Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

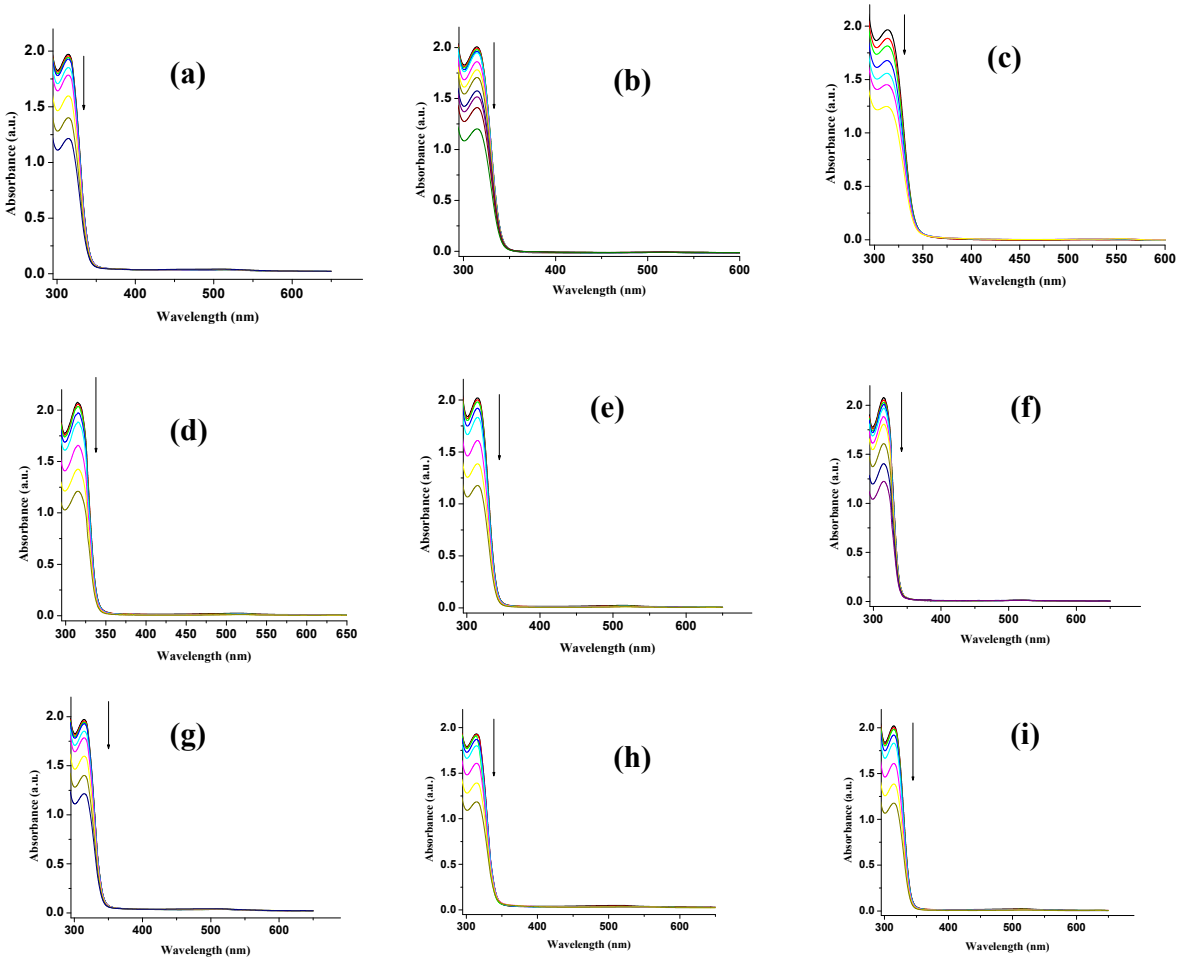
Rhodamine appended tripodal receptor as a ratiometric probe for Hg^{2+} ions

Kumaresh Ghosh*[a], Tanmay Sarkar[a], Asmita Samadder[b]

[a]Department of Chemistry, University of Kalyani, Kalyani-741235, India.
Email: ghosh_k2003@yahoo.co.in, Fax: +913325828282; Tel: +913325828750;
[b]Department of Zoology, University of Kalyani, Kalyani-741235.

---

1. Change in absorbance of receptor 1 with various metal ions in MeCN/water (4/1,v/v; 10 μM tris HCl buffer; pH = 7.0)



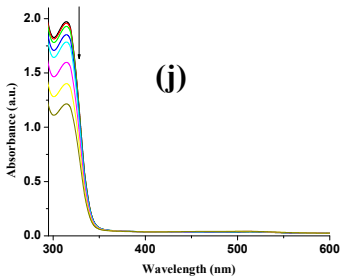
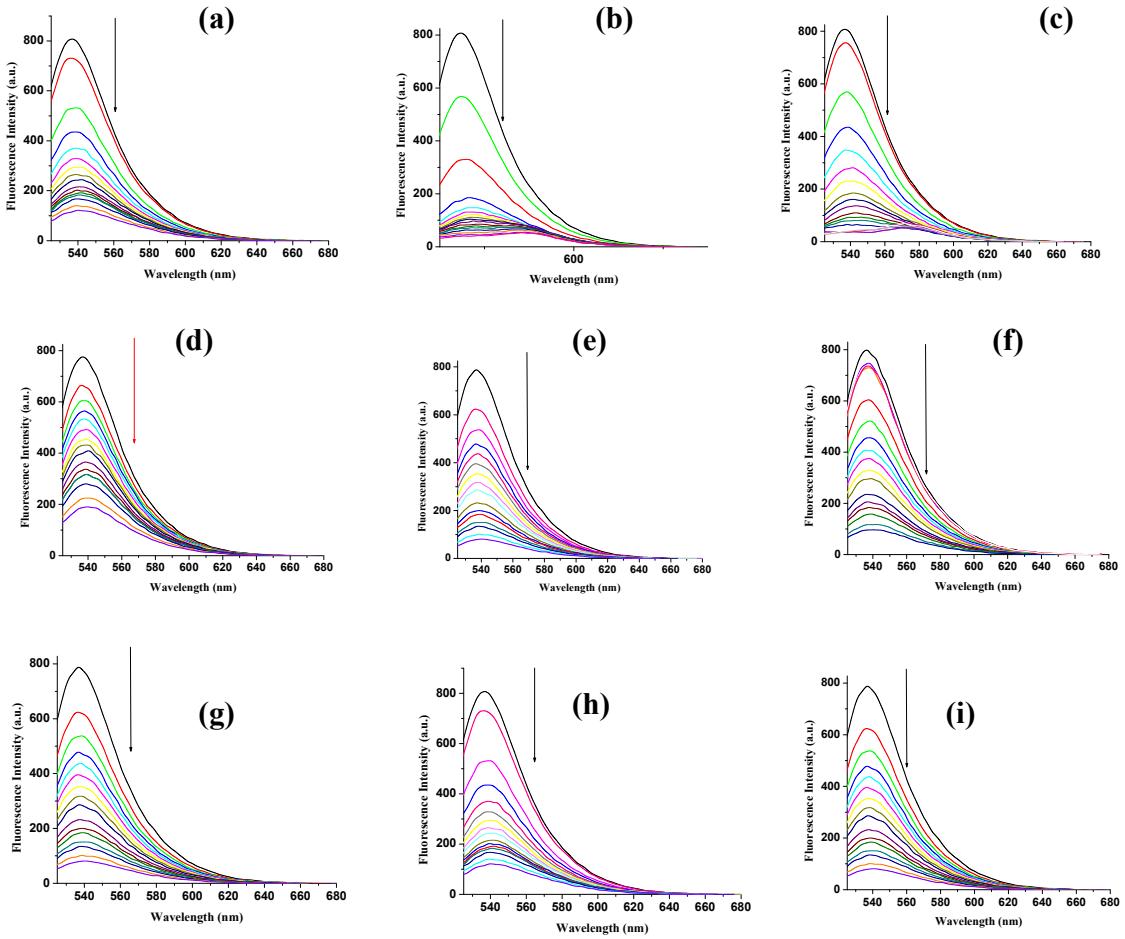


Figure 1S. Absorption titration spectra for **1** (c = 4.41 x 10^{-5} M) with (a) Co^{2+}, (b) Zn^{2+}, (c) Cu^{2+}, (d) Mg^{2+}, (e) Ni^{2+}, (f) Cd^{2+}, (g) Pb^{2+}, (h) Fe^{2+}, (i) $Mn^{2+}$and (j) Ag^{+} in MeCN/water (4/1,v/v; 10 µM tris HCl buffer; pH = 7.0) (in all cases [cation] = 8.82 x 10^{-4} M).

2.Change in emission of receptor 1 with Zn^{2+}, Cu^{2+}, Fe^{2+}, Cd^{2+}, Co^{2+}, Pb^{2+}, Mn^{2+}, Mg^{2+}, Ni^{2+}, Ag^{+} in MeCN/Water (4/1,v/v; 10 µM tris HCl buffer; pH 7.0).



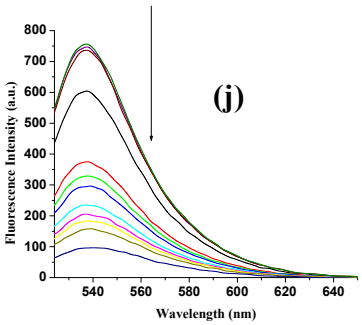


Figure 2S. Change in emission of receptor **1** (c = 4.41 x 10^{-5} M) upon addition of (a) Zn^{2+}, (b) Cu^{2+}, (c) Fe^{2+}, (d) Cd^{2+}, (e) Co^{2+}, (f) Pb^{2+}, (g) Mg^{2+}, (h) Mn^{2+}, (i) Ni^{2+} , (j) Ag^{+} in MeCN/Water (4/1, v/v; 10 µM tris HCl buffer; pH = 7.0) (in all cases [cation] = 8.82 x 10^{-4} M) [λ_{exc} = 510 nm].

3. Change in fluorescence ratio at 536 nm.

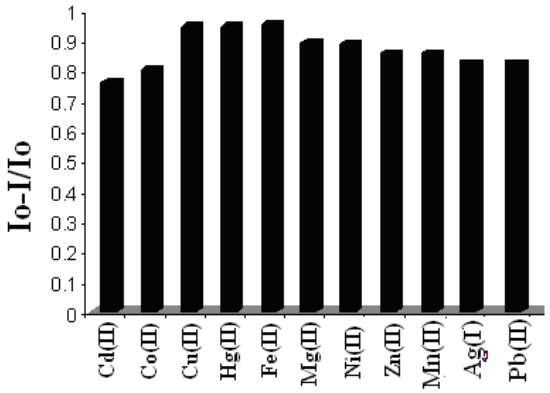


Figure 3S. Change in fluorescence ratio of **1** (c = 4.41 x 10^{-5} M) at 536 nm upon addition of 18 equiv. amounts of cations.

4. UV Job plot for 1 with Hg^{2+}mesured at 556 nm.

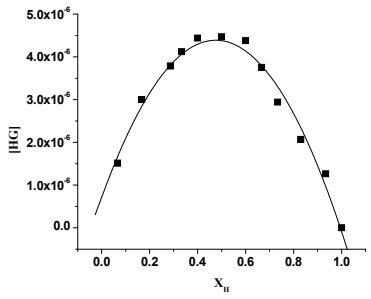


Figure 4S. UV Job plot for **1** with Hg^{2+} in MeCN/Water (4/1,v/v; 10 µM tris HCl buffer; pH = 7.0) ([H] = [G] = 4.41 x 10^{-5} M).

5. Emission titration spectra of 1 with Hg^{2+} in MeCN/Water (4/1,v/v; 35 μM tris HCl buffer, pH 7.0)

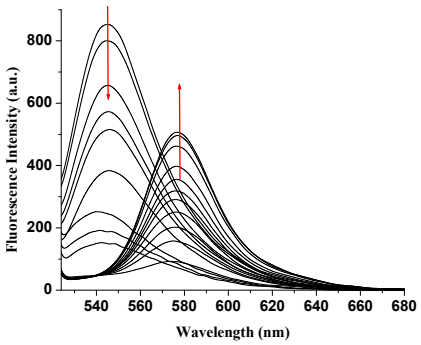


Figure 5S. Change in fluorescence spectra of **1** (c = 4.35 x 10^{-5} M) in MeCN/Water (4/1,v/v; 35 μM tris HCl buffer, pH 7.0) upon addition of Hg^{2+}.

6. Emission titration spectra of 1 with different concentrations of Hg^{2+} ions

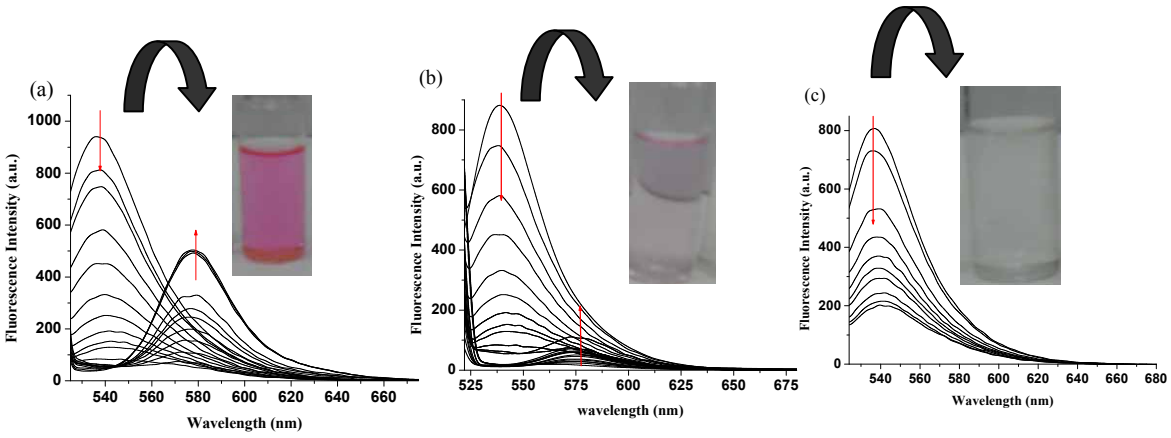


Figure 6S. Change in fluorescence spectra of **1** (c = 4.35 x 10^{-5} M) in MeCN/Water (4/1,v/v; 10 μM tris HCl buffer, pH 7.0) upon addition of (a) Hg^{2+} (c = 8.7 x 10^{-4} M); (b) Hg^{2+} (c = 8.7 x 10^{-5} M); (c) Hg^{2+} (c = 8.7 x 10^{-6} M).

7. Test of reversibility in the binding process

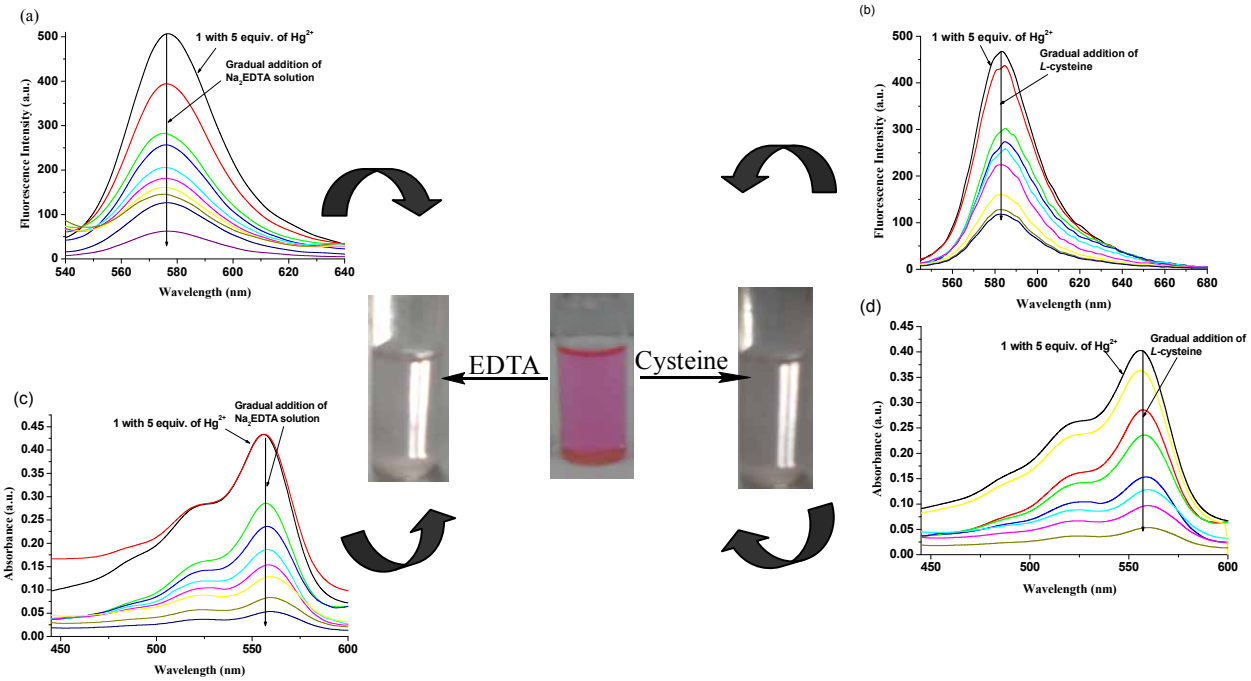


Figure 7S. Change in fluorescence spectra of **1- Hg^{2+}** complex (c = 6.5x 10^{-5} M) in MeCN/Water (4/1,v/v; 10 µM tris HCl buffer, pH 7.0) upon addition of (a) Na_2EDTA (c = 4.5 x 10^{-3} M); (b) Cysteine (c = 4.5 x 10^{-3} M)**.** Change in absorbance of **1-**Hg^{2+} complex in CH_3CN/H_2O (4/1, v/v; 10 µM tris HCl buffer; pH 7.0) upon addition of (c) Na_2EDTA (c = 4.5 x 10^{-3} M); (d) Cysteine (c = 4.5 x 10^{-3} M) and associated colour changes.

8. ^{1}H NMR of 1 ($CDCl_3$, 400 MHz):

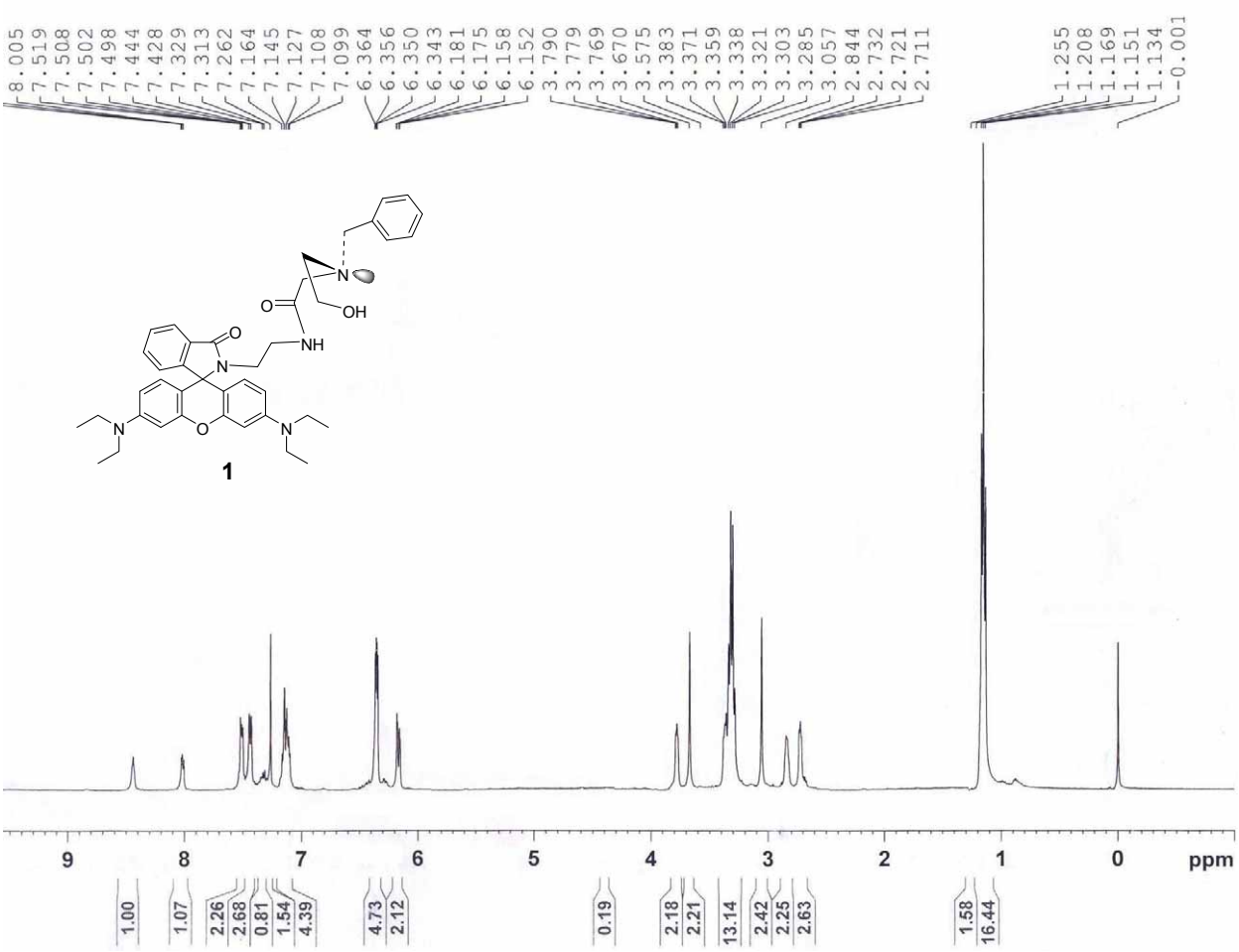


Figure 8S. ^{1}H NMR spectrum of receptor **1.**

9. ^{13}C NMR of 1 ($CDCl_3$, 100 MHz):

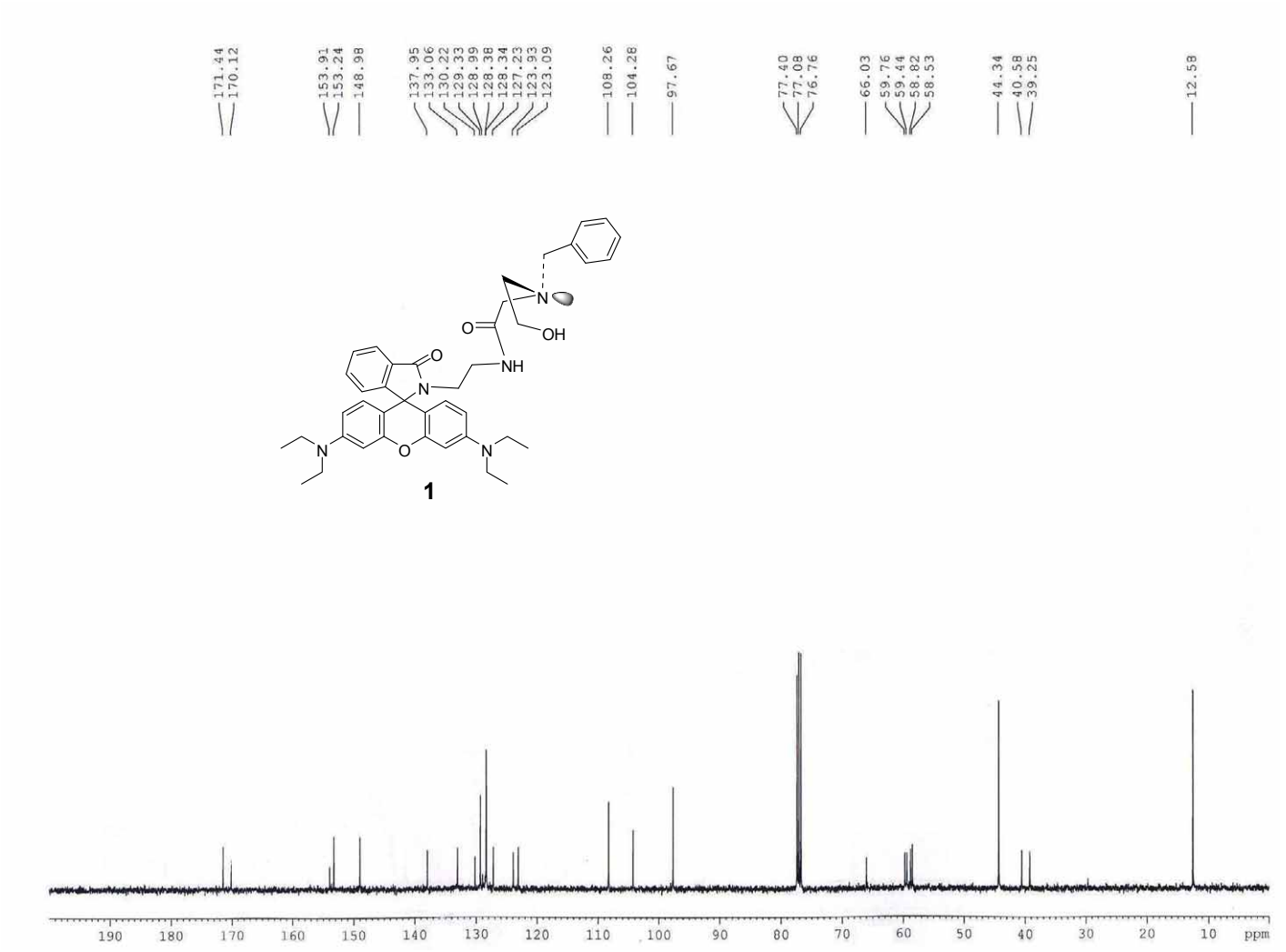
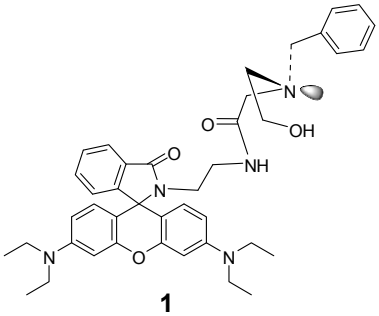
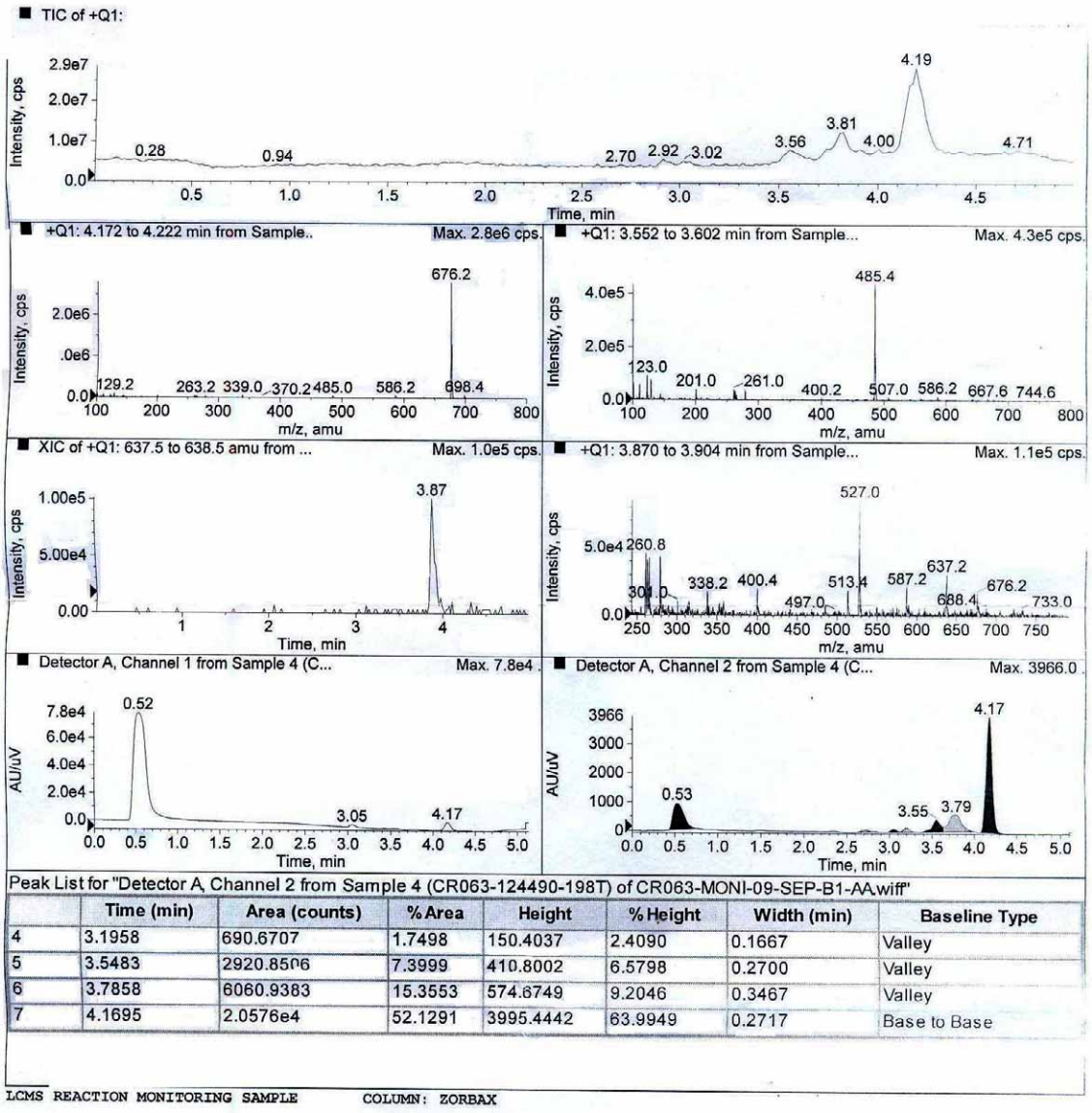


Figure 9S. ^{13}C NMR spectrum of receptor **1.**

10. Mass of 1



1



Peak List for "Detector A, Channel 2 from Sample 4 (CR063-124490-198T) of CR063-MONI-09-SEP-B1-AA.wiff"

	Time (min)	Area (counts)	% Area	Height	% Height	Width (min)	Baseline Type
4	3.1958	690.6707	1.7498	150.4037	2.4090	0.1667	Valley
5	3.5483	2920.8506	7.3999	410.8002	6.5798	0.2700	Valley
6	3.7858	6060.9383	15.3553	574.6749	9.2046	0.3467	Valley
7	4.1695	2.0576e4	52.1291	3995.4442	63.9949	0.2717	Base to Base

Figure 10. LCMS spectrum of receptor **1.**

11. ^{13}C NMR of 1 and 1 with 1.2 equiv. amounts of $Hg(ClO_4)_2$ ($CDCl_3$, 100 MHz):

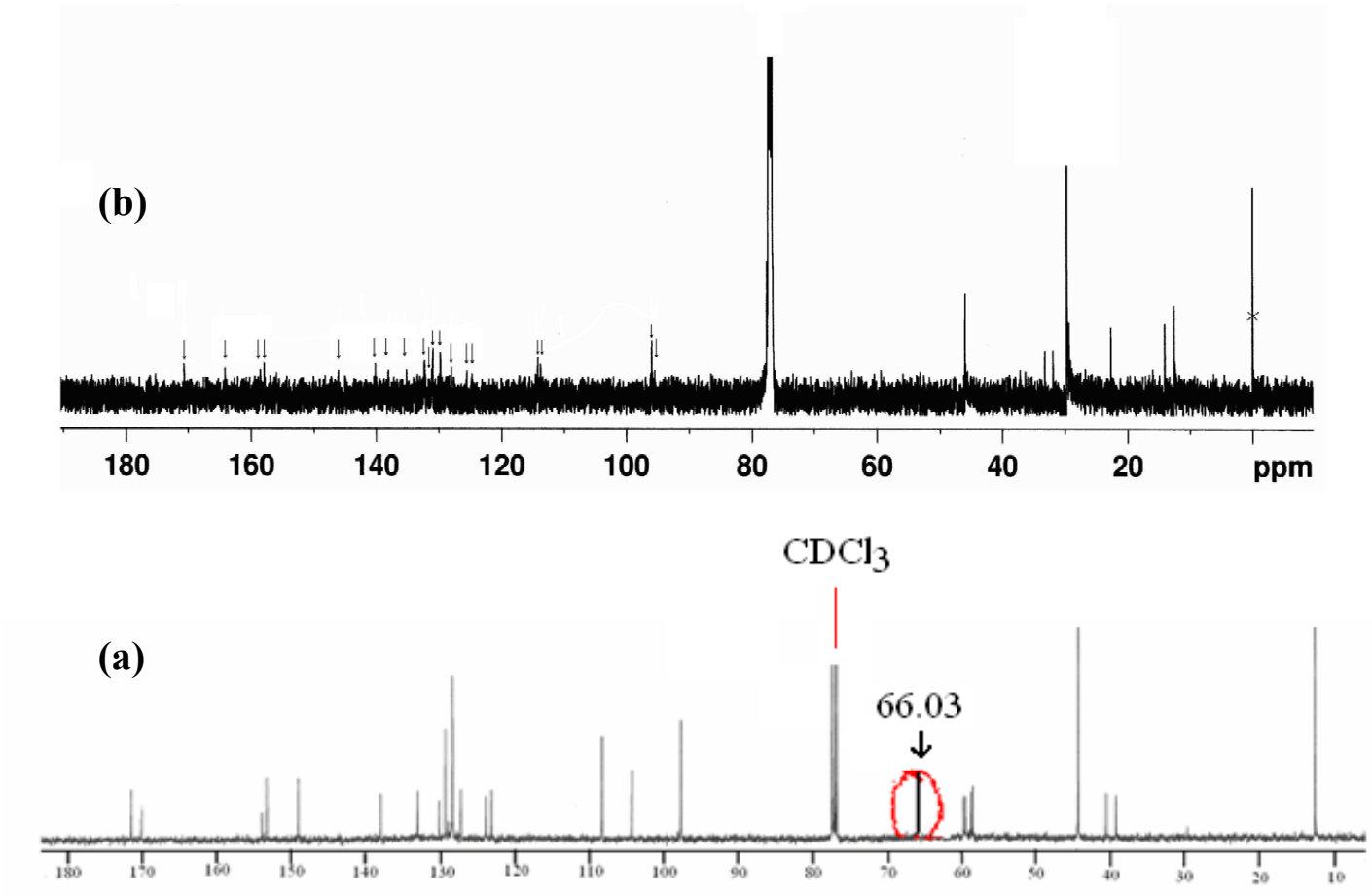


Figure 11S. ^{13}C NMR spectrum of (a) receptor **1**and (b) **1** with 1.2 equiv. amount of $Hg(ClO_4)_2$.