

## Supporting information:

# A novel water-soluble naked-eye probe with a large Stokes Shift for selective optical sensing of Hg<sup>2+</sup> and its application in water samples and living cells

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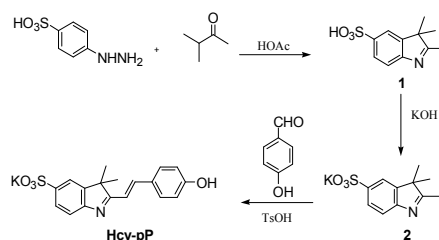
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## Contents:

### 1. Synthesis of Hcy-pP

A solution of compound **2** (0.160 g, 0.5 mmol), 4-dihydroxy-1-benzaldehyd(0.249 g, 1.5 mmol) and p-methyl benzenesulfonic acid (0.175g, 1.0 mmol) in anhydrous ethanol (10.0 mL) were refluxed for 3 h, then the mixture was cooled to room temperature. The precipitate was filtered off, washed with anhydrous ethanol and dried in vacuum to give **Hcy-pP** as a red solid mixture. (0.211 g, 73%). mp = 227~228 °C. The structure of Hcy-mP was confirmed by <sup>1</sup>H NMR: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>): δ 1.61 (s, 6H, CH<sub>3</sub>), 6.93-6.94 (d, J = 9.8 Hz, 1H, Ar-H), 7.10-7.12 (d, J = 15.5 Hz, 1H, CH=CH), 7.26-7.29 (d, J = 9.7 Hz, 1H, Ar-H), 7.47-7.48 (d, J = 8.9 Hz, 1H, Ar-H), 7.51-7.52 (d, J = 8.7 Hz, 1H, Ar-H), 7.72-7.73 (d, J = 9.1 Hz, 1H, ArH), 7.83-7.84 (d, J = 9.1 Hz, 1H, ArH), 7.90 (s, 1H, Ar-H), 8.18-8.21 (d, J = 15.6 Hz, 1H, CH=CH), 10.63 (s, 1H, OH).



Scheme S.1 The synthetic routes of probe Hcy-pP

## 2. Supplementary Figures

**Figure S-1** Benesi-Hildebrand plot from fluorescence titration data of **Hcy-mP** (10  $\mu\text{M}$ ) in HEPES buffer solution.

**Figure S-2** The Stern-Volmer curve of **Hcy-mP** with different concentrations of  $\text{Hg}^{2+}$ .

**Figure S-3** The effect of pH on the fluorescence intensity changes of **Hcy-mP** and **Hcy-mP** +  $\text{Hg}^{2+}$  at 517 nm in HEPES buffer solution.

**Figure S-4** ESI-MS of [**Hcy-mP** +  $\text{Hg}^{2+}$ ].

**Figure S-5** ESI-MS of [**Hcy-mP** +  $\text{Hg}^{2+}$  +  $\text{K}^+$  +  $\text{H}^+$ ].

**Figure S-6**  $^1\text{H}$  NMR of **Hcy-pP**

**Figure S-7**  $^1\text{H}$  NMR of **Hcy-mP**

**Figure S-8**  $^{13}\text{C}$  NMR of **Hcy-mP**

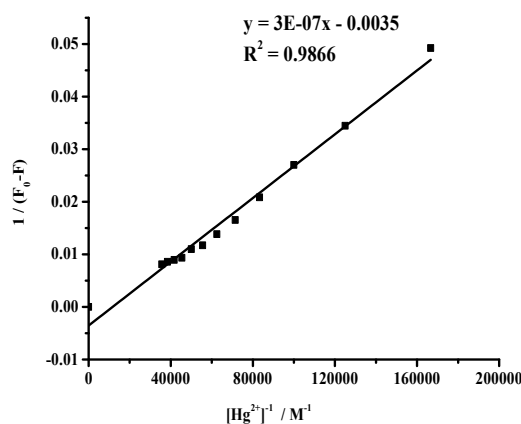
**Figure S-9** IR of **Hcy-mP**

### 3. Table S1 Application in water samples

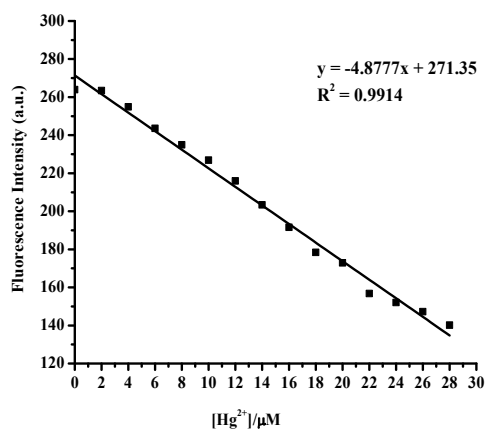
Sample	Added ( $\mu\text{M}$ )	Deteced( $\bar{x} \pm \text{SD}^{\text{b}}$ )( $\mu\text{M}$ )	Recovery(%)	RSD(%)
Tap Water	1.00	$0.99 \pm 0.013$	99	1.2
	3.00	$3.11 \pm 0.018$	103	0.9
	5.00	$4.98 \pm 0.021$	99.6	0.7
Drinking Water	1.00	$1.01 \pm 0.014$	100.5	0.8
	3.00	$2.85 \pm 0.021$	95	1.1
	5.00	$5.11 \pm 0.031$	102.5	1.3
Lake Water	1.00	$0.97 \pm 0.027$	97	1.0
	3.00	$3.08 \pm 0.011$	102	1.3
	5.00	$5.03 \pm 0.027$	100	2.3

<sup>a</sup> Mean of three determination

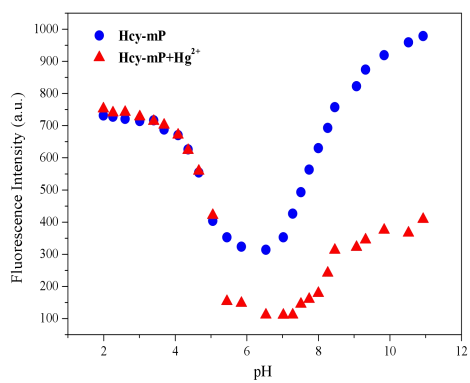
<sup>b</sup> SD: Standard deviation



**Figure S.1** Benesi-Hildebrand plot from fluorescence titration data of **Hcy-mP** (10  $\mu\text{M}$ ) in HEPES buffer solution.



**Figure S.2** The Stern-Volmer curve of **Hcy-mP** with different concentrations of **Hg<sup>2+</sup>**.



**Fig S.3** The effect of pH on the fluorescence intensity changes of **Hcy-mP** and **Hcy-mP+Hg<sup>2+</sup>** at 517 nm in HEPES buffer solution.

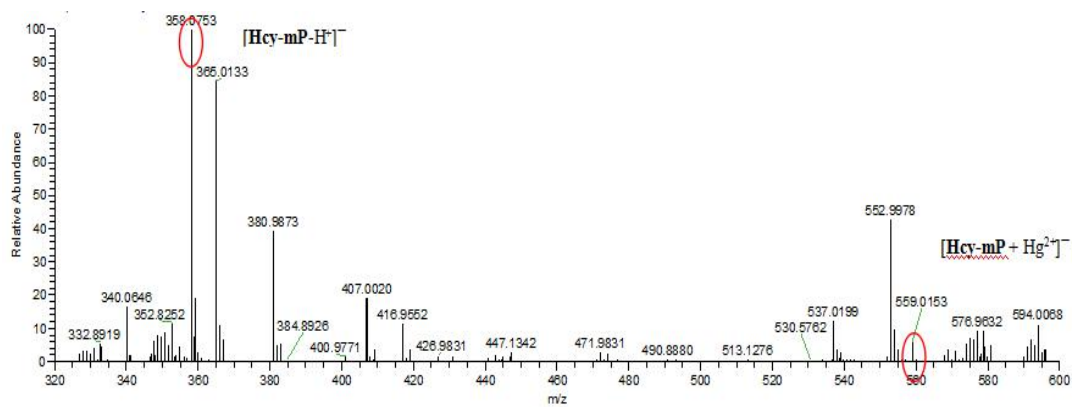


Fig S.4 ESI-MS of  $[\text{Hcy-mP} + \text{Hg}^{2+}]^-$

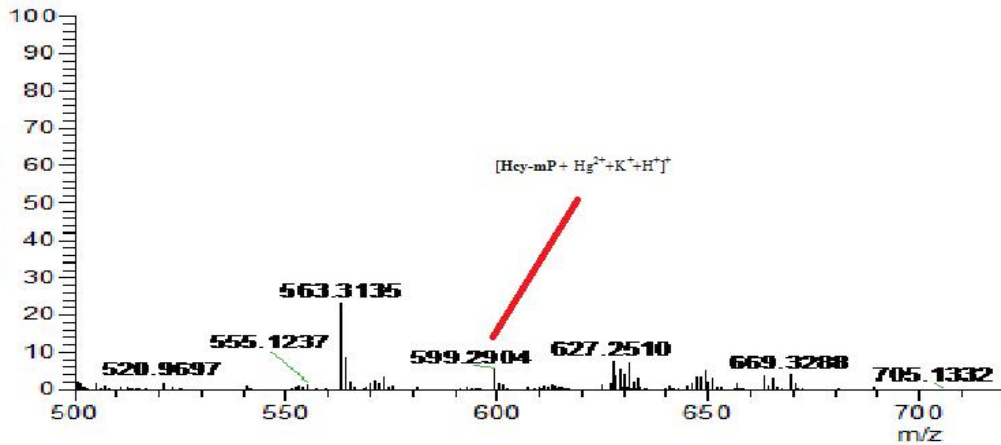


Figure S.5 ESI-MS of  $[\text{Hcy-mP} + \text{Hg}^{2+} + \text{K}^+ + \text{H}^+]^+$

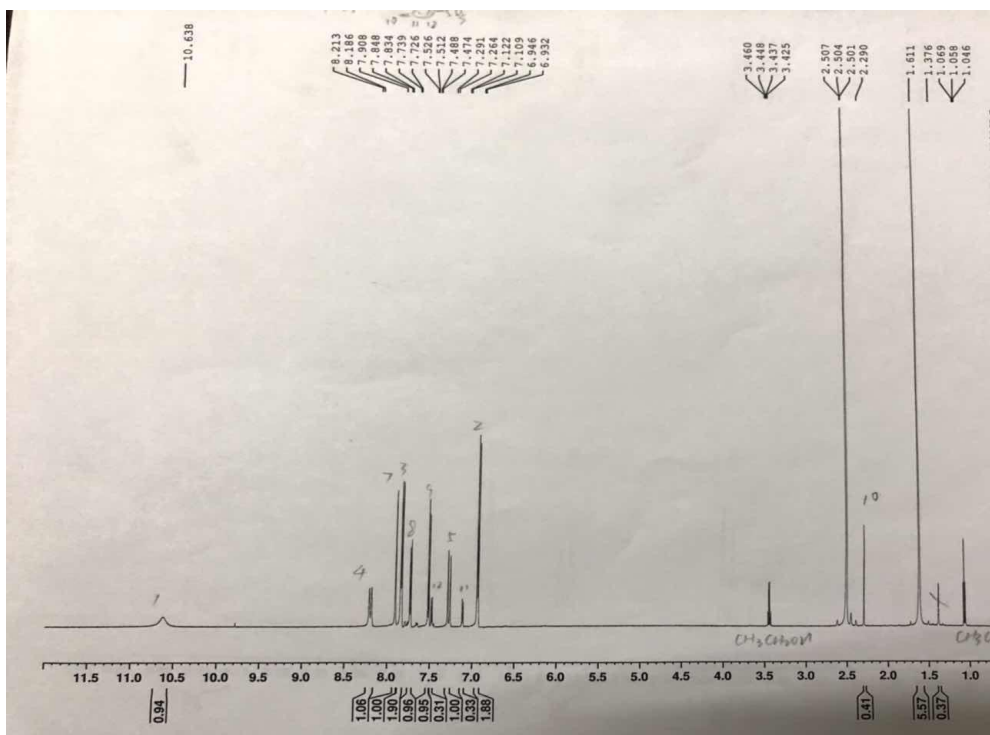


Figure S.6 <sup>1</sup>H NMR of Hcy-pP

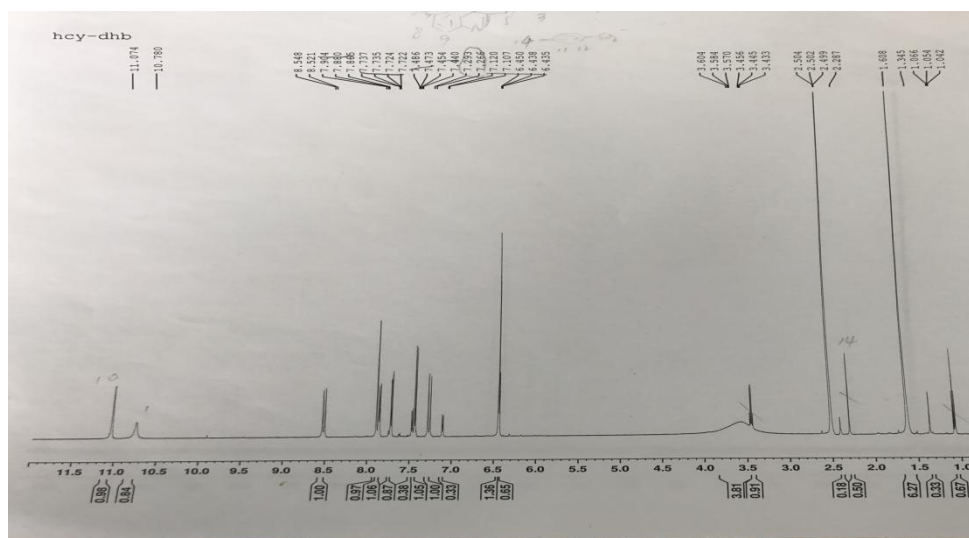


Figure S.7 <sup>1</sup>H NMR of Hcy-mP

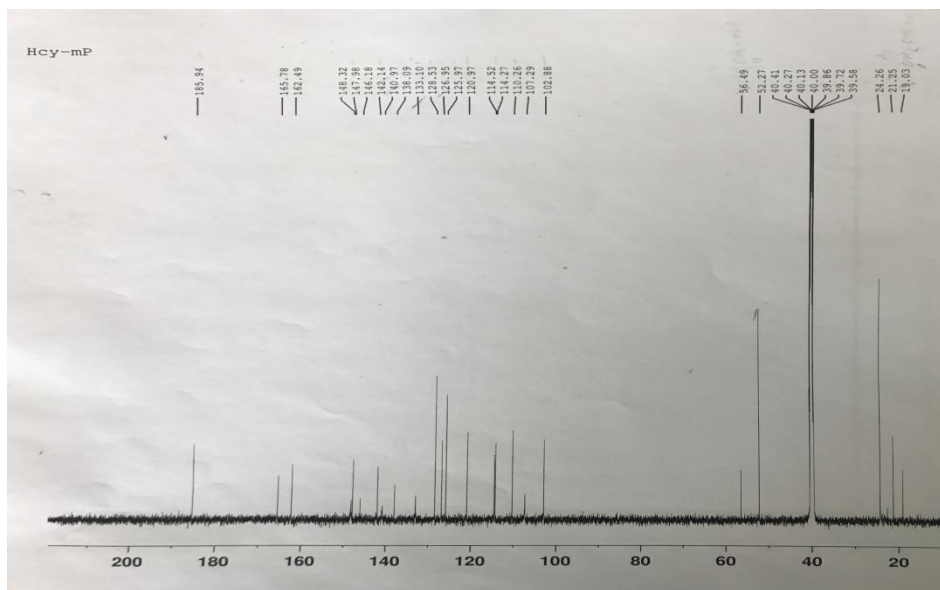


Figure S.8  $^{13}\text{C}$  NMR of Hcy-mP

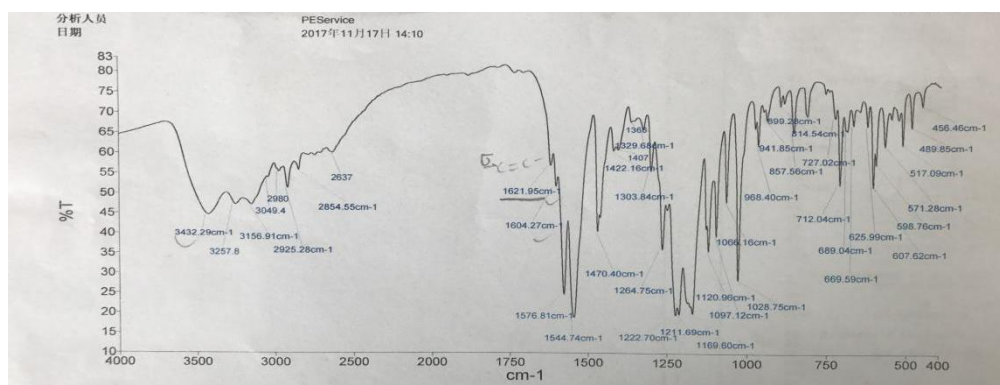


Figure S.9 IR of Hcy-mP