

Electronic Supplementary Information

Incorporation of triazole into a quinoline-rhodamine conjugate imparts iron (III) selective complexation permitting detection at nano molar levels

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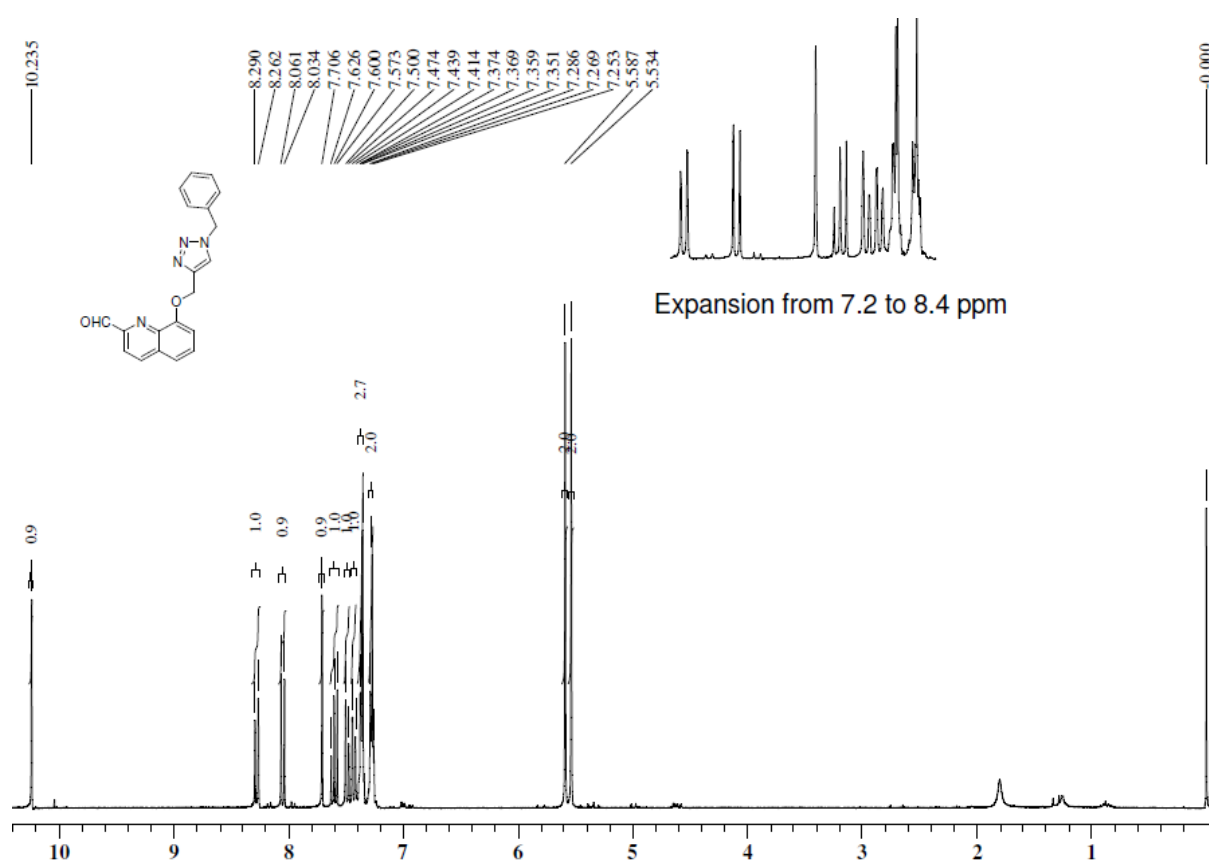


Fig. S1. ^1H NMR spectrum of C in CDCl_3

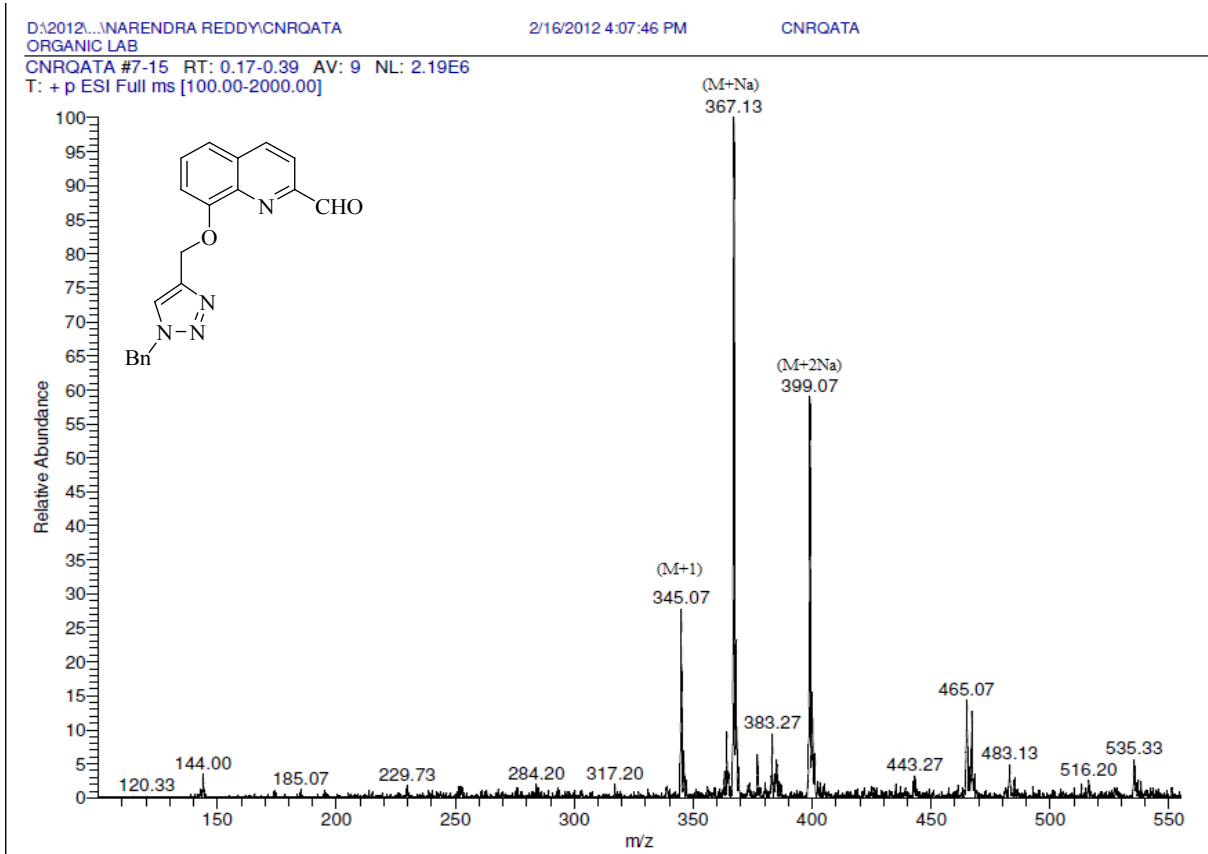


Fig. S2. ESI Mass spectrum of C

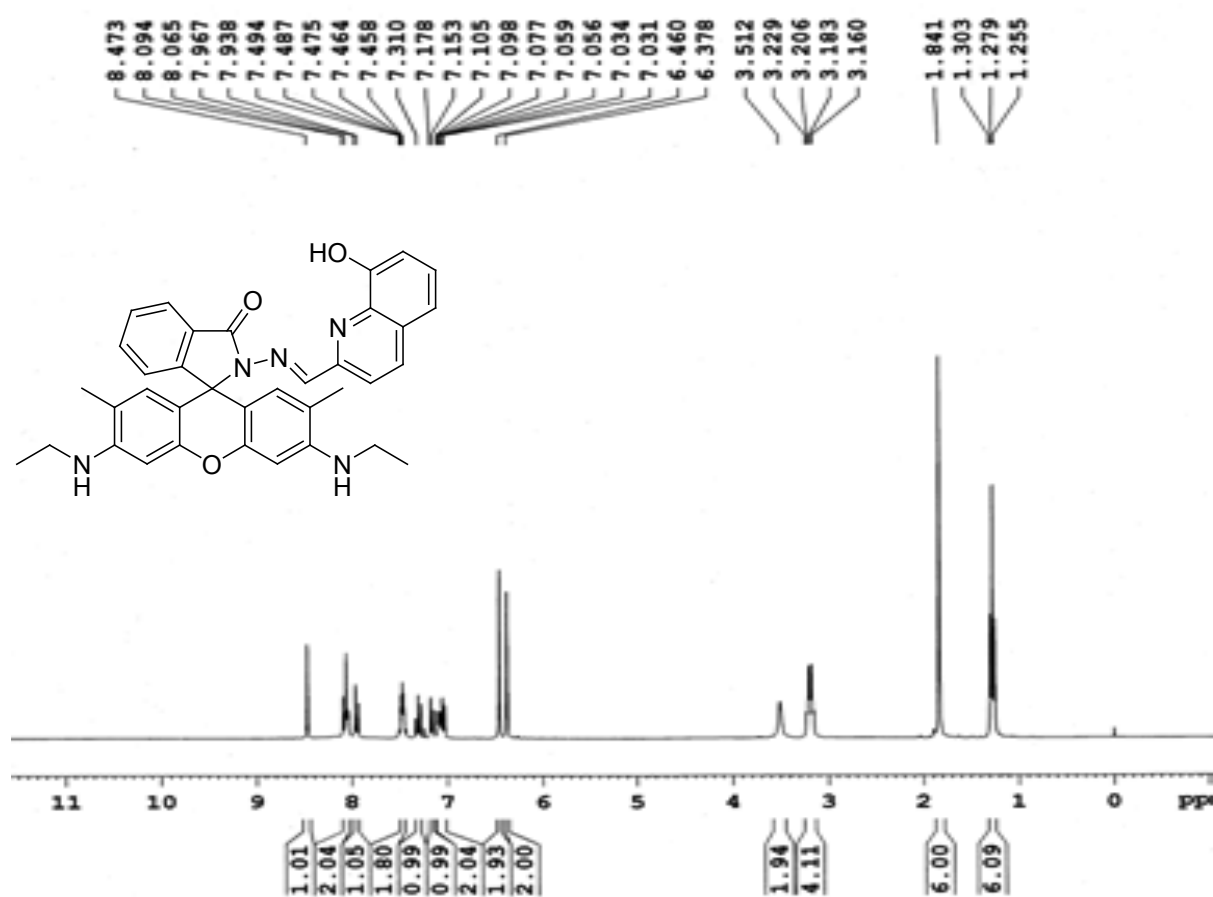


Fig. S3. ^1H NMR spectrum of **1** in CDCl_3

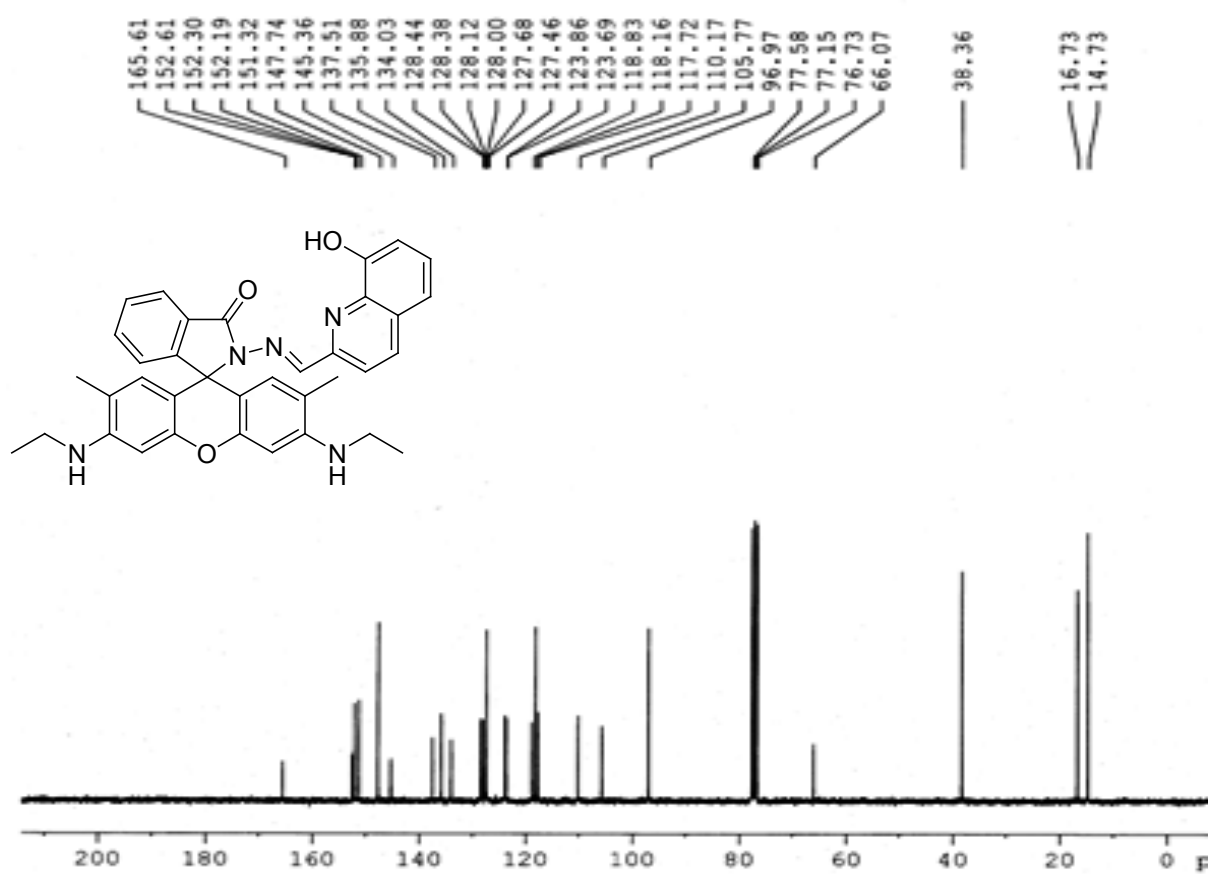


Fig. S4. ^{13}C NMR spectrum of 1 in CDCl_3

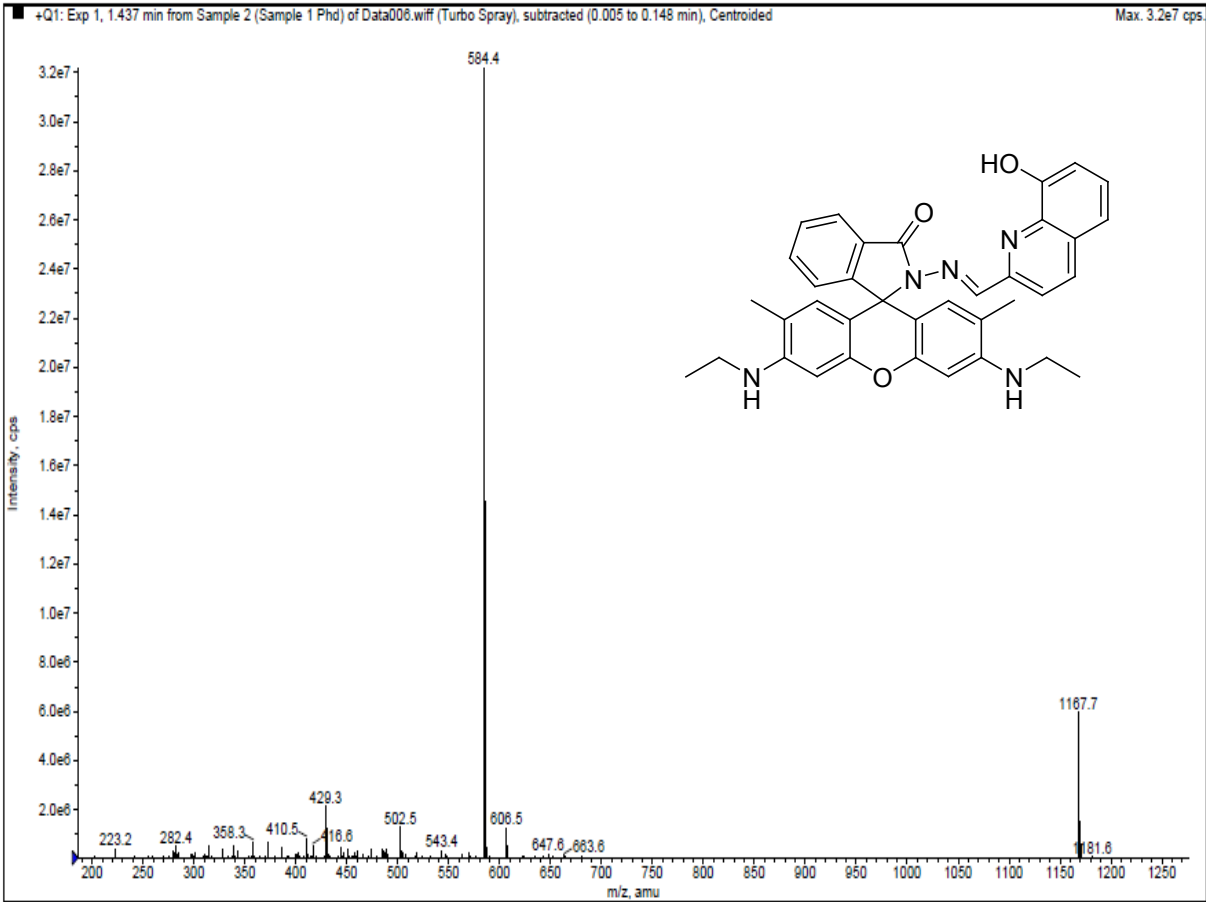


Fig. S5. ESI Mass spectrum of 1

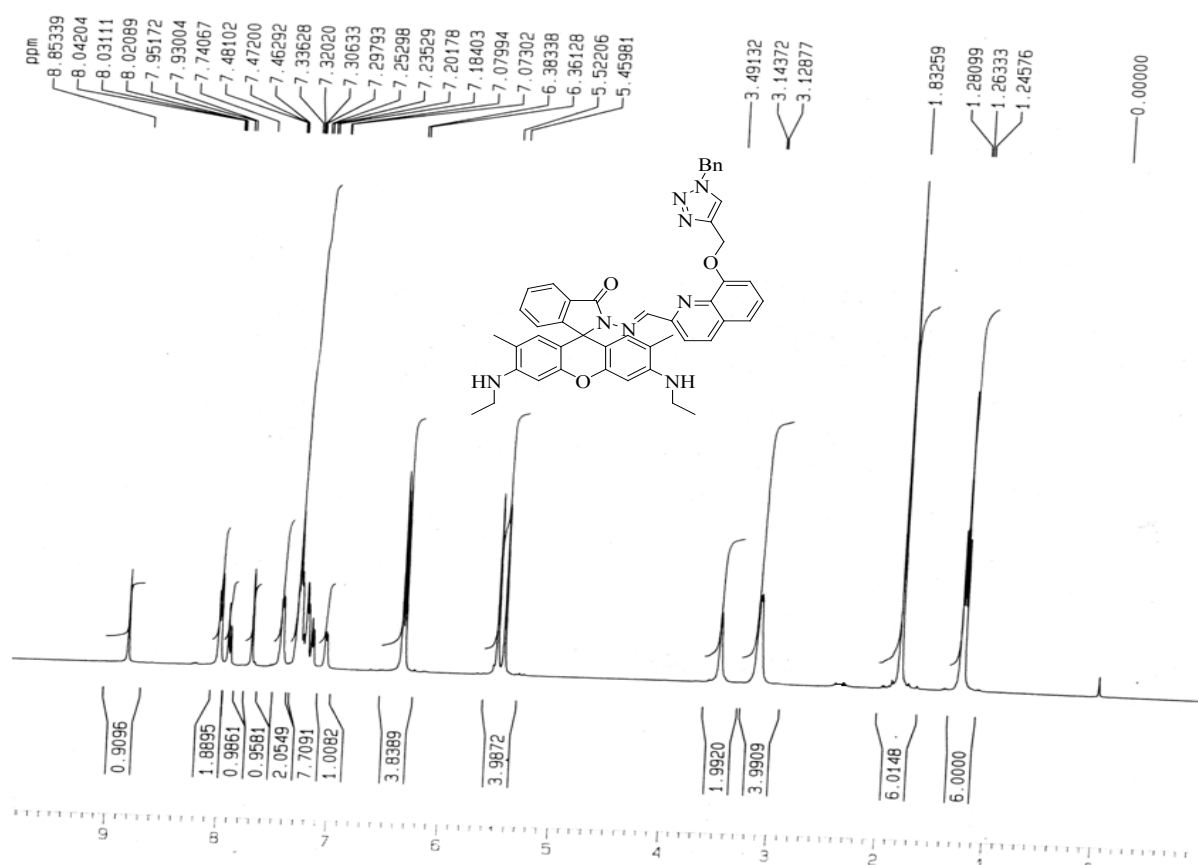


Fig. S6. ¹H NMR spectrum of 2 in CDCl₃

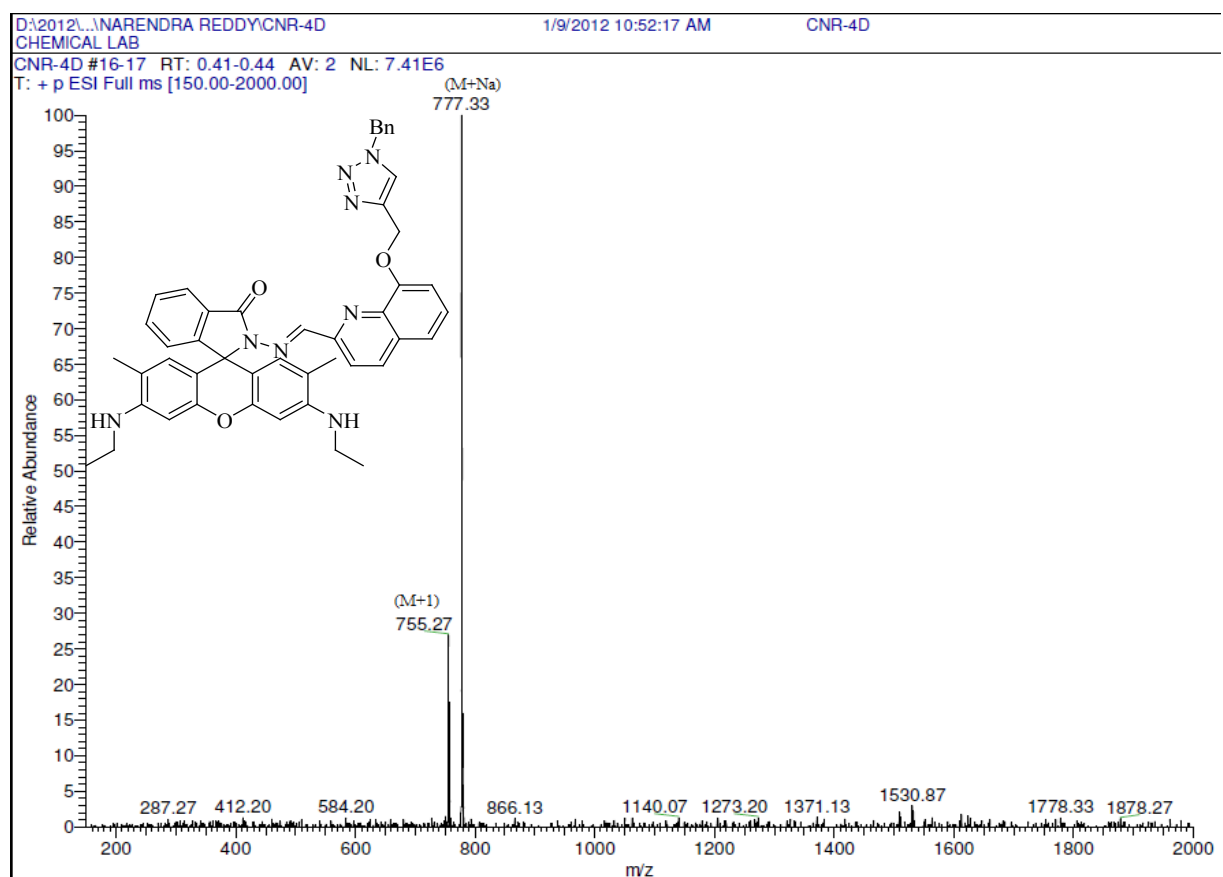
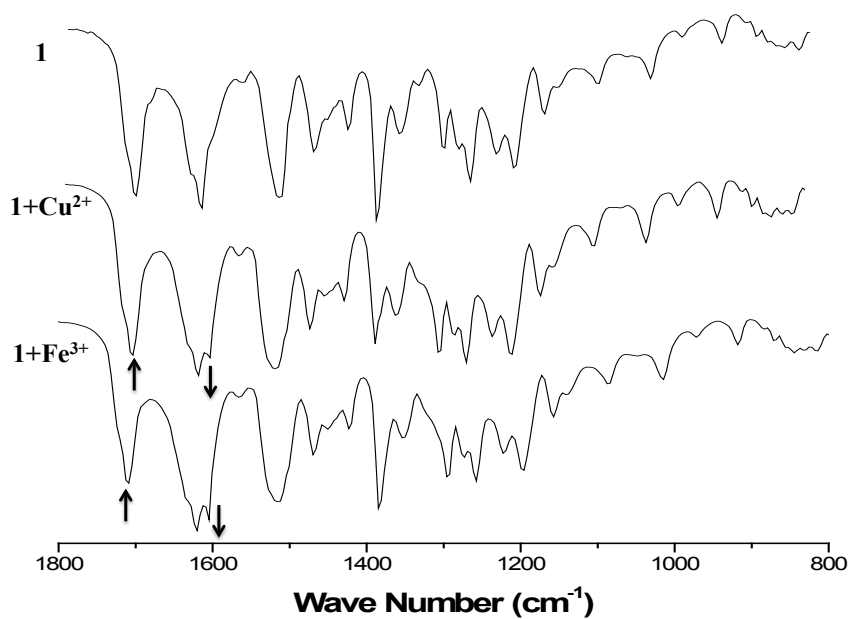
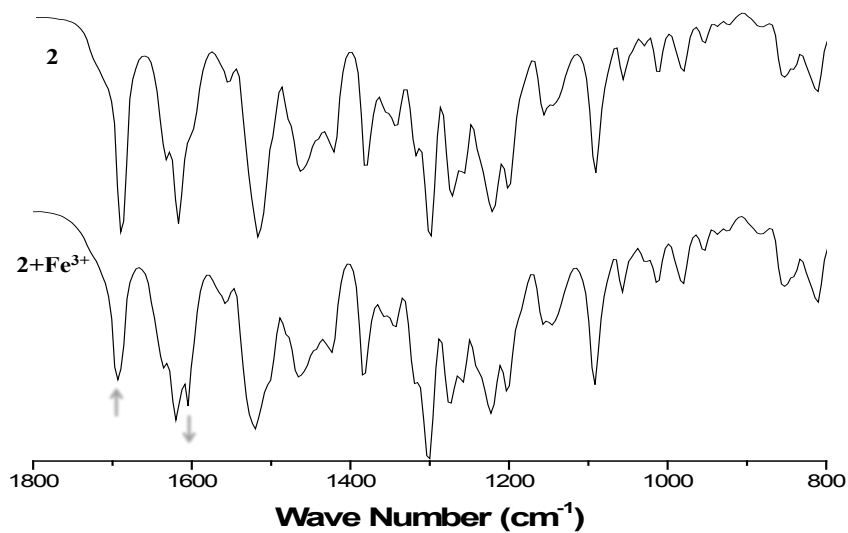


Fig. S8. ESI Mass spectrum of 2



(a)



(b)

Fig. S9. IR spectra of 2 mM probe **1** (a), probe **2** (b) alone and upon addition of 1mM metal ions. Upward arrow shows the decrement in the intensity of spitolactam ring 'C=O' and downward arrow shows the increment in the intensity of metal bound ring opened 'C-O'.

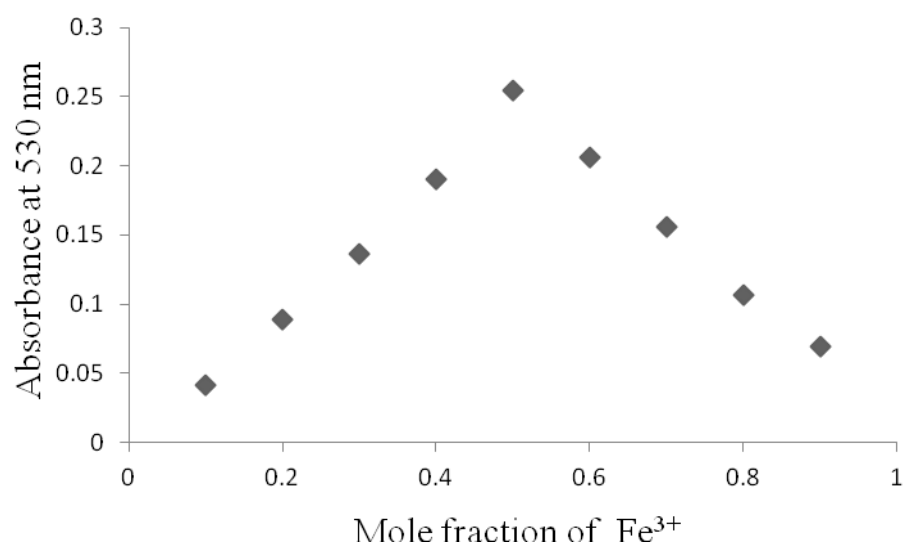


Fig. S10. Job plot of **2**-Fe³⁺ complex

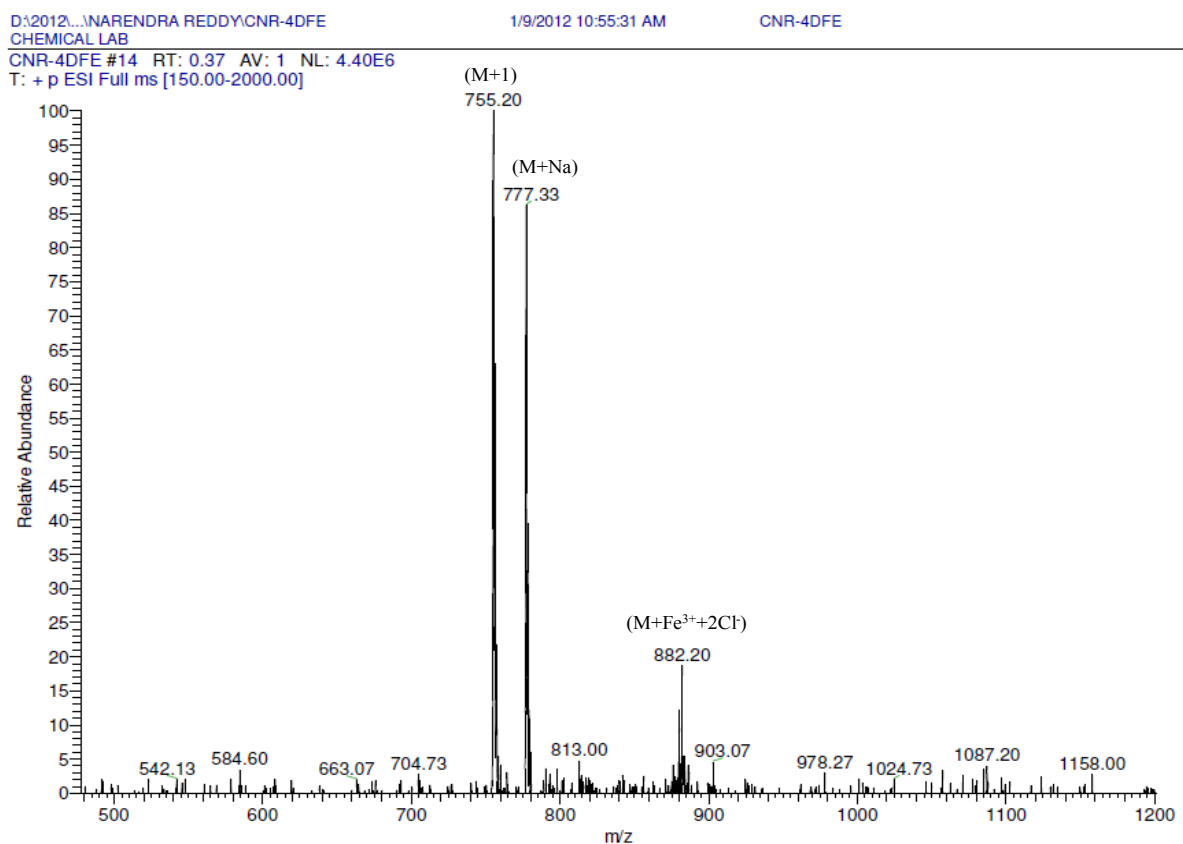


Fig. S11. ESI Mass spectrum of **2-Fe³⁺** complex

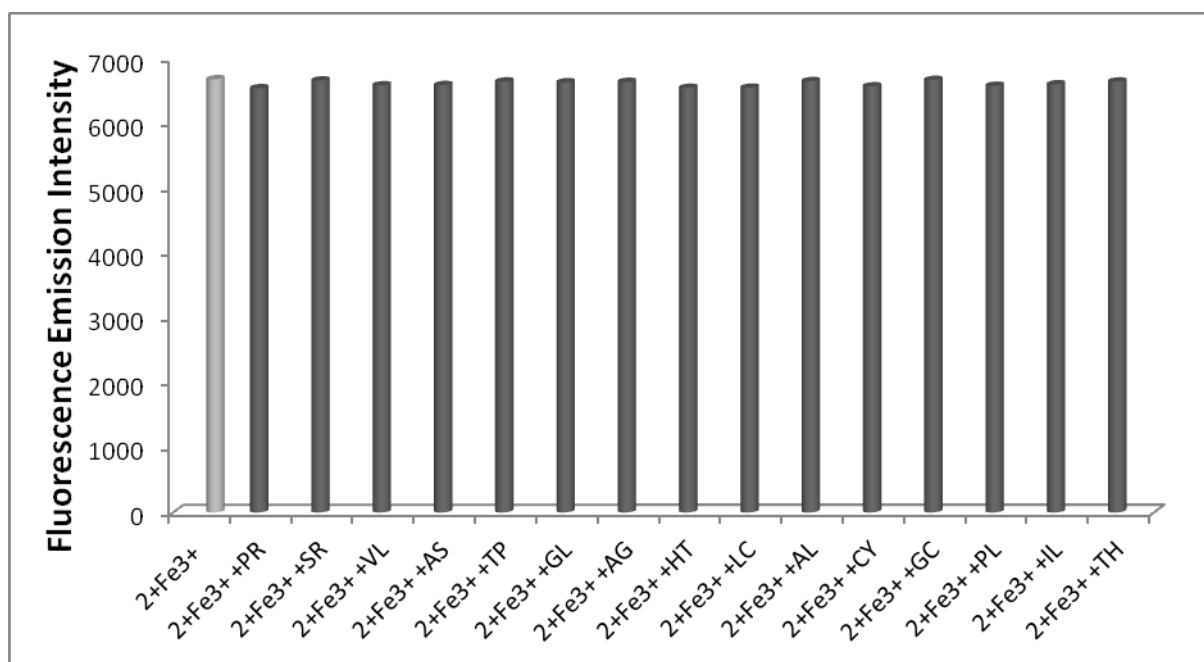


Fig. S12. Fe^{3+} ion selectivity of **2** (10 μM) in 1:1v/v 0.01M Tris HCl- CH_3CN pH 7.4 in the presence of various amino acids. The grey bar shows the fluorescence emission intensity upon addition of 1 equiv of Fe(III) to **2** (10 μM). The dark bars represent the fluorescence emission upon addition of 1 equiv of Fe(III) to a solution containing **2** (10 μM) and 5 equiv of the amino acid of interest.

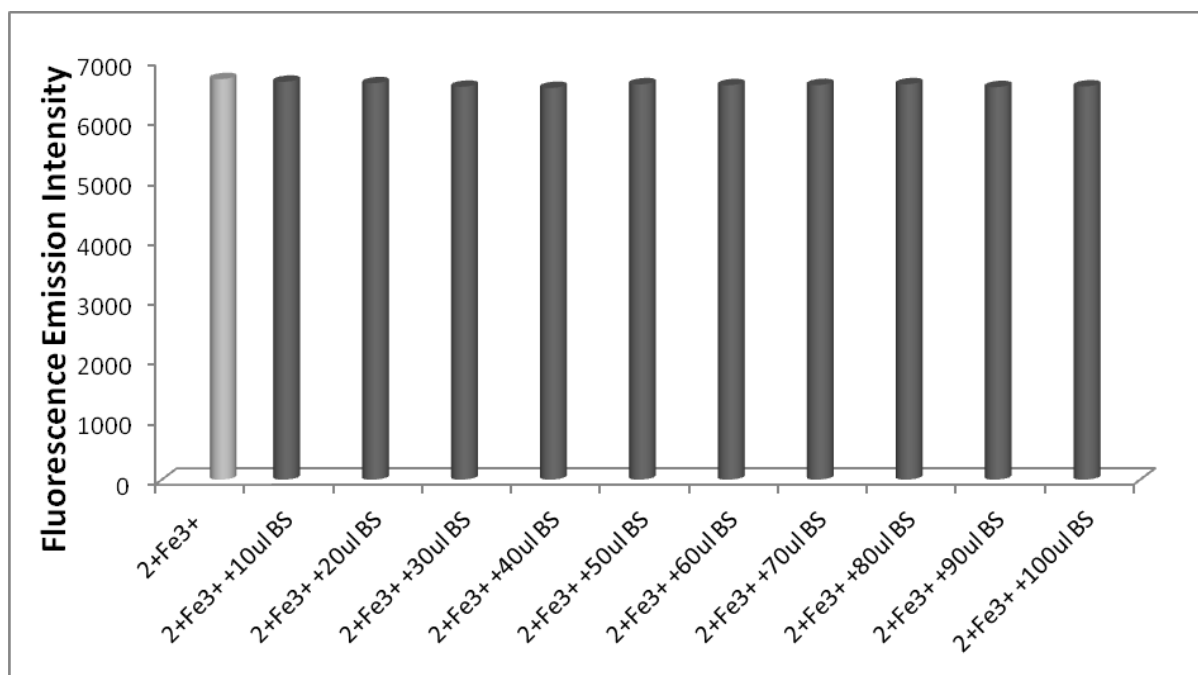


Fig. S13. Fe^{3+} ion selectivity of **2** ($10\ \mu\text{M}$) in 1:1v/v 0.01M Tris HCl- CH_3CN pH 7.4 in the presence of various amounts of human blood serum. The grey bar shows the fluorescence emission intensity upon addition of 1 equiv of Fe(III) to **2** ($10\ \mu\text{M}$). The dark bars represent the fluorescence emission upon addition of 1 equiv of Fe(III) to a solution of **2** ($10\ \mu\text{M}$) and various amounts of human blood serum.

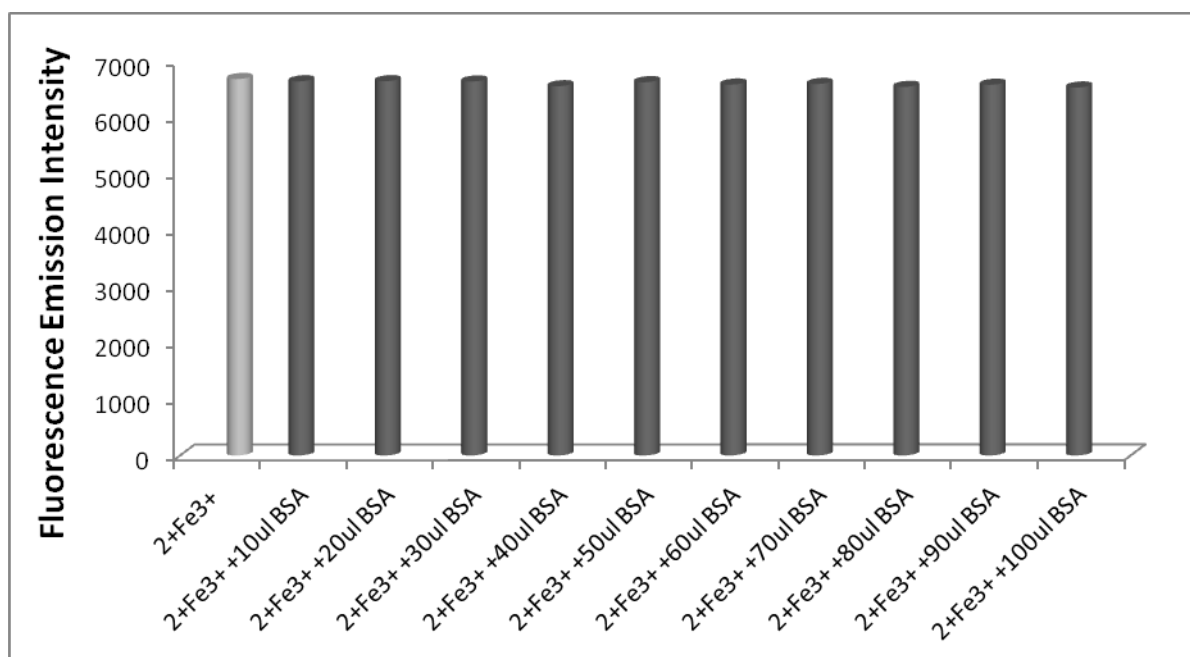


Fig. S14. Fe^{3+} ion selectivity of **2** ($10\ \mu\text{M}$) in 1:1v/v 0.01M Tris HCl- CH_3CN pH 7.4 in the presence of various amounts of Bovine Serum Albumin (BSA). The grey bar shows the fluorescence emission intensity upon addition of 1 equiv of Fe(III) to **2** ($10\ \mu\text{M}$). The dark bars represent the fluorescence emission upon addition of 1 equiv of Fe(III) to a solution of **2** ($10\ \mu\text{M}$) and various amounts of BSA.

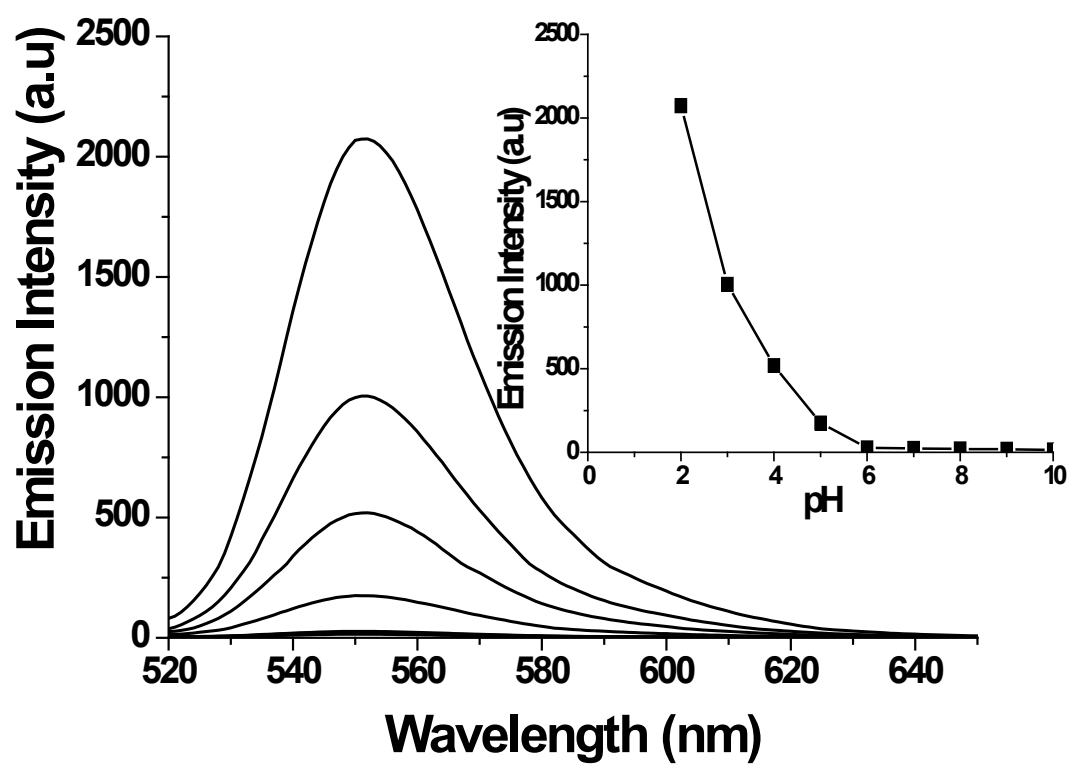


Fig. S15. pH dependant variation in fluorescence intensity of **2** (10 μM).

Cell viability assay

The cell viability assay of probe **2** on NIH3T3 cells was determined by MTT (3-(4, 5-Dimethylthiazol-2-yl)-2, 5- diphenyltetrazolium bromide) assay (*J Immunol Methods*, 1983, **65**, 55.). The NIH3T3 cells were trypsinised and seeded in 48-well flat-bottom culture plates at a density of 4×10^3 cells per well in 250 μ L DMEM supplemented with 10% FBS, 100 IU/mL penicillin, 100 μ g/mL streptomycin, 30 μ g/mL gentamicin. The cells were allowed for 24 hours to adhere and grow at 37 °C in CO₂ incubator. Then the medium was replaced with 250 μ L fresh medium containing various concentrations of probe **2** (0 to 6 μ M) and incubated for 12 hours in a humidified chamber with 5% CO₂ after which the medium was removed. The cells were further incubated for 3 hours with 250 μ L of fresh medium containing 1 mg/mL MTT reagent. The medium was then removed to eliminate non-reacted MTT reagent. DMSO (100 μ L) was added into each well to dissolve the formazan precipitate formed and was measured spectrophotometrically using a microplate reader at 570 nm. The assay was performed in quadruplet for each concentration. The cytotoxicity of the probe **2** was expressed in terms of percentage of cell viability relative to the untreated control cells which was taken as 100 percent viable.