Supplementary Information

An efficient naphthalimide based receptor for selective detection of $Hg^{2+}$and Pb^{2+}ions

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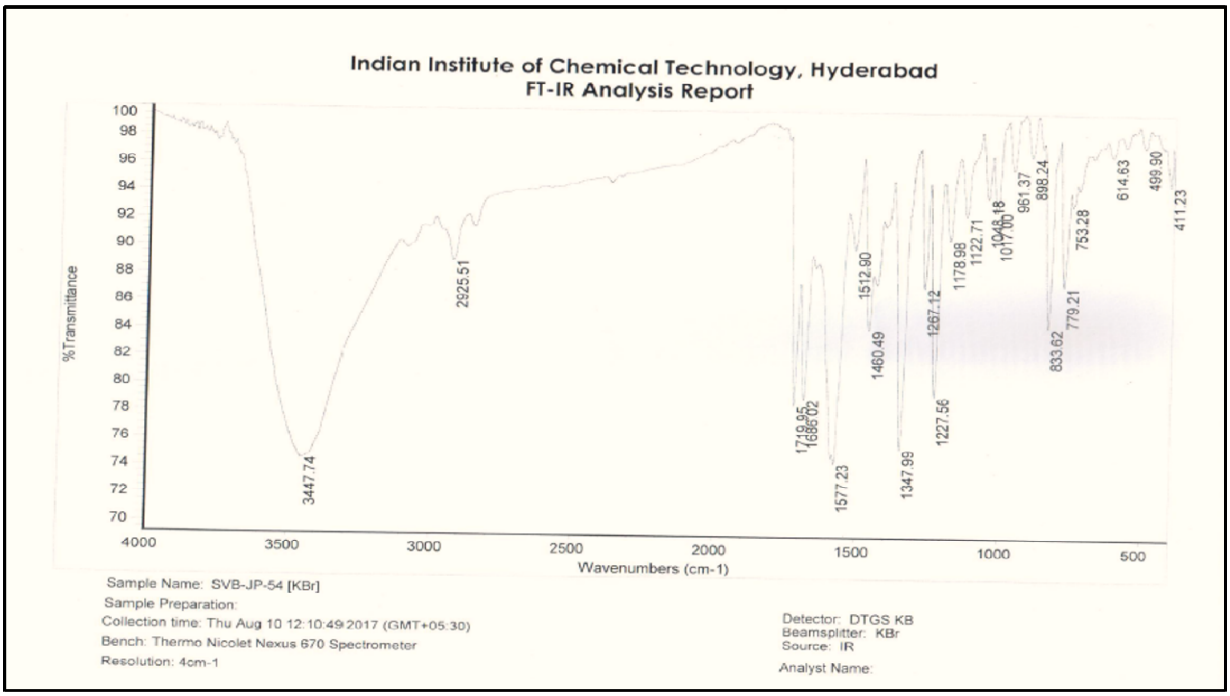

Figure S1. FT-IR of compound **C.**

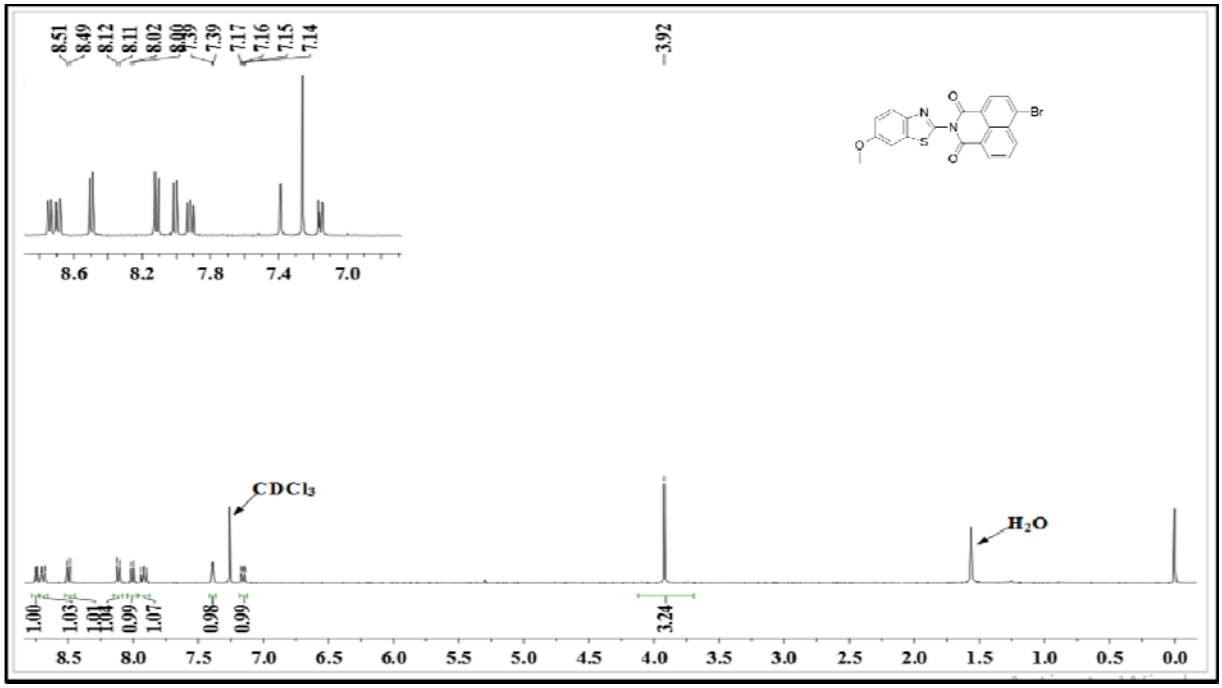

Figure S2.[1]HNMR spectra ofcompound **C**in $CDCl_3$**.**

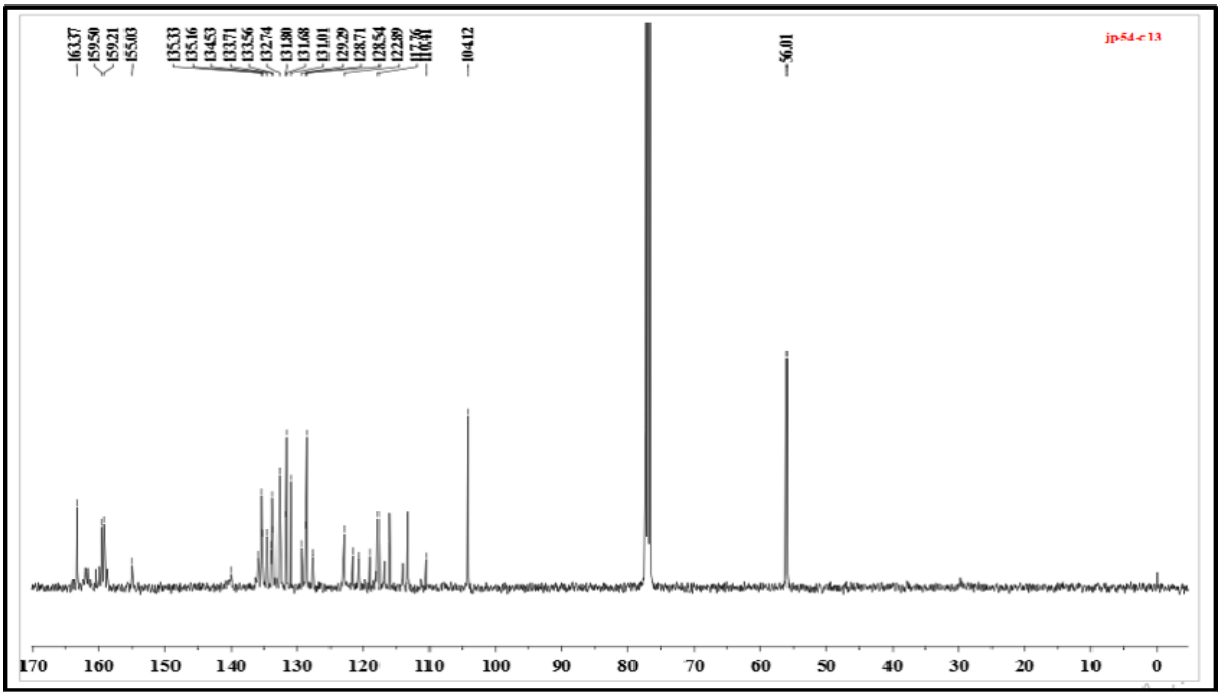

Figure S3. ^{13}CNMR spectra ofcompound **C**in $CDCl_3$**.**

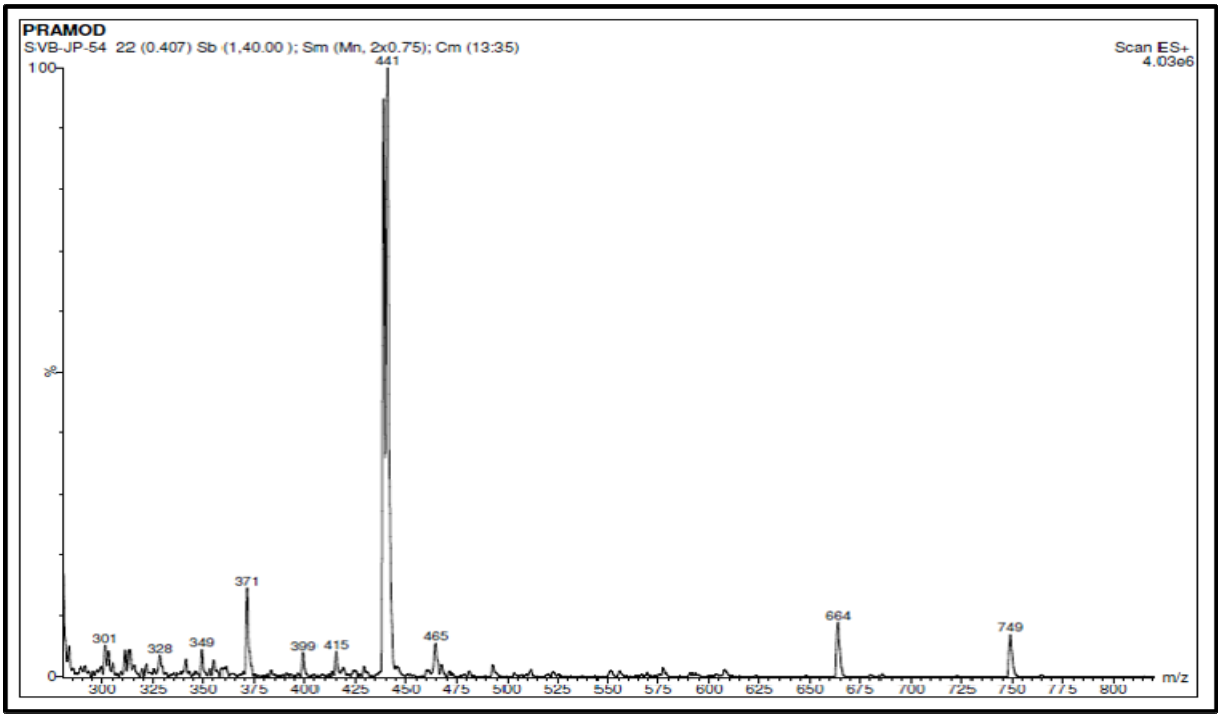

Figure S4. ESI-MASS spectrum of compound **C.**

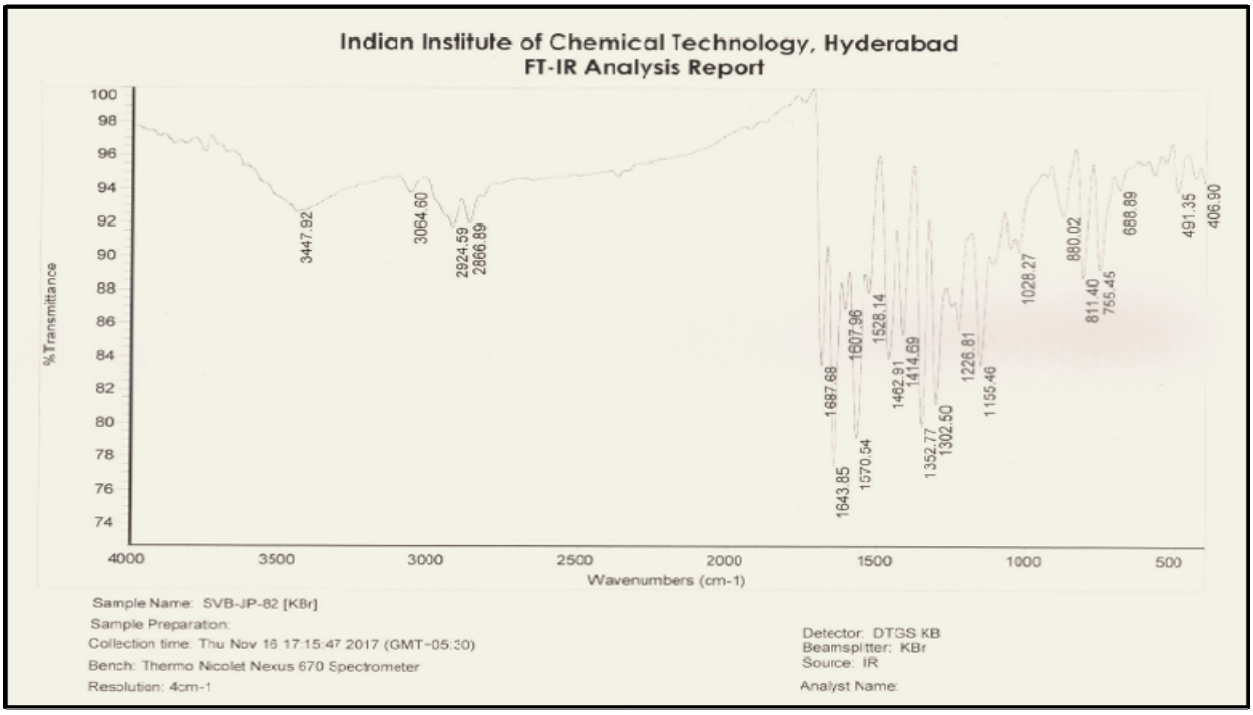

Figure S5. FT-IR spectra of receptor **1.**

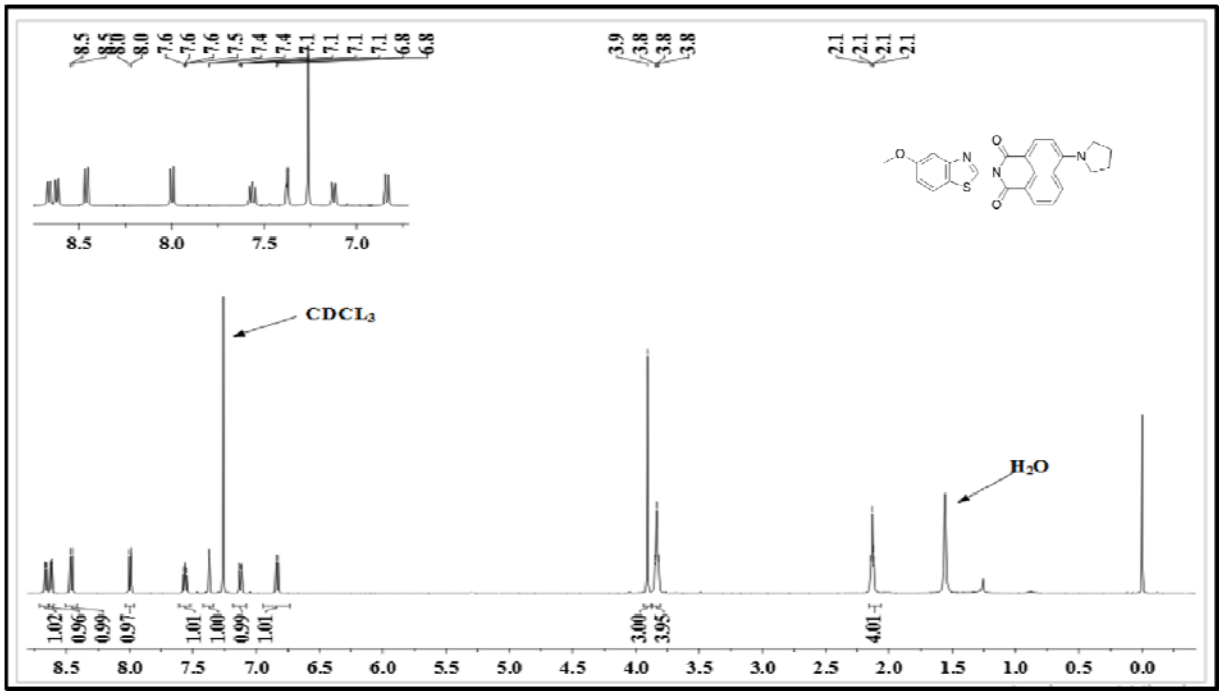

Figure S6. ^{1}HNMR spectra of receptor **1**in $CDCl_3$**.**

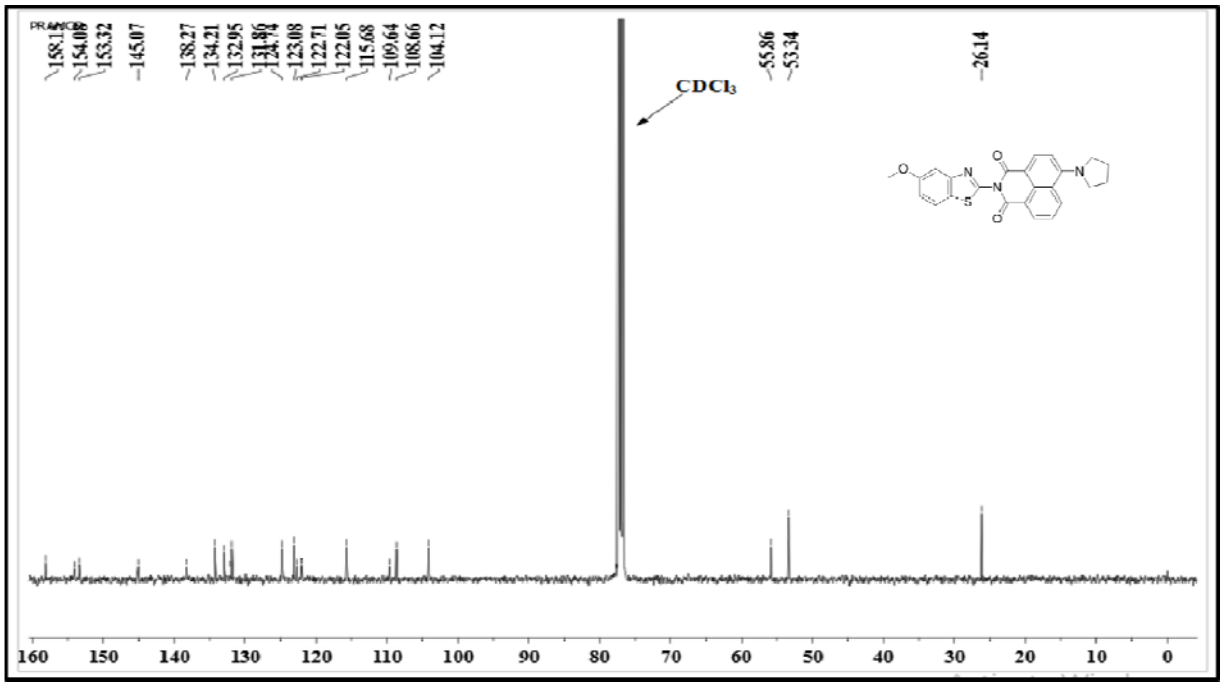

Figure S7. ^{13}CNMR spectra of receptor **1**in $CDCl_3$**.**

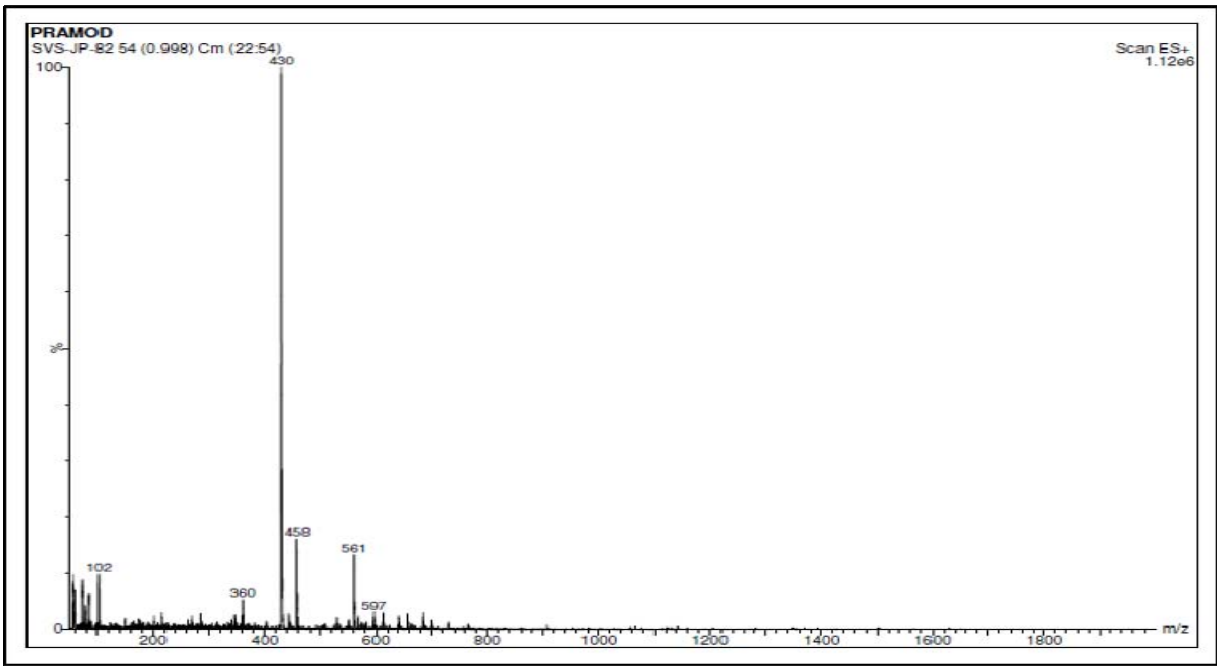

Figure S8. ESI-MASS spectrum ofreceptor **1.**

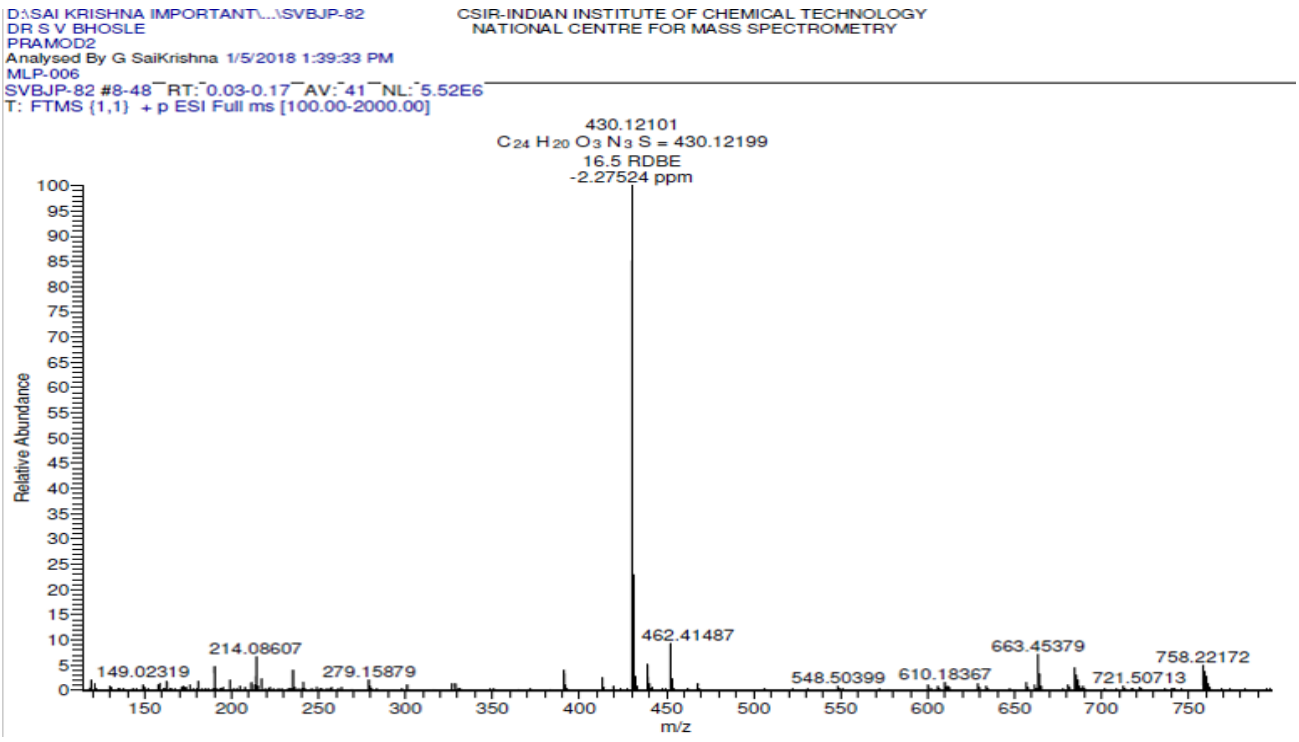

Figure S9.HRMSspectrumof receptor **1.**

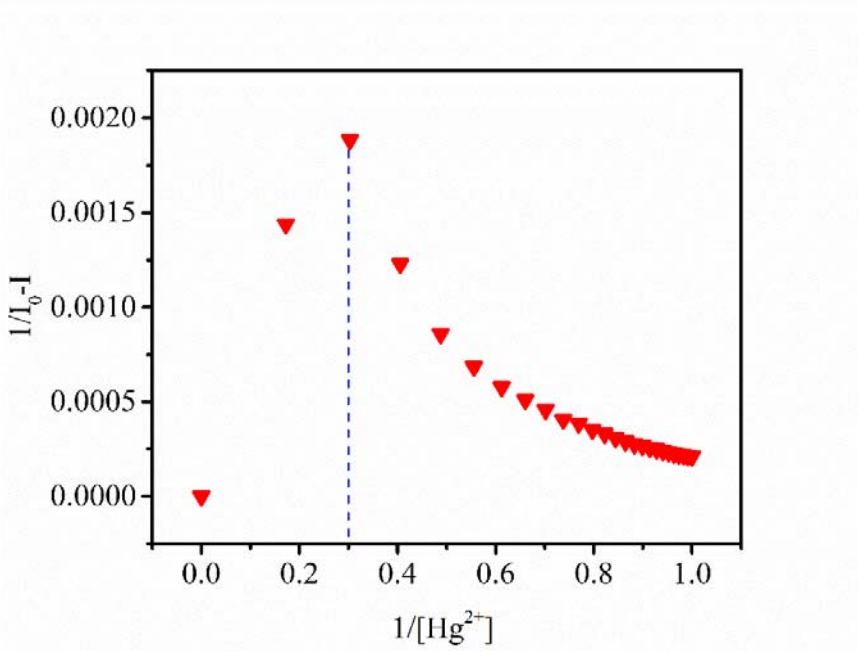

Figure S10. Job's plot for **1** with analyte Hg^{2+} at 600 nm. (λ_{ex} = 460 nm)

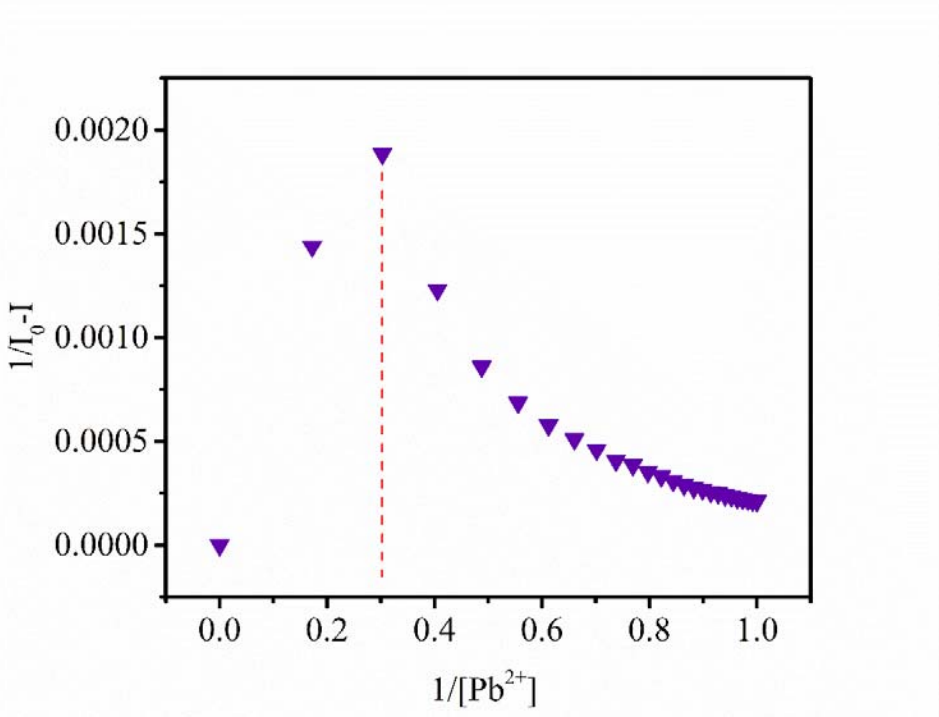

Figure S11. Job's plot for **1** with analyte Pb^{2+} at 600 nm (λ_{ex} = 460 nm)

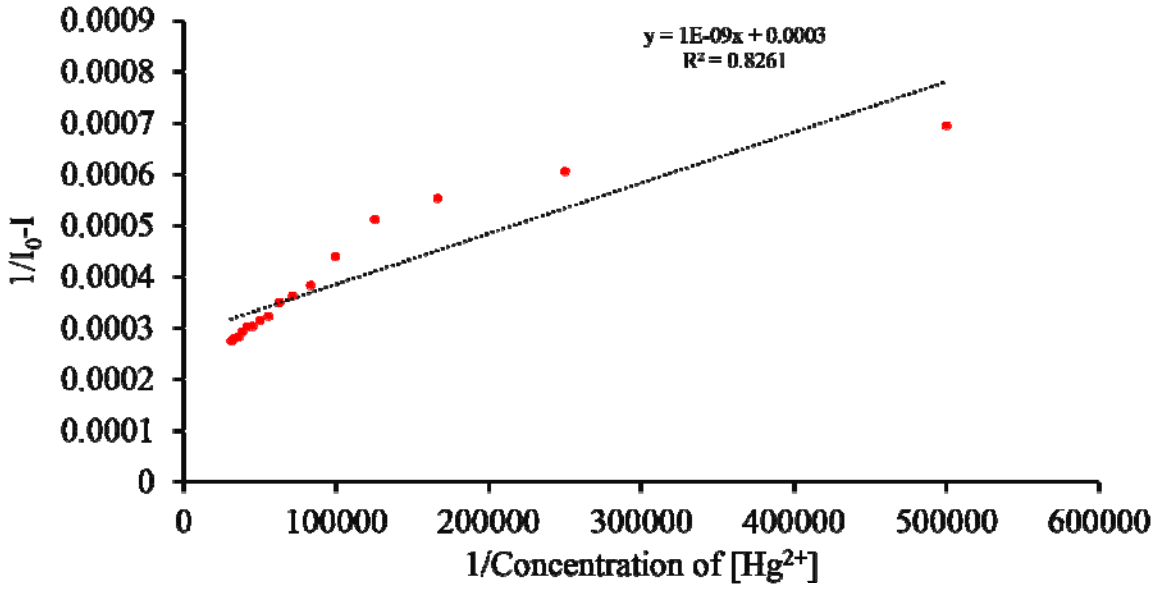

Figure S12. Benesi-Hildebrand plot of receptor **1** in presence of Hg^{2+}.

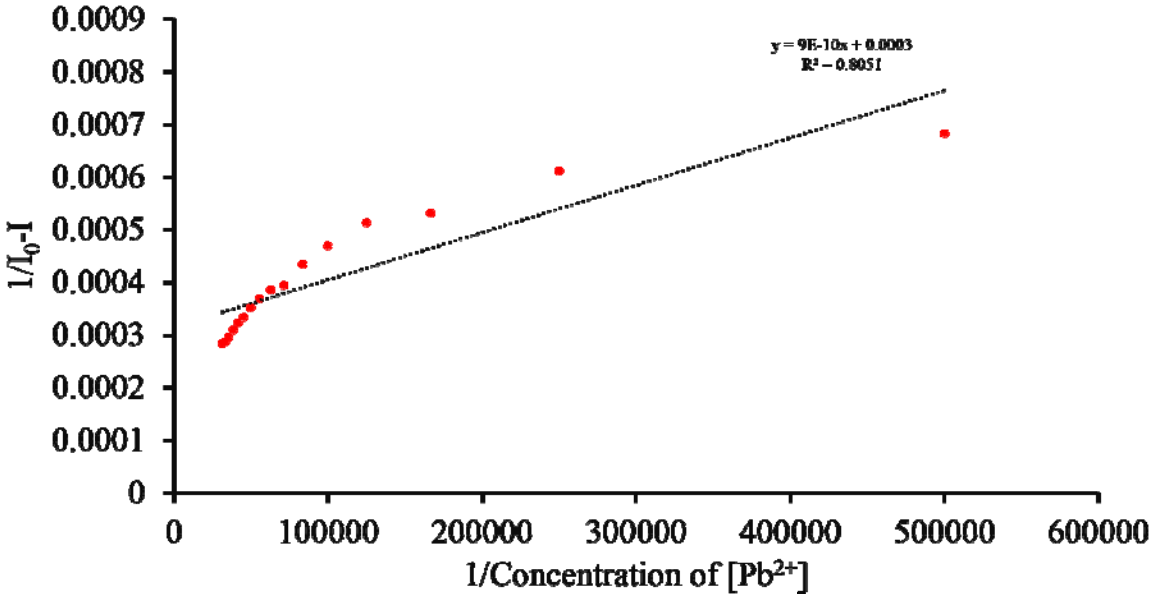

Figure S13. Benesi-Hildebrand plot of receptor **1** in presence of Pb^{2+}.

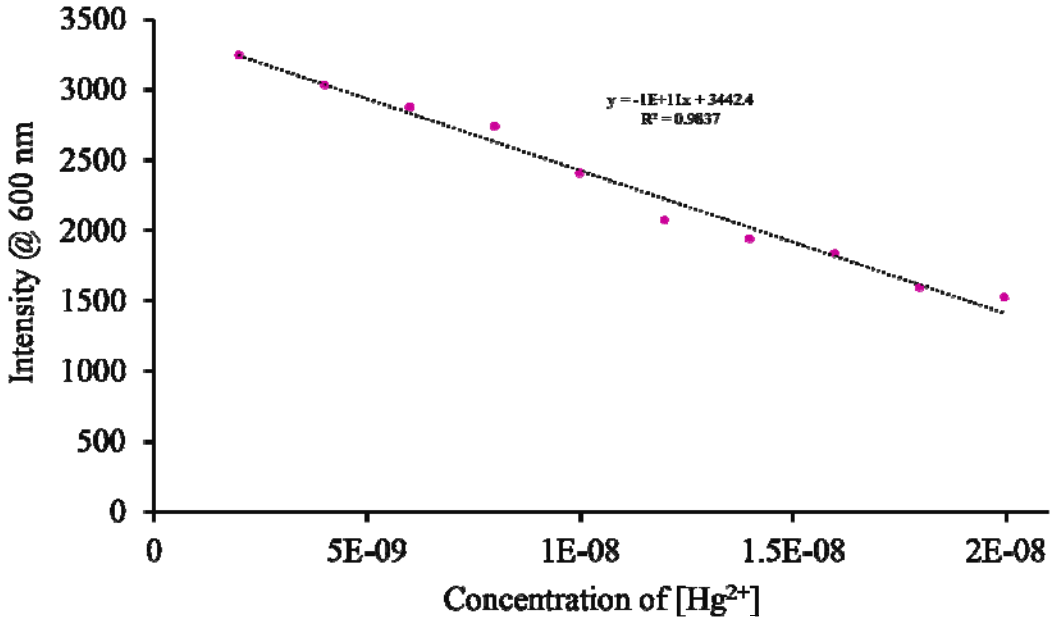

Figure S14. Calibration curve of receptor **1** in acetonitrile solution with the addition of increasing concentration ofHg^{2+}.

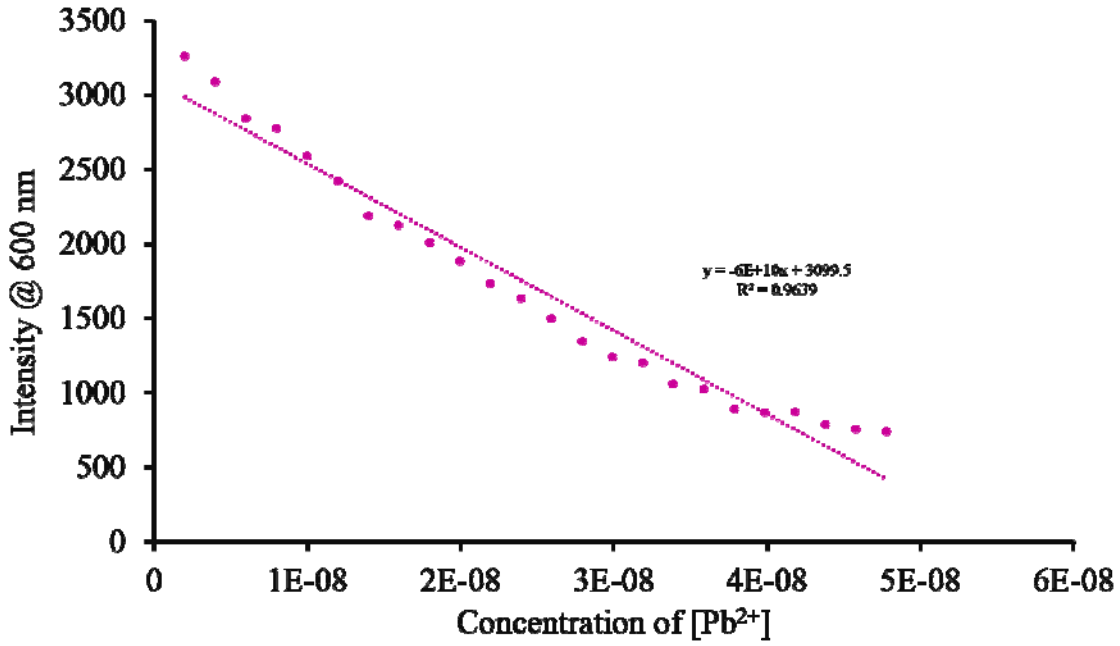

Figure S15. Calibration curve of receptor **1** in acetonitrile solution with the addition of increasing concentration ofPb^{2+}.

Table S1: Fluorescent sensor forHg^{2+} and Pb^{2+} analytes based on organic chromophores.

Analyte (ions)	**Organic Chromophores**	**Solvent**	**LOD**	**Ref.**
Hg^{2+}	Coumarin	HEPS buffer solution (20 mM HEPES, pH 7.2, EtOH:H_2O = 1:1, *v/v*)	1×10^{-5} M	1
Hg^{2+}	Rhodamine B derivatives	DMSO-HEPES buffer (0.02 mol/L, pH 7.4; *v/v* = 6:4) Milli-Q water	2.36×10^{-6} M	2
Hg^{2+}	Non-sulfur rhodamine derivatives	Acetonitrile	2×10^{-7} M	3
Hg^{2+}	Rhodamine C	HEPS buffer solution (20 mM HEPES, pH 7.0, EtOH:H_2O = 7:3, *v/v*)	7.4×10^{-8} M	4
Hg^{2+}	Fluorescein and rhodamine B	Dichloromethane	2.02×10^{-8} M	5
Hg^{2+}	Rhodol-coumarin	MeOH:H_2O = 1:1, *v/v*)	5.5×10^{-9} M	6
Hg^{2+}	Dansyl-Met-NH_2	HEPS buffer solution (10 mM HEPES, pH 7.4)	5×10^{-9} M	7
Pb^{2+}	1,3,6-trihydroxy xanthone	DMSO:H2O solution (2:1 ratio, *v/v*)	1.8×10^{-7} M	8
Pb^{2+}	Rhodamine hydroxamate derivative	HEPS buffer solution (10 mM HEPES, pH 6.5)	2.5×10^{-7} M	9
Pb^{2+}	BODIPY fluorophore	PBS buffer (0.1 M, pH 7.2)	1.34×10^{-8} M	10
Pb^{2+}	Rhodamine trimethoxy benzaldehyde conjugate derivative	HEPS buffer solution (pH 7.54)	1.5×10^{-8} M	11
Pb^{2+}	Rhodamine 6G derivatives	HEPS buffer solution (10 mM	2.7×10^{-9} M	12

		HEPES, pH 7.4)		
Pb^{2+}	Coumarin	Phosphate buffer (20 mM, 1:9 DMSO/H_2O (*v/v*), pH 8.0	1.9×10^{-9} M	13
Pb^{2+}	Coumarin	HEPES buffer solution (CH_3CN:H_2O = 95:5, v/v, 10 mM, pH 7.2)	3.36×10^{-11} M	14
Hg^{2+} and Pb^{2+}	Rhodamine 6G hydrazide	HEPS buffer solution (10 mM HEPES, pH 7.2, EtOH:H_2O = 9:1, *v/v*)	Hg^{2+} =1.6×10^{-8} M Pb^{2+} = 1.2×10^{-8} M	15
Hg^{2+} and Pb^{2+}	Benzothiazole-naphthalimide-pyrrolidine conjugate	Acetonitrile	Hg^{2+} = 7.44×10^{-10} M Pb^{2+} = 1.26×10^{-9} M	This work

Table S2. The singlet electronic transitions of **1** as calculated using TD-DFT at B3LYP def2-TZVP def2/J RIJCOSX level of theory.

	Excited states	E (nm)	f_{Osc}
1	HOMO→LUMO (87%)	446.3	0.35124
2	H-1→LUMO (100%)	510.1	0.00004
3	HOMO→L+1 (99%)	408.9	0.00193
4	H-2→LUMO (97%)	393.1	0.00044
5	H-3→LUMO (40%), HOMO→L+3 (55%)	307.5	0.00438
6	HOMO→L+2 (81%)	298.2	0.55728
7	H-5→LUMO (90%)	303.7	0.00148
8	H-4→LUMO (50%), H-3→LUMO (18%), HOMO→L+3 (17%)	282.1	0.08390

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