Supplementary data for:

A BODIPY-based Colorimetric and Fluorometric Chemosensor for Hg(II) Ions and its Application to Living Cell Imaging

Mani Vedamalai and Shu-Pao Wu*

Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan 300, Republic of China

Tel.: +886-3-5712121-ext56506

Fax: +886-3-5723764

E-mail: spwu@mail.nctu.edu.tw

Contents

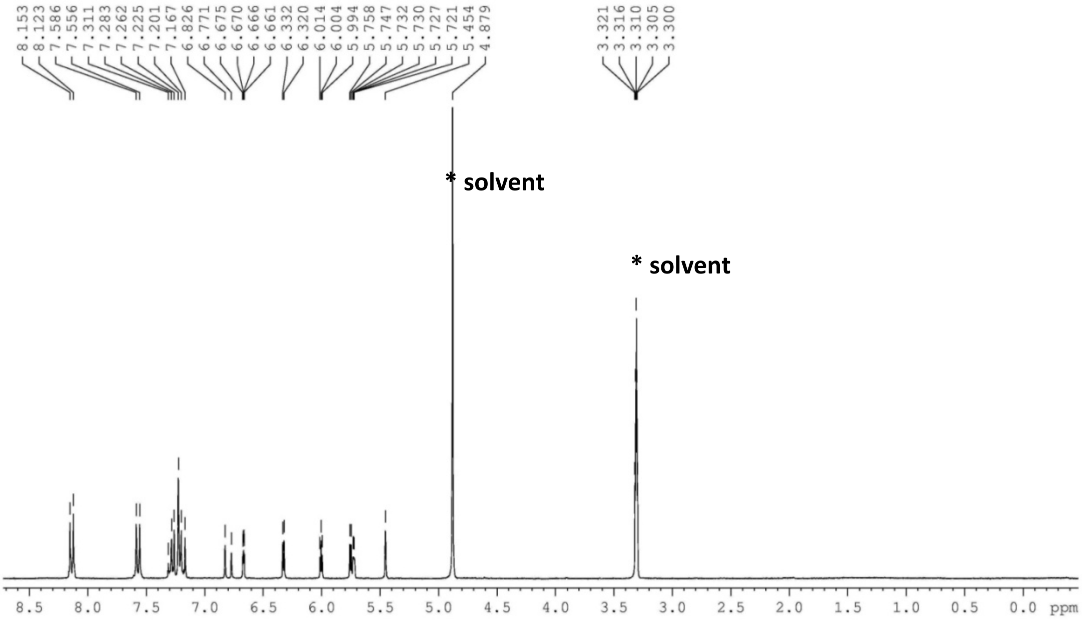

Figure S1. ^{1}H NMR spectra (300 MHz) of compound **2** in CD_3OD.

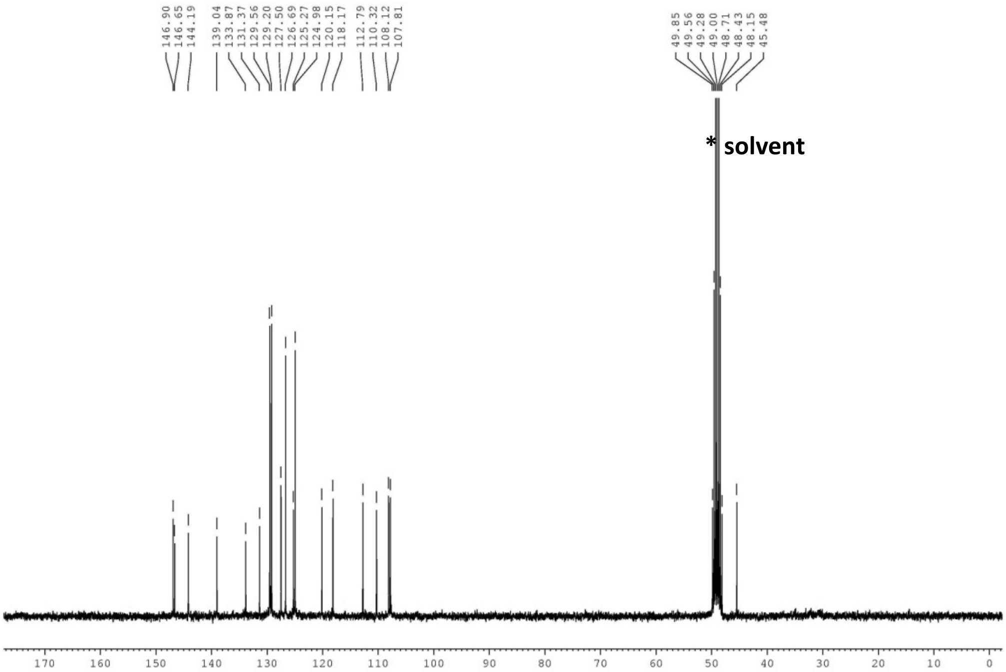

Figure S2. ^{13}C NMR spectra (75 MHz) of compound **2** in CD_3OD

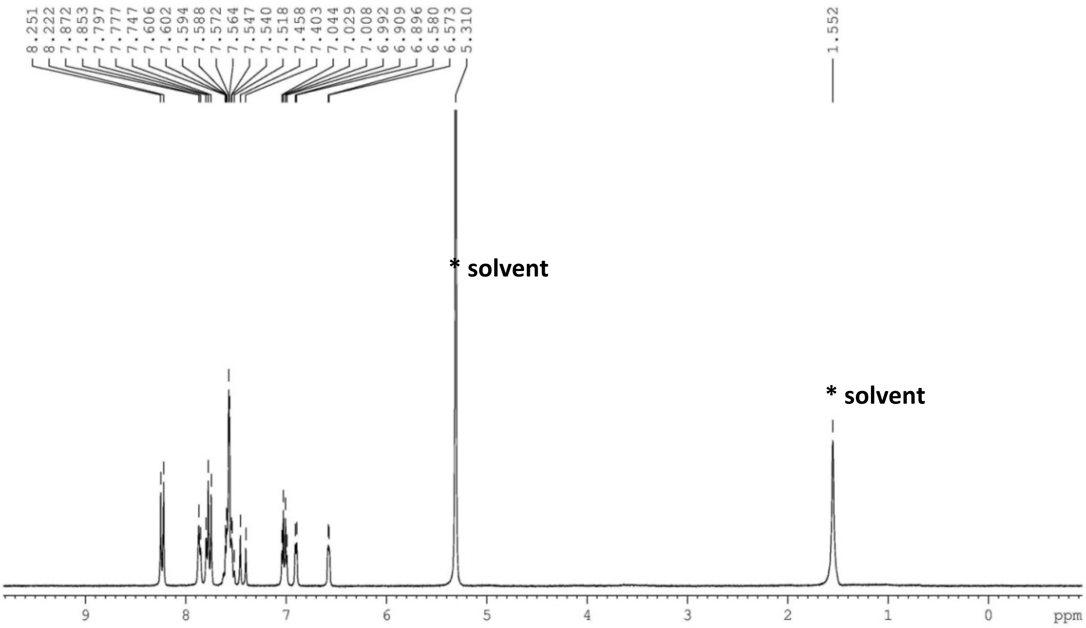

Figure S3. ^{1}H NMR spectra (500 MHz) of compound **3** in CD_2Cl_2.

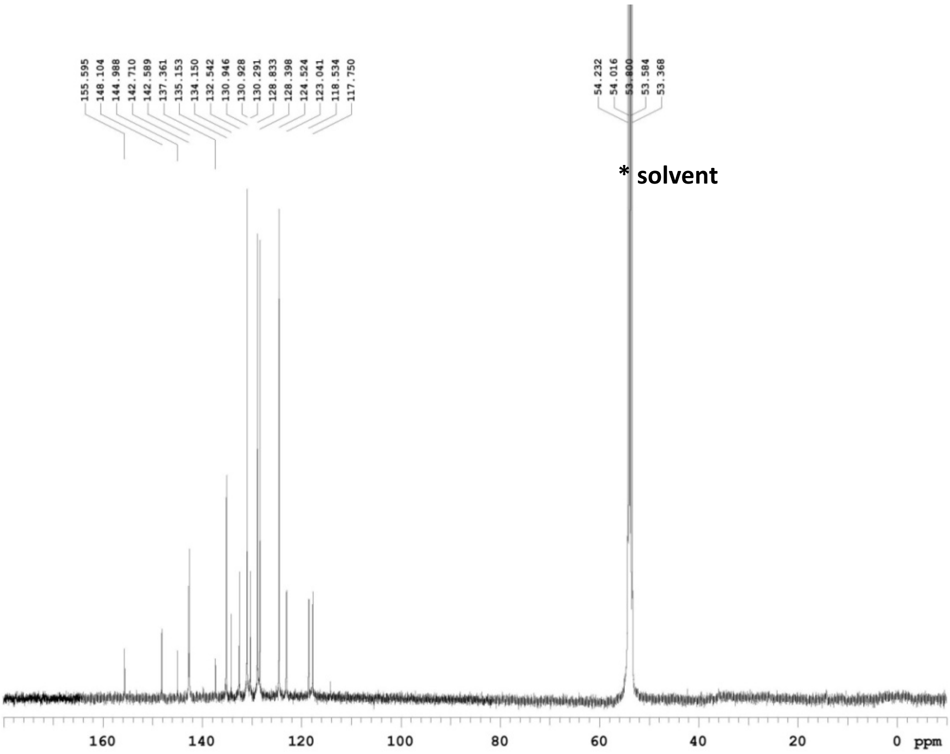

Figure S4. ^{13}C NMR spectra (125 MHz) of compound **3** in CD_2Cl_2

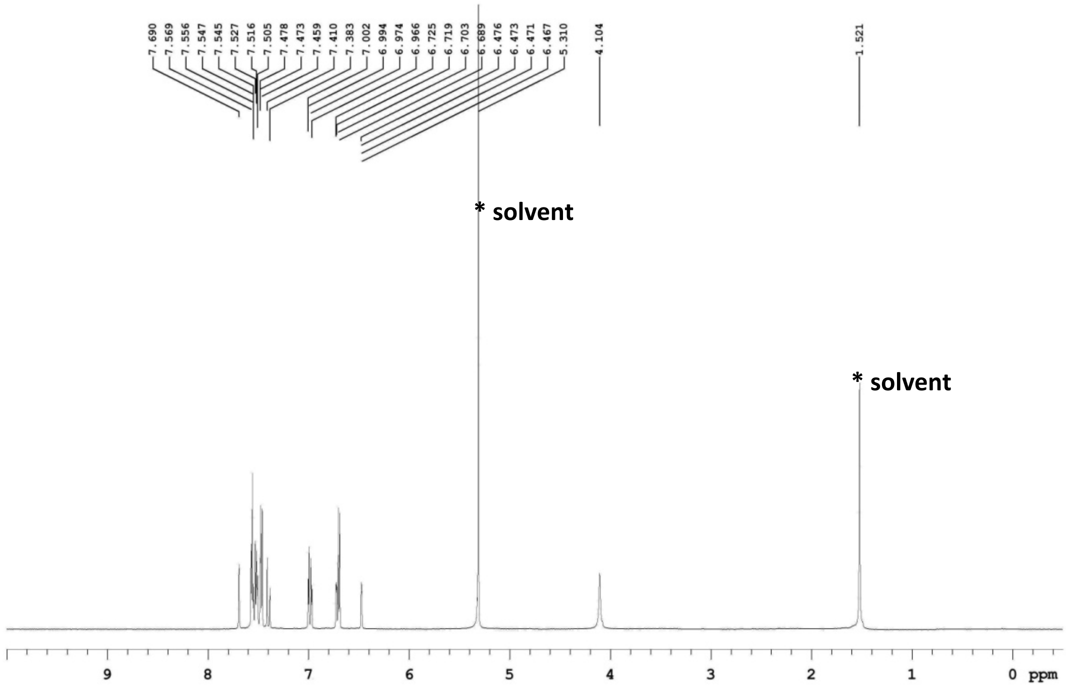

Figure S5. [1]H NMR spectra (600 MHz) of compound **4** in CD_2Cl_2

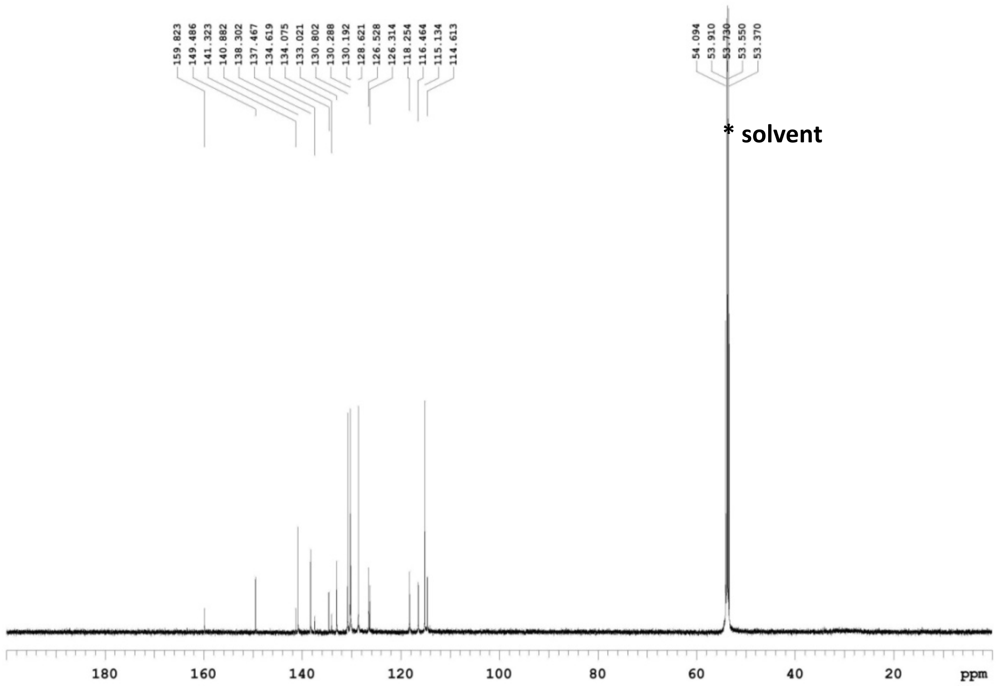

Figure S6. [13]C NMR spectra (150 MHz) of compound **4** in CD_2Cl_2

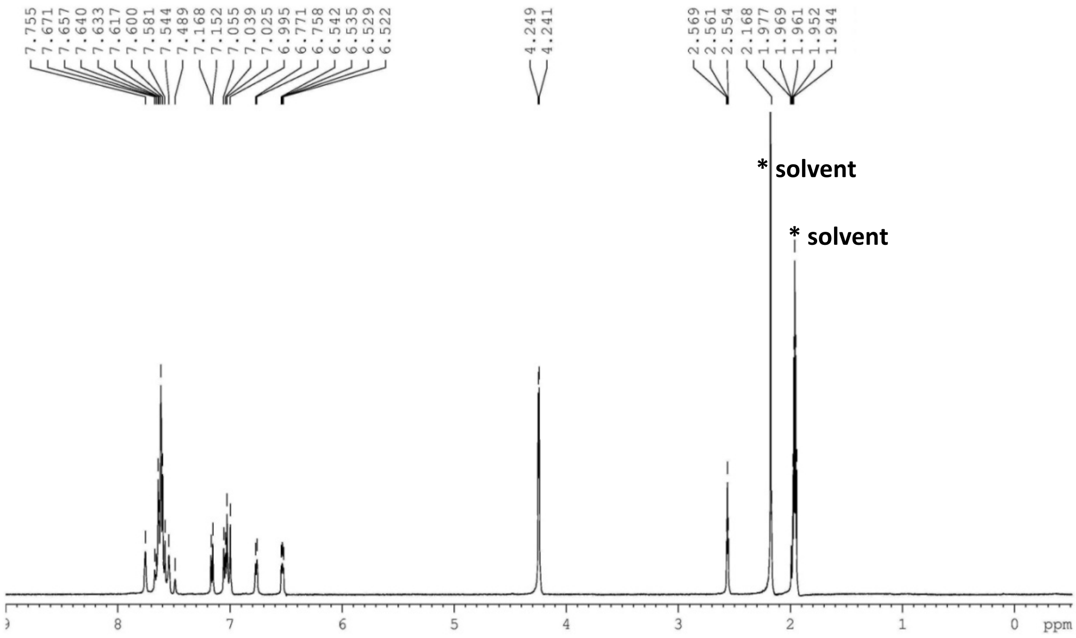

Figure S7. [1]H NMR spectra (300 MHz) of **5** in CD_3CN.

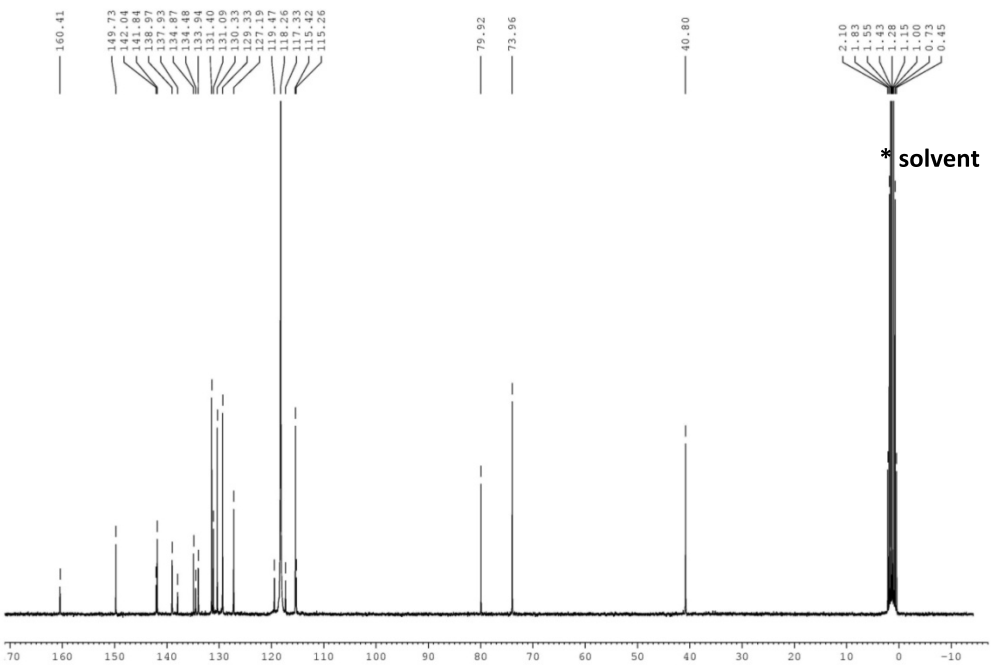

Figure S8. [13]C NMR spectra (75 MHz) of **5** in CD_3CN.

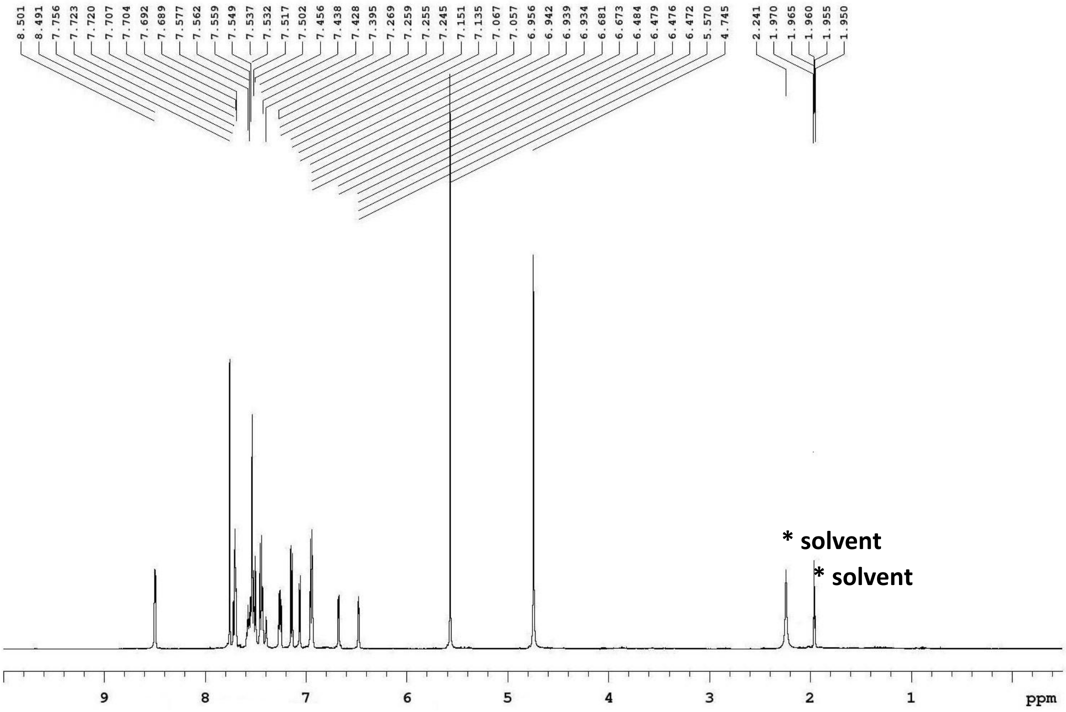

Figure S9. [1]H NMR spectra (500 MHz) of **MS1** in CD_3CN.

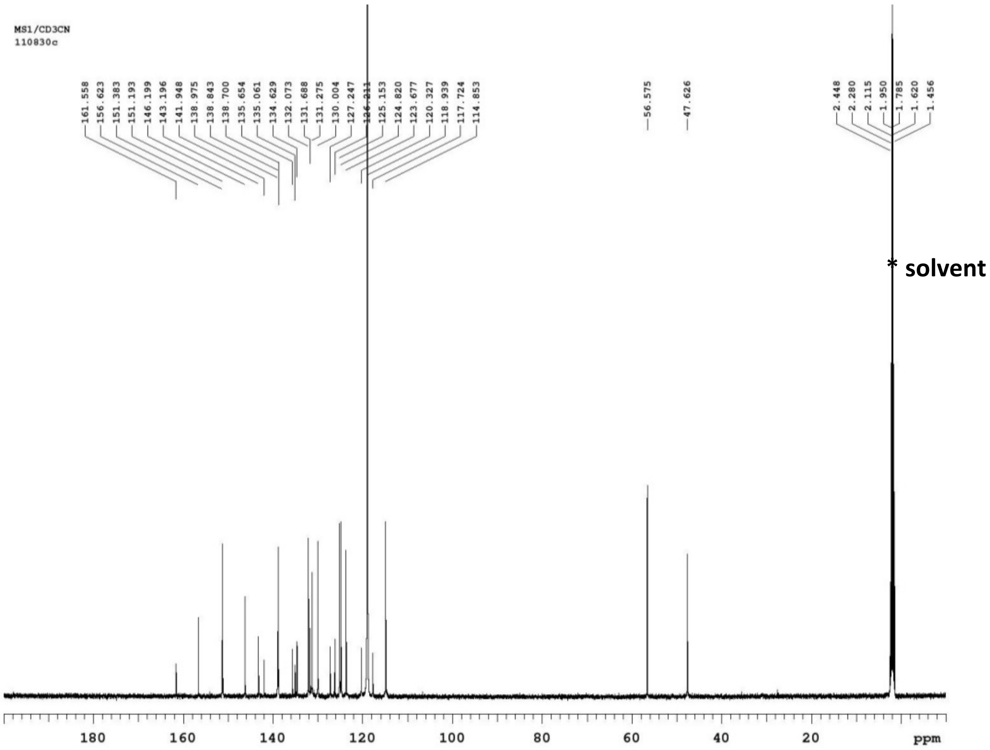

Figure S10. [13]C NMR spectra (125 MHz) of **MS1** in CD_3CN.

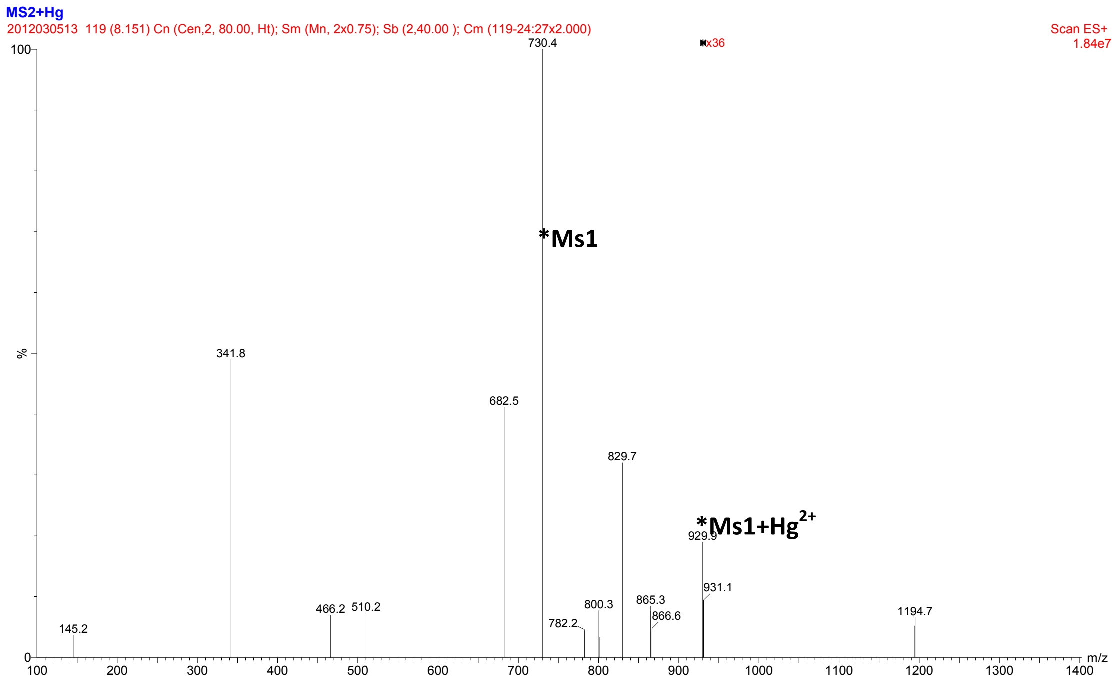

Figure S11. ESI-Mass of **MS1**-Hg^{2+} complex.

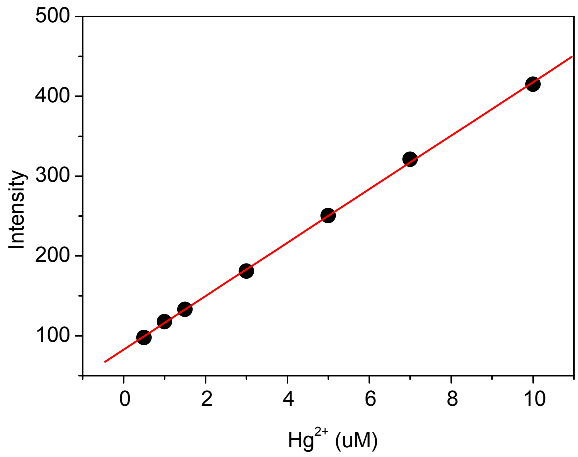

Figure S12. Calibration curve of **MS1**-Hg^{2+} in acetonitrile-water (v/v = 9/1, 2.5 mM Hepes, pH 7.0) solutions. The excitation wavelength was 550 nm, and the monitored emission wavelength was 650 nm.

Linear Regression Data

Y = A + S * X

Parameter	Value	Error	R	SD	N	P
A	82.56453	1.51151	0.99981	2.52755	7	<0.0001
S	33.51315	0.29283				

The detection limit (DL) of Hg^{2+} ions using chemosensor **MS1** was determined from the following equation:

DL = K * SD / S

Where K = 3: SD is the standard deviation of the blank solution; S is the slope of the calibration curve. DL = 3* 2.52755 / 33.51315 = 0.226 (μM)