Rhodamine based "off-on" probe for selective detection of Hg(II) and subsequent L-Proline and 4-Hydroxyproline discrimination.

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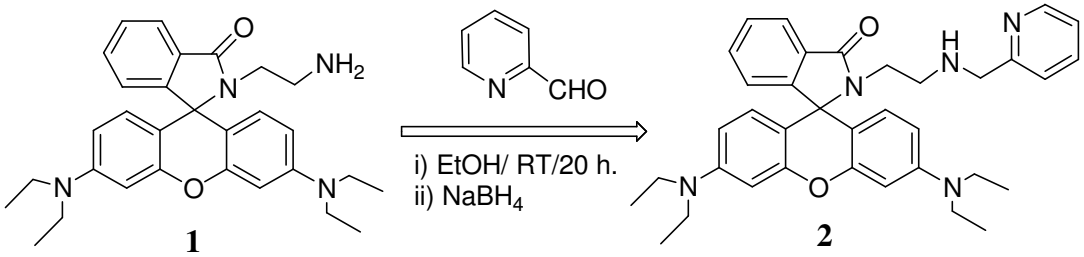
Electronic Supplementary Information

Synthesis of Probe 2



Scheme S1: Synthetic route to compound **2**

To an ethanolic solution(10 mL) of **1** (0.2325g, 0.479 mmol), Pyridine-2-carboxaldehyde (0.6mL, excess) was added and stirred at room temperature for 20 h. The Schiff base thus formed was reduced upon addition of $NaBH_4$ in portions. The reaction mixture was allowed to react for 5 h at room temperature followed by reflux for 1h to ensure complete reduction. The solvent was then evaporated to dryness under reduced pressure. Distilled water was added to the solid mass and the organic part was collected after extraction with $CHCl_3$ (3× 30 mL). Each organic layer was dried over anhydrous Na_2SO_4, filtered and the combined filtrate was evaporated under reduced pressure to get a solid mass which was purified and separated through column chromatography using neutral alumina with 1% MeOH in $CHCl_3$.

Yield: 0.233 g (84%); ESI-MS, m/z^+ (%): 576.3 $[M+1]^+$, (100%); ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS, δ): 8.453 (d, J = 3.6 Hz, 1H), 8.379 (d, J = 4.4 Hz, 2H), 7.812 (m, 2H), 7.507 (t, J = 1.2 Hz, 2H), 7.333 (dd, J_1 = 2.8 Hz, J_2 = 2.8Hz 3H), 7.146 (d, J = 7.6 Hz, 2H), 6.979 (m, 4H), 6.394 (s, 2H), 6.359 (s, 3H), 6.285 (d, J = 2.4Hz,4H), 6.135(dd, J = 2.4Hz, 3H), 3.659 (s, 4H), 3.226 (t, J = 6.8 Hz, 10H), 2.408 (t, J = 6.4 Hz, 4H), 1.051 (t, J = 6.8 Hz, 14 H); ^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C, TMS, δ): 168.75, 159.41, 153.39, 148.89, 136.53, 132.54, 131.17, 128.13, 123.91, 122.22, 121.93, 120.59, 108.21, 105.51, 97.89, 65.22, 54.48, 47.81, 44.47, 40.23, 29.81, 12.72; Anal. Calcd. for $C_{36}H_{41}N_5O_2$, %: C, 75.1, H, 7.18, N, 12.16. Found: C, 75.34, H, 7.97, N 11.73.

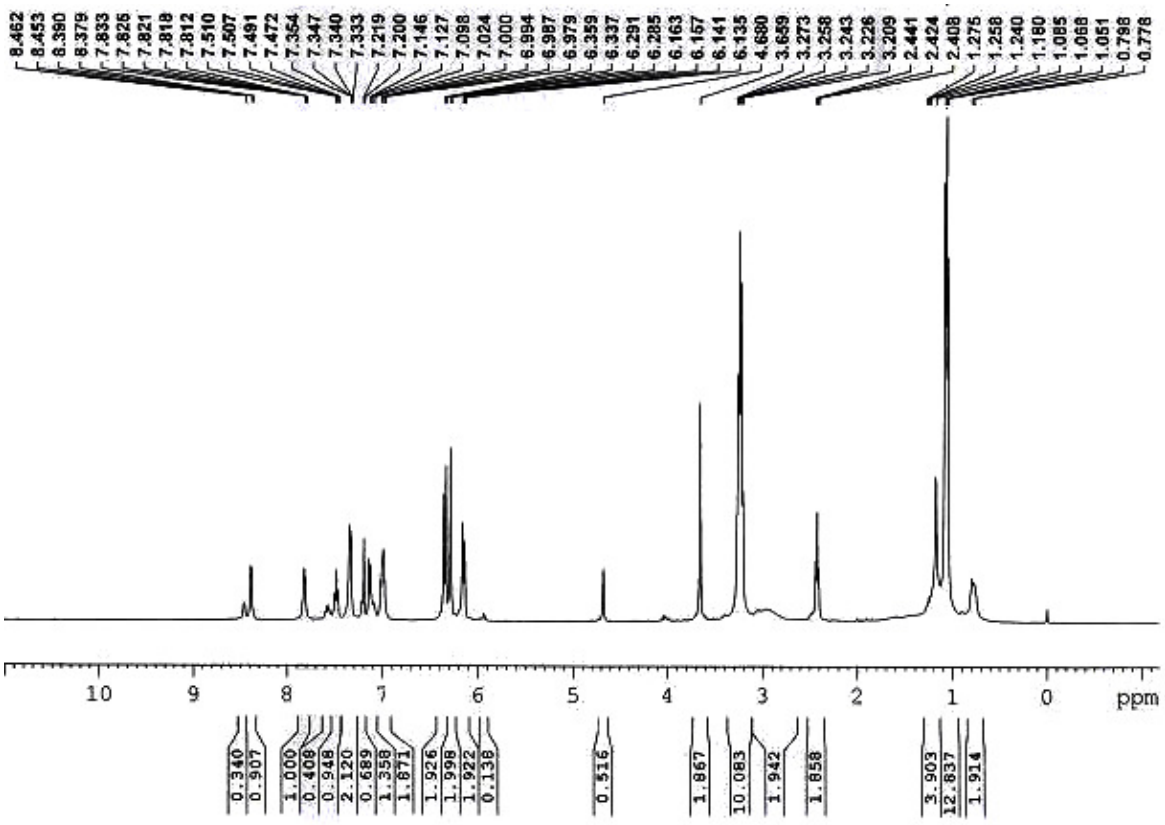


Fig. S1: ^{1}H NMR Spectrum of probe **2** in $CDCl_3$

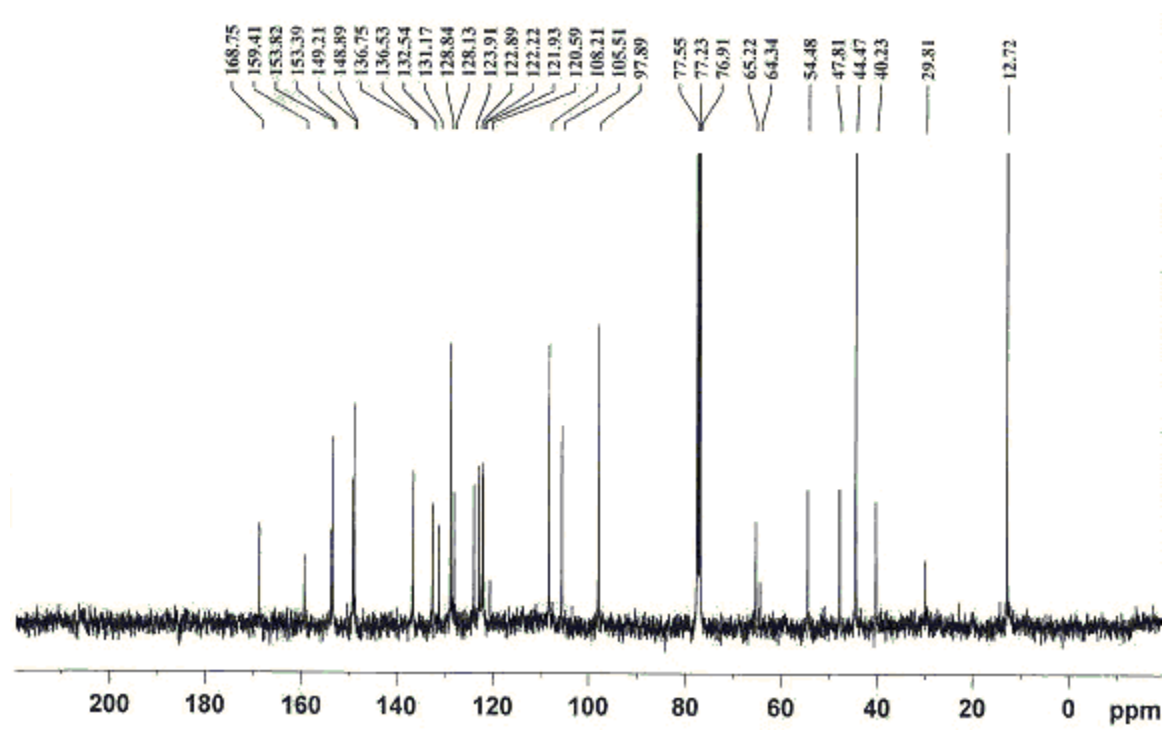


Fig. S2: ^{13}C NMR Spectrum of probe **2** in $CDCl_3$

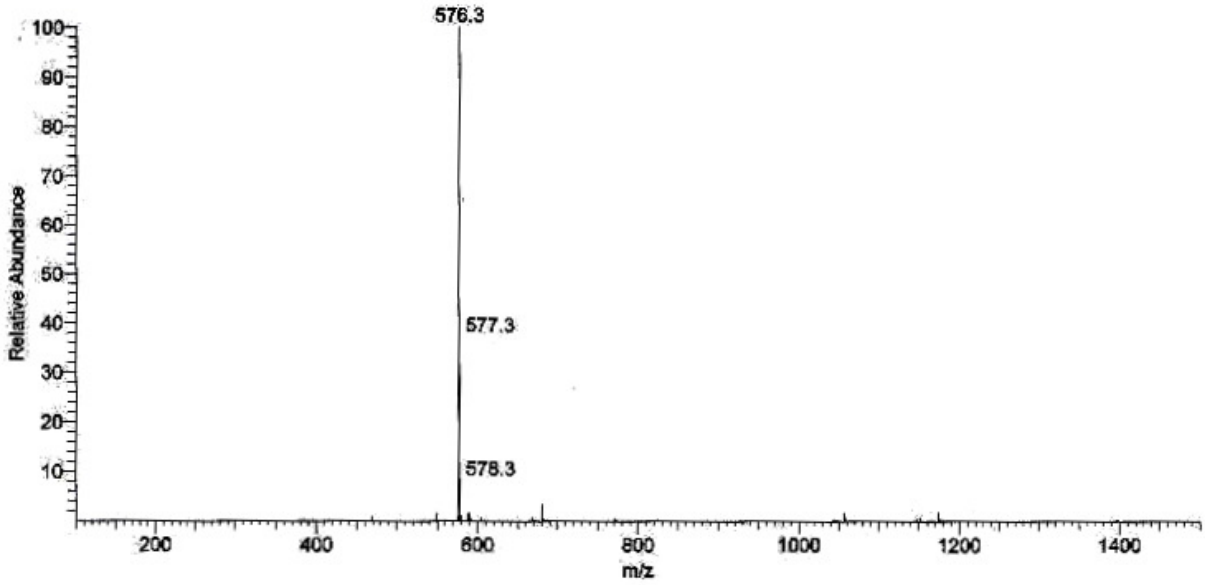


Fig. S3: ESI Mass Spectrum of probe **2**

Absorption and Emission Studies

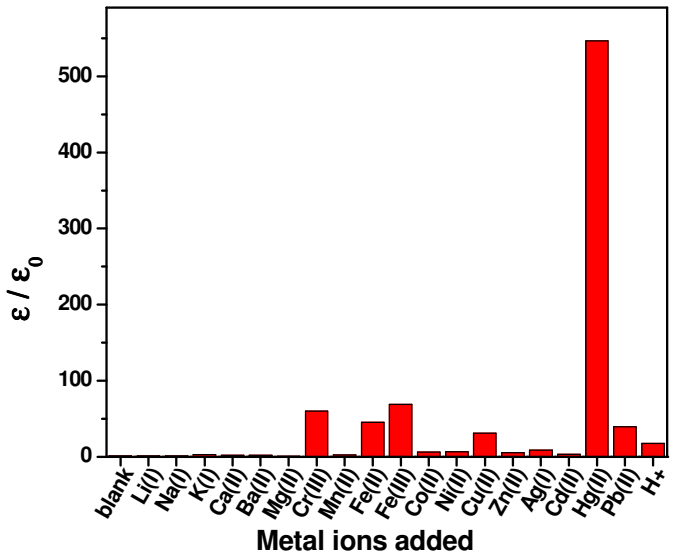


Fig. S4: Bar diagram corresponding to absorption spectral profile of **2**, before and after addition of various metal ions in MeCN-H_2O (1:1 v/v, Tris-HCl, pH 7.2). [**2**] = 1×10^{-4} M.

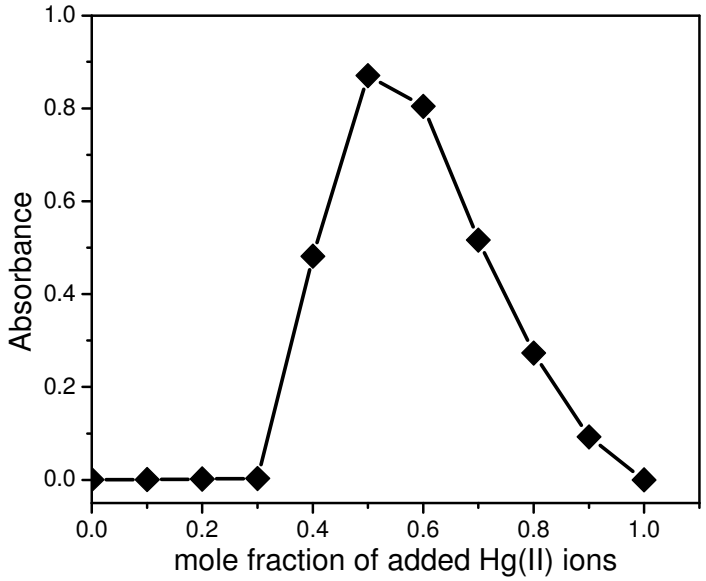


Fig. S5: Plot of absorbance of **2** observed at 558nm against mole fractions of added Hg(II) ions in MeCN-H_2O (1:1 v/v), [**2**] = 1×10^{-4}M.

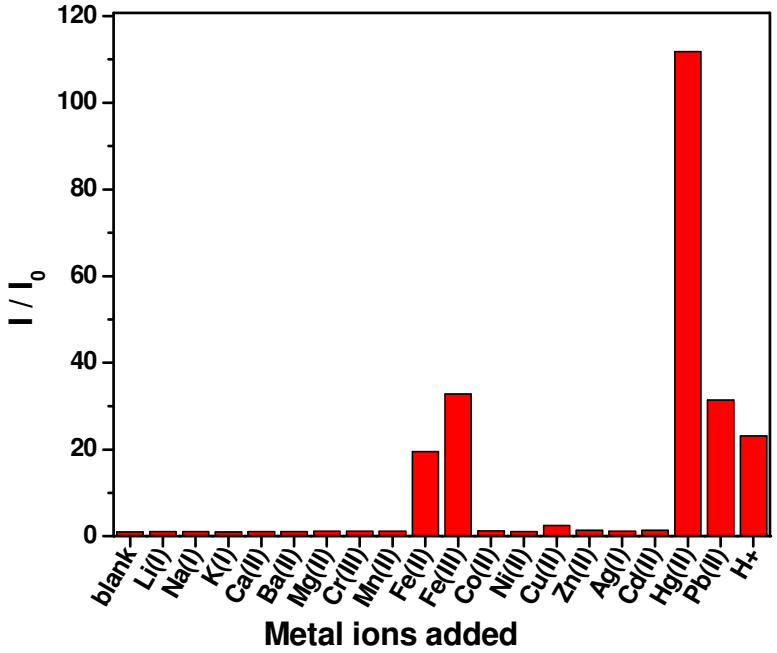


Fig. S6: Bar diagram corresponding to fluorescence of **2** before and after addition of various metal ions in MeCN-H_2O (1:1 v/v), λ_{ex} = 500 nm, ex. and em. b. p. = 5nm, RT, [**2**] = 1×10^{-6}M.

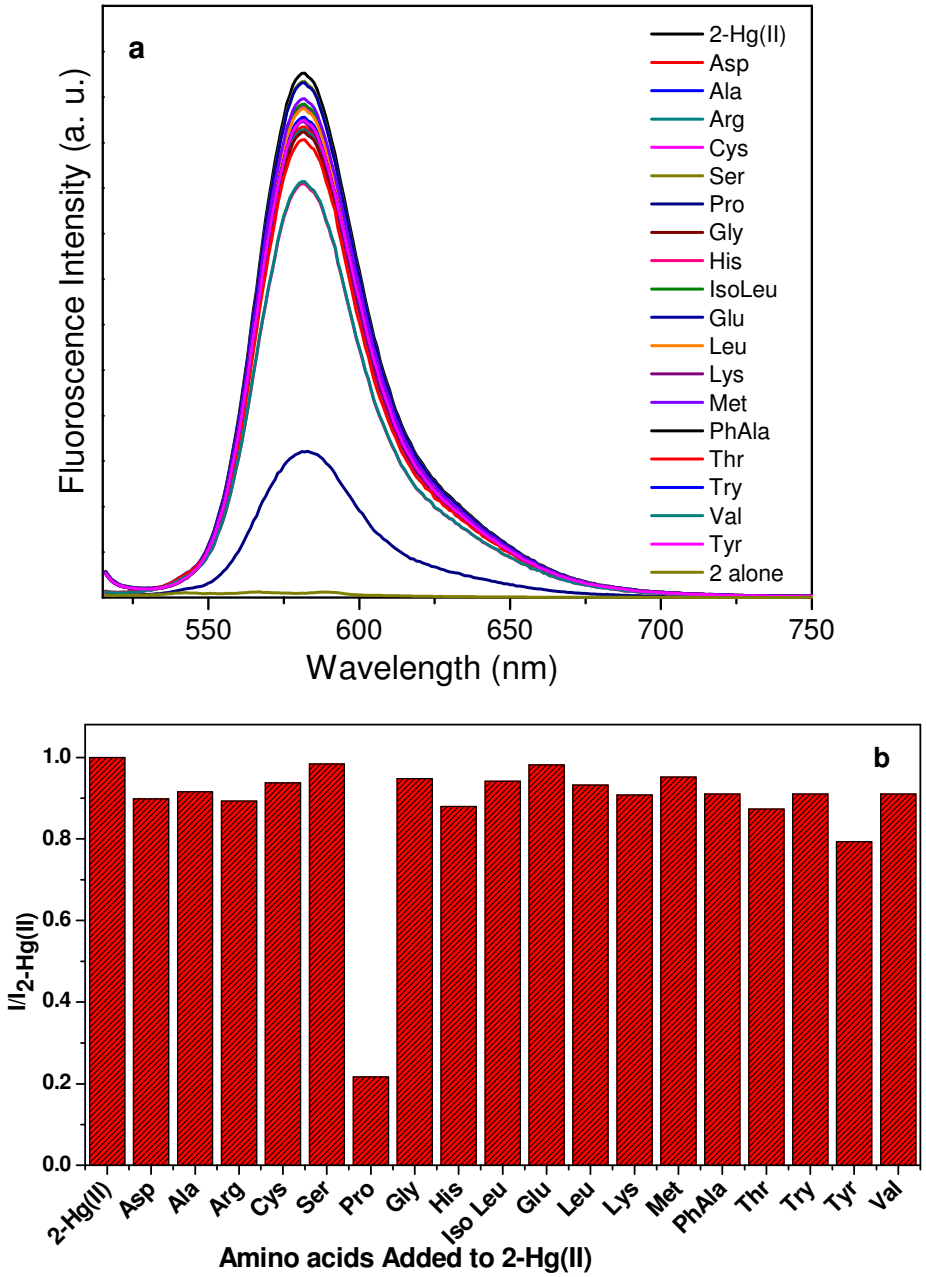


Fig. S7: (a) Fluorescence spectra of **2**-Hg(II) with addition of amino acids and (b) the corresponding bar diagram corresponding to the emission of **2**-Hg(II) + (Amino acids) at ~580 nm in MeCN-H_2O (1:1 v/v), [**2**] = 1×10^{-6}M, λ_{ex} = 500 nm, ex. and em. b. p. = 5nm, RT.

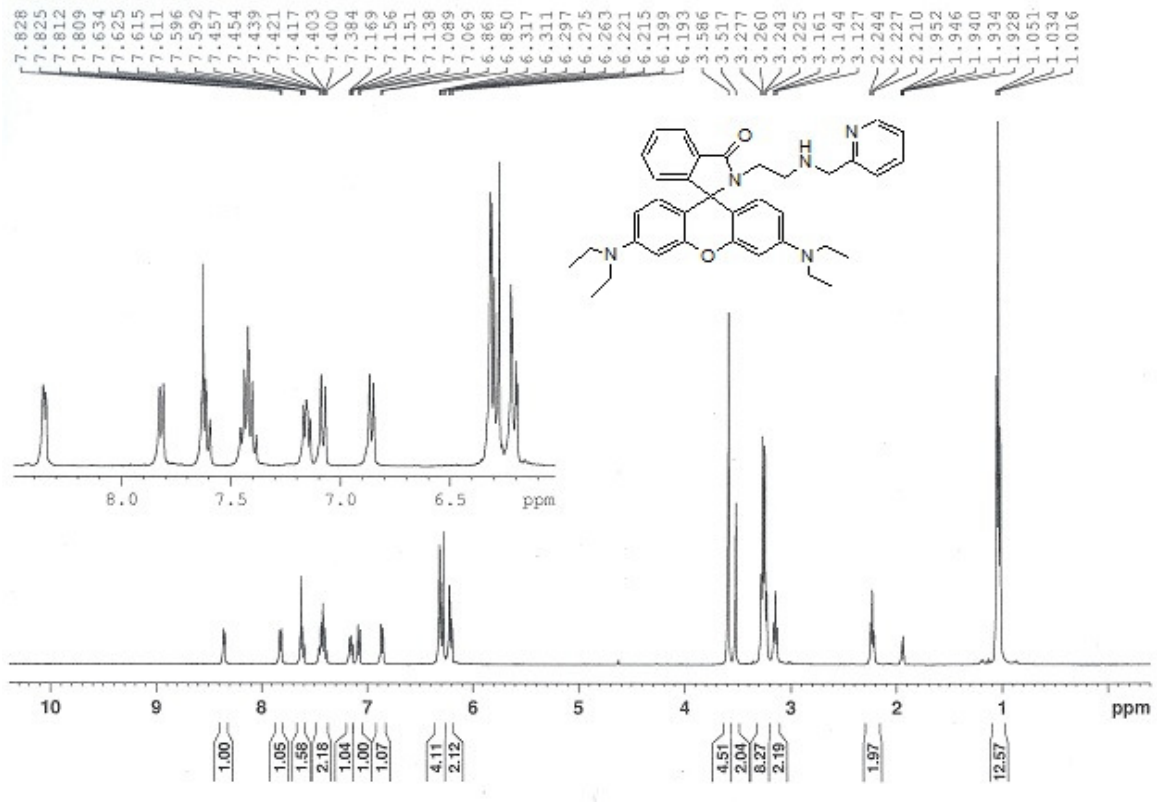


Fig. S8: ^{1}H NMR Spectrum of probe **2** in CD_3CN-D_2O (1:1 v/v).

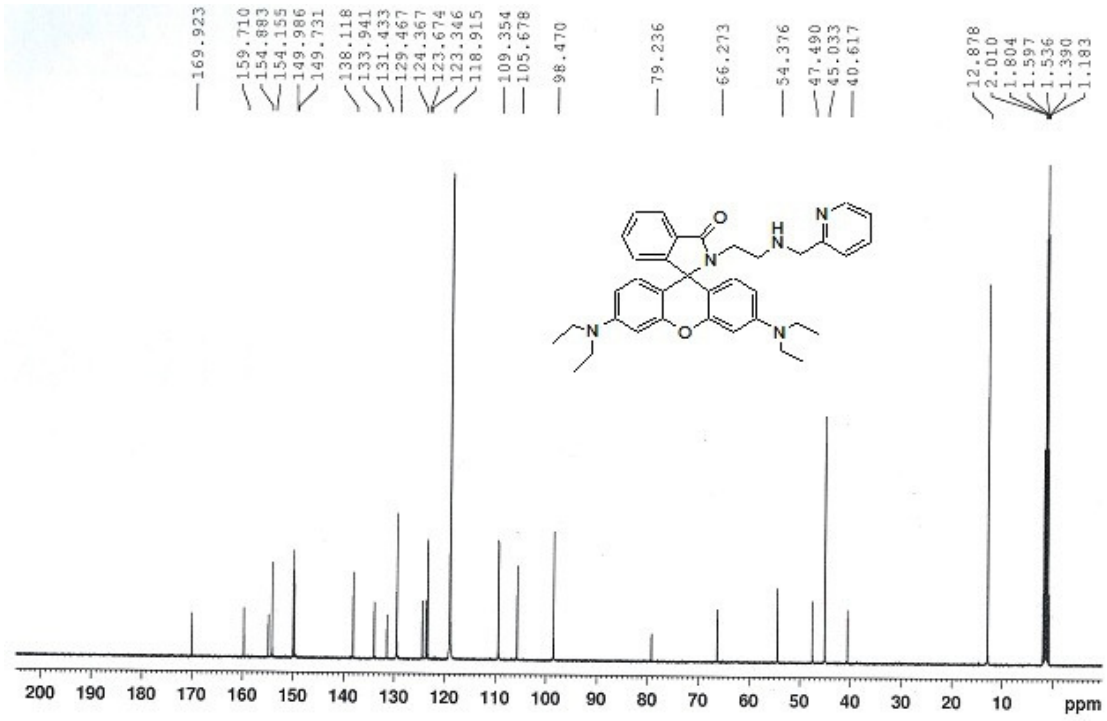


Fig. S9: ^{13}C NMR Spectrum of probe **2** in CD_3CN-D_2O (1:1 v/v).