Copillar[5]arene-rhodamine conjugate as a selective sensor for Hg^{2+} ions

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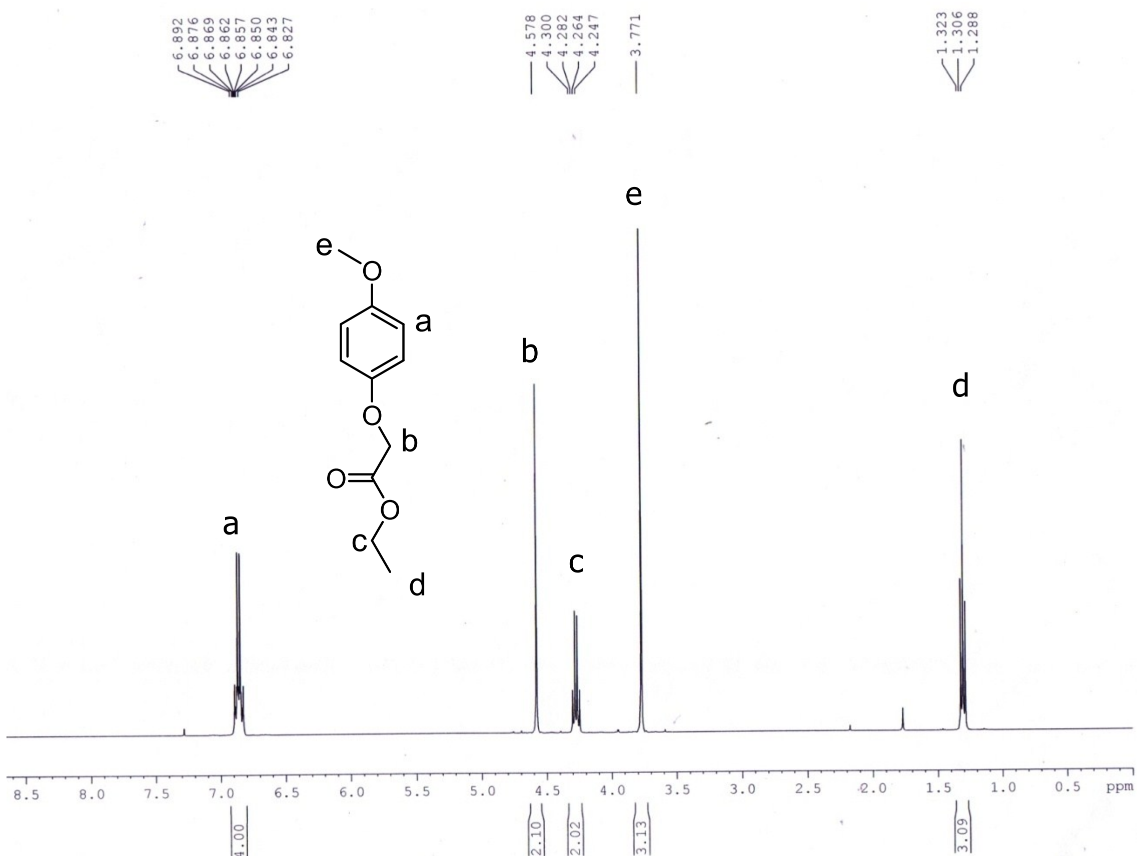


Figure S1. ^{1}H NMR spectrum of compound **3.**

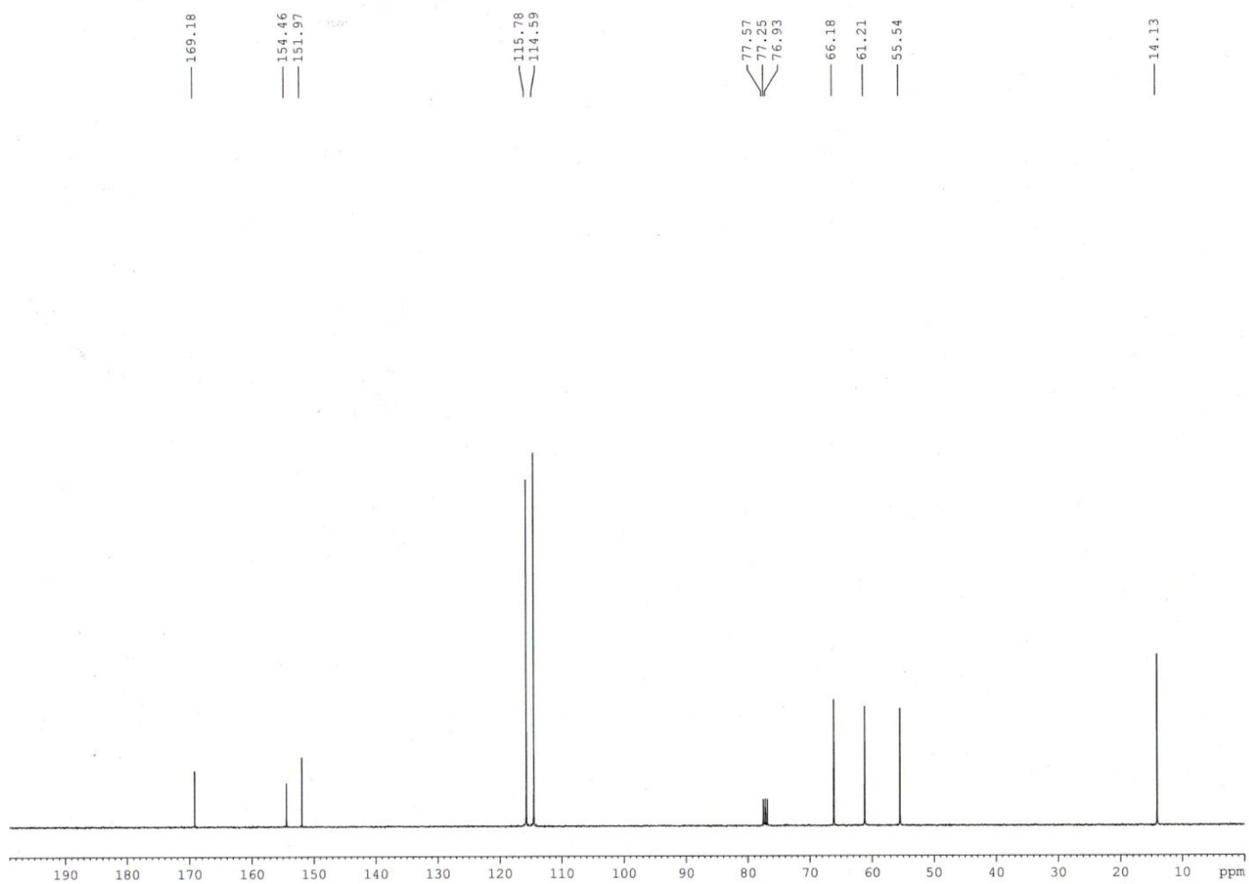


Figure S2. ^{13}C NMR spectrum of compound **3** in $CDCl_3$**.**

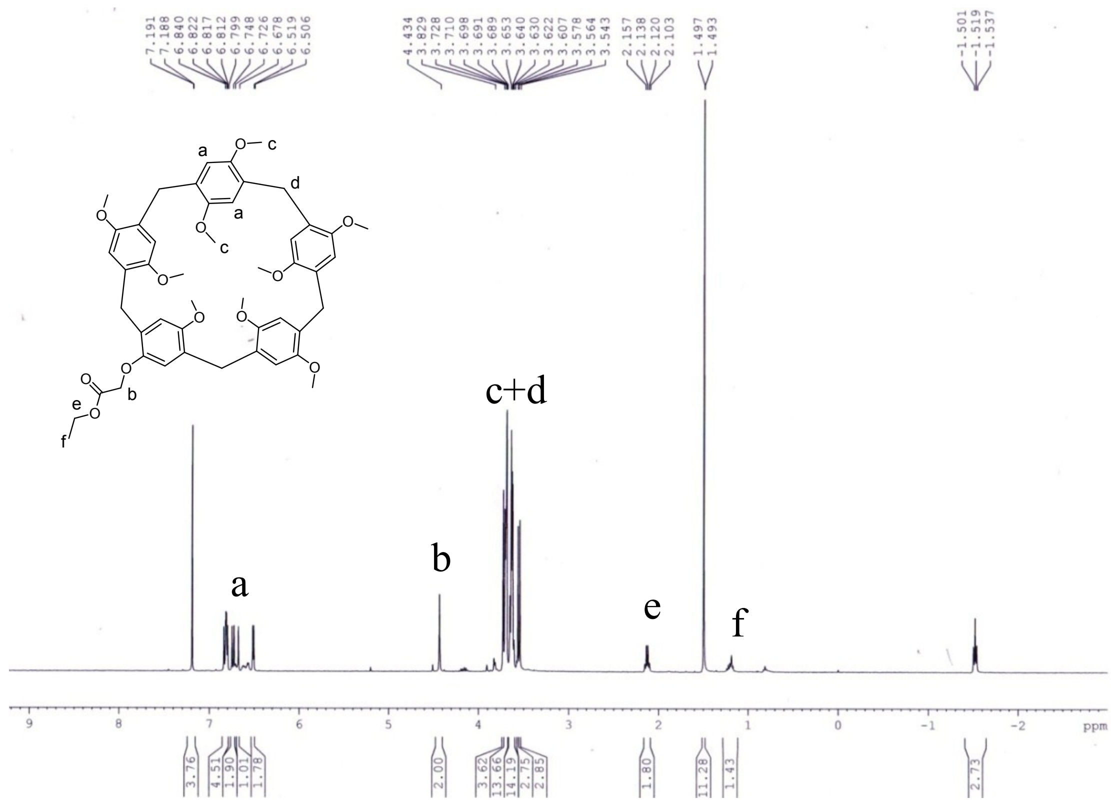


Figure S3. [1]H NMR spectrum of compound **4** in $CDCl_3$**.**

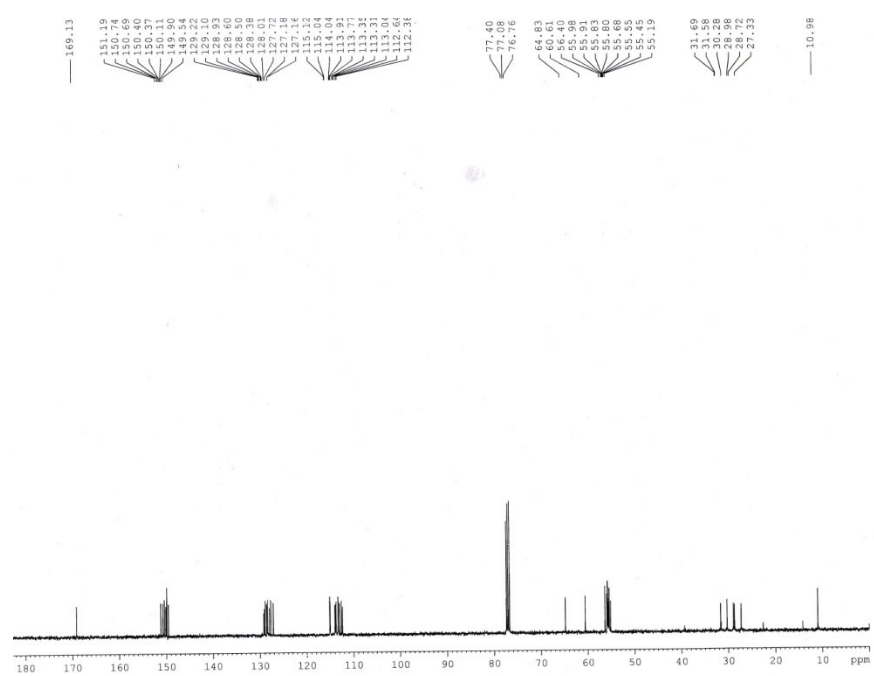


Figure S4. [13]C NMR spectrum of compound **4 in** $CDCl_3$**.**

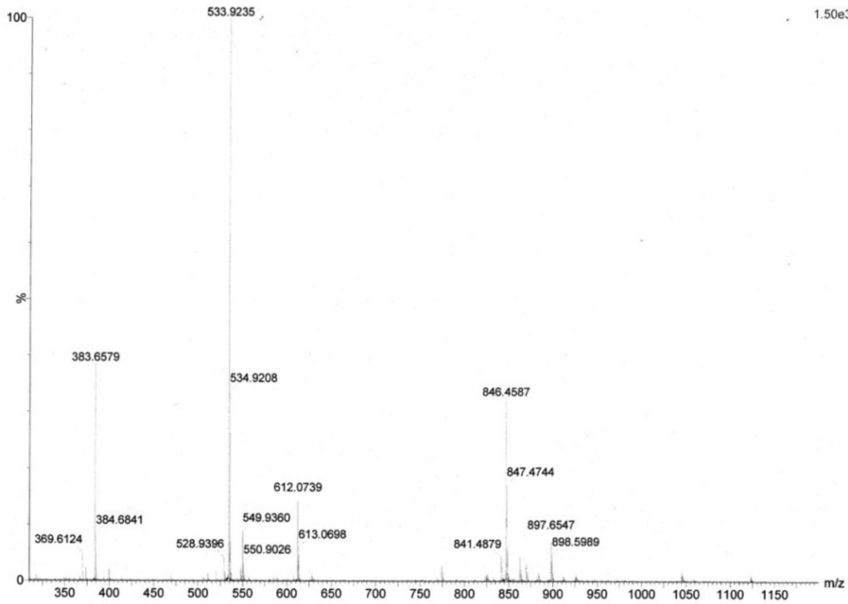


Figure S5. Electrospray ionization mass spectrum of compound (ESI MS) **4**. Assignment of the main peak: *m/z* 846.45 $[M+ Na]^+$ (40%).

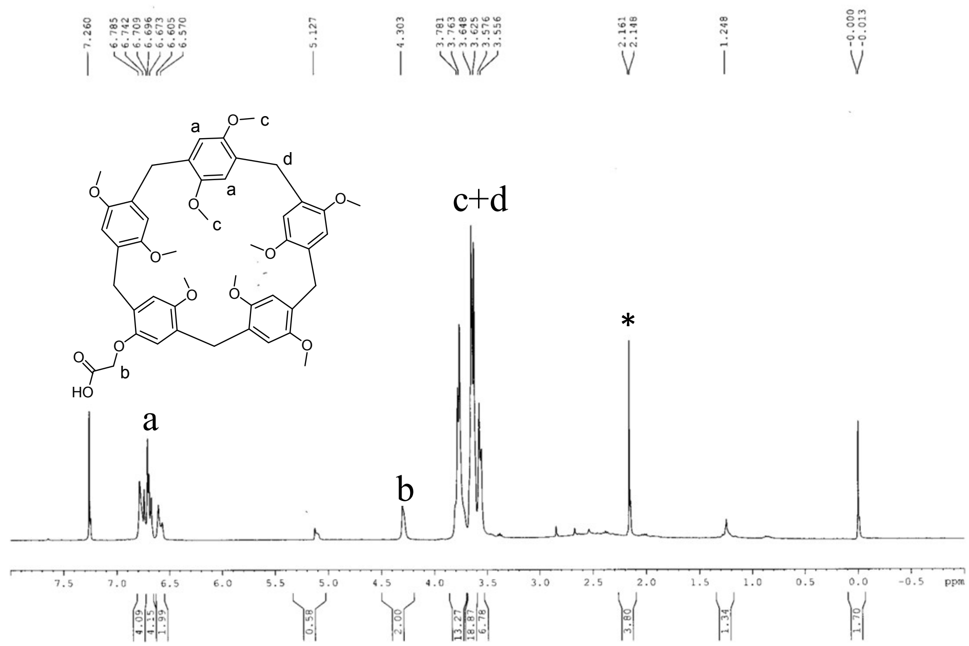


Figure S6. ^1H NMR spectrum of compound **5** in $CDCl_3$ (* Represents the appearance of peak due to CH_3COCH_3).

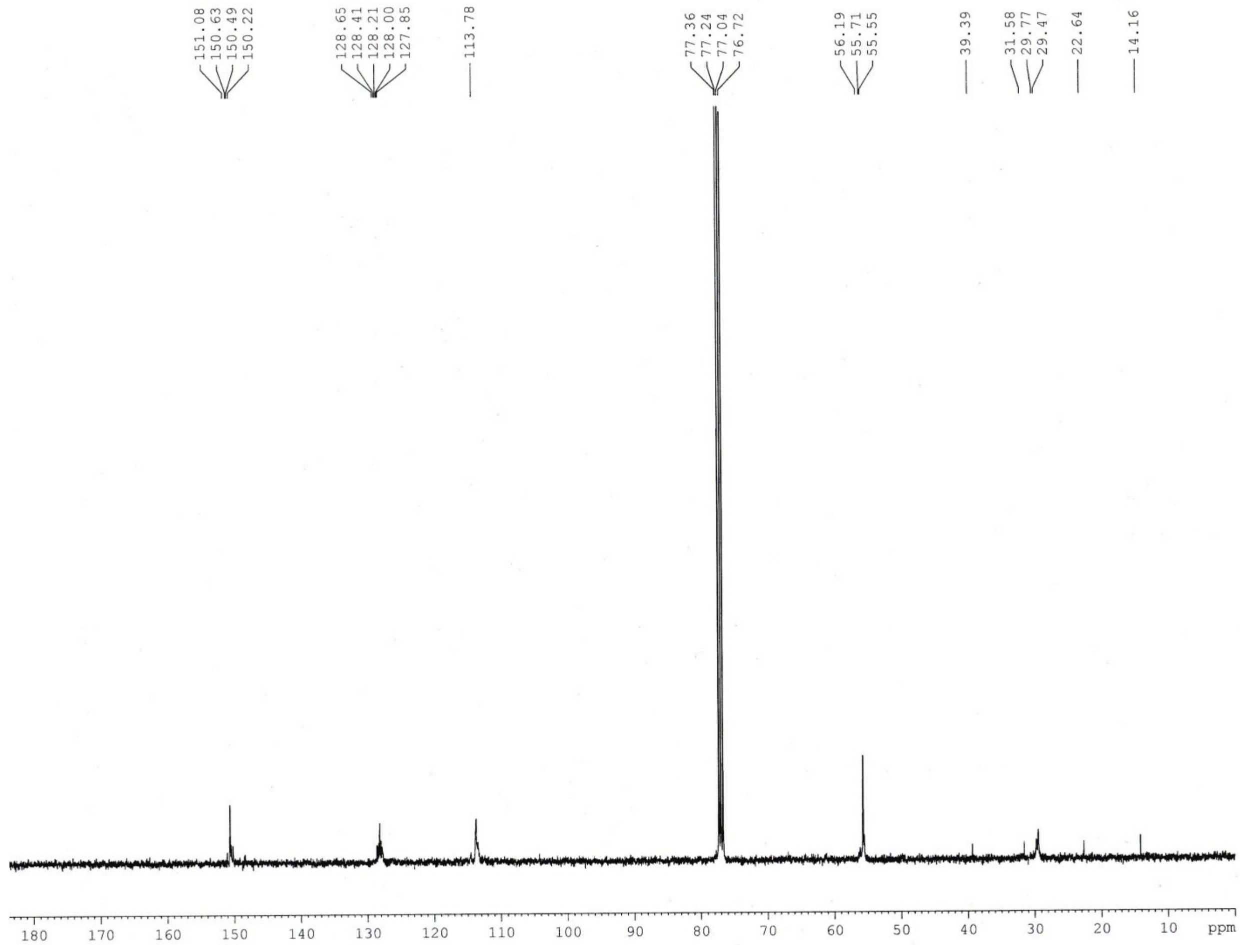


Figure S7. ^{13}C NMR spectrum of compound **5** in $CDCl_3$.

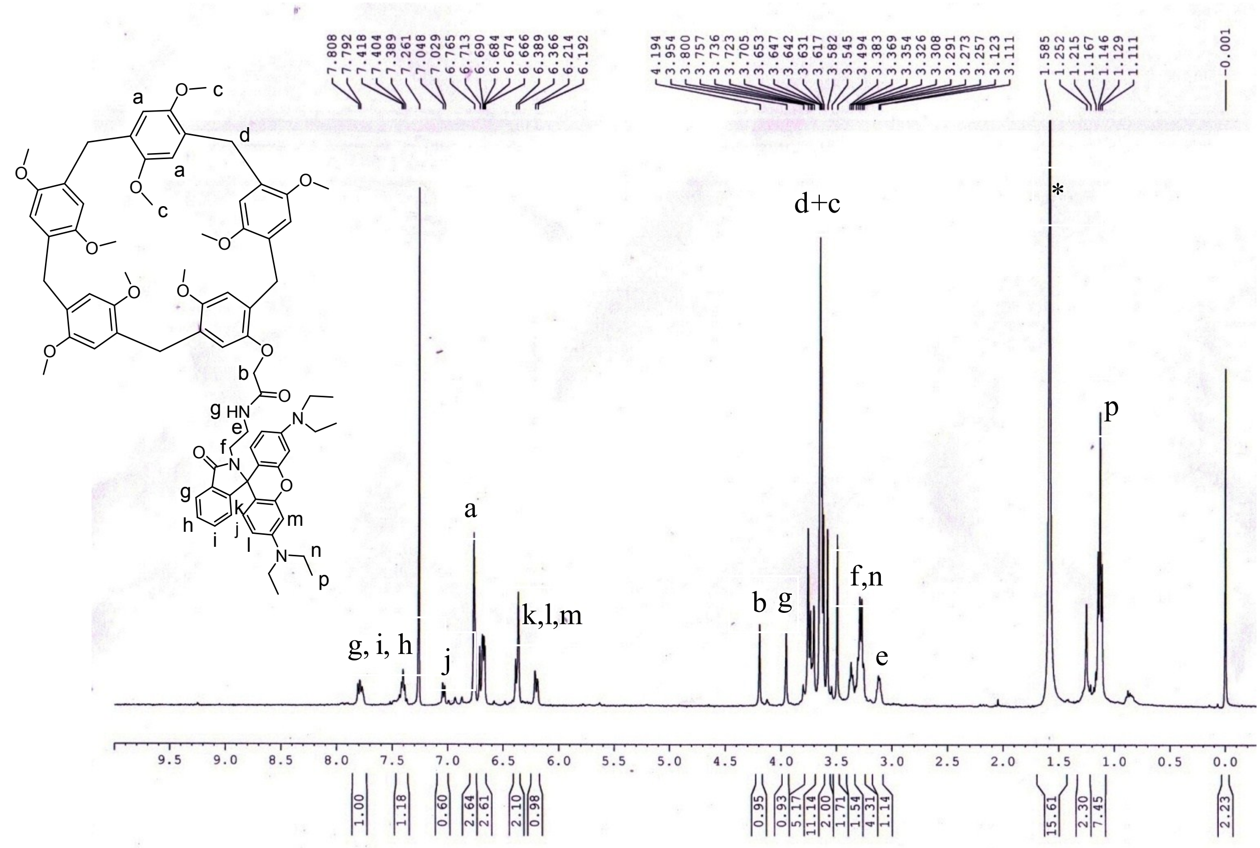


Figure S8. ^{1}H NMR spectrum of receptor **1** in $CDCl_3$ (* Represents the appearance of peak due to H_2O).

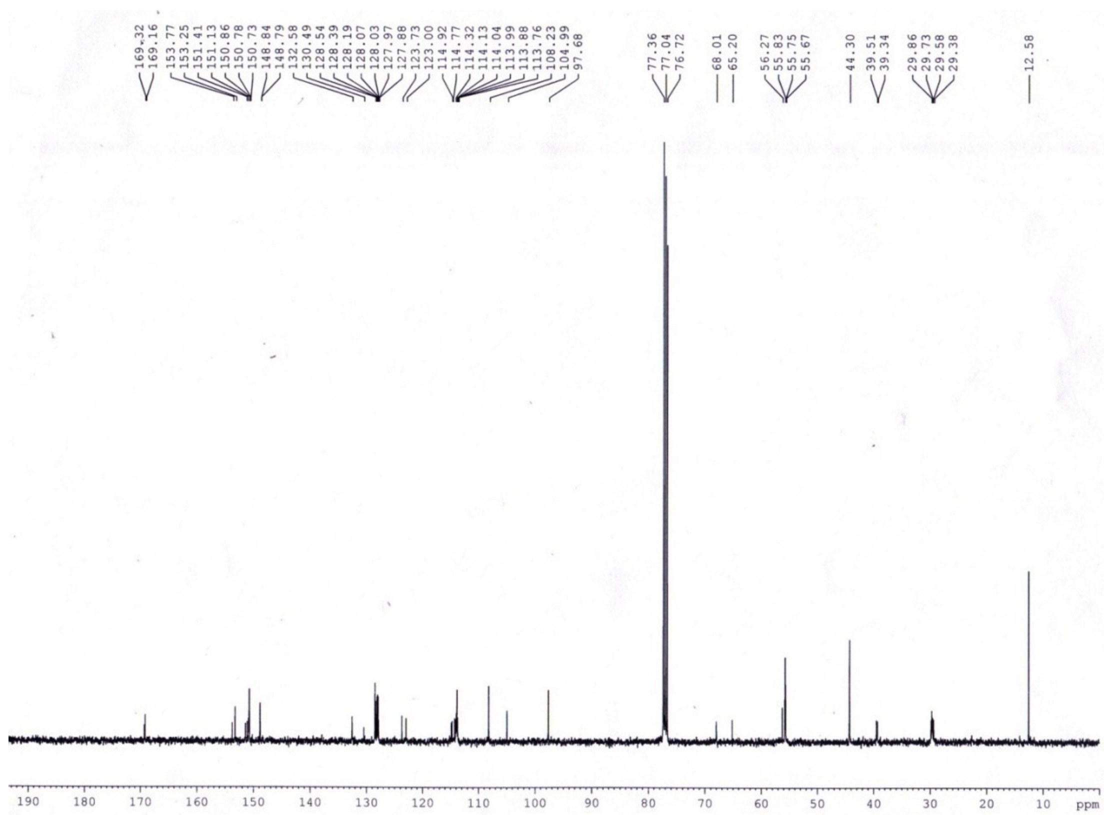


Figure S9. ^{13}C NMR spectrum of receptor **1** in $CDCl_3$.

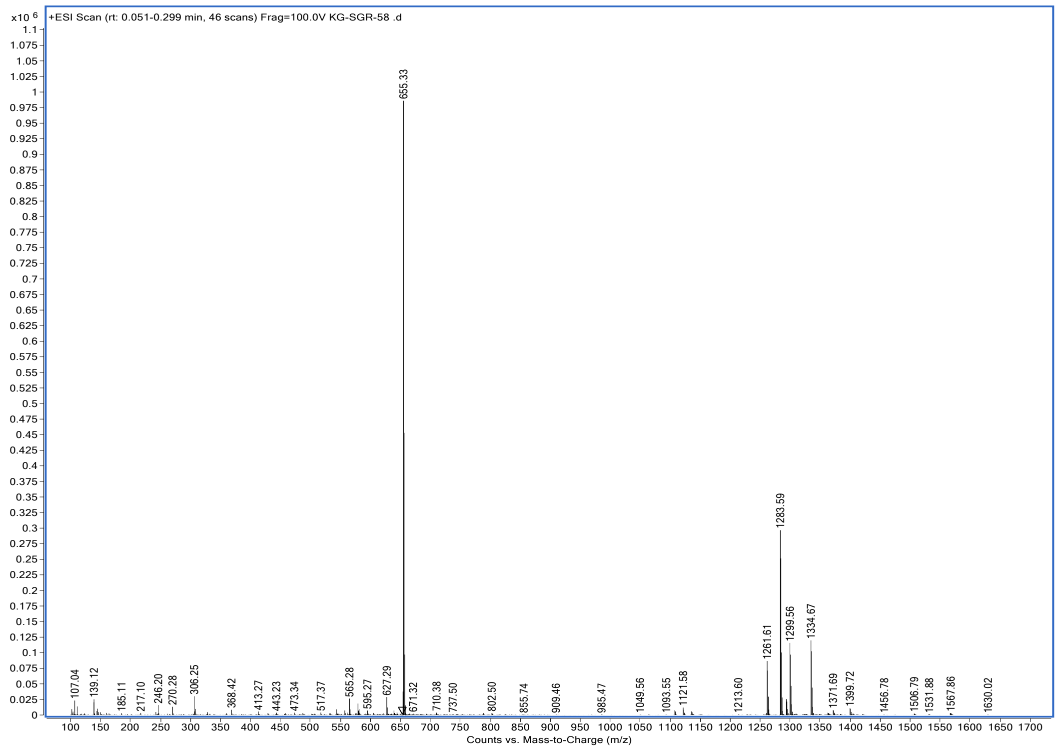


Figure S10. ESI MS of receptor **1.** Assignment of the main peak: *m*/*z* 1283.59 [M+ Na]$^+$ (30%).

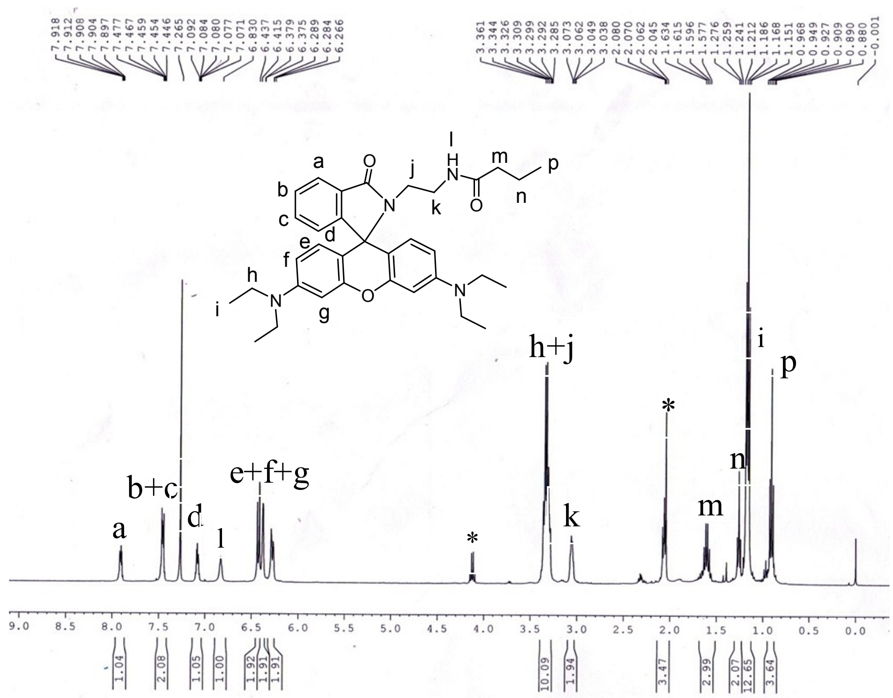


Figure S11. ^{1}H NMR spectrum of receptor **2** in $CDCl_3$.

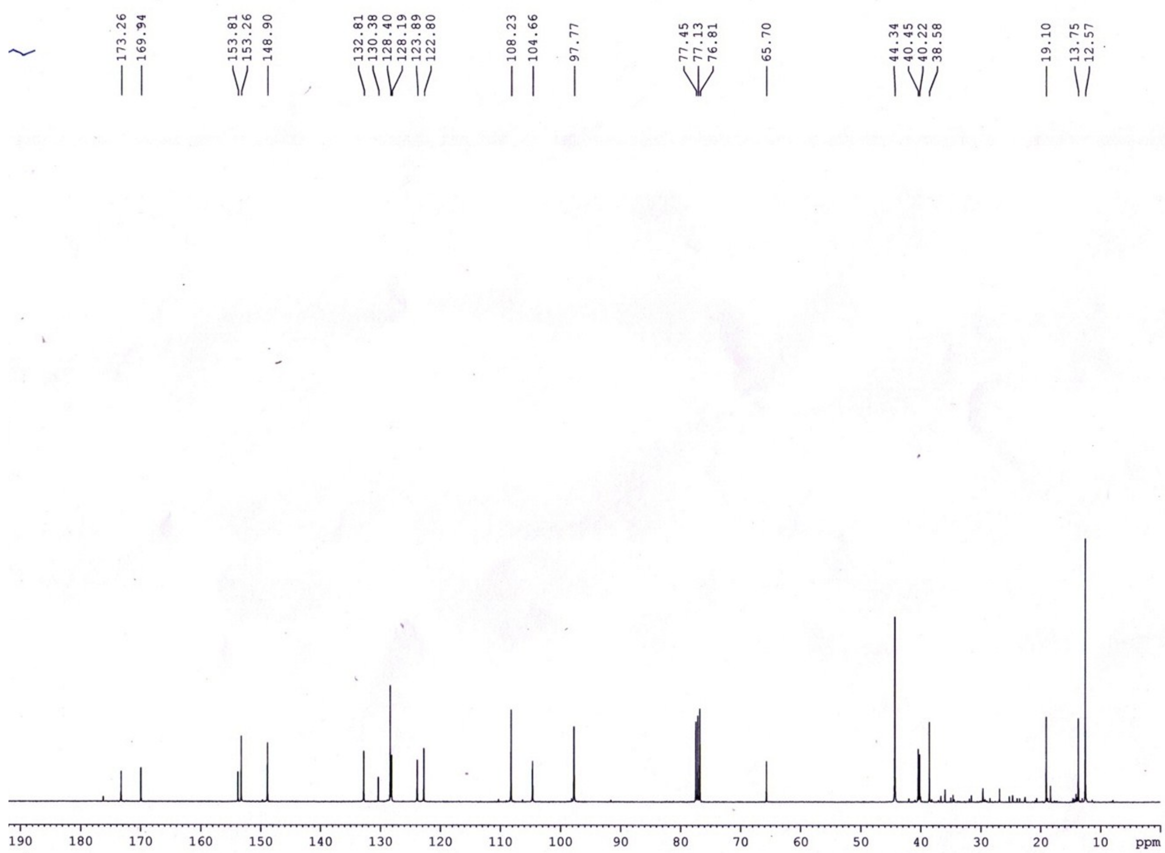


Figure S12. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

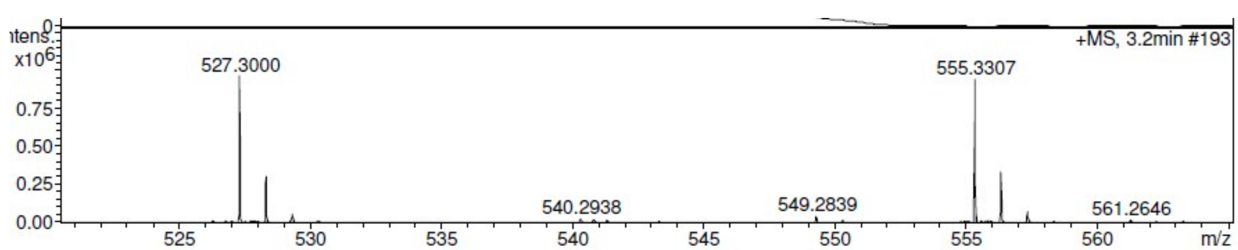


Figure S13. ESI-MS spectrum of compound **2**.

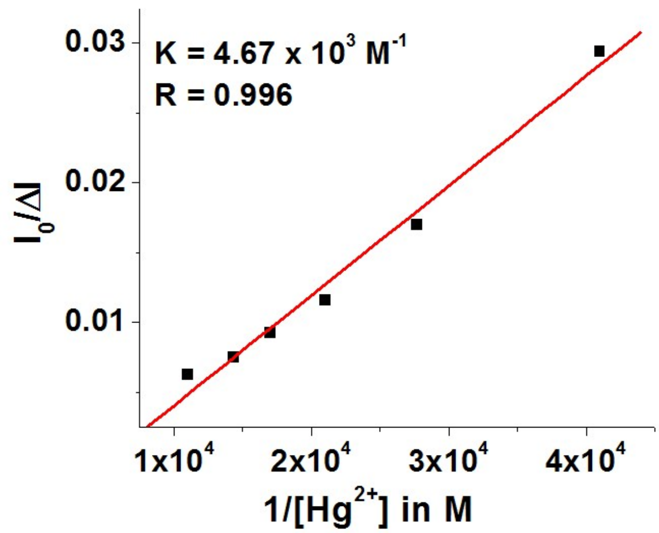


Figure S14. UV-Vis Benesi-Hilderband plot for receptor 1 with Hg^{2+} ([H] = [G] = 2.5×10^{-5} M).

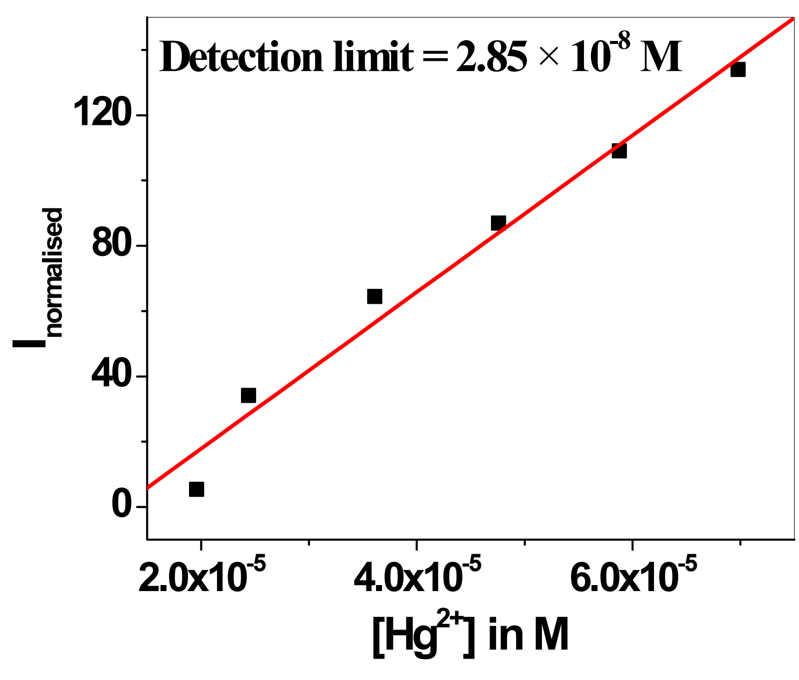


Figure S15. Linear binding constant curve for receptor **1** (c = 2.5×10^{-5} M) with Hg^{2+} (c = 1×10^{-3} M).

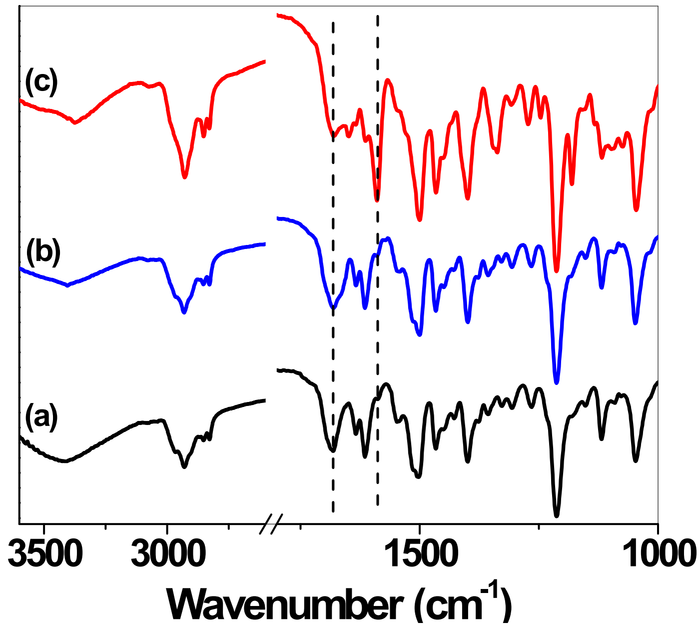


Figure S16. Partial IR spectrum of (a) receptor **1,** (b) receptor **1** in presence of equivalent amount of $Cu(ClO_4)_2$ and (c) receptor **1** in presence of equivalent amounts of $Hg(ClO_4)_2$.

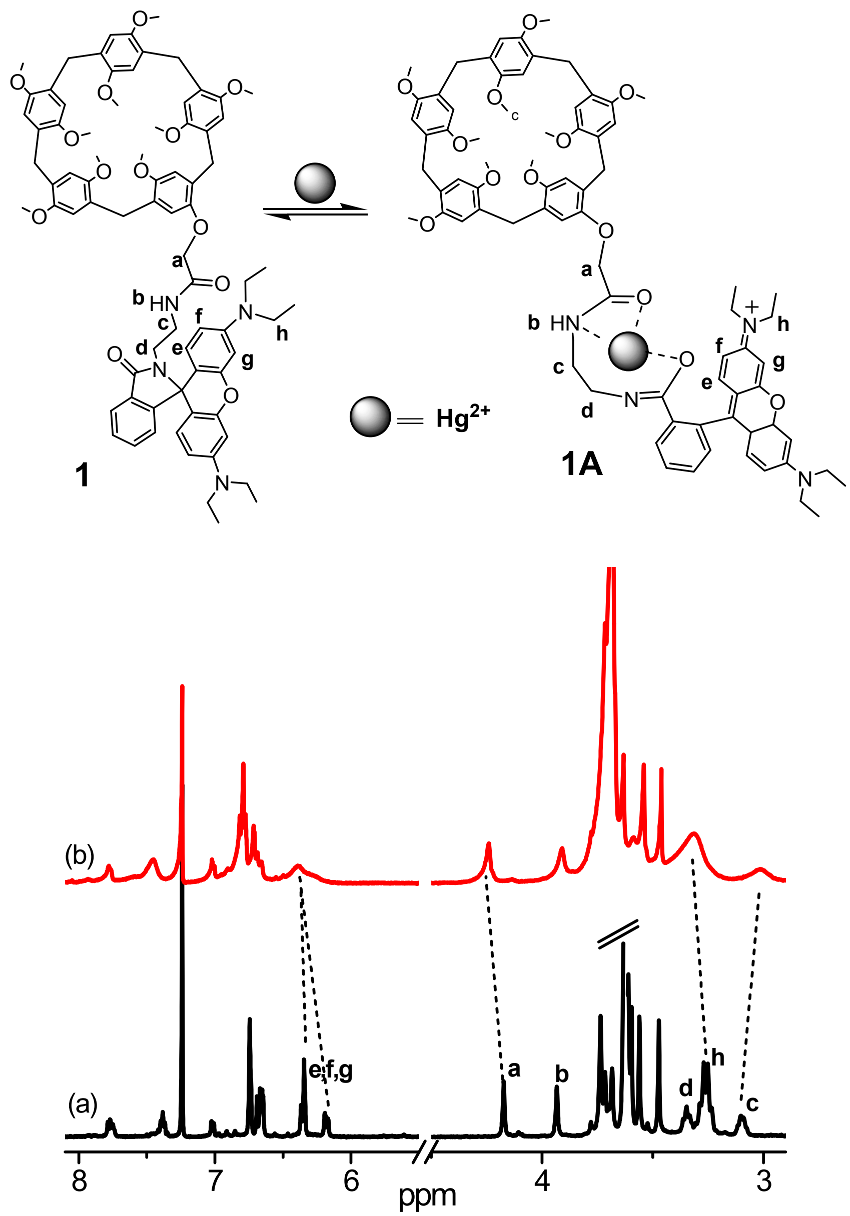


Figure S17. (a) Suggest mode of binding of receptor **1** with Hg^{2+}, and partial ^{1}H NMR spectra of receptor **1** ($c = 2.5 \times 10^{-3}$ M) (a) in absence and (b) presence of 1 equiv. of Hg^{2+} ion in $CDCl_3$.

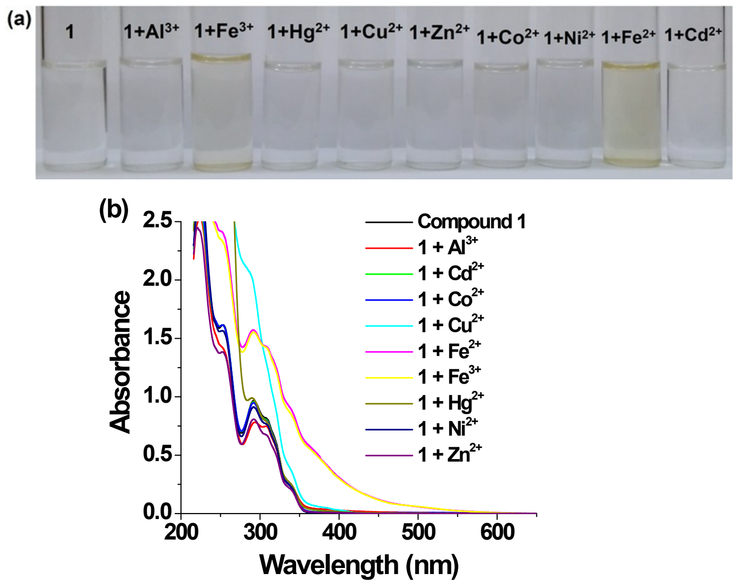
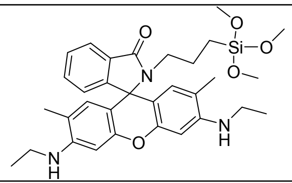
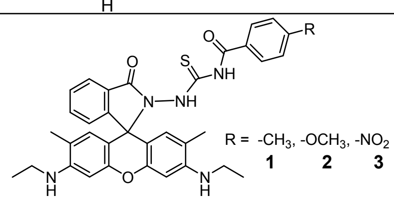
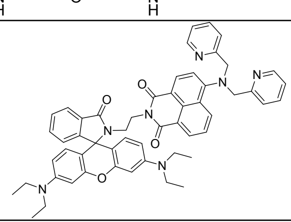
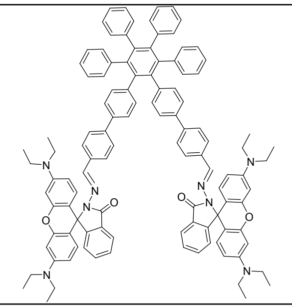
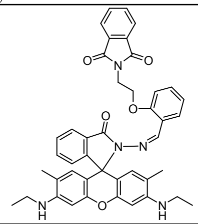
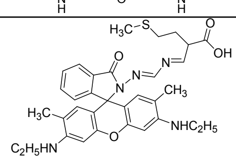
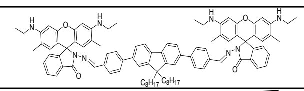
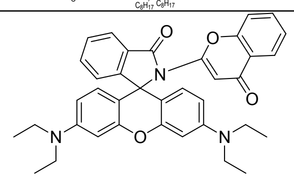
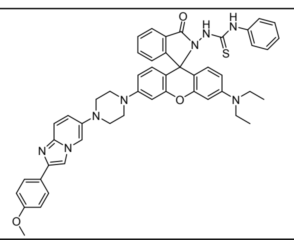
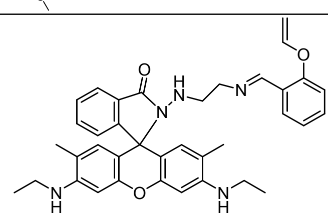
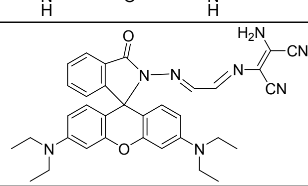
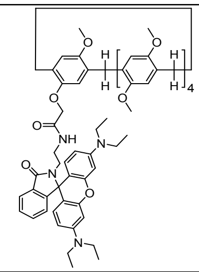


Figure S18: Color change of solution of compound **1** (c = 2.5 × 10^{-5} M) in CH_3CN-H_2O (3:1, v/v, 10 mM Tris-HCl Buffer, pH = 6.5) after addition of 50 equiv. amounts of different metal ions (taken as perchlorate salt); (b) Change in absorption spectra of **1** (c = 2.5 × 10^{-5} M) upon addition of 50 equiv. amounts of different metal ions in CH_3CN-H_2O (3:1, v/v, 10 mM Tris-HCl Buffer, pH = 6.5).

Table S1: Reported Rhodamine-based structures in Hg^{2+} sensing

Entry	Structure of compounds	Selectivity	Medium	Detection limit (M)	Ref.
1.		Hg^{2+} ion	Water/ethanol (1:4, v/v, PBS buffer, pH 7)	2.59 x 10^{-9}	1
2.		Hg^{2+} ion	DMF–H_2O (1:1, v/v, pH 7.2)	(**1**) 1.46×10^{-8} (**2**) 1.69×10^{-8} (**3**) 1.64×10^{-7}	2
3.		Hg^{2+} and Fe^{3+} ion	EtOH/PBS buffer (1:1, v/v,pH 7.4)	2.72 × 10^{-6}	3

4.		Hg^{2+} ion	HEPES/CH_3CN (1:1, pH 7.0)	1×10^{-7}	4
5		Hg^{2+} ion	CH_3CN/H_2O (7:3 v/v) in HEPES buffer at pH 7.2	1.62×10^{-9}	5
6.		Hg^{2+} ion	CH_3CN/H_2O (1:1, v/v, 10 mM, Tris-HCl buffer pH 7.04)	2.63×10^{-8}	6
7.		Hg^{2+} ion	DMF:H_2O (2:8, v/v).	7.48×10^{-9}	7
8.		Dual detection of Al^{3+} and Hg^{2+} ion	CH_3CN/H_2O (3:1, v/v; 10 mM HEPES buffer ; pH = 6.85	1.9×10^{-7} for Al^{3+} ion and 1.26×10^{-7} ion for Hg^{2+} ion	8
9.		Hg^{2+} ion	PBS/C_2H_5OH (9/1, v/v)	9.1×10^{-9}	9
10.		Hg^{2+} ion	$CH_3CN:H_2O$ (3:7)	136×10^{-7}	10
11.		Ga^{3+} and Hg^{2+} ion	methanol−HEPES (1:1, v/v, pH 7.0)	6.34×10^{-9} for Hg^{2+} 3.52 $\times 10^{-9}$ for Ga^{3+}	11

12.		Hg^{2+} ion	CH_3CN	2.85×10^{-8}	Present work

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