Supporting Information

Fluorometric Sensing of Hg^{2+} ions in aqueous medium by nano-aggregates of a tripodal receptor

Ajnesh Singh[a,†], Simanpreet Kaur[b,†], Narinder Singh[a,*] Navneet Kaur [b,*]

[a] Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Panjab 140001, India.
[b] Centre for Nanoscience & Nanotecnology, Panjab University, Chandigarh, 160014, India.

[†] both authors have equal contributed

∗ Corresponding author: E-mail address; nsingh@iitrpr.ac.in (N. Singh), navneetkaur@ pu.ac.in (N. Kaur), Tel.: +91 1881242176/+91-1722534464.

Table of contents

Figure S1. FT IR spectrum of compound **1**.

Figure S2. ^{1}H NMR spectrum of compound **1**.

Figure S3. ^{13}C NMR spectrum of compound **1**.

Figure S4. ESI Mass spectrum of compound **1**.

Figure S5. FT IR spectrum of compound **2**.

Figure S6. ^{1}H NMR spectrum of compound **2**.

Figure S7. ^{13}C NMR spectrum of compound **2**.

Figure S8. ESI Mass spectrum of compound **1**.

Figure S9: Effect of water content (0-100%) on the formation of nanoparticles.

Figure S10. Determination of LOD

Figure S11. Fluorescence spectra of nano-aggregates **N1** on addition on various tetrabutylammonium anions (F^-, Cl^-, Br^-, I^-, PO_4^{3-}, ClO_4^-, HSO_4^-, CN^- and CH_3COO^-).

Figure S12. Fluorescence spectra of nano-aggregates **N2** on addition on various tetrabutylammonium anions (F^-, Cl^-, Br^-, I^-, PO_4^{3-}, ClO_4^-, HSO_4^-, CN^- and CH_3COO^-).

Figure S13. Fluorescence spectra of nano-aggregates **N1** at different pH values.

Figure S14. Fluorescence spectra of nano-aggregates **N1**at different concentrations of TBA nitrate to evaluate the salt effect.

Figure S15. ESI Mass spectrum of complex [**1**.Hg^{2+}.$(NO_3)_2$].H_2O.

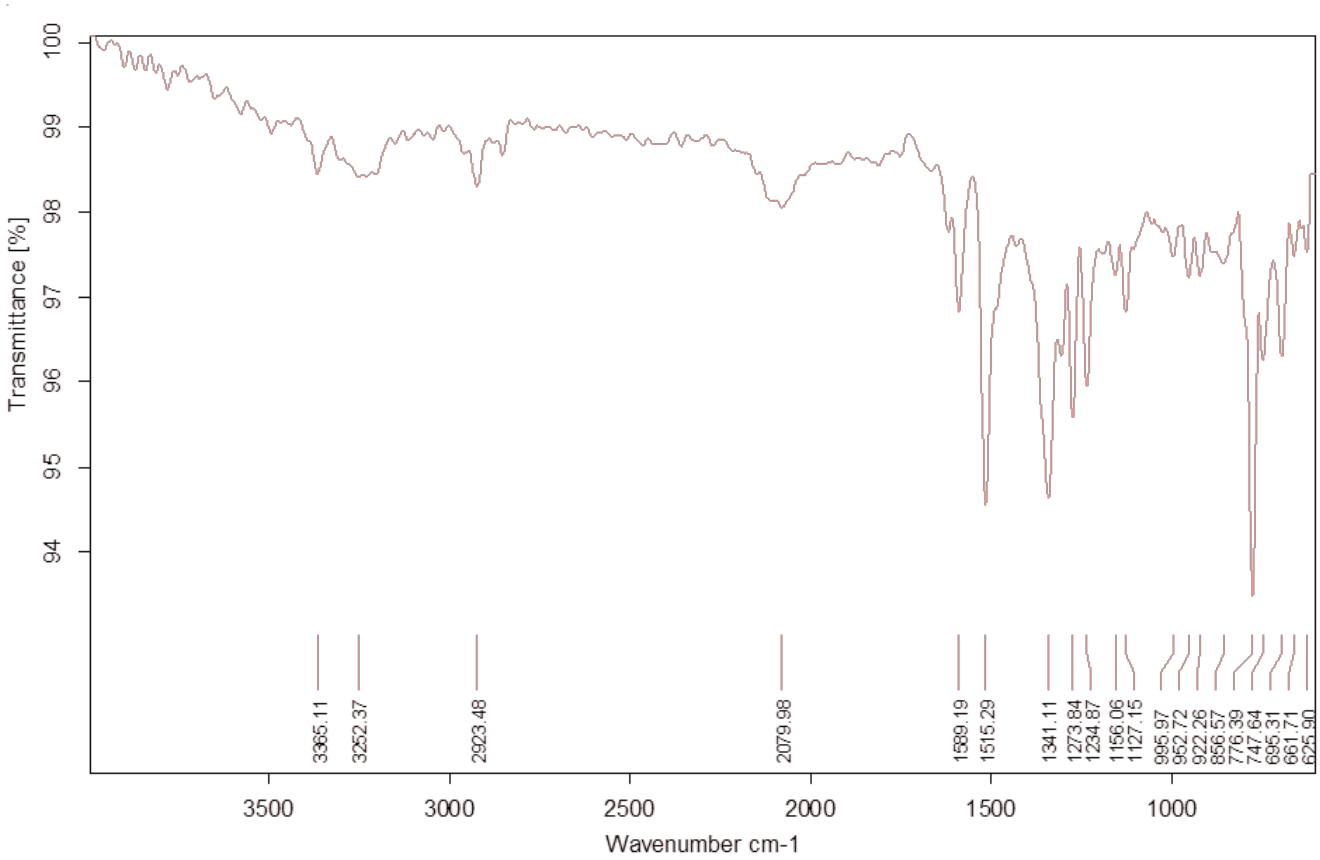

Figure S1. FT IR spectrum of compound **1**.

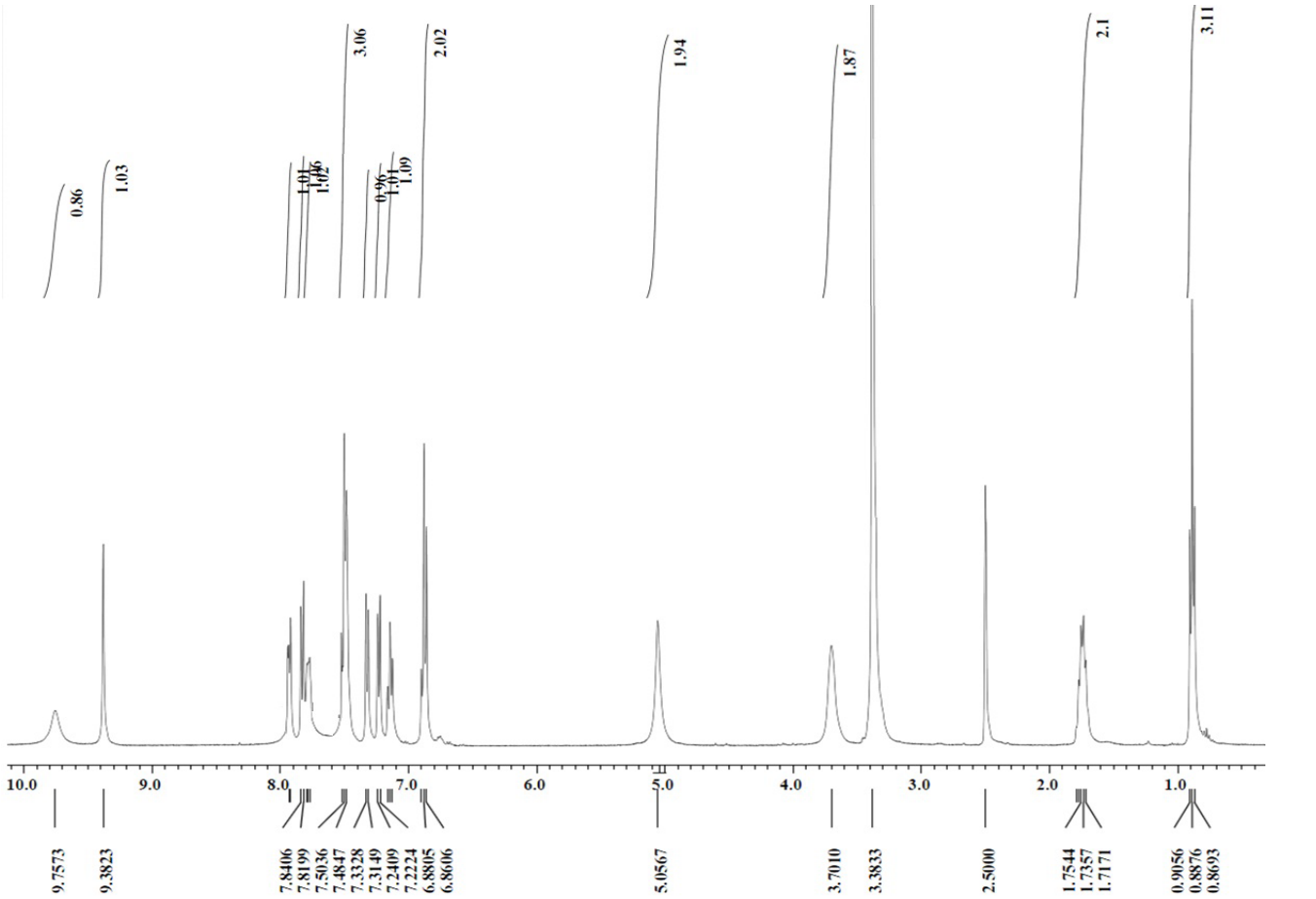

Figure S2. ^{1}H NMR spectrum of compound **1**.

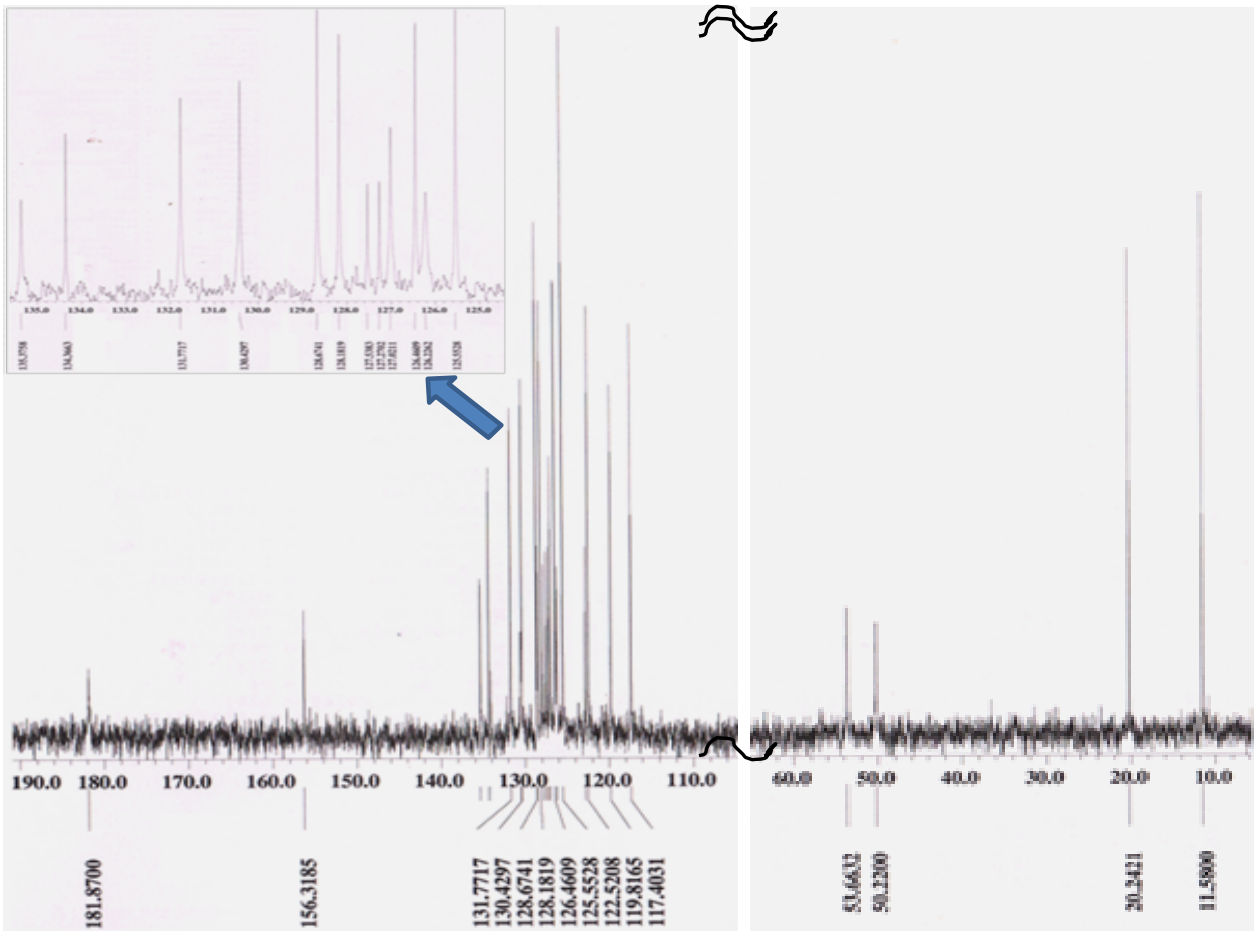

Figure S3. ^{13}C NMR spectrum of compound **1**.

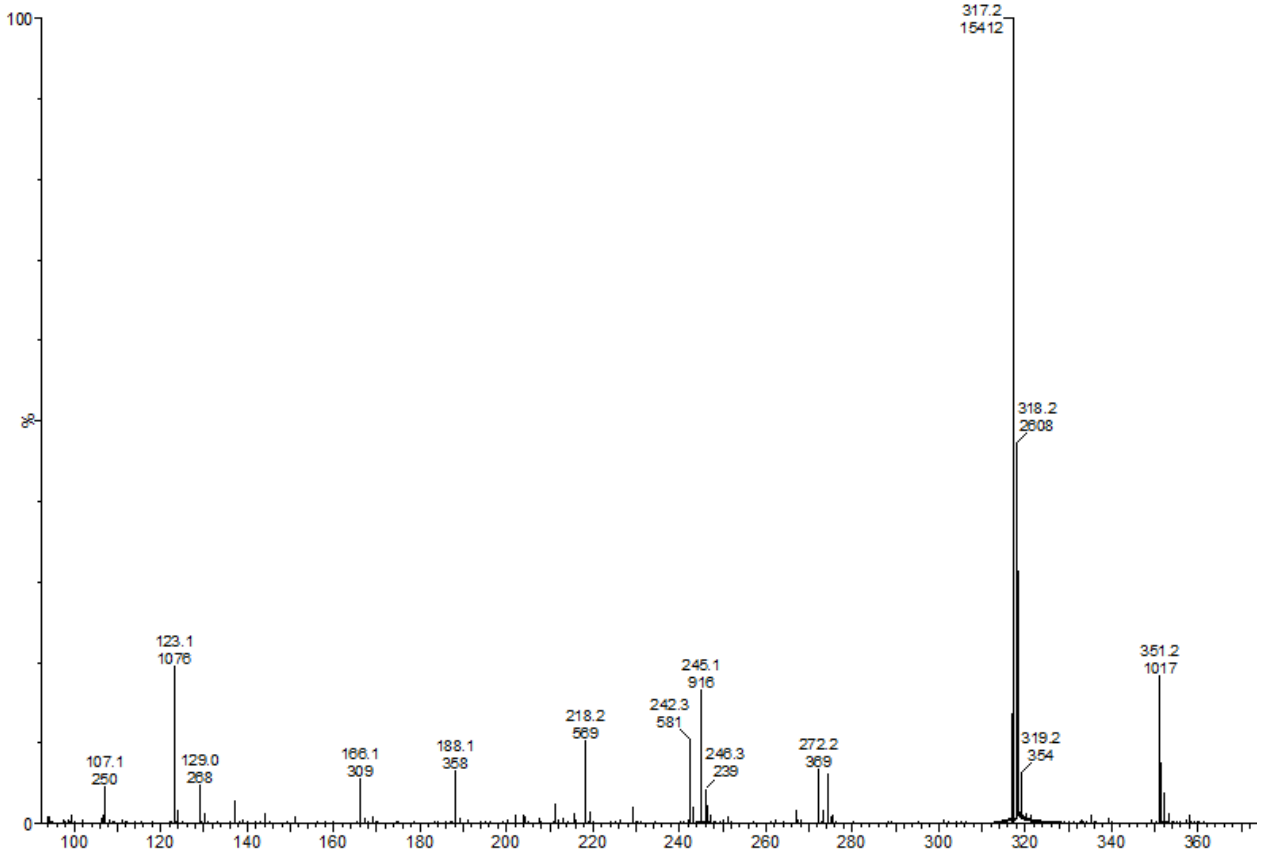

Figure S4. ESI Mass spectrum of compound **1**.

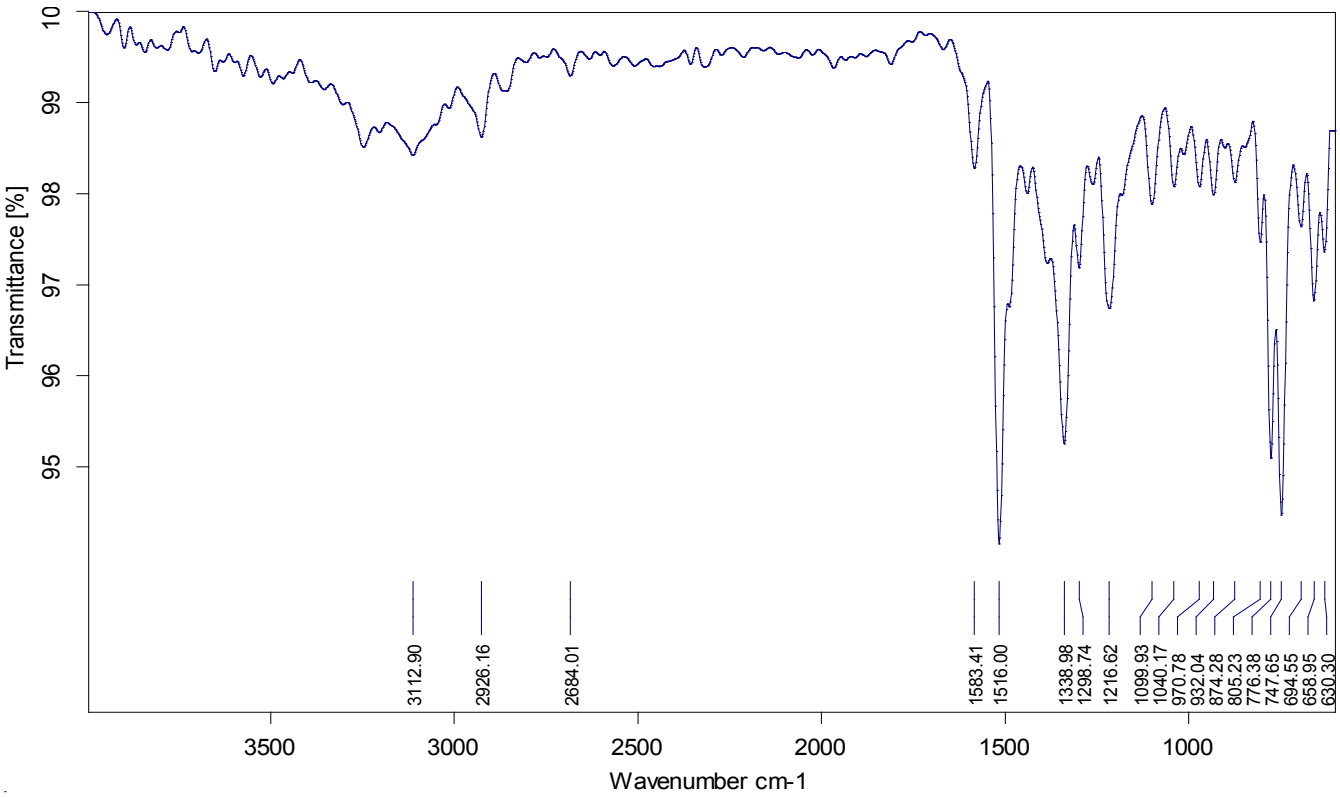

Figure S5. FT IR spectrum of compound **2**.

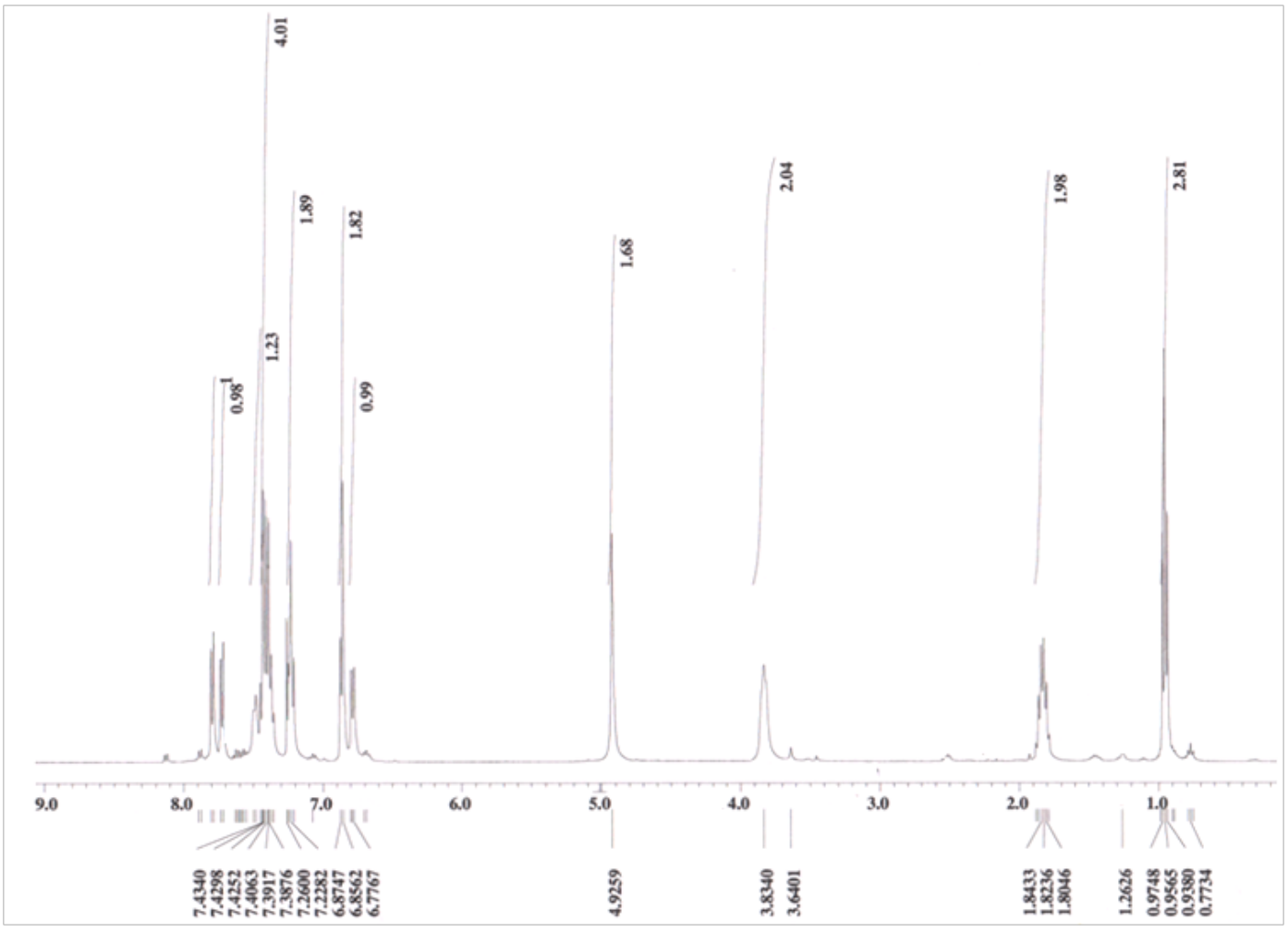

Figure S6. ^{1}H NMR spectrum of compound **2**.

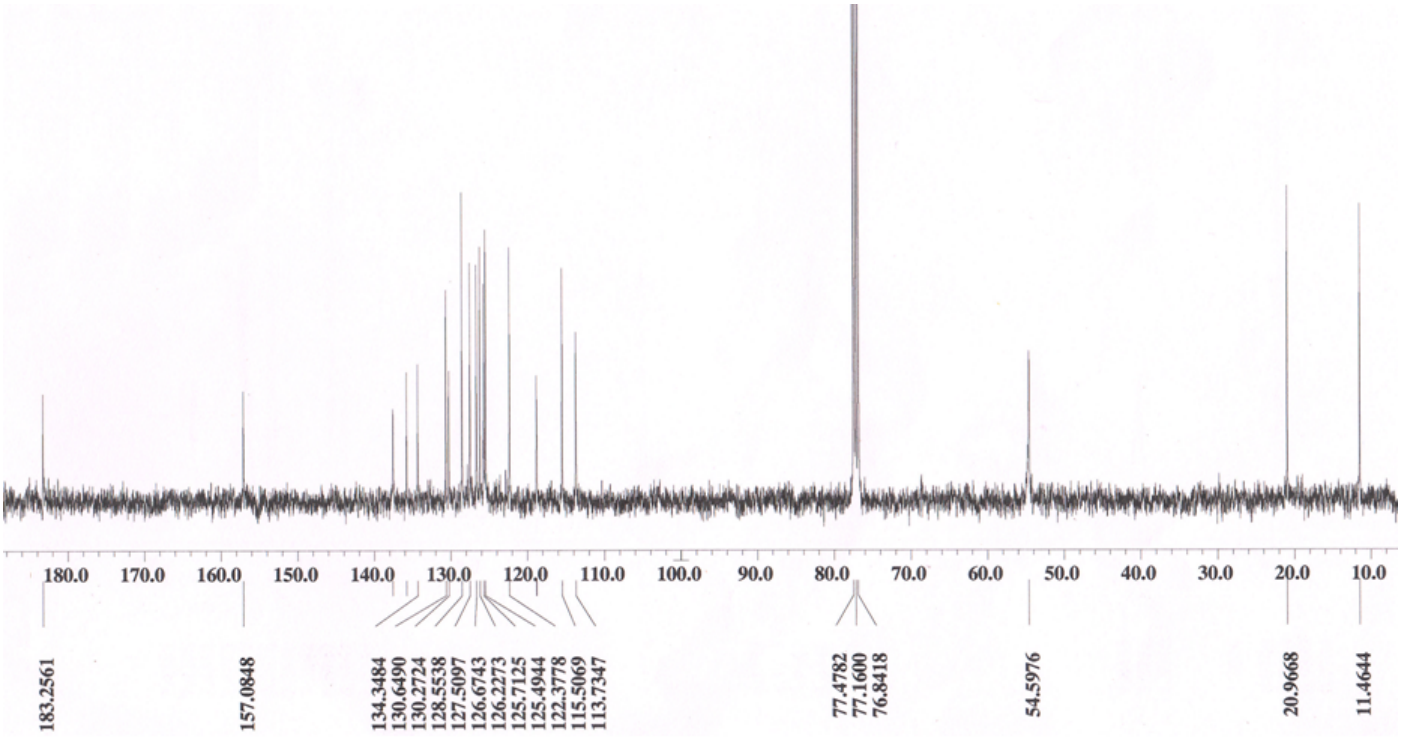

Figure S7. ^{13}C NMR spectrum of compound **2**.

Figure S8. ESI Mass spectrum of compound **2**.

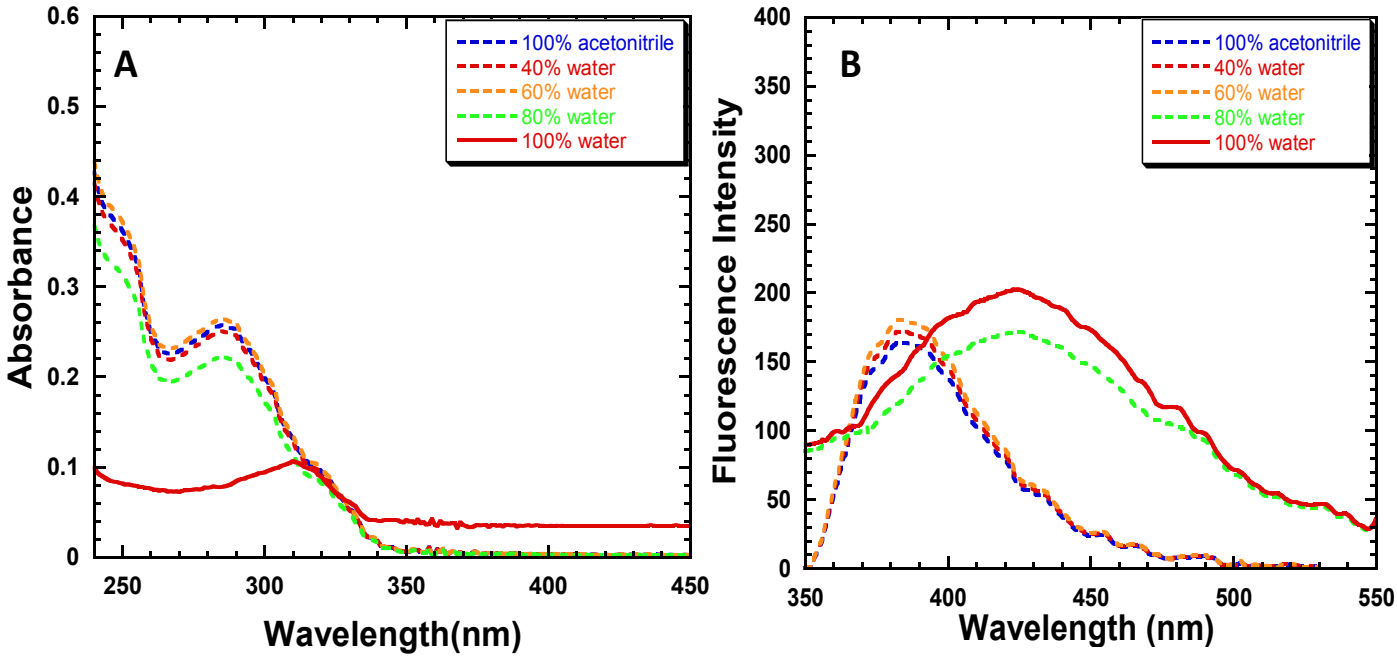

Figure S9: Effect of water content (0-100%) on the formation of nanoparticles.

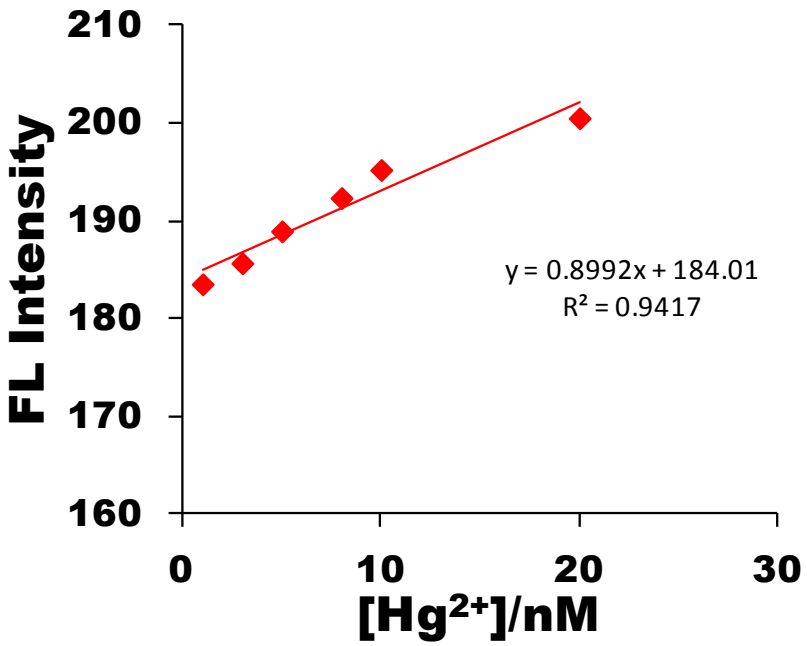

Figure S10. Fluorescence Intensity (380 nm, excited at 285nm) of nano-aggregates **N1**(25μM) as a function of Hg^{2+} concentration. The calibration curve in this concentration range is linear. The standard deviation (σ) of the emission intensity without any Hg^{2+} was determined to be 0.7237. Therefore, the detection limit was determined to be 2.41×10^{-9} M according to the 3σ method.

Determination of the detection limit.

The detection limit (DL) of nano-aggregates of **1** for Hg^{2+} was determined from the following equation:

$$DL = \frac{KS_{b1}}{S}$$

Where K = 3; *Sb1* is the standard deviation of the blank solution; *S* is the slope of the calibration curve.

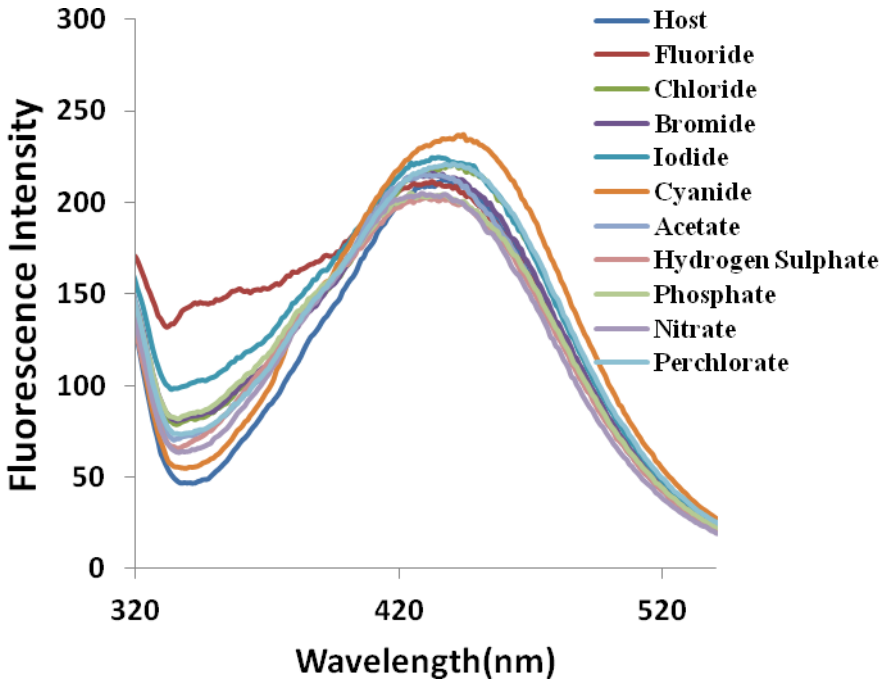

Figure S11. Fluorescence spectra of nano-aggregates **N1** on addition on various tetrabutylammonium anions (F^-, Cl^-, Br^-, I^-, PO_4^{3-}, ClO_4^-, HSO_4^-, CN^- and CH_3COO^-).

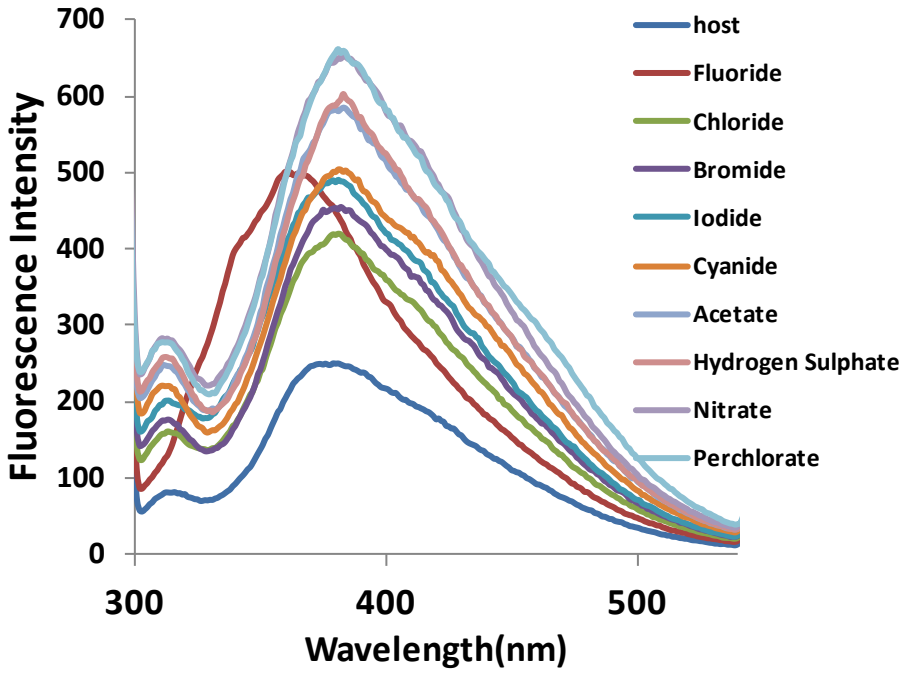

Figure S12. Fluorescence spectra of nano-aggregates **N2** on addition on various tetrabutylammonium anions (F^-, Cl^-, Br^-, I^-, PO_4^{3-}, ClO_4^-, HSO_4^-, CN^- and CH_3COO^-).

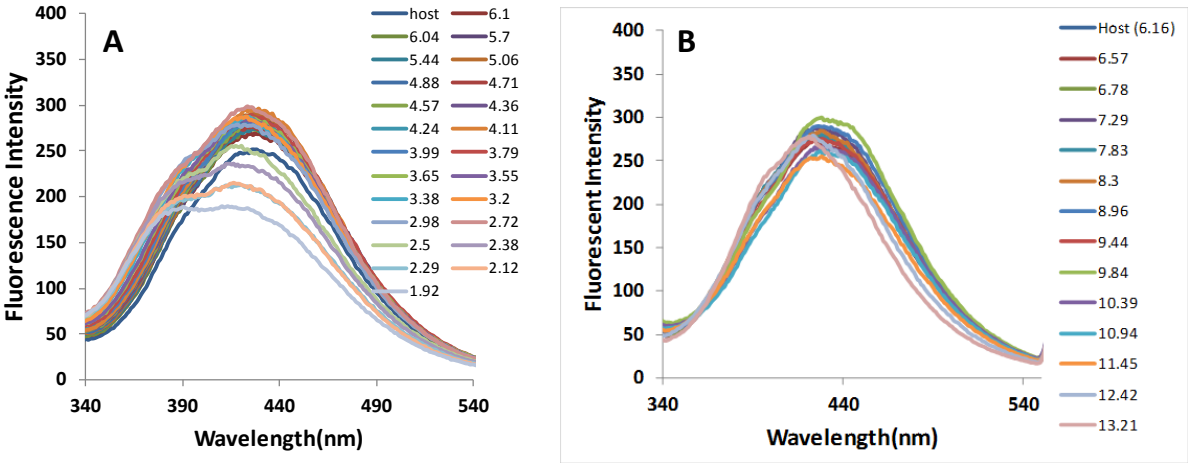

Figure S13. Fluorescence spectra of nano-aggregates **N1**at different pH values.

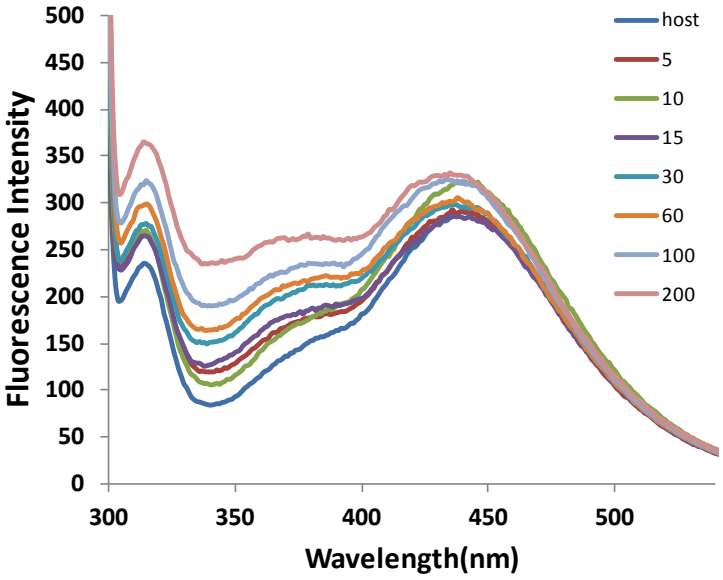

Figure S14. Fluorescence spectra of nano-aggregates **N1**at different concentrations of TBA nitrate to evaluate the salt effect.

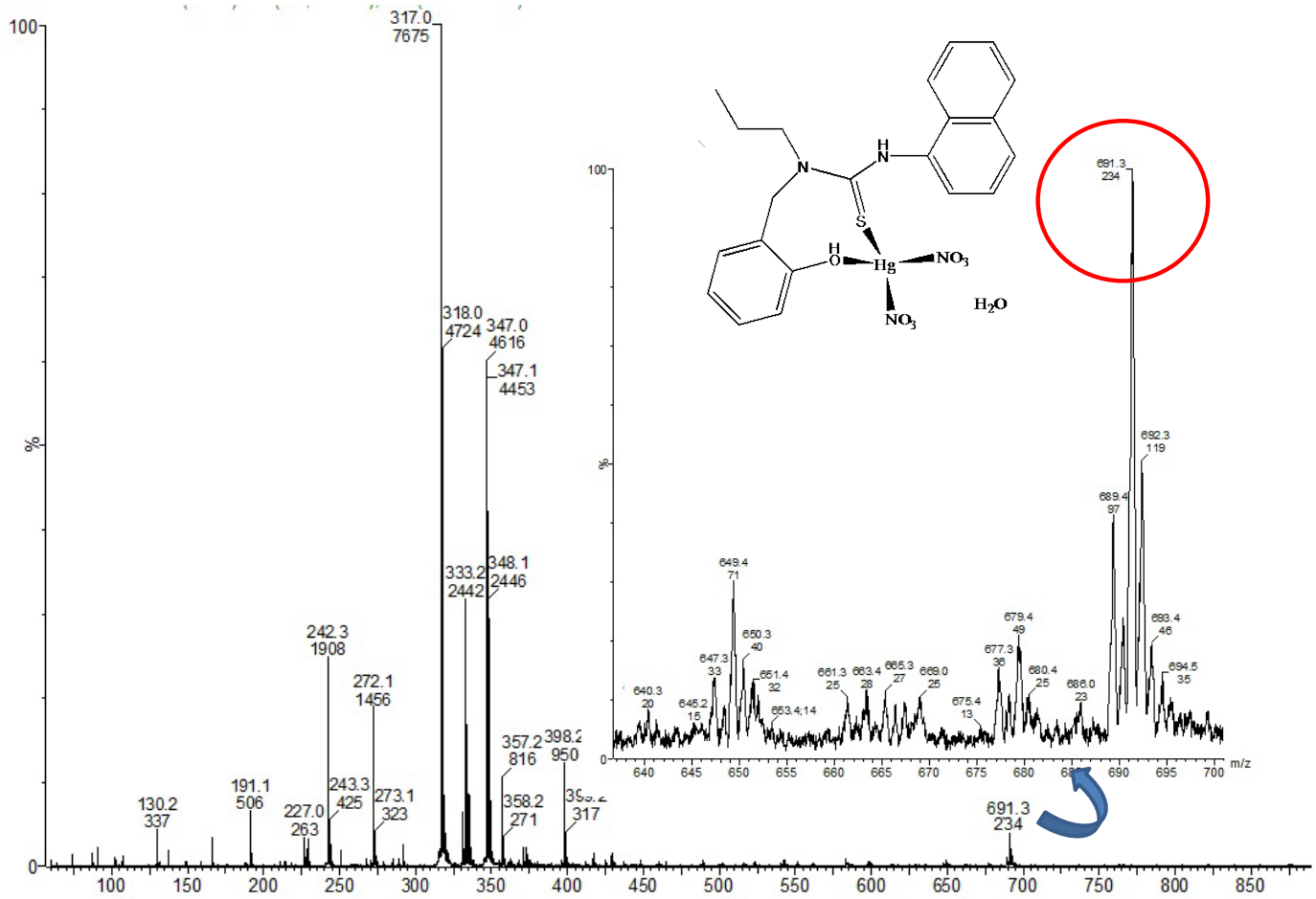

Figure S15. ESI Mass spectrum of complex [**1**.Hg^{2+}.$(NO_3)_2$].H_2O.

Table S1: A comparison between the reported probes and present work.

Solvent System	**Linear range** (μM)	**LOD**	**Working mechanism**	**Ref. No.**
CH_3CN–HEPES buffer	0.001-1	7.4 nm	Fluorescence on	14
Dichloromethane	0-2.0	50 nm	Fluorescence on	15
Water:MeOH (1:2)	0.3-1.0	30 nm	FRET	16
THF-Water (95:5)	NA	NA	Bond energy Transfer	17
H_2O–MeCN(99:1)	0.01-4.5	2.1nm	Fluorescence on	18
Tris-HCl buffer	0.1-20	0.5 ppb	Fluorescence off	19
HEPES buffer	NA	200 nm	Fluorescence on	20
THF/H_2O (9:1)	NA	4.5 nm	Fluorescence off	21
Phosphate buffer	0-30	0.2 μM	Fluorescence off	22
Acetonitrile :water (4:1)	NA	1.74 μM	Fluorescence off	23
Methanol	NA	15 μM	Fluorescence off	24
Water	**1-10**	**2.4 nM**	**Fluorescence on**	**Present work**