

## Supplementary Information

### A red-emitting fluorescent probe for detecting Hg<sup>2+</sup> in aqueous medium, living cells and organism with a large Stokes shift

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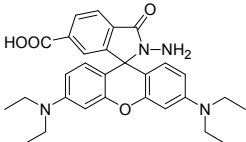
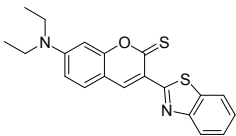
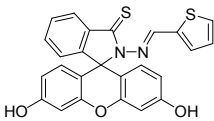
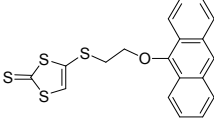
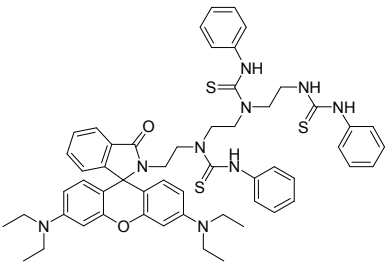
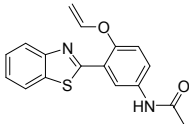
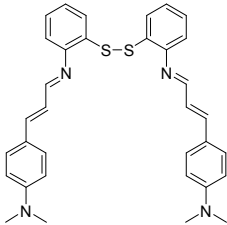
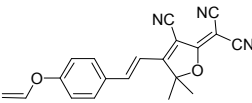
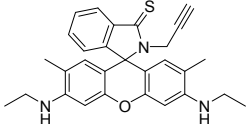
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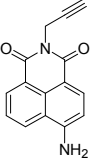
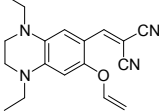
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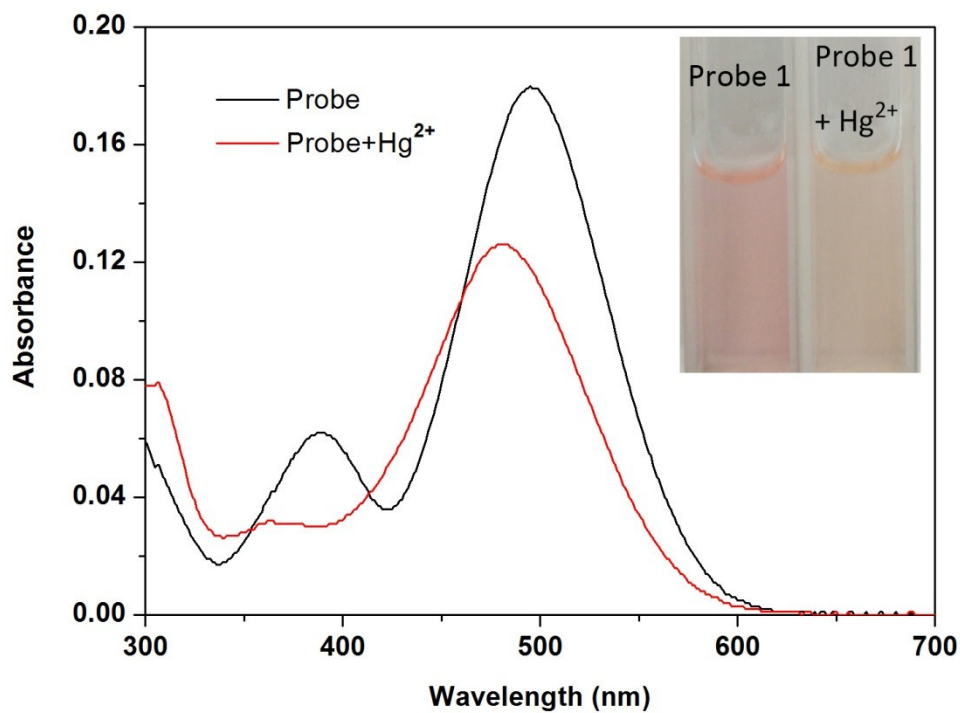
**Table S1** Comparison of Fluorescent Probes for Hg<sup>2+</sup>.

Probe	$\lambda_{\text{ex}}/\lambda_{\text{em}}$ (nm)	Stokes shift (nm)	Detection limit (nM)	Analytical applications	Literature
	520/573	53	97	River water, pond water and living cells	Analytica Chimica Acta, 2016, 934, 218- 225
	487/511	24	1700	No	Chem. Commun., 2009, 3560-3562
	509/529	20	39	Living cells	Talanta, 2017, 170, 103–110
	370/418	48	50	No	Chem. Commun., 2005, 2161–2163
	520/583	63	304	Pond water and tap water	Dyes and Pigments, 2016, 127, 94-99
	365/500	135	100	No	Org. Lett., 2011, 13, 3422-3425
	380/458	78	80	No	Org. Lett., 2012, 14, 6084-6087
	560/613	53	10	River water and living cells	Sensors and Actuators B, 2014, 191, 605– 611
	534/566	32	39	Living cells	Chem. Commun., 2010, 46, 3529–3531

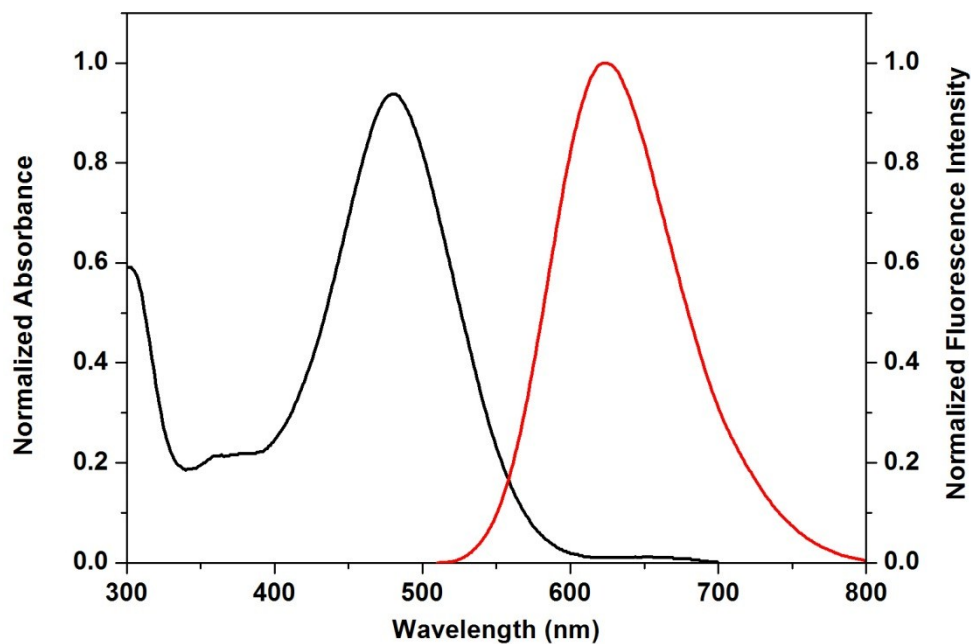
	420/480	66	50	No	Org. Lett., 2010, 22, 5310-5313
	475/625	150	7.1	Water samples, living cells and organism	This work

**Table S2** Determination of Hg<sup>2+</sup> in water samples.

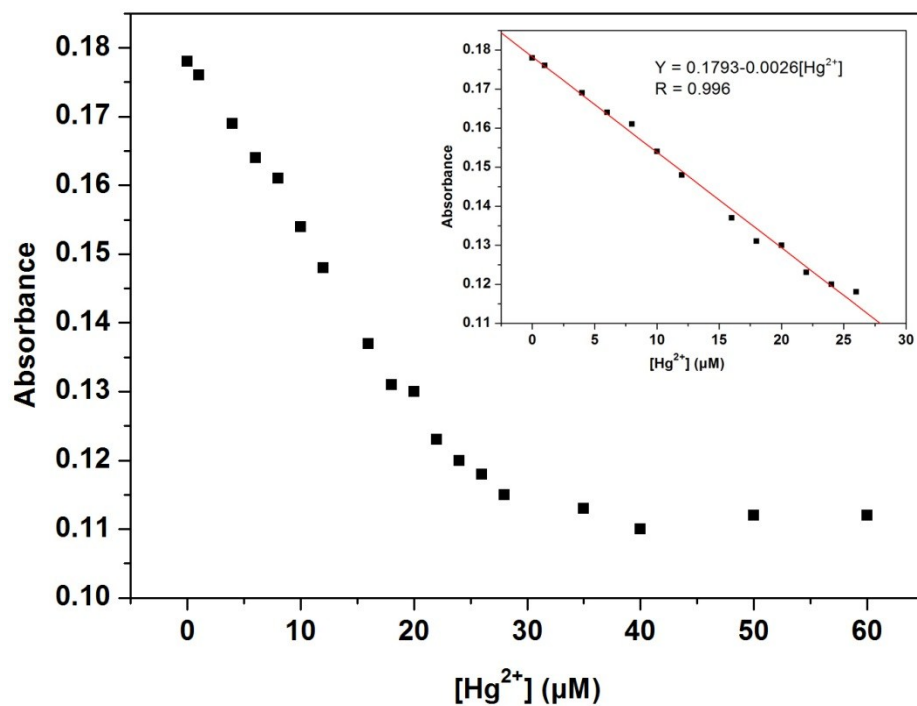
Sample	HgCl <sub>2</sub> spiked (μM)	HgCl <sub>2</sub> recovered (μM)	Recovery (%)
Tap water	0	not detected	
	2	2.07 ± 0.03	103
	4	3.82 ± 0.12	95
	6	5.78 ± 0.13	96
	8	7.78 ± 0.09	97
	10	10.50 ± 0.07	105
	12	12.61 ± 0.21	105
	14	13.48 ± 0.19	96
	16	16.51 ± 0.14	103
	18	17.74 ± 0.19	99
	20	19.48 ± 0.03	97
Yangtze River water	0	not detected	
	2	2.24 ± 0.09	109
	4	3.82 ± 0.05	96
	6	5.69 ± 0.12	95
	8	7.76 ± 0.20	97
	10	10.18 ± 0.16	102
	12	12.64 ± 0.19	105
	14	13.95 ± 0.22	100
	16	16.37 ± 0.06	102
	18	17.47 ± 0.08	97
	20	19.90 ± 0.15	99
Xiang River water	0	not detected	
	2	1.82 ± 0.13	91
	4	3.81 ± 0.21	95
	6	5.48 ± 0.19	91
	8	7.69 ± 0.07	96
	10	10.23 ± 0.06	102
	12	12.36 ± 0.08	103
	14	13.75 ± 0.11	98
	16	16.34 ± 0.12	102
	18	17.92 ± 0.07	99
	20	19.86 ± 0.20	99



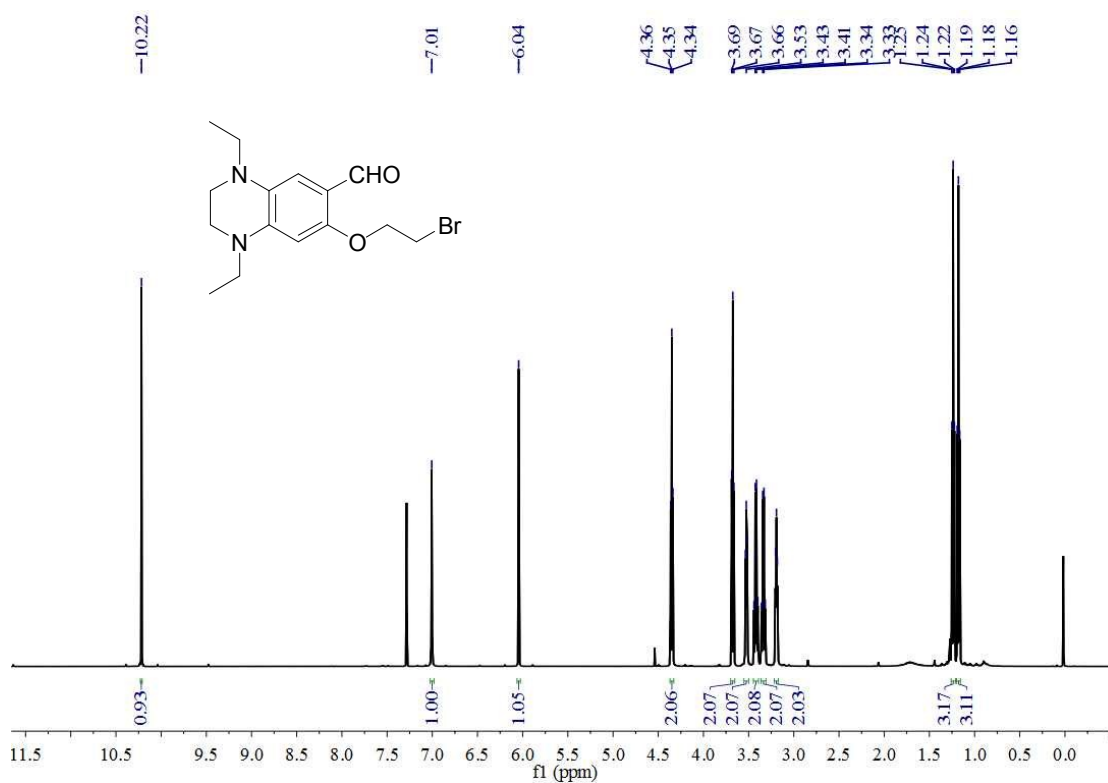
**Fig. S1** Absorption spectra of Probe 1 (10.0  $\mu\text{M}$ ) in the presence/absence of  $\text{Hg}^{2+}$  (5.0 equiv.) in HEPES buffer (20 mM, pH=7.4, containing 30% EtOH) incubation at room temperature for 60 min. Inset: photographs of Probe 1 without (left) and with (right) 5.0 equiv. of  $\text{Hg}^{2+}$ .



**Fig. S2** Absorption (black) and emission spectra (red) of dye 5 (10.0  $\mu\text{M}$ ) in HEPES buffer (20 mM, pH=7.4, containing 30% EtOH).



**Fig. S3** Absorbance at 495 nm of Probe **1** (10.0  $\mu\text{M}$ ) versus the concentration of  $\text{Hg}^{2+}$  in HEPES buffer (20 mM, pH=7.4, containing 30% EtOH). Inset: the linear relationship between the absorbance of the solution of Probe **1** and  $\text{Hg}^{2+}$  concentration (0.0-25.0  $\mu\text{M}$ ).



**Fig. S4**  $^1\text{H}$  NMR spectrum of compound **3** in  $\text{CDCl}_3$ .

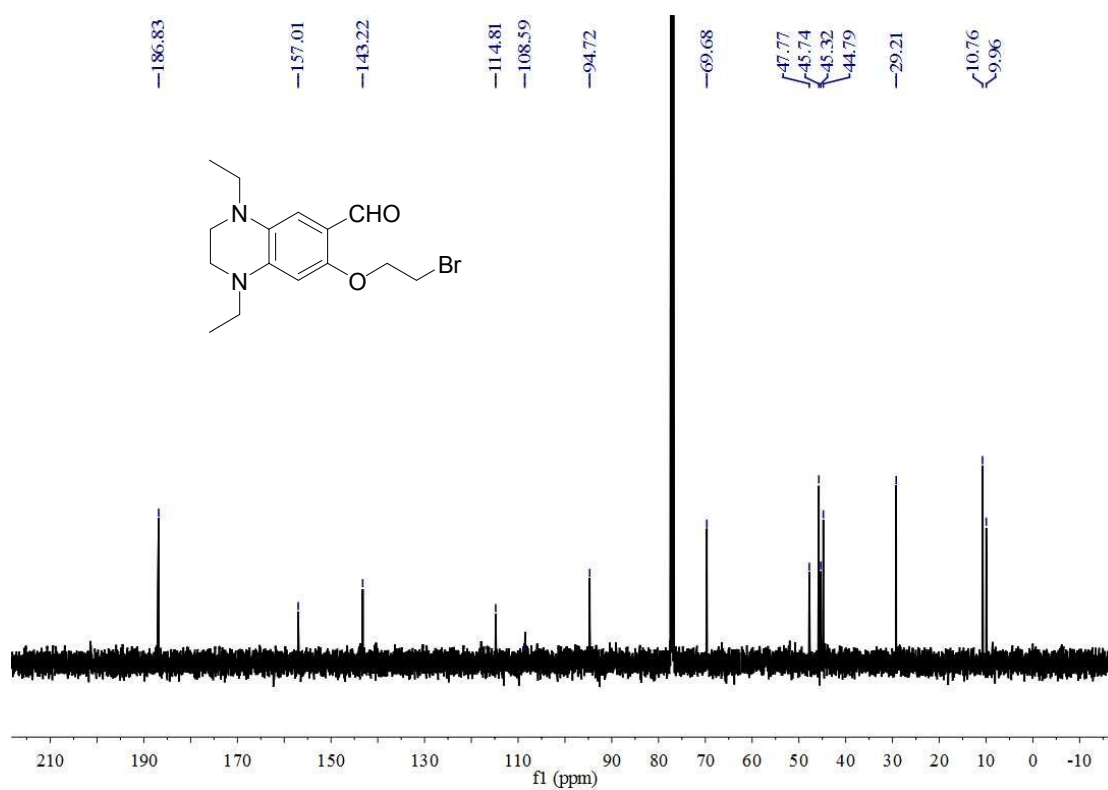


Fig. S5 <sup>13</sup>C NMR spectrum of compound 3 in CDCl<sub>3</sub>.

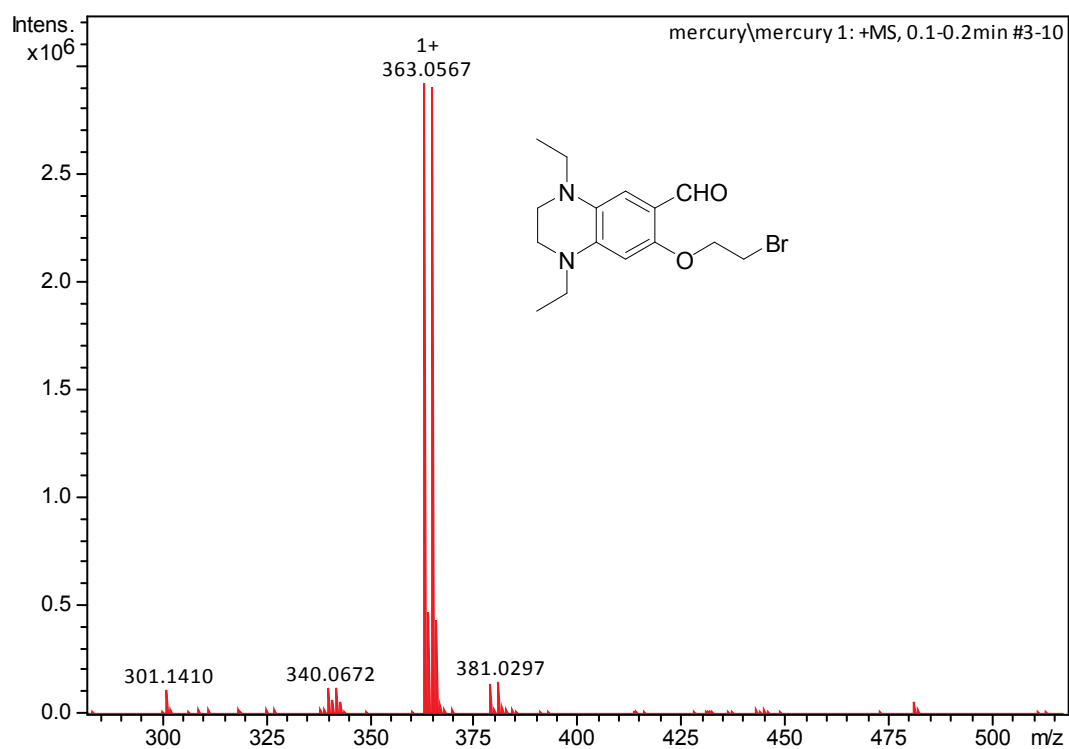


Fig. S6 HRMS spectrum of compound 3.

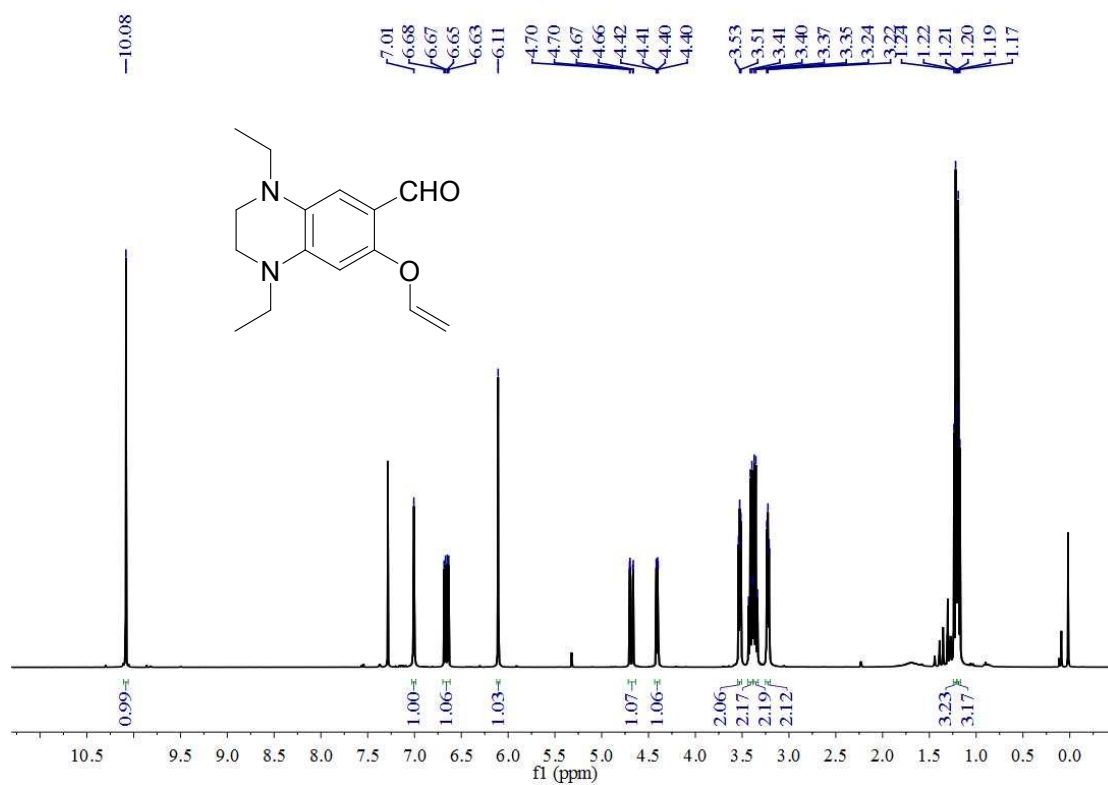


Fig. S7 <sup>1</sup>H NMR spectrum of compound 4 in CDCl<sub>3</sub>.

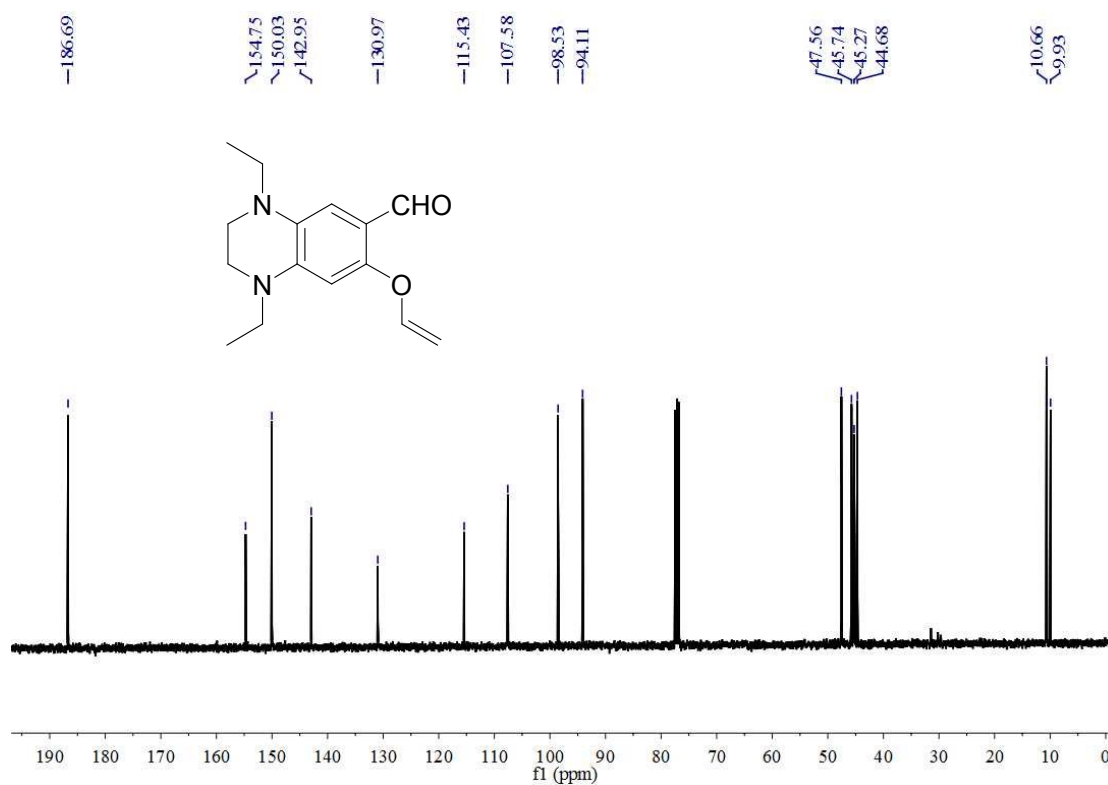


Fig. S8 <sup>13</sup>C NMR spectrum of compound 4 in CDCl<sub>3</sub>.

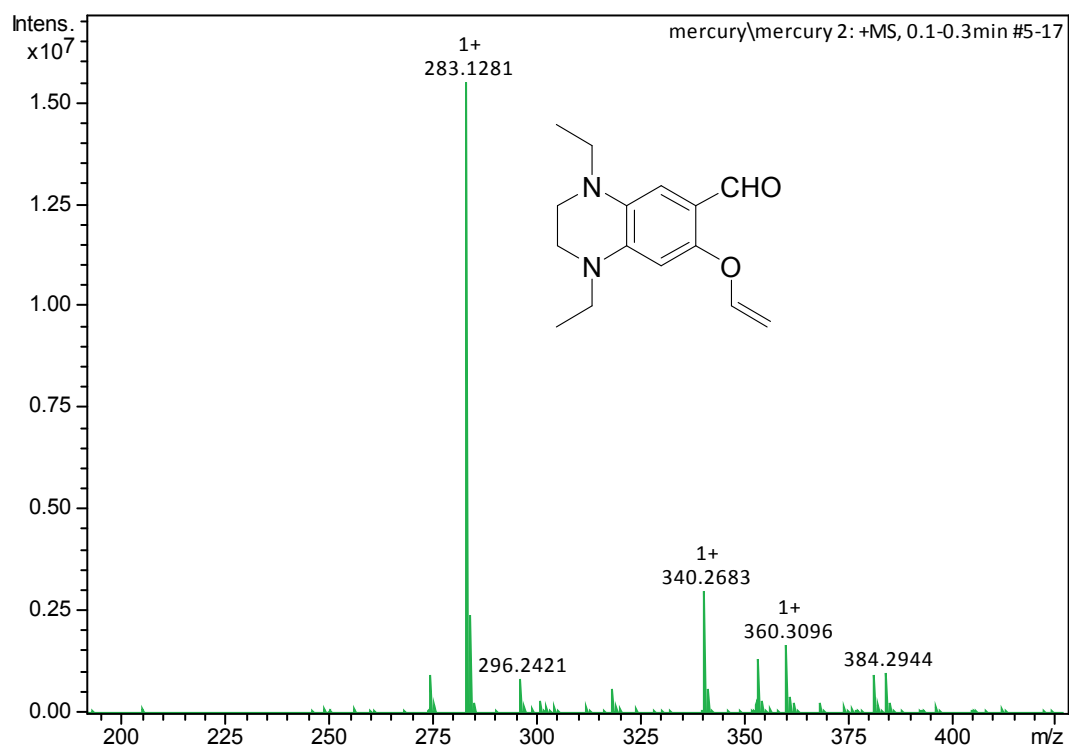


Fig. S9 HRMS spectrum of compound 4.

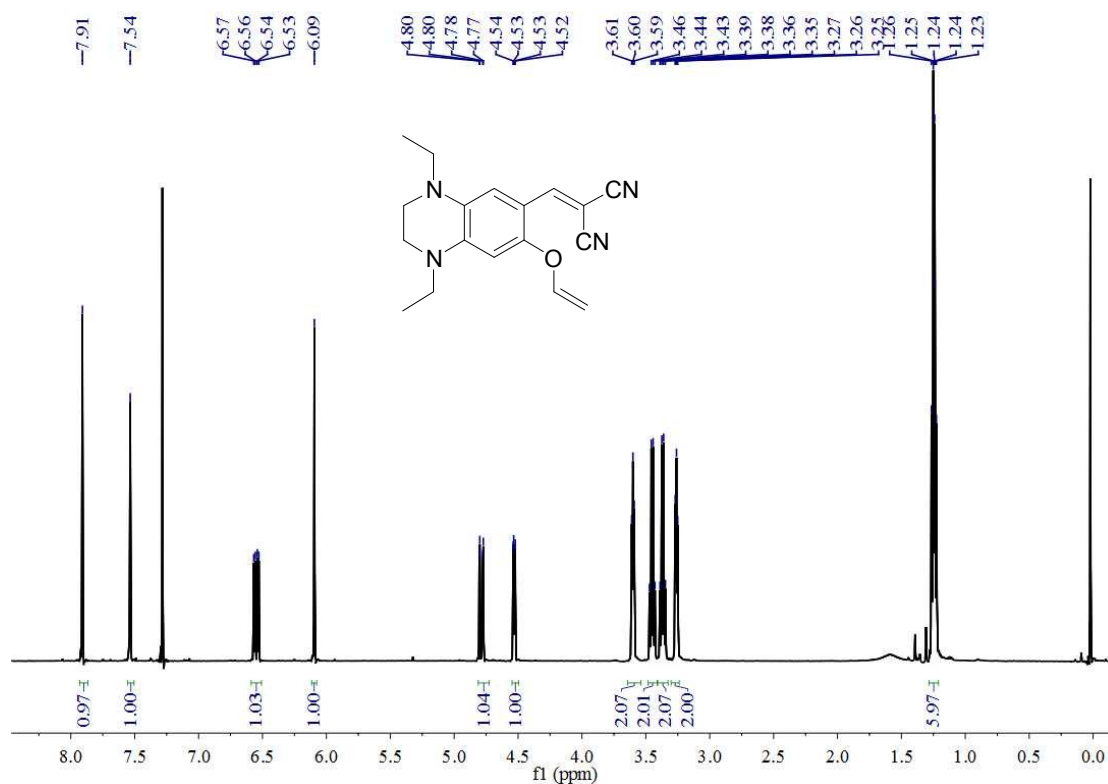
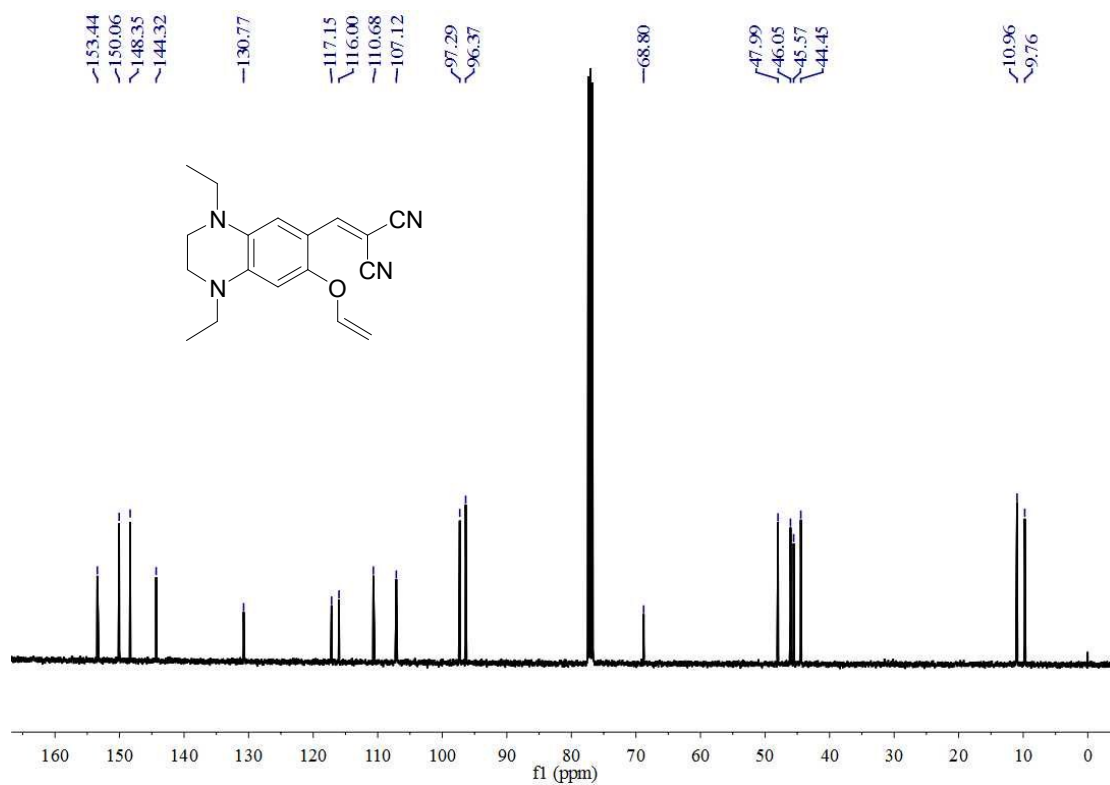
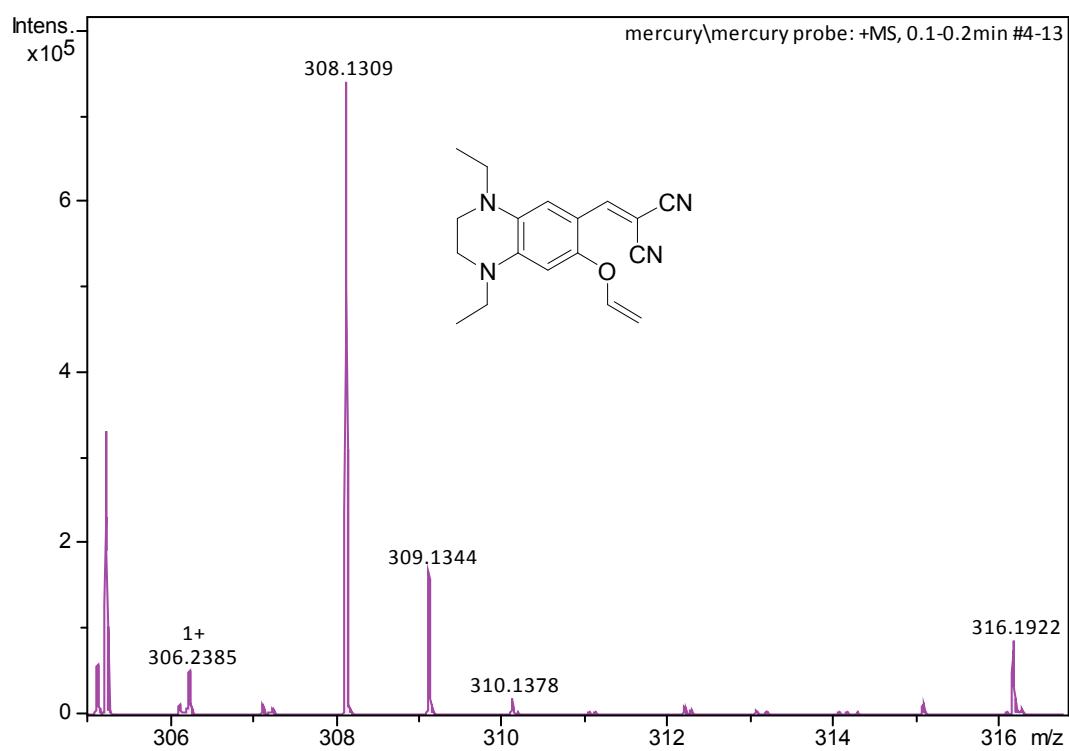


Fig. S10 <sup>1</sup>H NMR spectrum of Probe 1 in CDCl<sub>3</sub>.

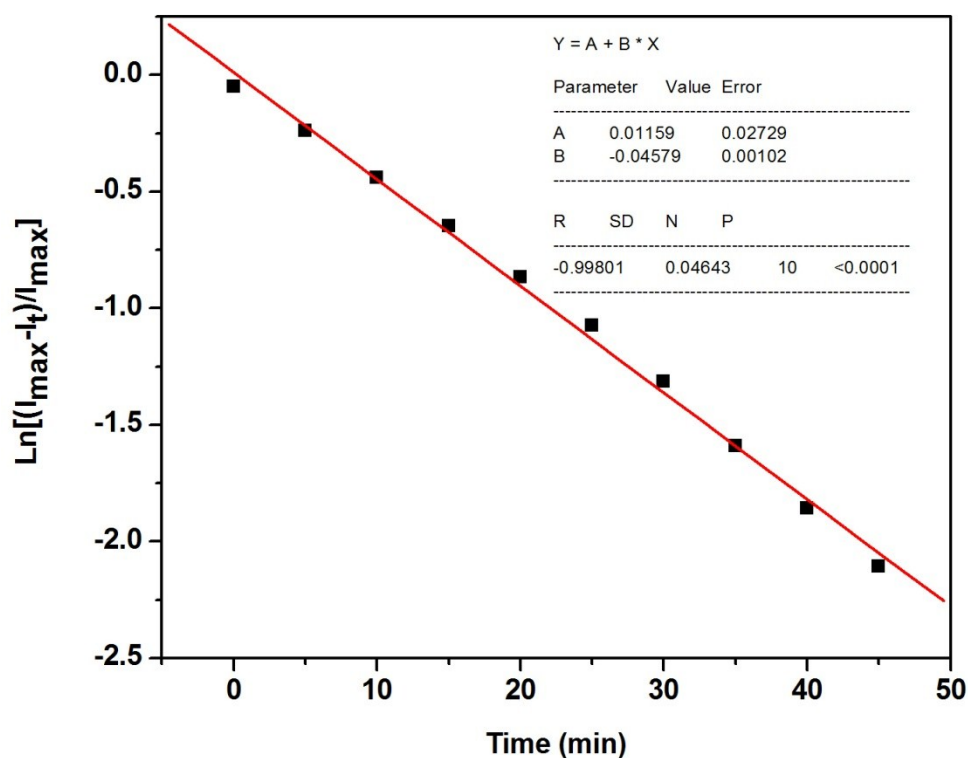




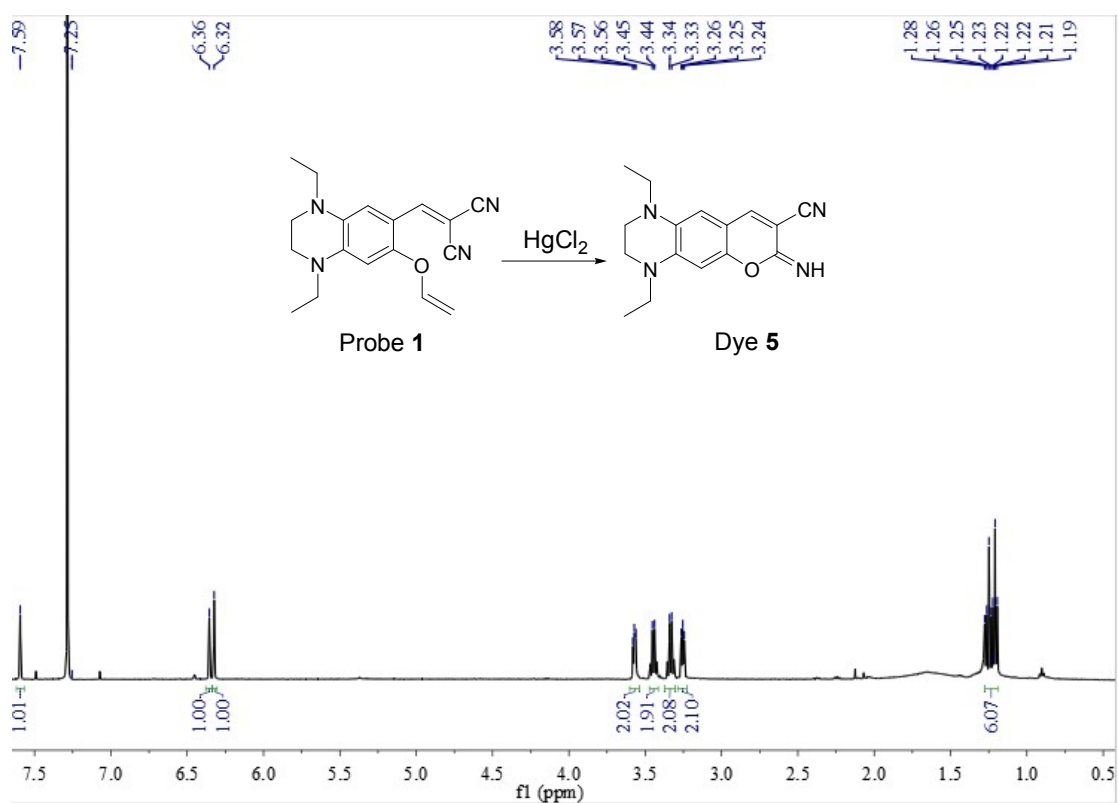
**Fig. S11** <sup>13</sup>C NMR spectrum of Probe 1 in CDCl<sub>3</sub>.



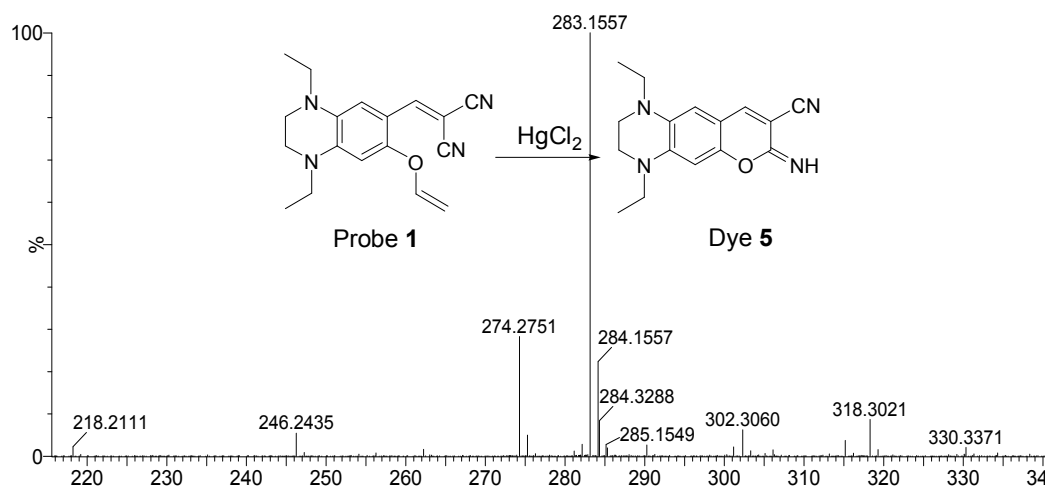
**Fig. S12** HRMS spectrum of compound Probe 1.



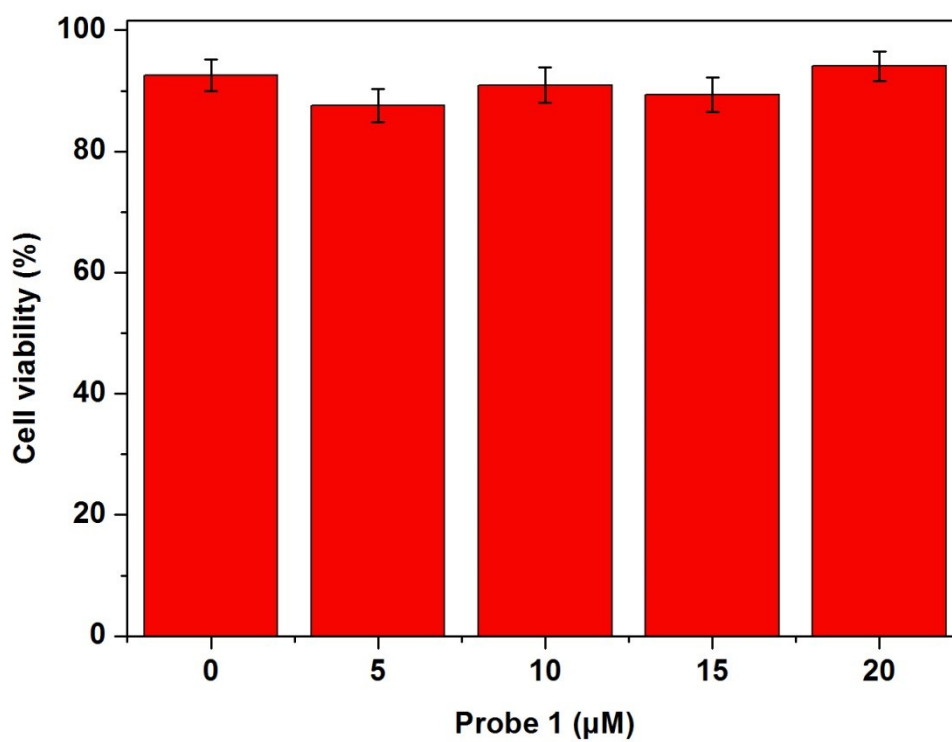
**Fig. S13** Plot of the natural log of fluorescence intensity change for Probe **1** (10.0  $\mu\text{M}$ ) with  $\text{Hg}^{2+}$  (5.0 equiv.) as a function of the reaction time in HEPES buffer (20 mM, pH=7.4, containing 30% EtOH).  $k_{\text{obs}} = 0.04579 \text{ min}^{-1}$ .



**Fig. S14**  $^1\text{H}$  NMR spectrum of the reaction product between Probe **1** and  $\text{Hg}^{2+}$  in  $\text{CDCl}_3$ .



**Fig. S15** HRMS spectrum of the reaction product between Probe 1 and  $\text{Hg}^{2+}$ .



**Fig. S16** Cytotoxicity assay of Probe 1 at different concentration for HeLa cells.