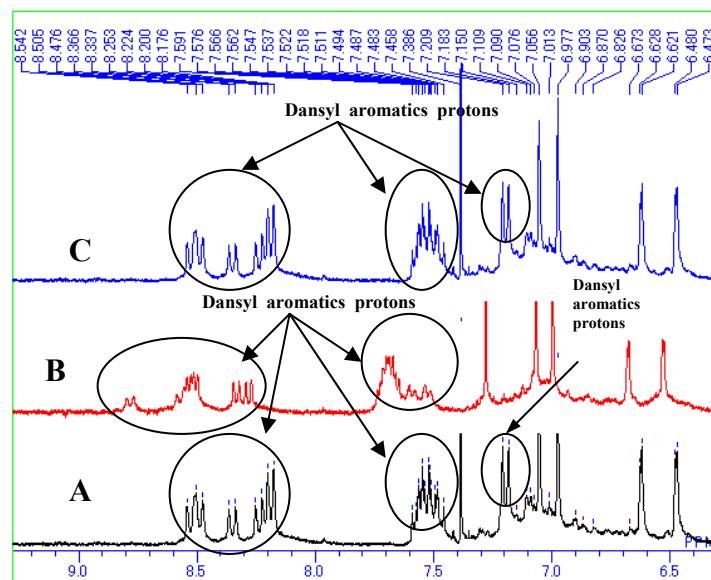


Figure S6. ¹H NMR of (A) 3; (B) 3 + 2. equiv Hg²⁺ ions; (C) 3 + 2. equiv Hg²⁺ ions + 4 equiv. Cl⁻ ions in CDCl₃: CD₃CN (8:2).

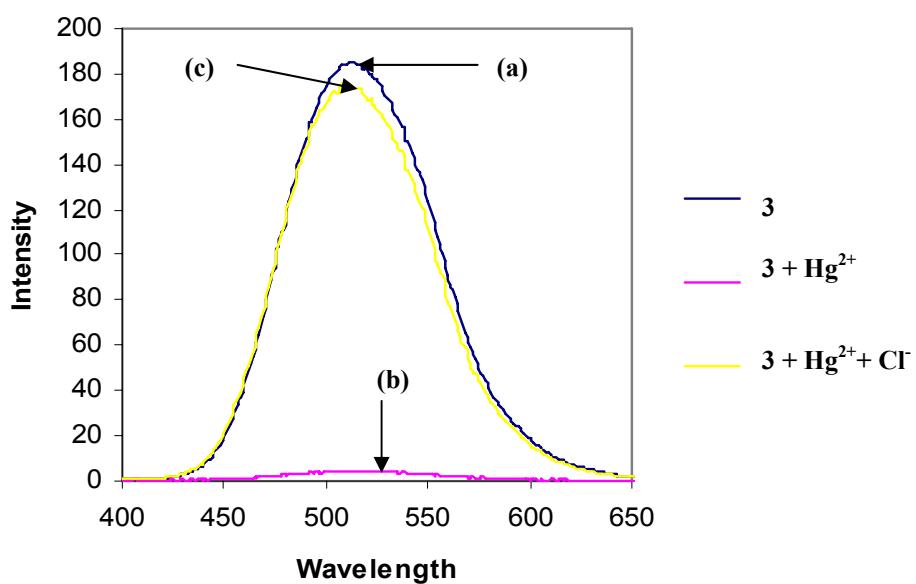


Figure S7. Fluorescence emission spectra of (a) **3**; (b) **$3 + \text{Hg}^{2+}$** ; (c) **$3 + \text{Hg}^{2+} + \text{Cl}^-$** in THF:H₂O (9:1,v/v) buffered with Universal Buffer, pH = 10 ; $\lambda = 338$ nm.

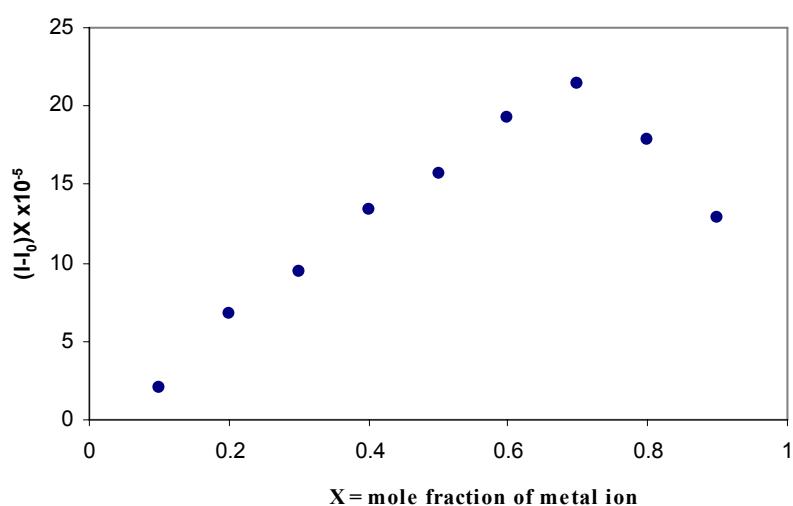


Figure S8. Job's plot of **3** toward Hg^{2+} ions.

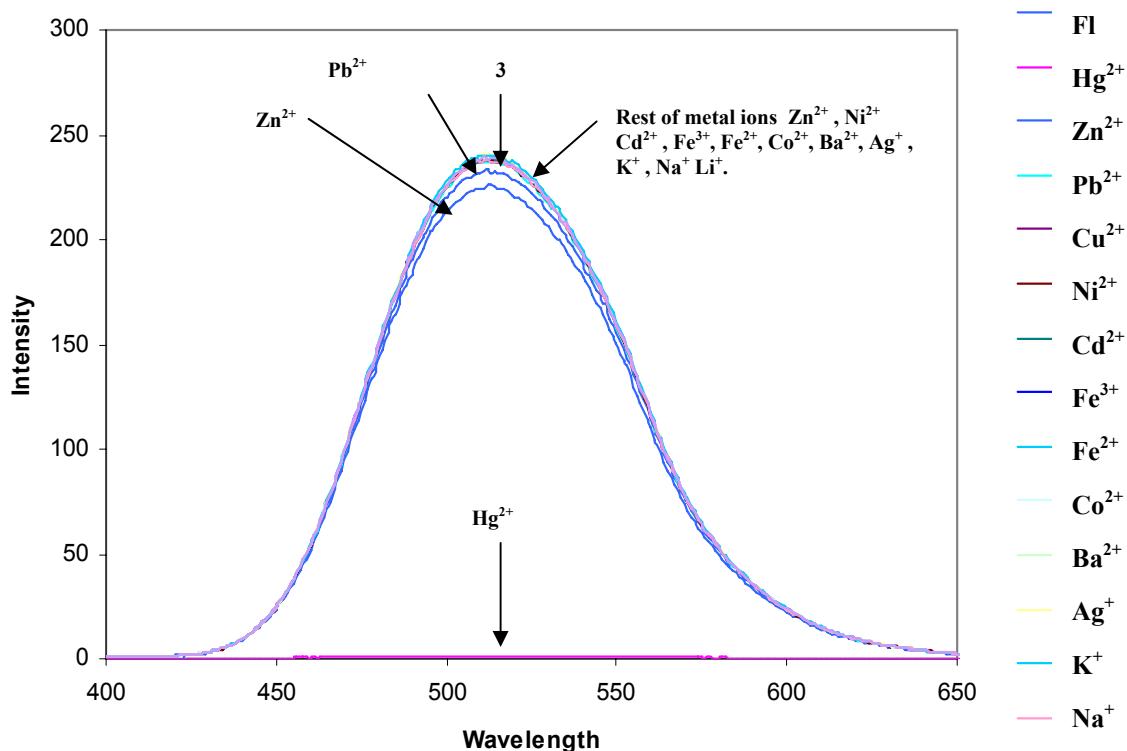


Figure S9. Fluorescence Spectra of **3** in the presence of various metal ions in THF:H₂O (9:1, v/v) buffered with Universal Buffer, pH = 7.0; $\lambda = 338$ nm.

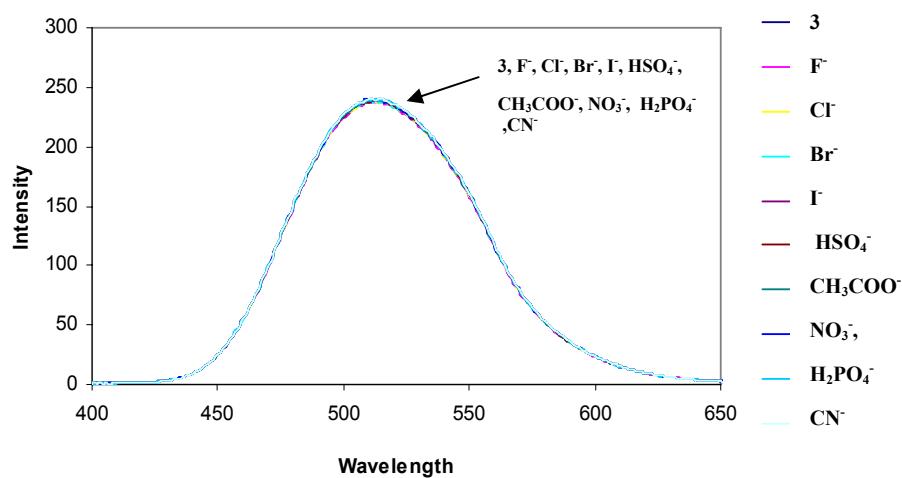


Figure S10 Fluorescence Spectra of **3** in the presence of various anions in THF:H₂O (9:1, v/v) buffered with Universal Buffer, pH = 7.0; $\lambda = 338$ nm.

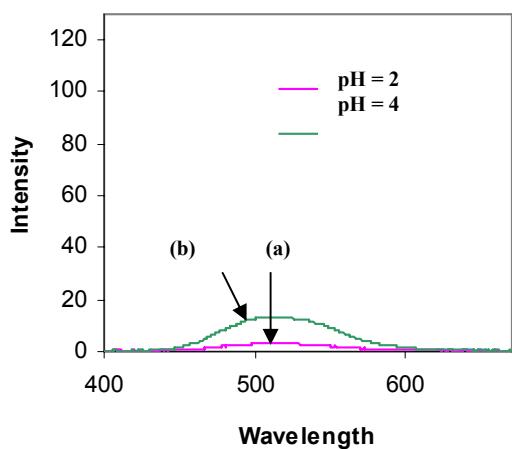


Figure S11. Fluorescence emission spectra of **3** at (a) pH value 2; (b) pH value 4 in THF:H₂O (9:1,v/v) buffered with Universal Buffer; $\lambda = 338$ nm.

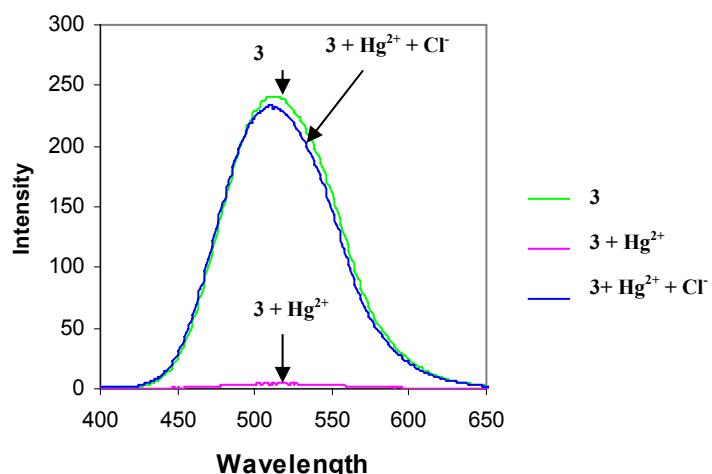


Figure S12. Fluorescence emission spectra of (a) 3; (b) 3 + Hg²⁺; (c) 3+ Hg²⁺ + Cl⁻ in THF:H₂O (9:1,v/v) buffered with Universal Buffer; pH = 7.0; λ = 338 nm.

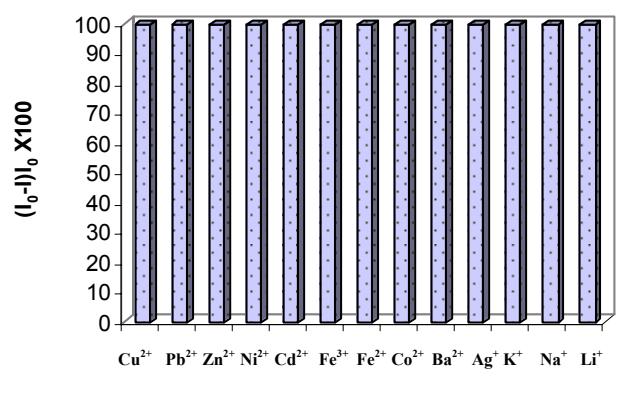


Figure S13. Fluorescence response of **3** ($1\ \mu\text{M}$) to Hg^{2+} ($23\ \mu\text{M}$) over other selected metal ($100\ \mu\text{M}$) ions.

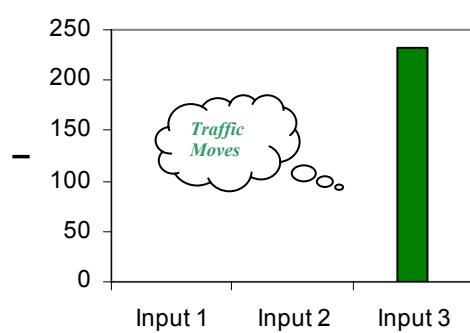


Figure 14. On addition of input 3 [$\text{Cl}^-/\text{Br}^-/\text{I}^-$ (green color)] to the solution of **3** the fluorescence emission remains ‘ON’ (*traffic movement on*); **I** is the fluorescence emission after addition of input 3 $\text{Cl}^-/\text{Br}^-/\text{I}^-$.

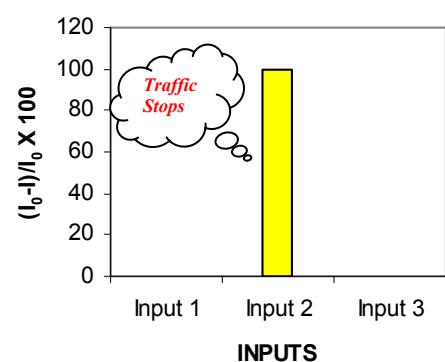


Figure 15. On addition of input 2 [Hg^{2+} ions (yellow color)] the fluorescence emission of **3** gets quenched (*traffic movement off*); I_0 is the fluorescence emission at 515 nm of free host and I is the fluorescence emission after adding Hg^{2+} ions.

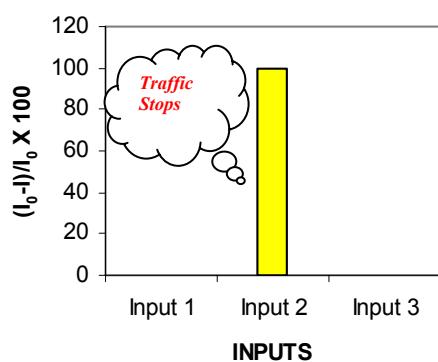


Figure 16. On addition of input 2 [Hg^{2+} ions (yellow color)] to the solution of **3** containing input 3 ($\text{Cl}^-/\text{Br}^-/\text{I}^-$), fluorescence emission gets quenched (*traffic movement off*); I_0 is the fluorescence intensity at 515 nm of free host and I is the fluorescence emission after adding Hg^{2+} ions.

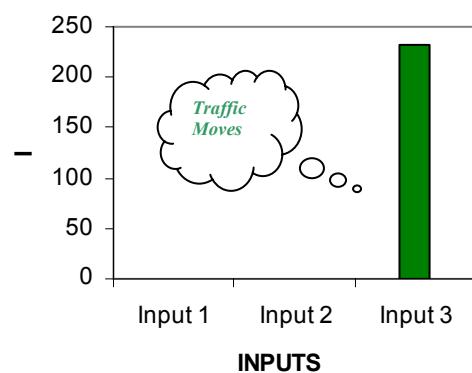


Figure 17. On addition of input 3 $[\text{Cl}^-/\text{Br}^-/\text{I}^-$ (green color)] to 3Hg^{2+} complex the fluorescence emission is restored and gets ‘ON’ (*traffic movement on*); **I** is the fluorescence emission after addition of input 3 $\text{Cl}^-/\text{Br}^-/\text{I}^-$.

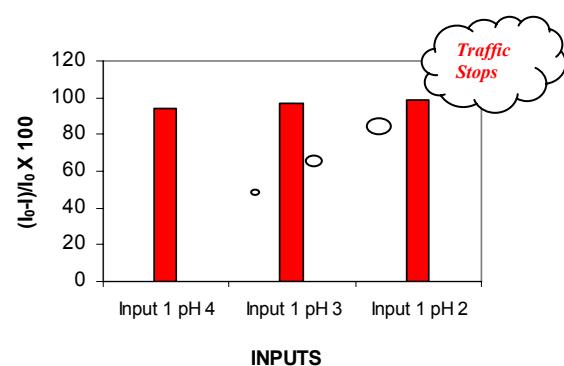
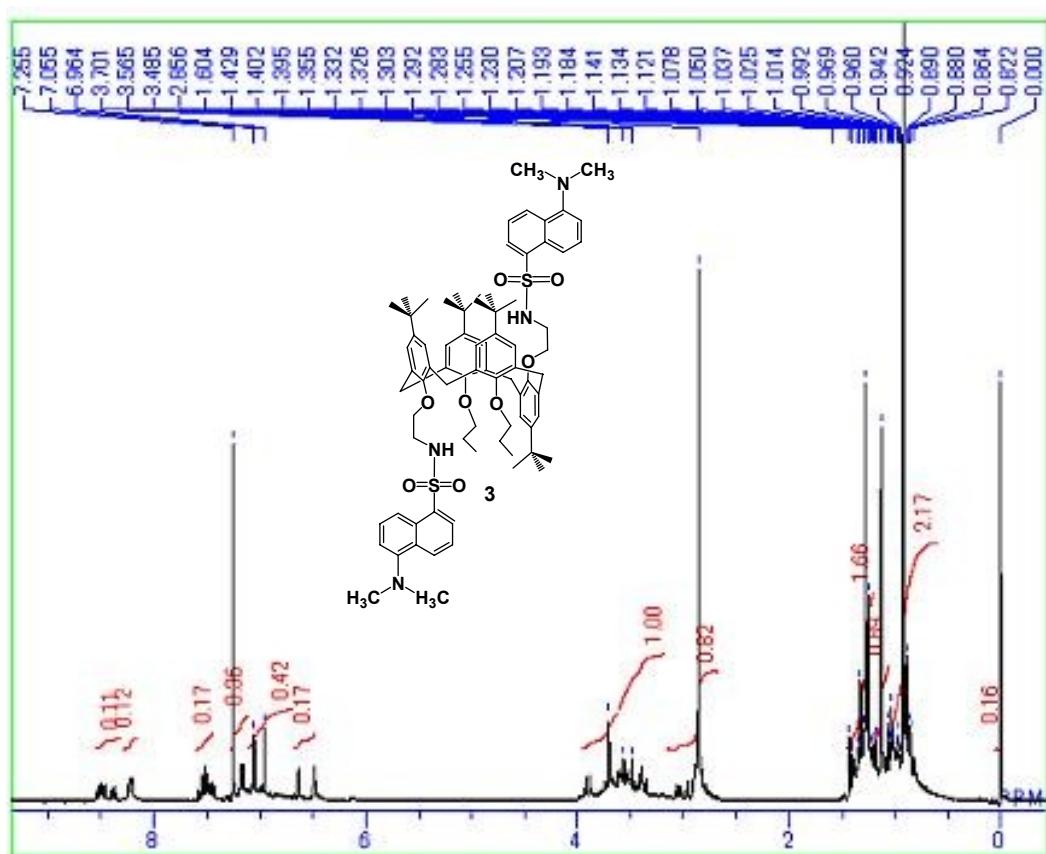
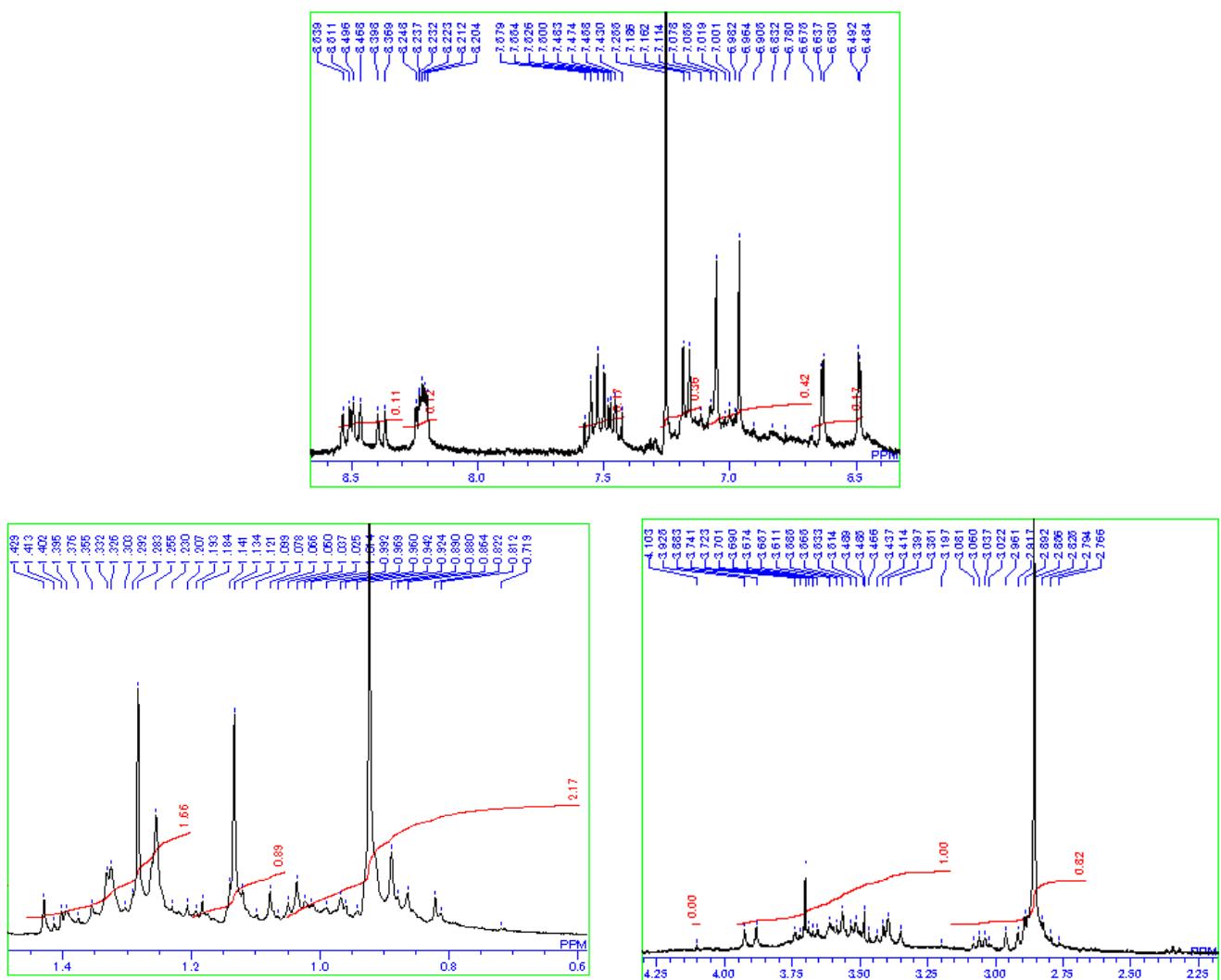


Figure 18. On $\text{pH} \leq$ (red signal) the fluorescence intensity is quenched (*traffic movement off*); I_0 is the fluorescence intensity at 515 nm of free host and I is the fluorescence emission after adding Hg^{2+} ions.

¹H NMR Spectrum of 3



Expanded ^1H NMR Spectrum of **3**



¹³C NMR Spectrum of 3

