Supporting Information

Highly selective colorimetric and fluorescent detection for Hg^{2+} in aqueous solutions using dipeptide-based chemosensor

Jooyoung Park, Byunggyu In, and Keun-Hyeung Lee*

Bioorganic Chemistry Lab, Center for Design and Applications of Molecular Catalysts, Department of Chemistry and Chemical Engineering, Inha University, Incheon, 402-751, South Korea.
E-mail: leekh@inha.ac.kr; Fax: +82-32-8675604; Tel: +82-32-8607674

Contents **Pages**

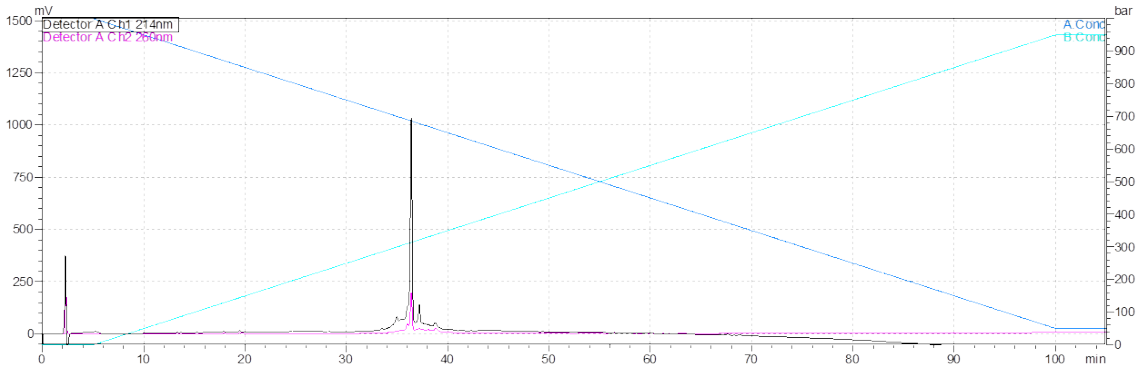

Fig. S1. HPLC chromatograph of **1**

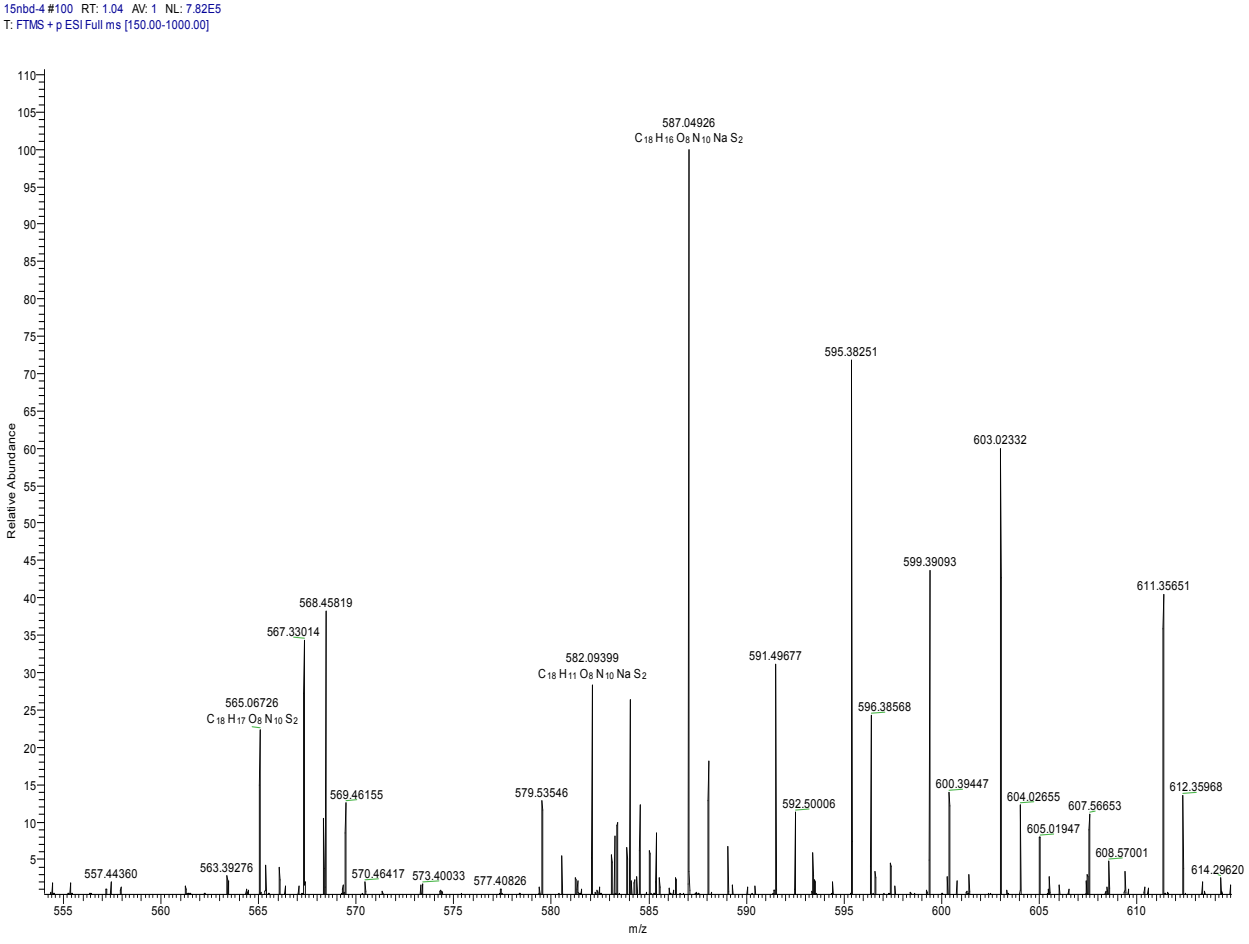

Fig. S2. ESI-HRMS spectrum of **1**

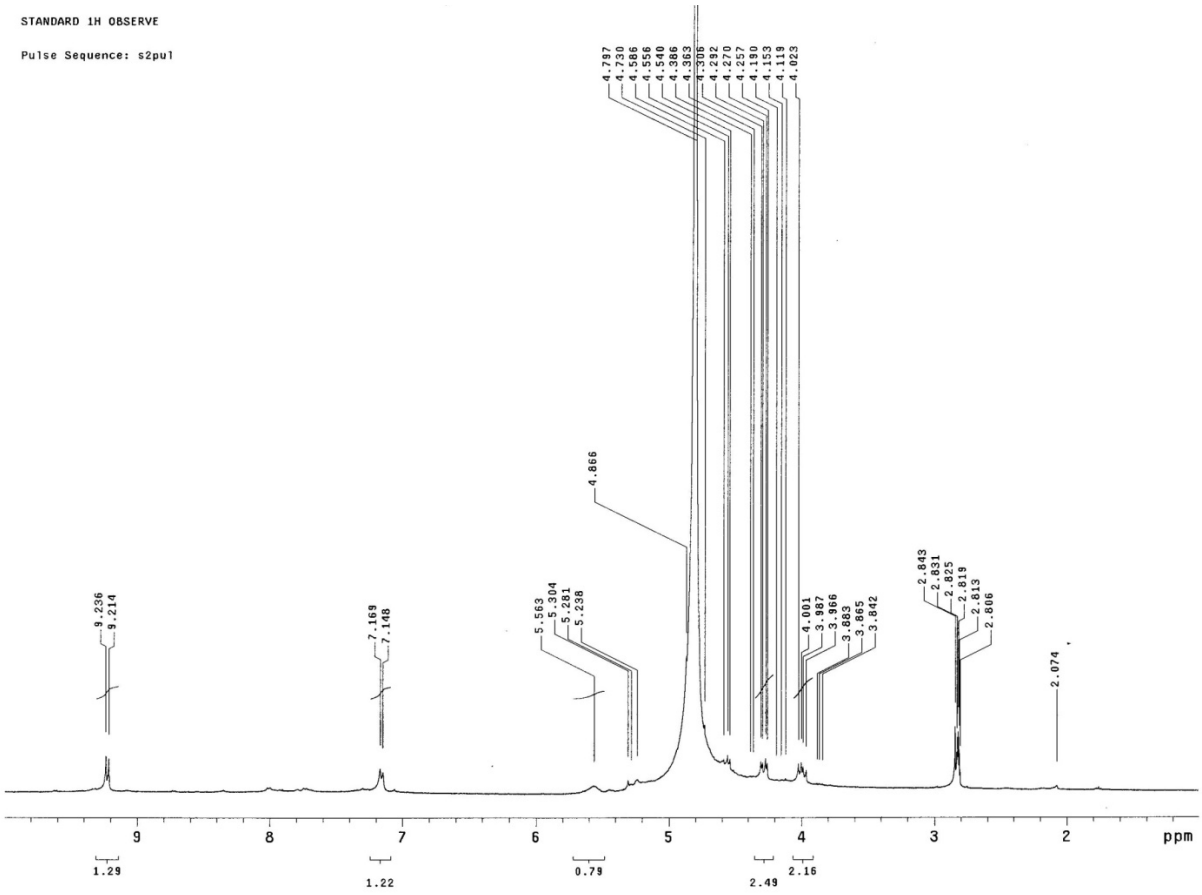

Fig. S3. ***¹H*** NMR of **1** in 50% CD_3CN/D_2O

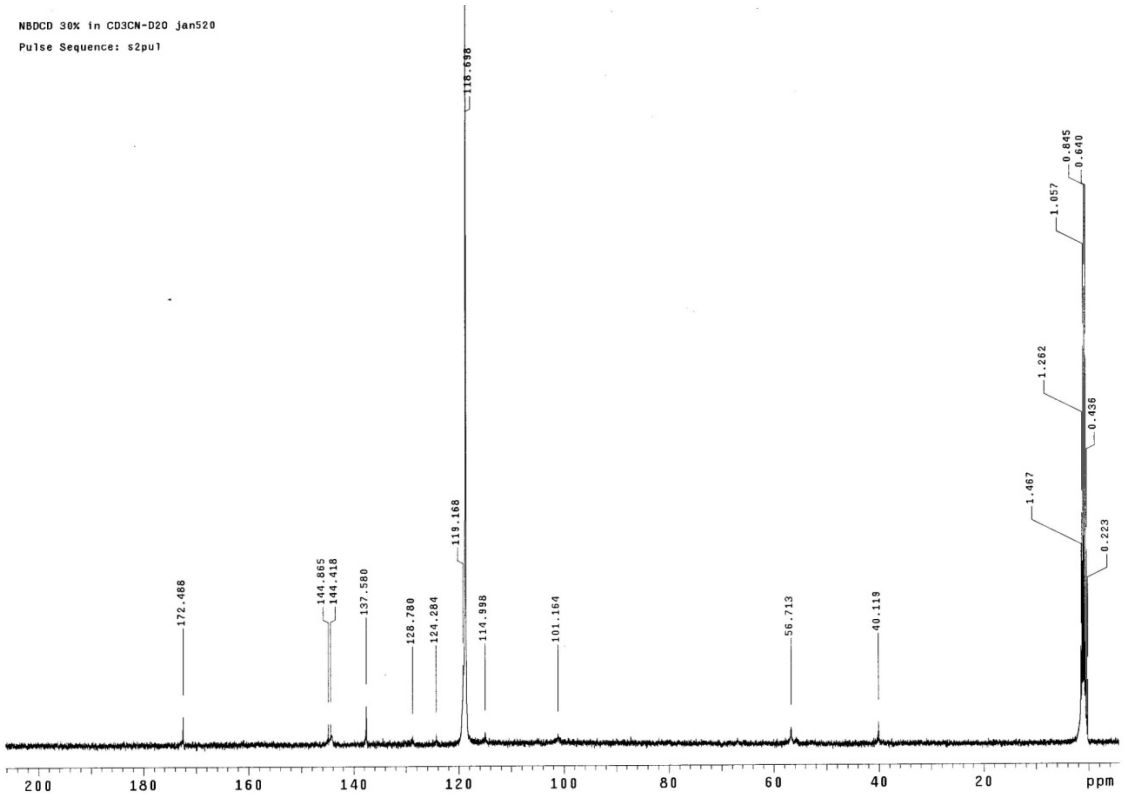

Fig. S4. ***^{13}C*** NMR of **1** in 50% CD_3CN/D_2O

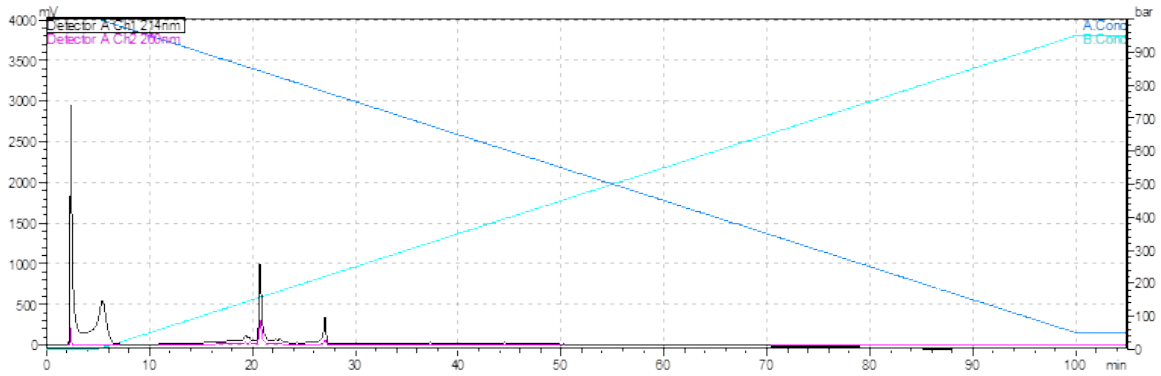

Fig. S5. HPLC chromatograph of **2**

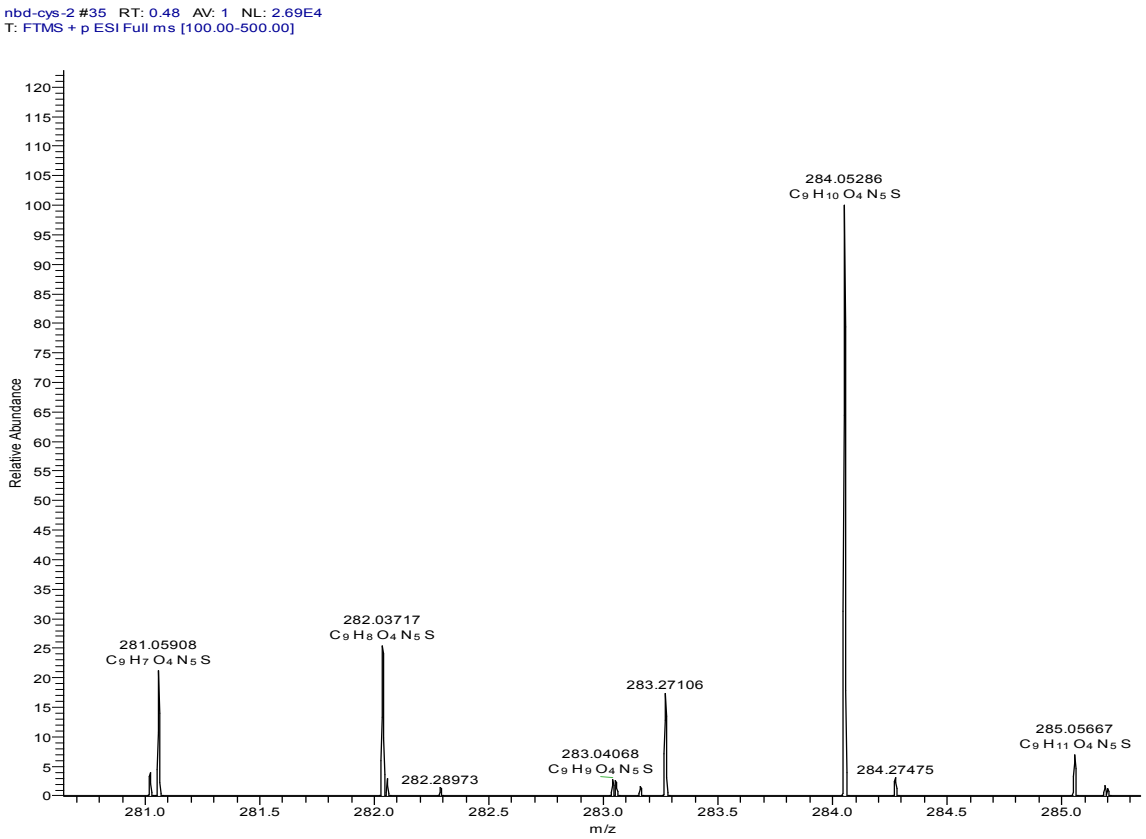

Fig. S6. ESI-HRMS spectrum of **2**

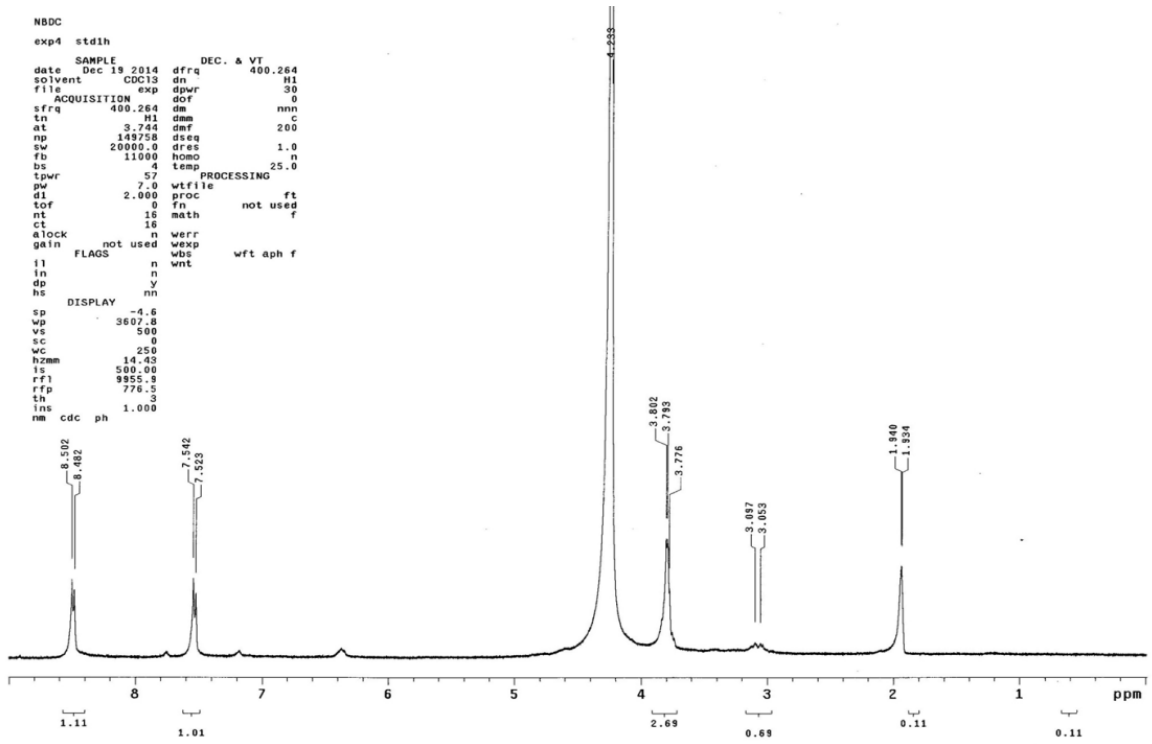

Fig. S7. ***[1]H*** NMR of **2** in 50% CD_3CN/D_2O

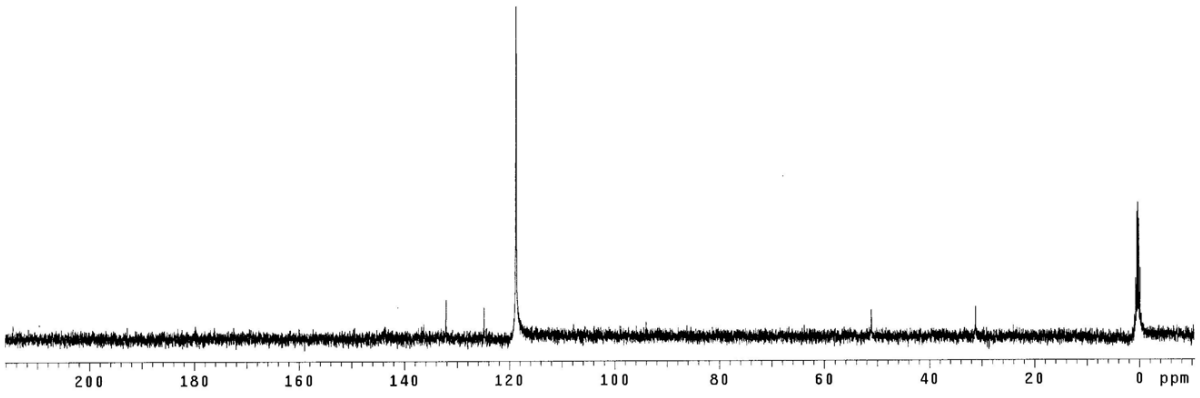

Fig. S8. ***[13]C*** NMR of **2** in 50% CD_3CN/D_2O

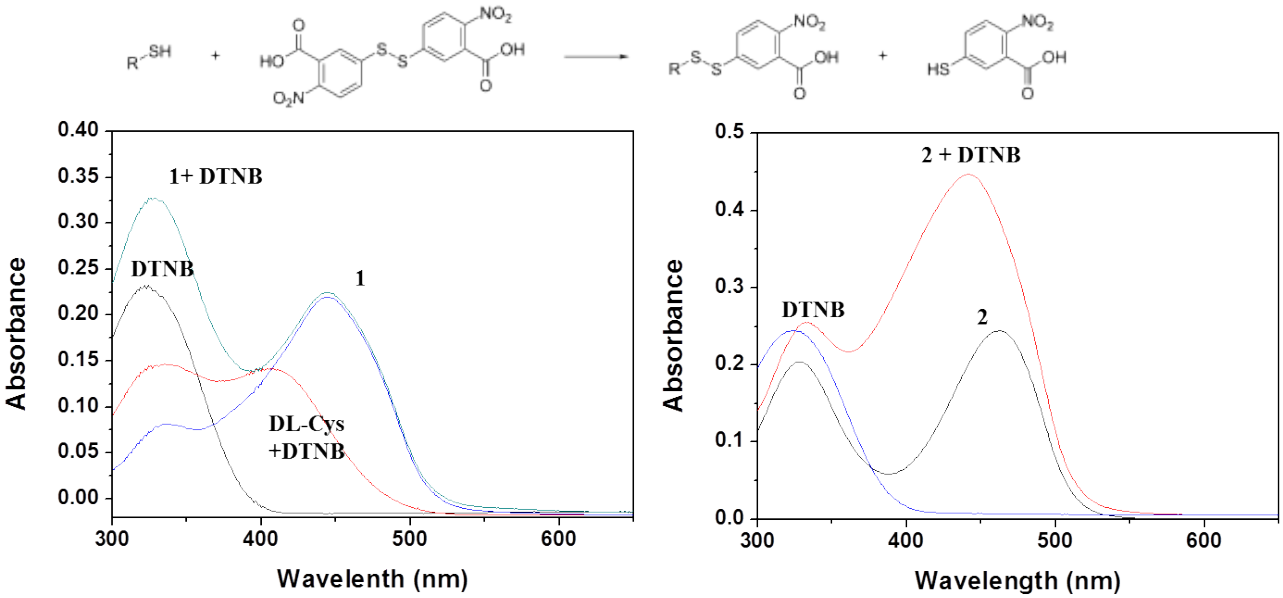

Fig. S9. UV/VIS Absorbance of (a) **1** and (b) **2** (10 μM) in the presence of DTNB (10 μM) in 10 mM Tris buffer solution (pH 8.0) containing 1% CH_3CN.

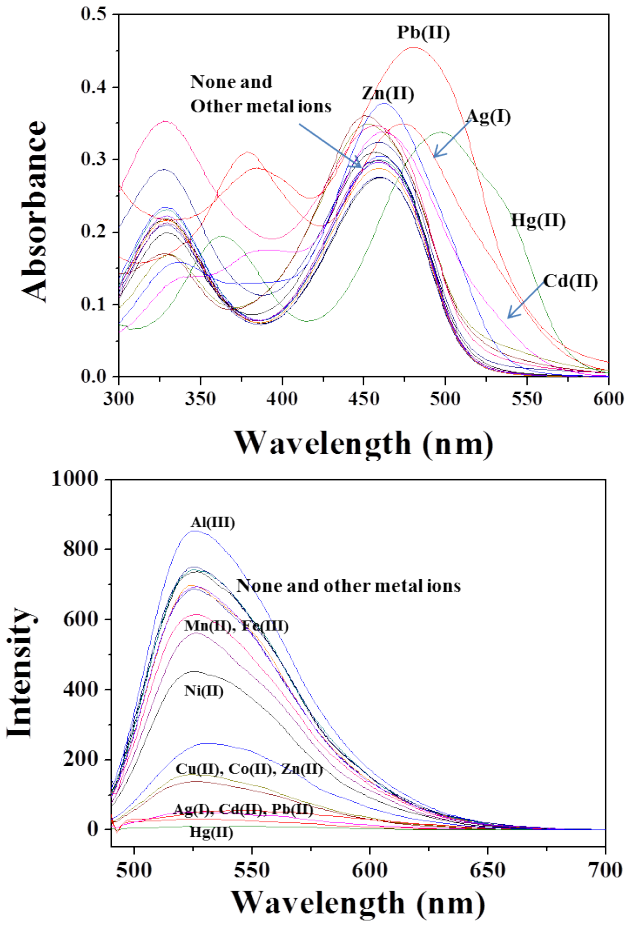

Fig. S10. UV-VIS absorbance and fluorescence emission spectra of **2** (15 μM) in aqueous buffered solution (10 mM HEPES, pH 7.4) containing 3% CH_3CN in the presence of various metal ions (60 μM).

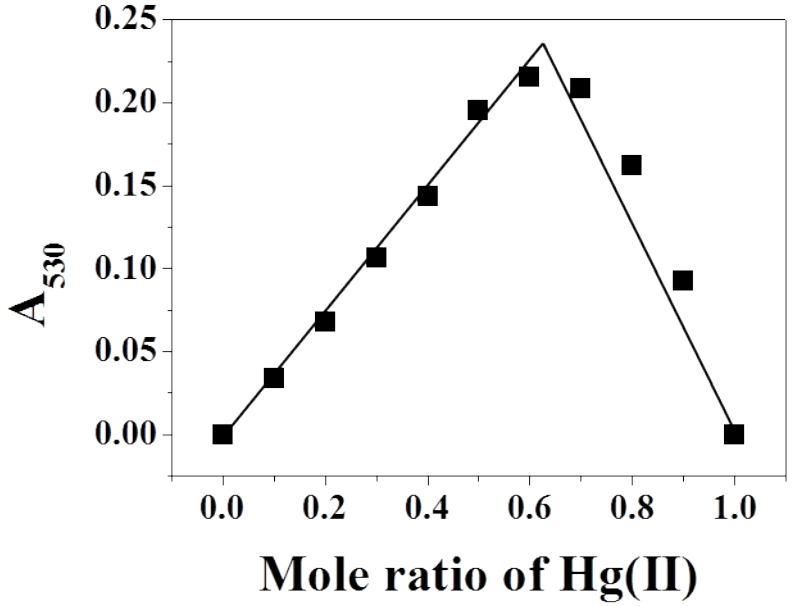

Fig. S11. A Job's plot for **1** (30 μM) with Hg^{II} in 10mM HEPES buffer solution (pH 7.4) containing 5% CH_3CN by absorbance change.

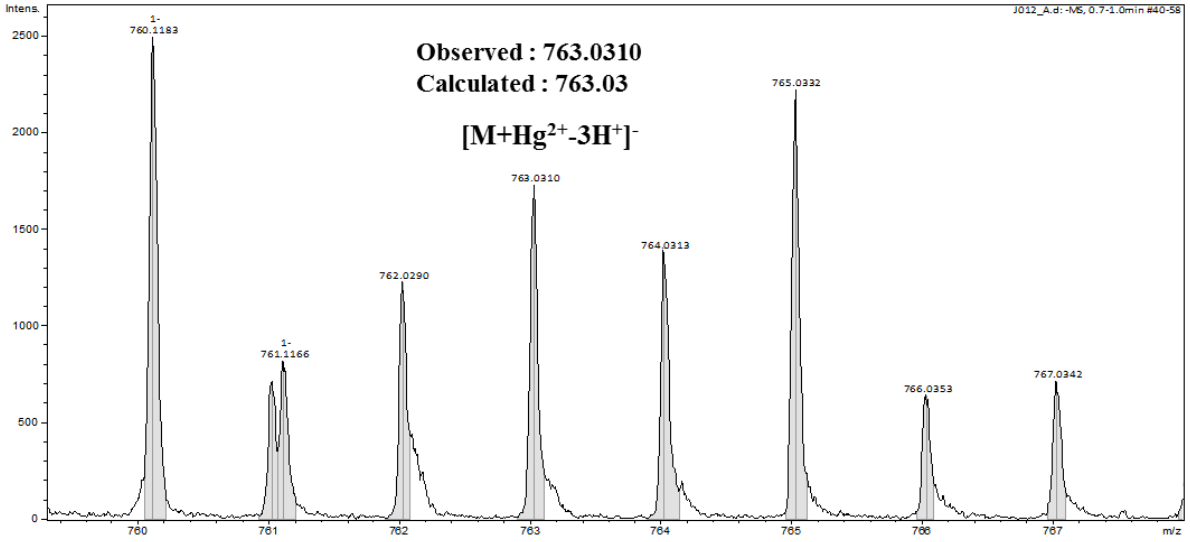

Fig. S12. ESI-HRMS spectrum of **1** (100 μM) with Hg^{II} (400 μM) in 50% CH_3CN/H_2O containing 10 mM ammonium carbonate.

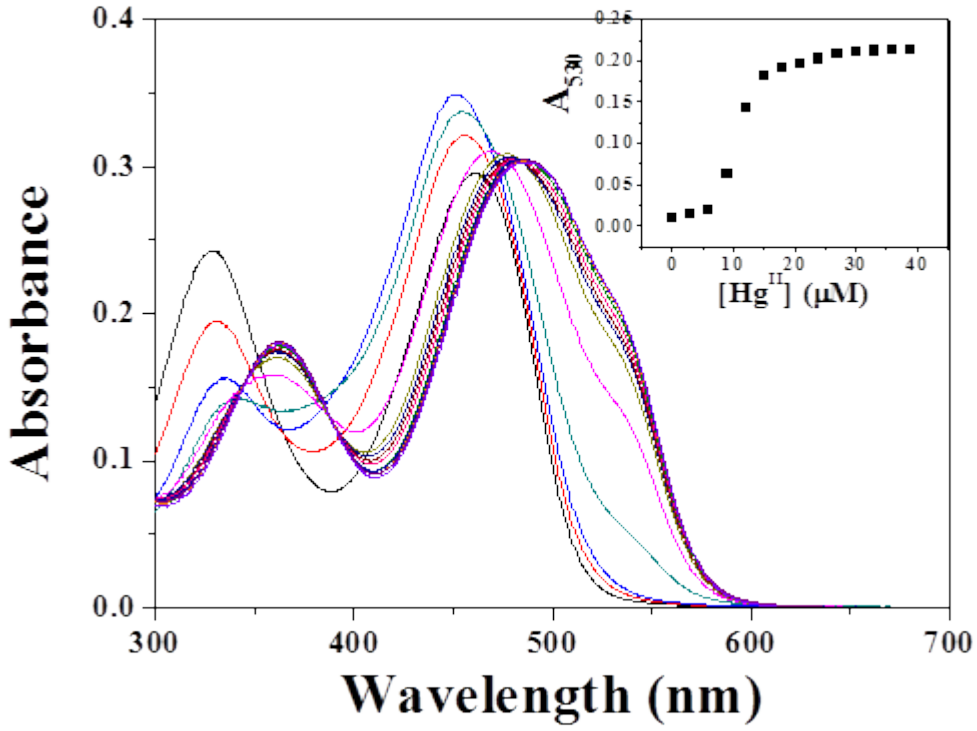

Fig. S13. UV-VIS absorbance titration curve of **2** (15 μM) in the presence of Hg^{II}, (0, 5, ..., 60 μM) in aqueous buffered solution (10 mM HEPES, pH 7.4) containing 3% CH_3CN.

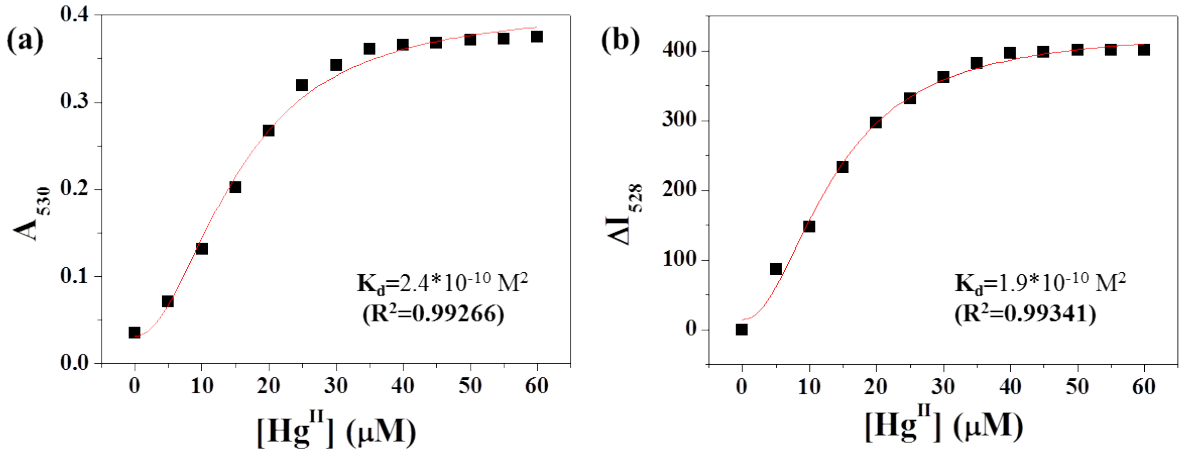

Fig. S14. (a) UV-VIS absorbance and (b) fluorescence emission titration curve of **1** (15 μM) in the presence of Hg^{II}, (0, 5, ..., 60 μM) in aqueous buffered solution (10 mM HEPES, pH 7.4) containing 3% CH_3CN. (λ_{ex} = 469 nm, Slit 5/10 nm)

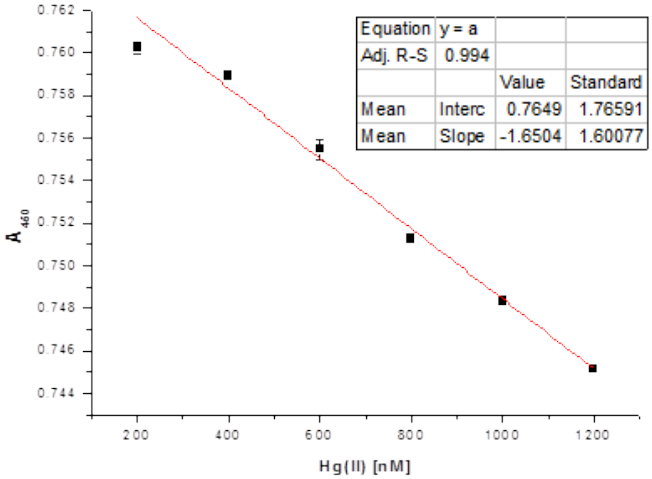

Fig. S15. Detection limit of **1** (15 μM) with Hg^{II} ions in 10 mM HEPES buffer solution (pH 7.4) containing 3% CH_3CN.

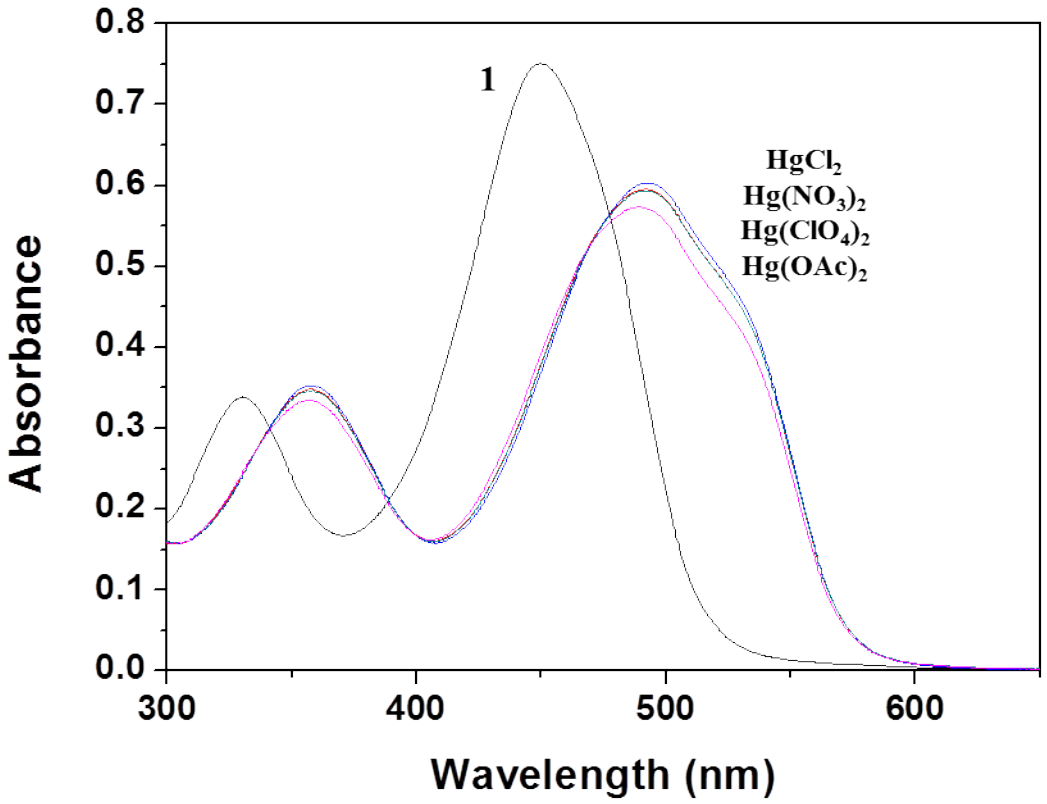

Fig. S16. UV-VIS absorbance spectra of **1** (15 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% CH_3CN in presence of Hg^{II} ($HgCl_2$, $Hg(OAc)_2$, $Hg(NO_3)_2$ and $Hg(ClO_4)_2$, 60 μM).

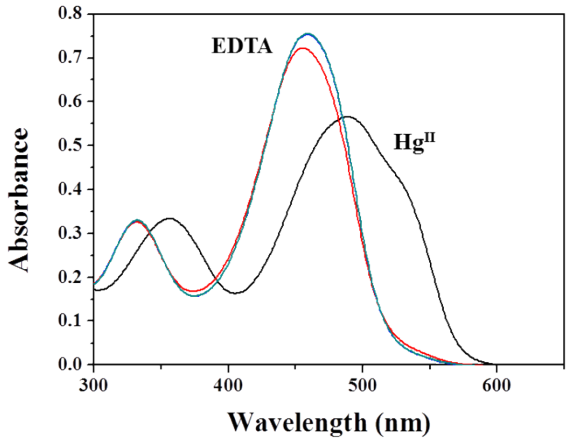

Fig. S17. UV-VIS absorbance spectra of **1** (15 μM) with Hg^{II} (30 μM) in the presence of EDTA (0, 15, 30, …, 75 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% CH_3CN.

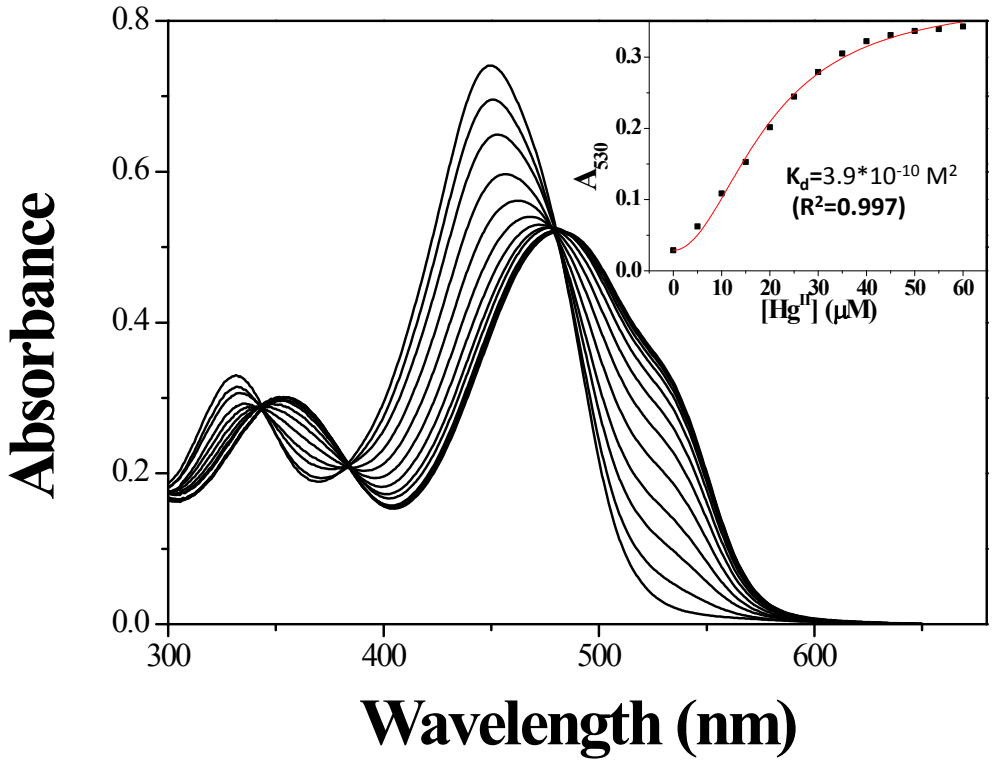

Fig. S18. UV-VIS absorbance and spectra of **1** (15 μM) in the presence of Hg^{2+} (0, 5, ..., 60 μM) in groundwater containing 3% CH_3CN and 10 mM HEPES (pH 7.4).

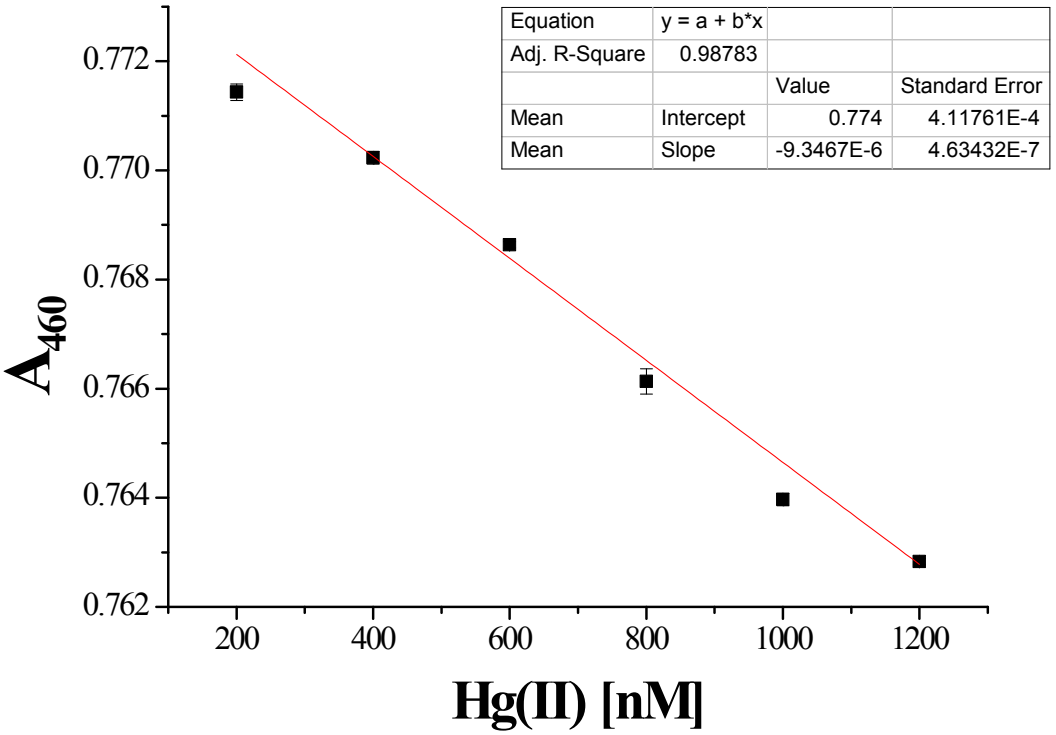

Fig. S19. Detection limit of **1** (15 μM) with Hg^{II} ions in groundwater containing 3% CH_3CN and 10 mM HEPES (pH 7.4).

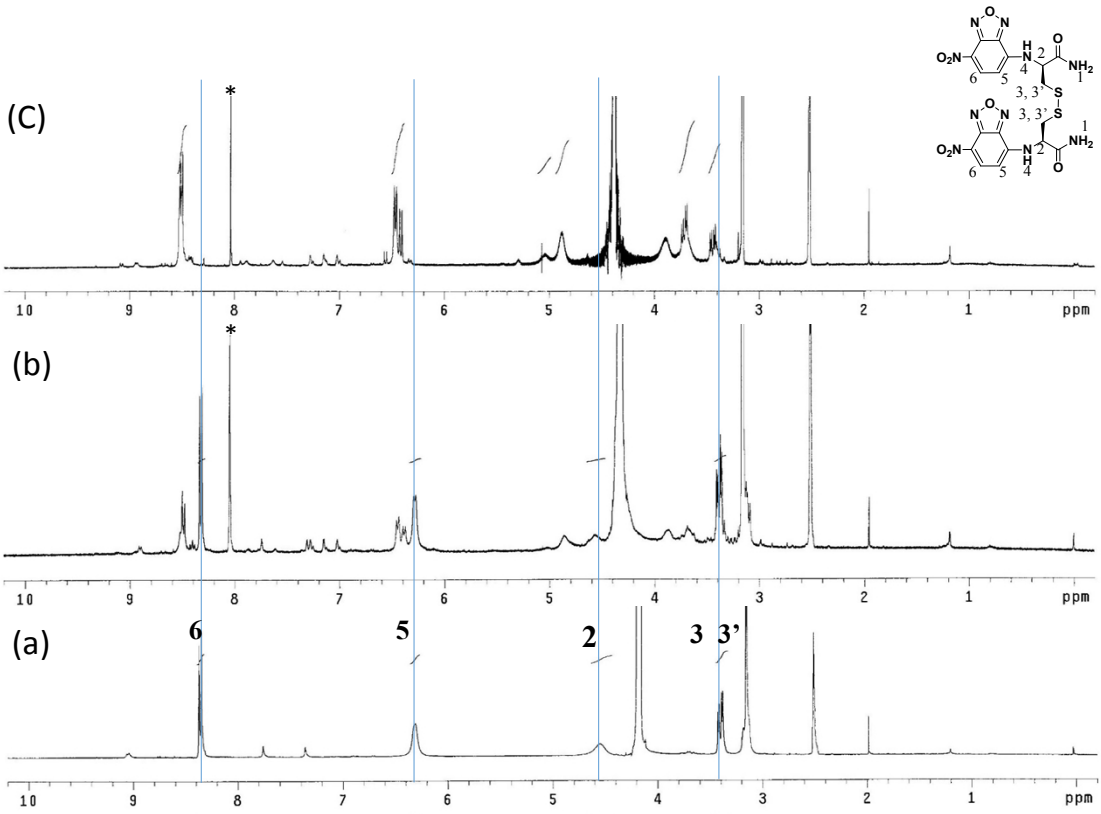

Fig. S20. Partial ^{1}H NMR spectra of (a) **1** (15 mM), (b) **1** in the presence of NH_4HCO_2 (1.5 equiv), and (c) **1** in the presence of NH_4HCO_2 (1.5 equiv) and $Hg(ClO_4)_2$ (6 equiv), in CD_3OD/DMSO-d6 (1:1, v/v). Ammonium format (NH_4HCO_2) was added for neutral pH and the peak (*) at 8.03 ppm corresponded to the proton of NH_4HCO_2.

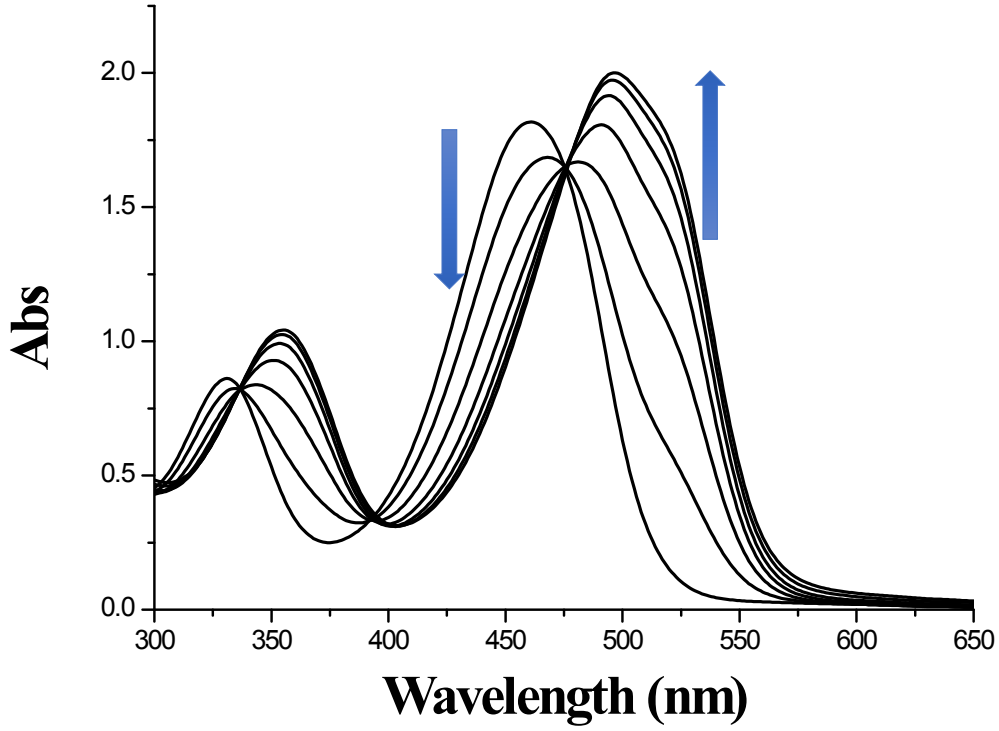

Fig. S21. UV-VIS absorbance spectra of NBDCD (30 μM) in the presence of Hg^{2+} (0, 60, 80, …., 360 uM) in DMSO/MeOH (1:1) containing 1mM ammonium formate.