

Electronic Supplementary Information

**A Novel Water Soluble Chemosensor Based on Carboxyl
Functionalized NDI Derivatives for Selective Detection and
Facile Removal of Mercury (II)**

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Materials and methods

All the cations Fe^{3+} , Hg^{2+} , Ag^+ , Ca^{2+} , Cu^{2+} , Co^{2+} , Ni^{2+} , Cd^{2+} , Pb^{2+} , Zn^{2+} , Cr^{3+} , and Mg^{2+} was added in the form of perchlorate salts, which were purchased from Alfa-Aesar Chemical, and stored in a vacuum desiccator. All other reagents and solvents were commercially available at analytical grade and were used without further purification. ^1H NMR spectra were recorded using a Mercury-400BB spectrometer at 400 MHz for ^1H NMR. The fluorescence spectra were recorded with a Shimadzu RF-5301 spectrofluorimeter. The IR was performed on a Digilab FTS-3000 FT-IR spectrophotometer. Mass spectra were recorded on an esquire 6000 MS instrument equipped with an electrospray (ESI) ion source and version 3.4 of Bruker Daltonics Data Analysis as the data collection system.

Synthesis of compound **M2**

Naphthalene dianhydride (750mg, 2.8mmol) and amino acetic acid (420mg, 5.6mmol) was suspended in about 20 mL DMF in a reaction flask equipped with a stir bar and the reaction mixture was stirred for 24 h at 140 °C under N₂ atmosphere (Scheme 1). The solids were dissolved in 50 mL of anhydrous MeOH. The reaction was heated to reflux for 16h. Then the reaction was cooled, filtered and the brown solid was suspended in ca. 20 mL of MeOH, filtered, and dried under high vacuum. The field gray solid was isolated pure in an 88% yield. Then the product was dissolved in NaOH aqueous solution and gained the **M2**. ¹H NMR (DMSO-*d*₆, 400 MHz): δ 8.73 (s, 4H, ArH), δ 4.73 (s, 4H, -CH₂). IR (KBr, cm⁻¹) ν: 1700.20 (-COOH), 3105.50 (-OH), 1803.40 (AR, C=O); ESI-MS calcd for [C₁₈H₁₀O₄N₂ + H]⁺ = 383.05; found: 383.05.

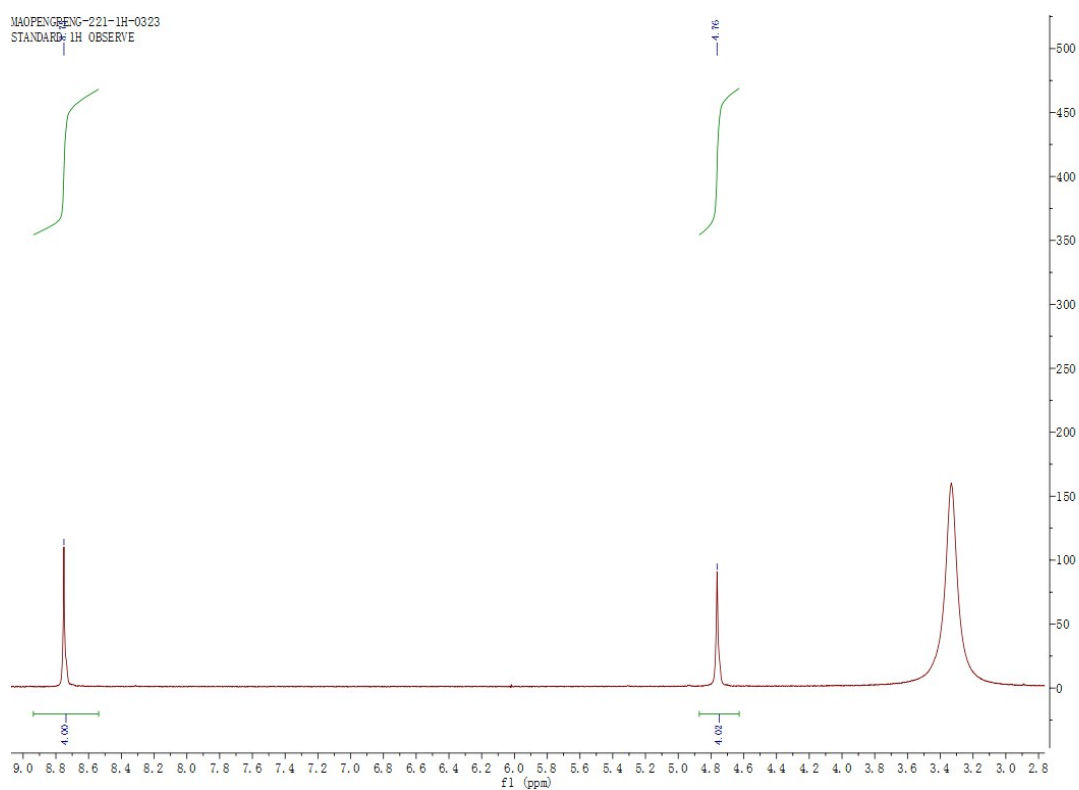


Fig. S1 ^1H NMR spectra of compound **M2**.

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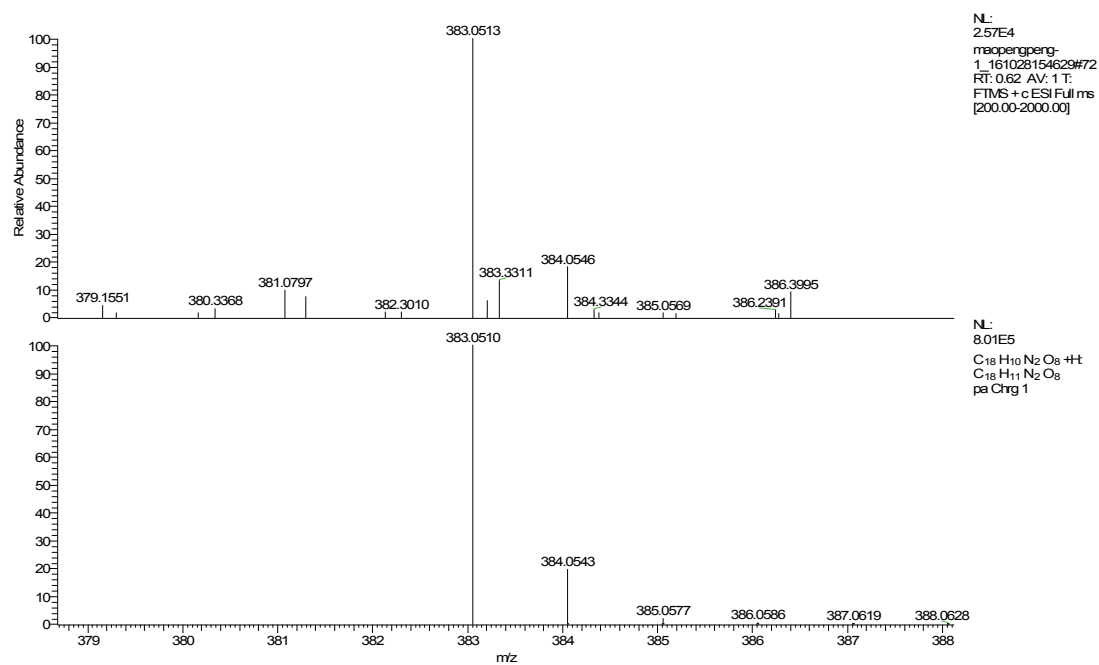


Fig. S2 ESI-MS spectrum of **M2**.

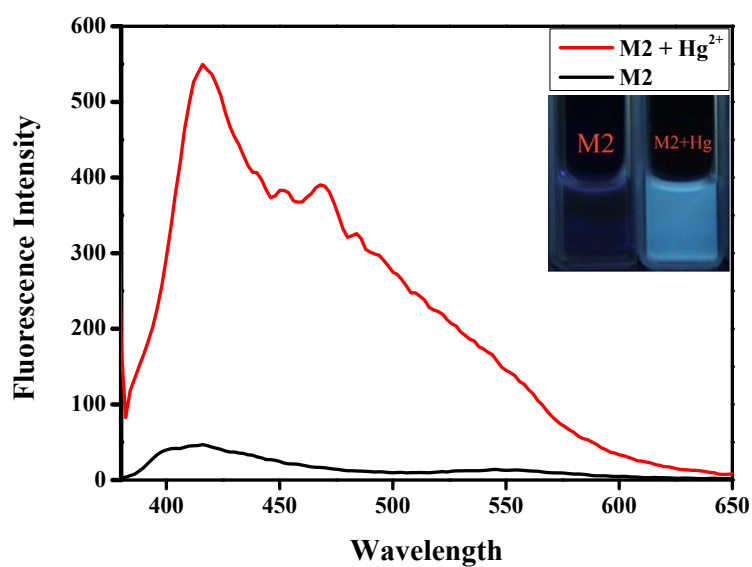


Fig. S3 Fluorescence spectra of **M2** (20 μ M) upon an excitation at 425 nm in H₂O (buffered with HEPES, pH = 7.2) solution in the presence of Hg²⁺ (10 equiv.). Inset: photograph from left to right shows the change in the fluorescence of **M2**, **M2**-Hg²⁺ (10 equiv.) in H₂O (buffered with HEPEPS, pH = 7.2) solution, which was taken under a UV-lamp (365nm).

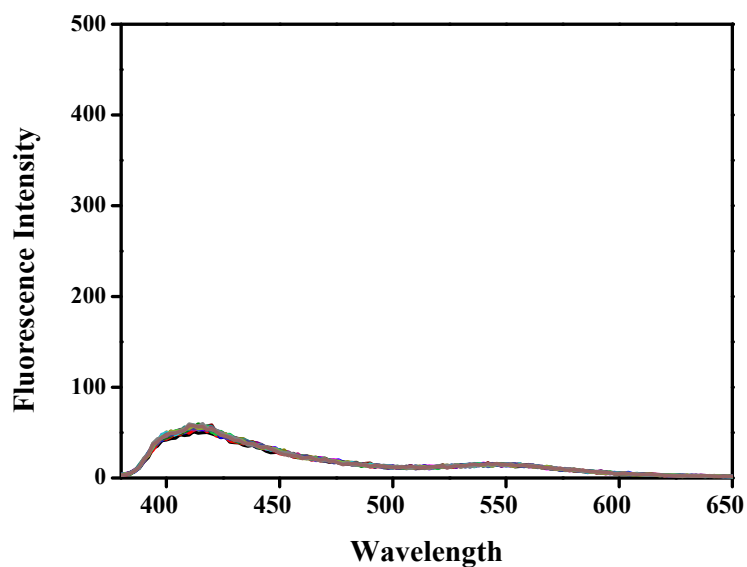


Fig. S4 Fluorescent spectral of blank tests was measured 20 times.

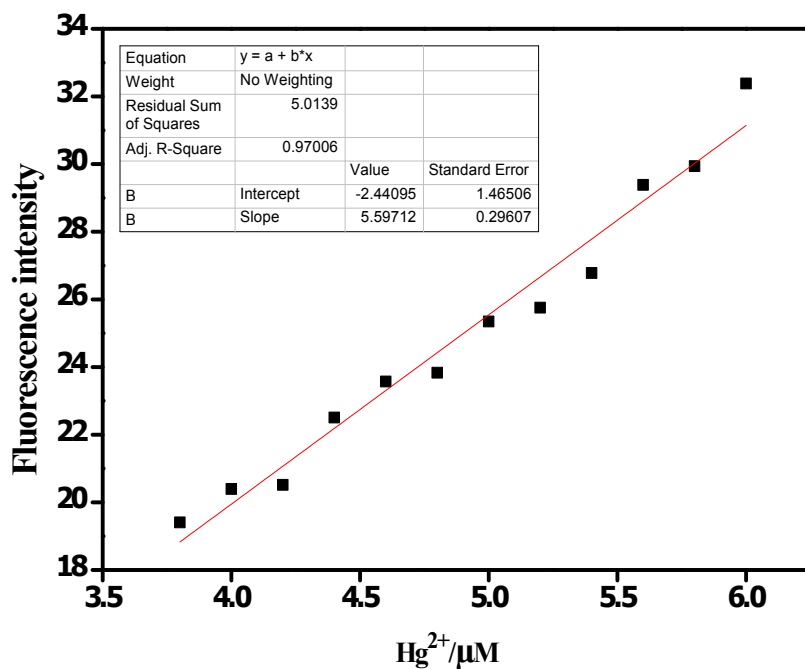


Fig. S5 Plot of the intensity at 365nm for a mixture of the sensor **M2** (20 μM) and Hg^{2+} in water (buffered with HEPES, pH = 7.2) in the range 0.00 to 16.50 μM . (λ_{ex} = 365 nm). The result of the analysis as follows:

Linear Equation: $Y = 5.5971 \times X - 2.44095$ $R^2 = 0.97006$

$$S = 5.59712 \times 10^6 \quad \delta = \sqrt{\frac{\sum (A_0 - A_1)^2}{N-1}} = 2.20875 (N=20) \quad K = 3$$

$$\text{LOD} = K \times \delta / S = 1.18 \times 10^{-6} \text{ M}$$

A_0 is the absorbance intensity of **M2**; A_1 is the average of the A_0 .

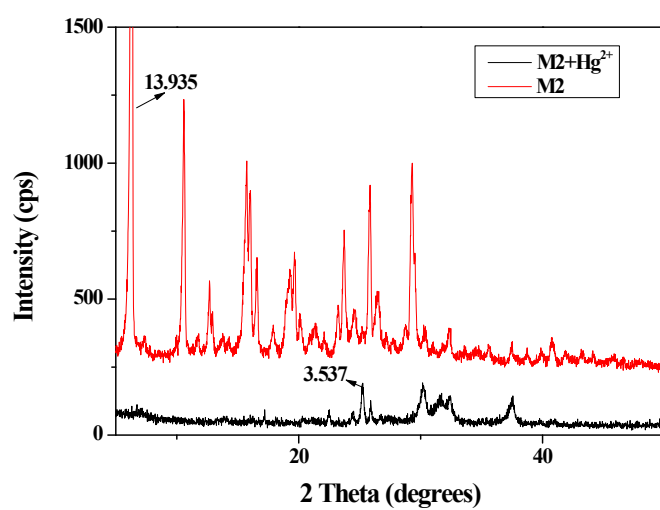


Fig. S6 Powder XRD patterns of the sensor **M2** and **M2-Hg²⁺**.

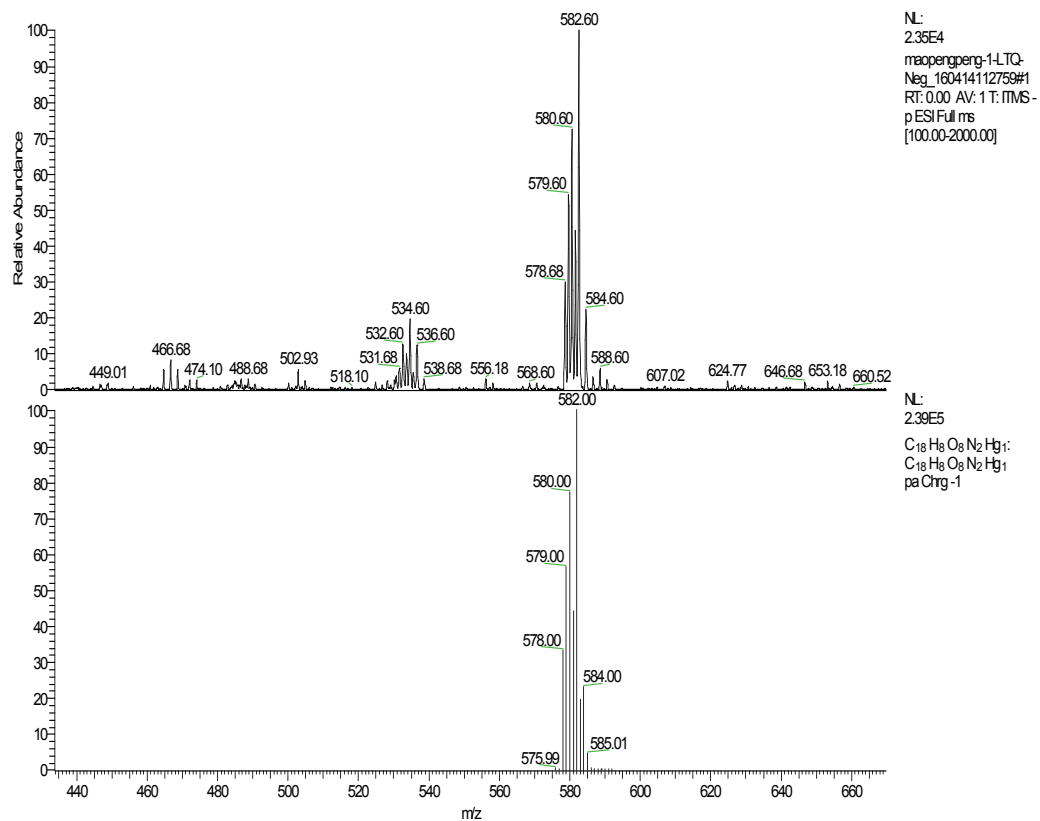


Fig. S7 ESI-MS spectrum of $M2-Hg^{2+}$.

Table S1 The ICP data of **M2** with different concentration of Hg^{2+} .

Test items	number of samples							
	10^{-4} -1:1	10^{-4} -1:2	10^{-5} -1:1	10^{-5} -1:2	10^{-6} -1:1	10^{-6} -1:2	10^{-7} -1:1	10^{-7} -1:2
content of Hg mg/L	2.82	0.26	ND	ND	ND	ND	ND	ND

Remark: ND means Hg element in the sample is not checked out (the content of Hg < 0.1 mg/L).

Measurement of fluorescence quantum yields

Fluorescence quantum yields were determined by the following equation.

$$\Phi = \Phi_R \times \frac{I}{I_R} \frac{A_R}{A}$$

Where Φ is fluorescence quantum yield, I is the integrated fluorescence intensity and A is the optical density (absorption). The subscript R refers to the reference of Quinine hemesulfate salt.

Determination of association constant

The association constants (K) were calculated based on the fluorescent titration curve of the probes with ions. Association constants were determined by a nonlinear least squares fit of the data with the following equation as referenced elsewhere. I is the observed the fluorescence intensity of **M2** at the fixed concentrations of Hg^{2+} . I_{\max} and I_{\min} are the corresponding maximum and minimum, respectively.

$$\log \frac{I - I_{\min}}{I_{\max} - I} = \log K + \log [\text{Hg}^{2+}]$$

$$K = 2.65 \times 10^9 \text{ M}^{-2}$$