Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

Rhodamine-labelled simple architectures for fluorometric and colorimetric sensing of Hg^{2} and Pb^{2} ions in semi-aqueous and aqueous environments

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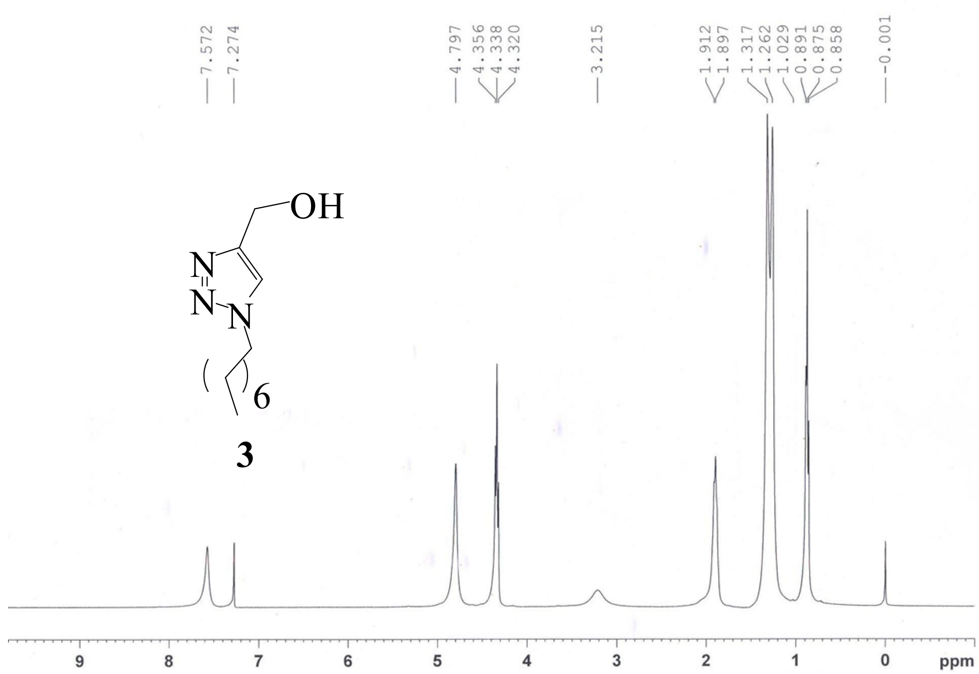
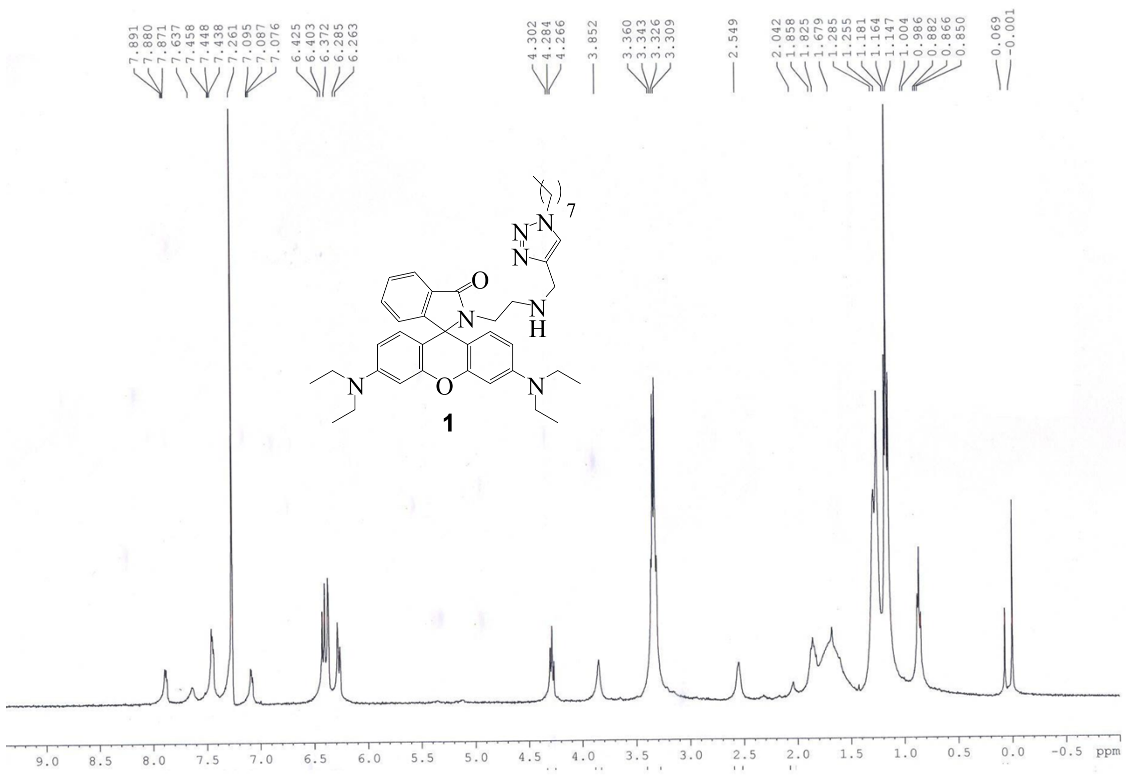
1. Spectral data of compounds

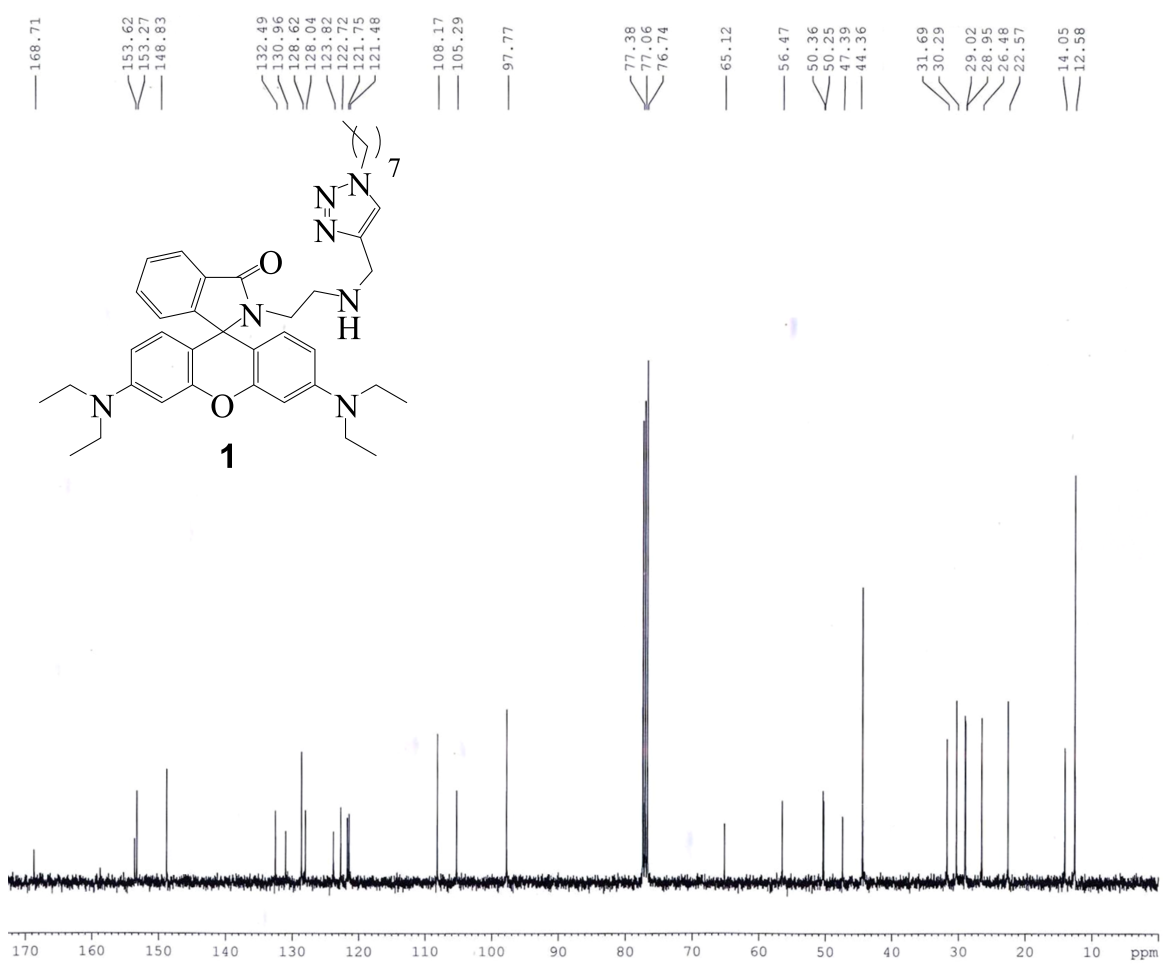
^{1}H NMR of 3 ($CDCl_3$, 400 MHz):



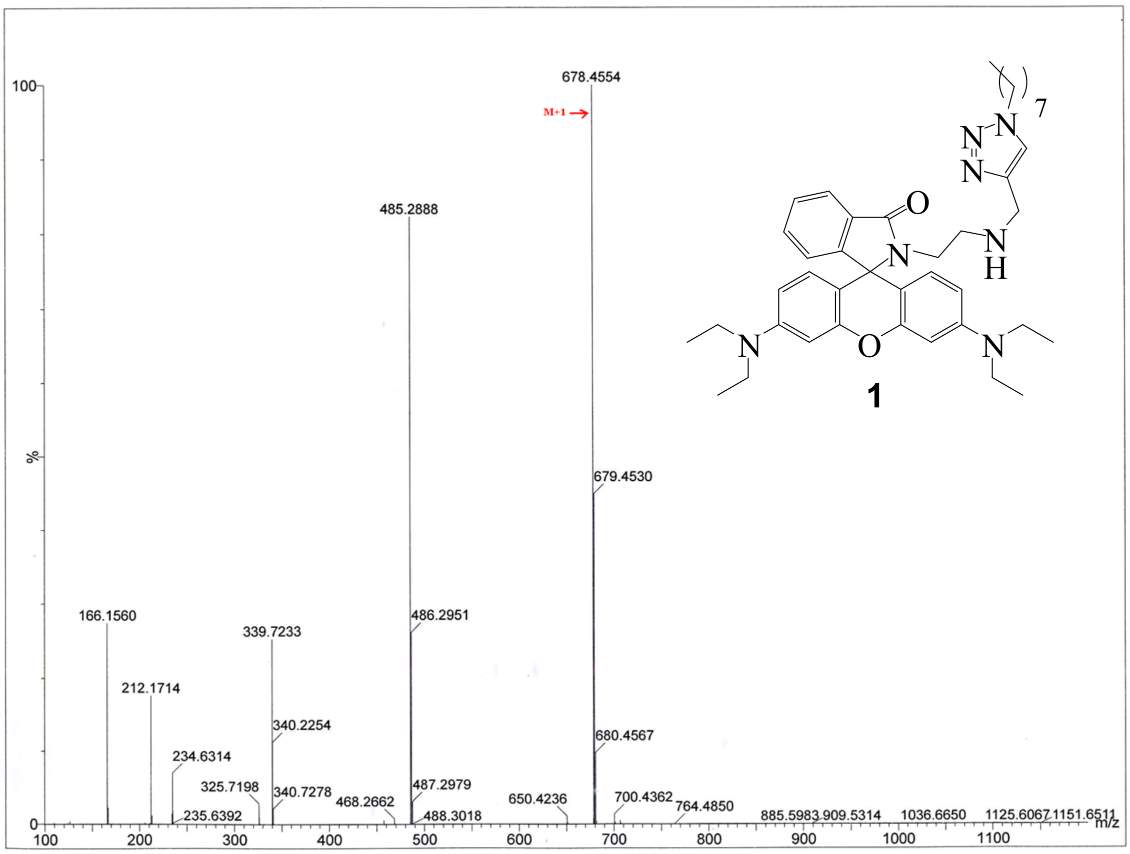
[1]H NMR of 1 ($CDCl_3$, 400 MHz):



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



Mass of 1:


678.4554
M+1
485.2888
679.4530
166.1560
339.7233
486.2951
212.1714
340.2254
680.4567
234.6314
325.7198
340.7278
468.2662
487.2979
650.4236
700.4362
764.4850
235.6392
488.3018
885.5983
909.5314
1036.6650
1125.6067
1151.6511
100
%
0
100
200
300
400
500
600
700
800
900
1000
1100
m/z
7
N
O
H
1

2. Change in emission of receptor 1 with Zn^{2+}, Fe^{3+}, Cd^{2+}, Co^{2+}, Pb^{2+}, Mg^{2+}, Ni^{2+}, Ag^{+} in MeCN/Water (4/1,v/v; 10 μM tris HCl buffer; pH 7).

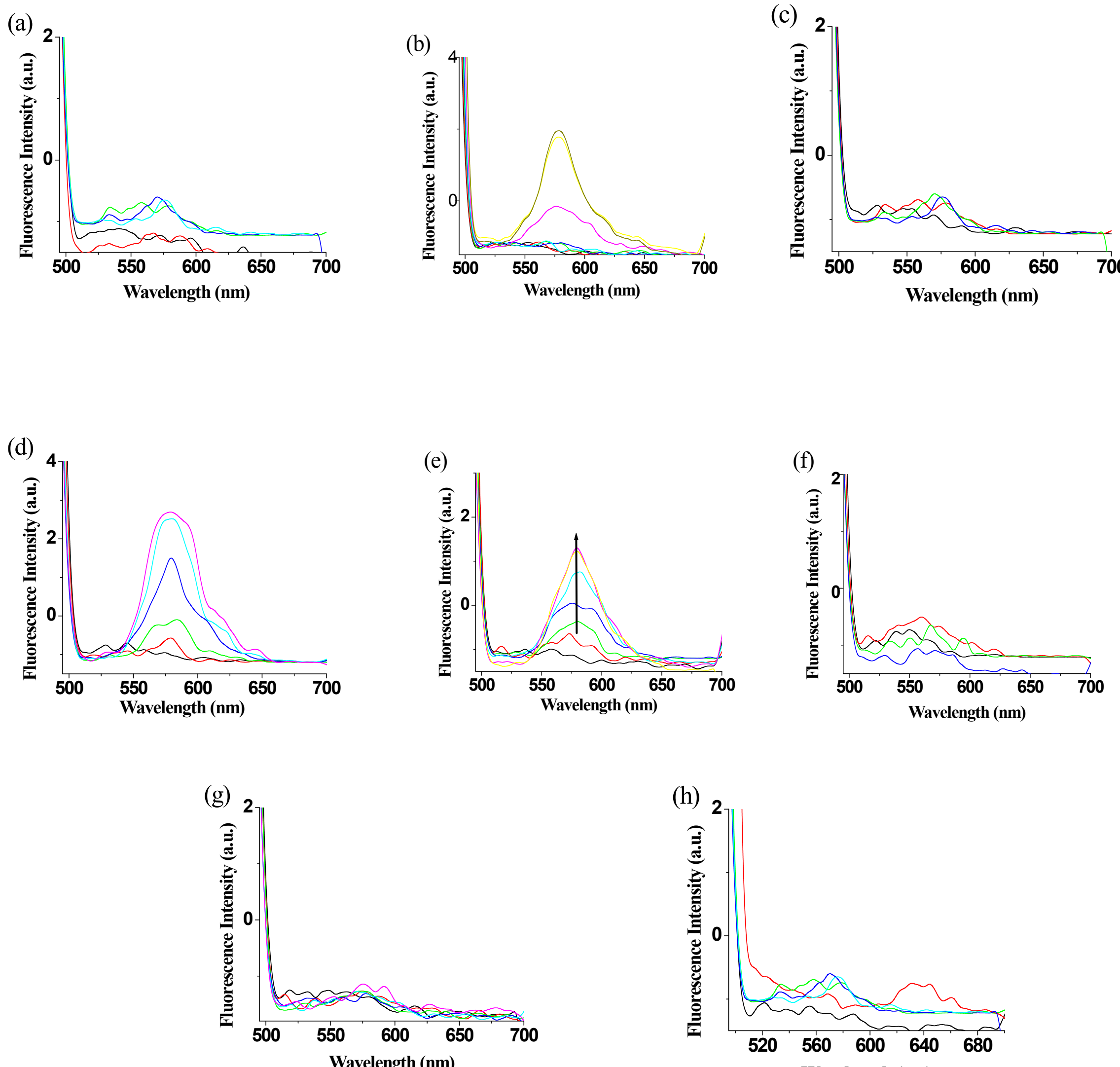


Figure S1. Change in emission of receptor **1** (c = 2.25 x 10^{-5} M) upon addition of (a) Zn^{2+}, (b) Fe^{3+}, (c) Cd^{2+}, (d) Co^{2+}, (e) Cu^{2+}, (f) Mg^{2+}, (g) Ni^{2+}, (h) Ag^{+} in MeCN/Water (4/1, v/v; 10 μM tris HCl buffer; pH = 7) (in all cases [cation] 4.5 x 10^{-4} M) [λ_{exc} = 490 nm].

3. Change in absorbance of receptor 1 with various metal ions in MeCN/water (4/1, v/v; 10 μM tris HCl buffer; pH = 7)

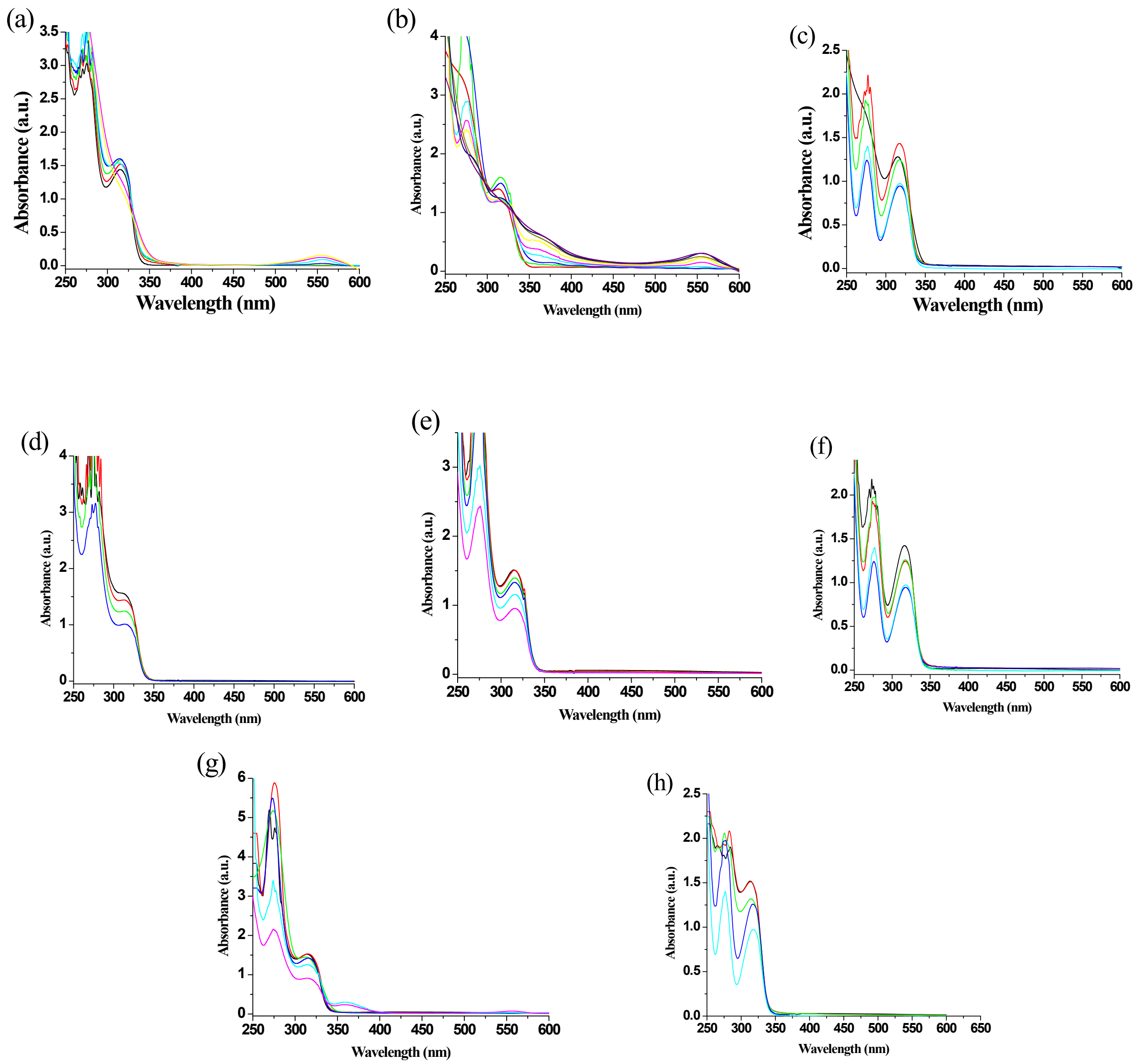


Figure S2. Absorption titration spectra for **1** (c = 2.25 x 10^{-5} M) with (a) Cu^{2+}, (b) Fe^{3+}, (c) Zn^{2+}, (d) Cd^{2+}, (e) Mg^{2+}, (f) Ni^{2+}, (g) Co^{2+} and (h) Ag^{+} in MeCN/water (4/1,v/v; 10 μM tris HCl buffer; pH =7) (in all cases [cation] =4.5 x 10^{-4} M).

4. ^{1}H NMR study, UV and Fluorescence Job plots for 1 with Hg^{2+} and Pb^{2+} measured at 556 nm.

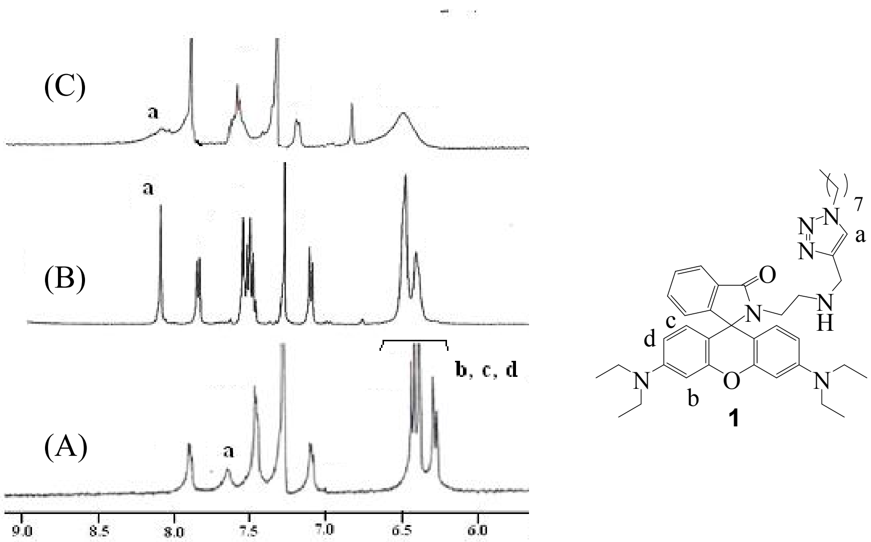


Figure S3a. Partial ^{1}H NMR (400 MHz, $CDCl_3$) of (A) **1** (5.21×10^{-3} M); (B) with 1 equiv. amount of $Pb(ClO_4)_2$ and (c) with 1 equiv. $Hg(ClO_4)_2$.

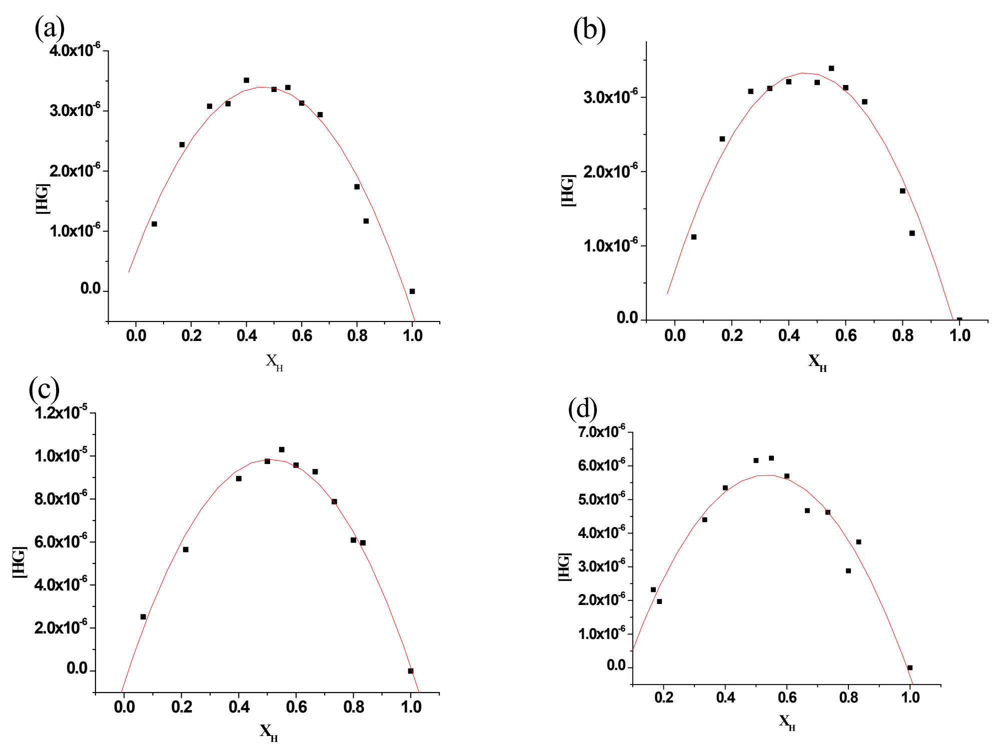


Figure S3b. Fluorescence Job plots for **1** with (a) Hg^{2+}; (b) Pb^{2+} ; UV Job plots for **1** with (c) Hg^{2+}, (d) Pb^{2+} in MeCN/Water (4/1,v/v; 10 μM tris HCl buffer; pH = 7) ([H] = [G] = 4.5×10^{-5} M).

5. Change in fluorescence spectra of (a) 1- Hg^{2+}, (b) 1- Pb^{2+} complex upon addition of KI

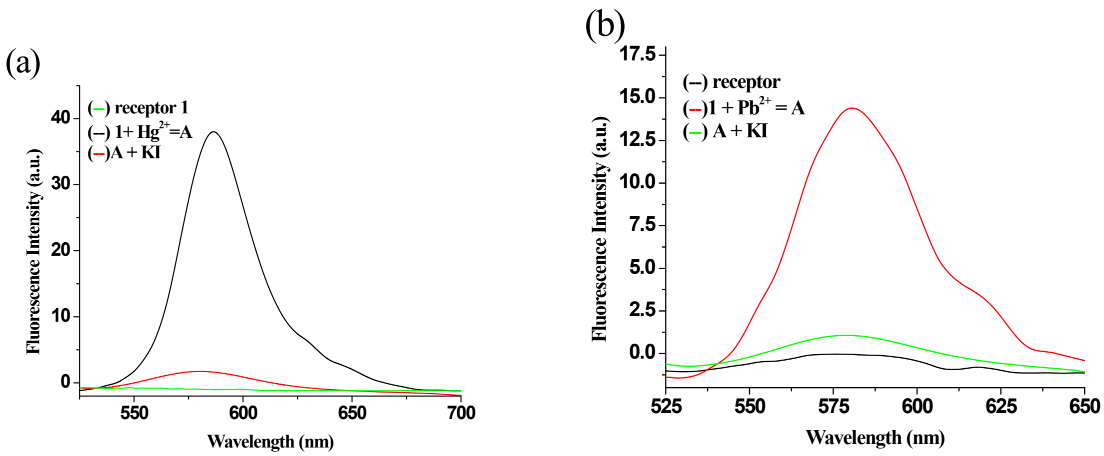
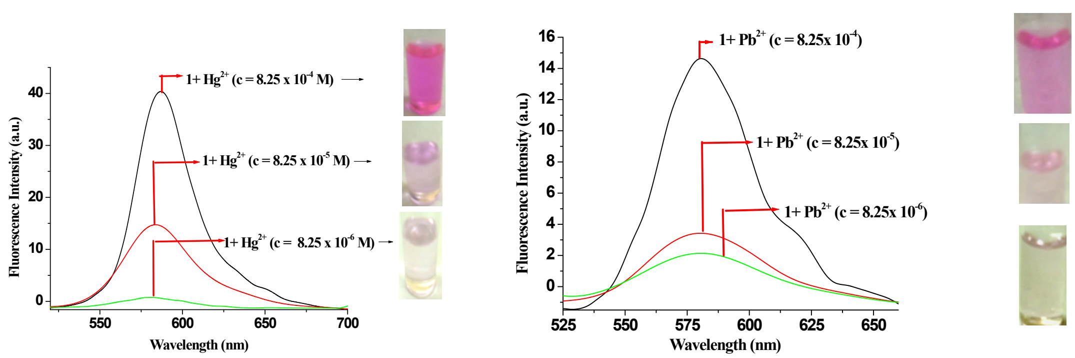


Figure S4: (a) Change in fluorescence spectra of (a)**1- Hg^{2+}, (b) 1- Pb^{2+}** complex (c = 4.1x 10^{-5} M) in MeCN/Water (4/1,v /v) 10 μM tris HCl buffer (pH 7) upon addition of (a) KI (c = 2.1 x 10^{-3} M).

6. Colorimetric change of 1 with Pb^{2+}:



(a) (b)

Figure S5: Change in fluorescence spectra of **1** (c = 2.25 x 10^{-5} M) in CH_3CN/water (4/1, v/v; 10 μM tris HCl buffer, pH = 7.0) upon addition of (a) Hg^{2+} and (b) Pb^{2+} of different concentrations.

7. MTT assay.

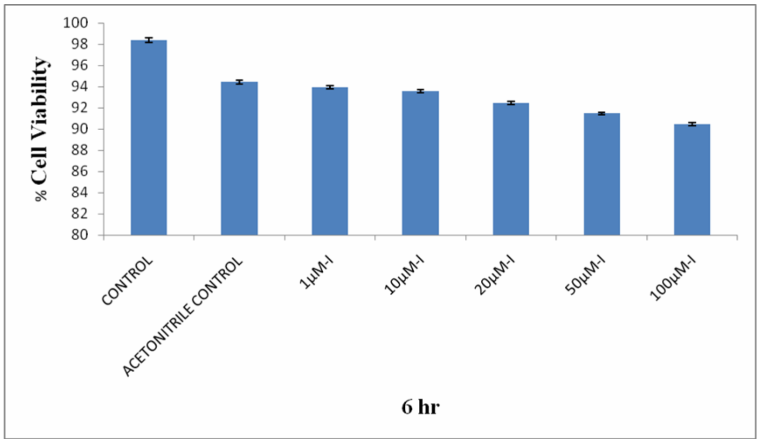


Figure S6. Cell viability of HeLa cells treated with different concentrations (1 μM-100 μM) of chemosensor **1** for six hrs determined by MTT assay.

8. FTIR spectra of 1, Merrifield resin and 2:

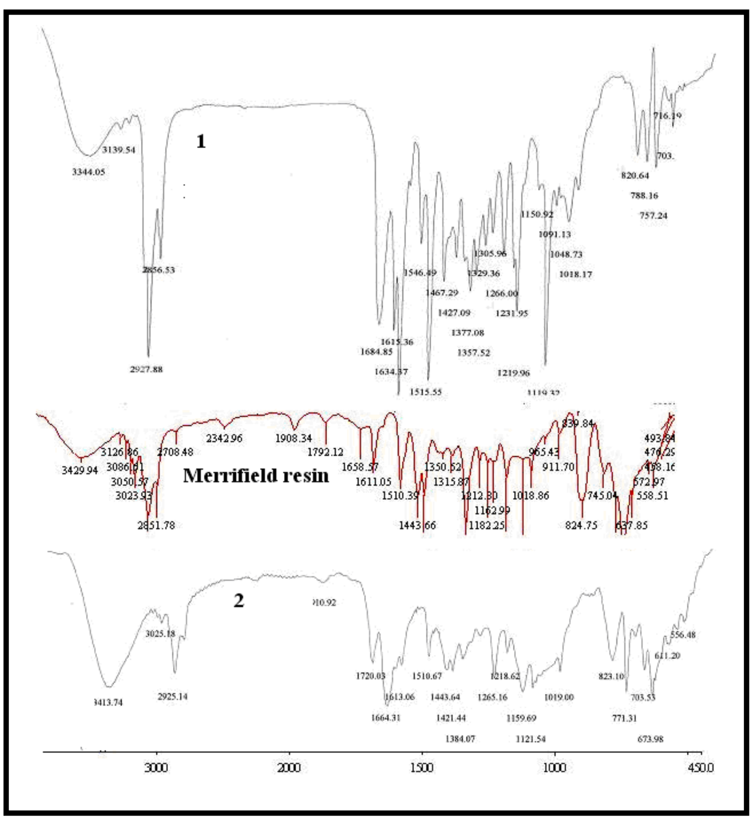


Figure S7. FTIR spectra of **1**, Merrifield resin and **2**.

9. FTIR spectra of 2, 2- Hg^{2+} and 2- Pb^{2+}complex:

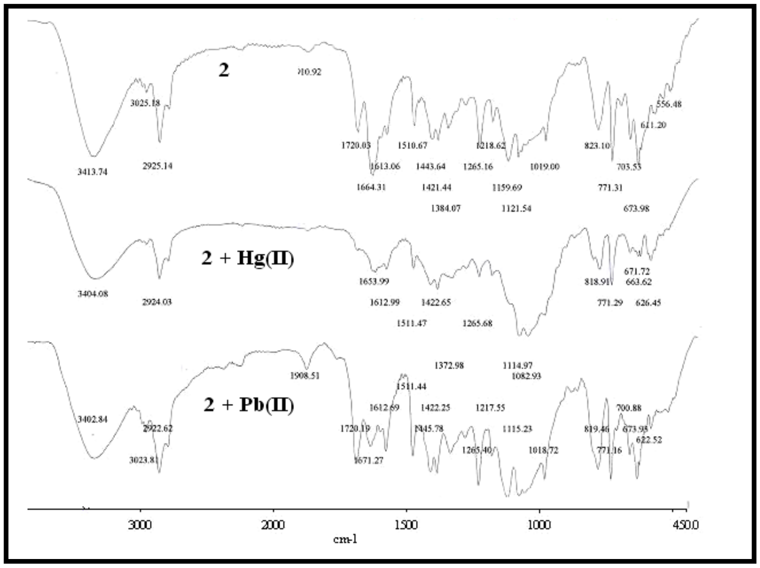


Figure S8. FTIR spectra of **2** and **2- Hg^{2+}**, **2- Pb^{2+}** complexes.

10. Reuse study:

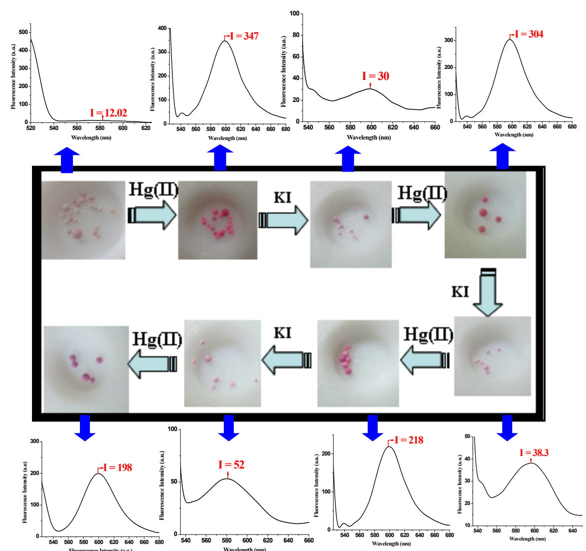


Figure S9. Reuse study of 2 for Hg^{2+} ions.