

## Supporting Information

### Naphthylthiourea-Modified Permethylcyclodextrin as a Highly Sensitive and Selective Turn-On Fluorescent Chemosensor for Hg<sup>2+</sup> in Water and Living Cells

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**Figure S1.** <sup>1</sup>H NMR spectrum (400 MHz) of **1** in D<sub>2</sub>O.

**Figure S2.** <sup>13</sup>C NMR spectrum (100 MHz) of **1** in CDCl<sub>3</sub>.

**Figure S3.** FT-IR spectrum of **1**.

**Figure S4.** ESI-MS of **1**.

**Figure S5.** <sup>1</sup>H NMR spectrum (400 MHz) of **2** in D<sub>2</sub>O.

**Figure S6.** <sup>13</sup>C NMR spectrum (75 MHz) of **2** in CDCl<sub>3</sub>.

**Figure S7.** HR-MS of **2**.

**Figure S8.** FT-IR spectrum of **2**.

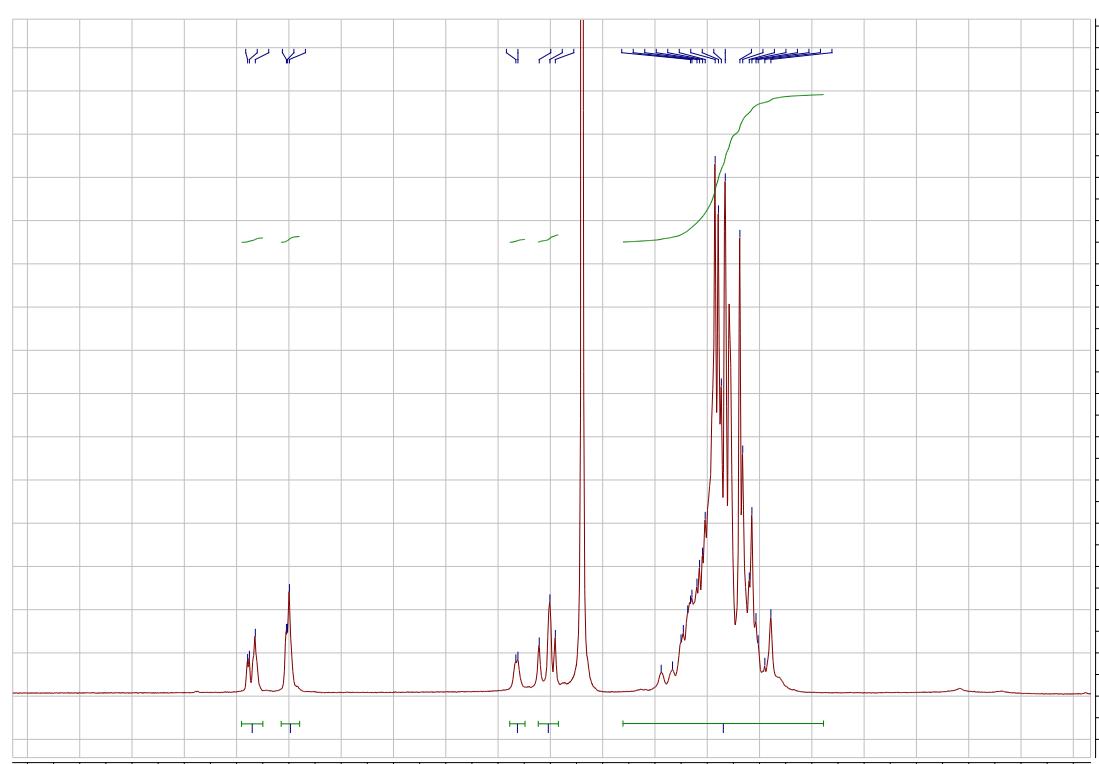
**Figure S9.** ESI-MS after addition of Hg<sup>2+</sup> ion into the aqueous solution of probe **1**.

**Figure S10.** ROESY spectrum between **1** and liposome.

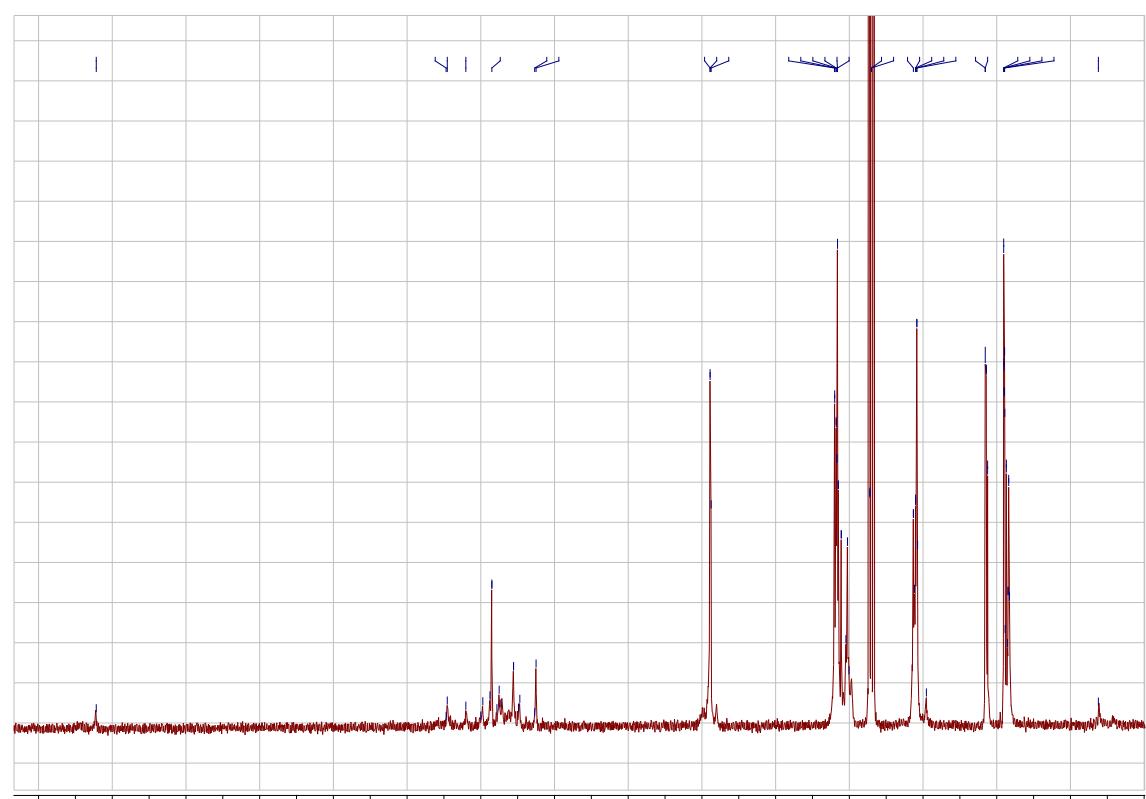
**Figure S11.** Fluorescence spectra of **1** and free 1-naphthyl isothiocyanate (5 μM in

H<sub>2</sub>O/MeCN) with and without the addition of Hg<sup>2+</sup> (200 equiv).

**Figure S12.** Fluorescence spectra of **1** (5 μM in H<sub>2</sub>O) with the addition of Ag<sup>+</sup> (200 equiv) within 72h.



**Figure S1.** <sup>1</sup>H NMR spectrum (400 MHz) of **1** in  $\text{D}_2\text{O}$ .



**Figure S2.** <sup>13</sup>C NMR spectrum (100 MHz) of **1** in  $\text{CDCl}_3$ .

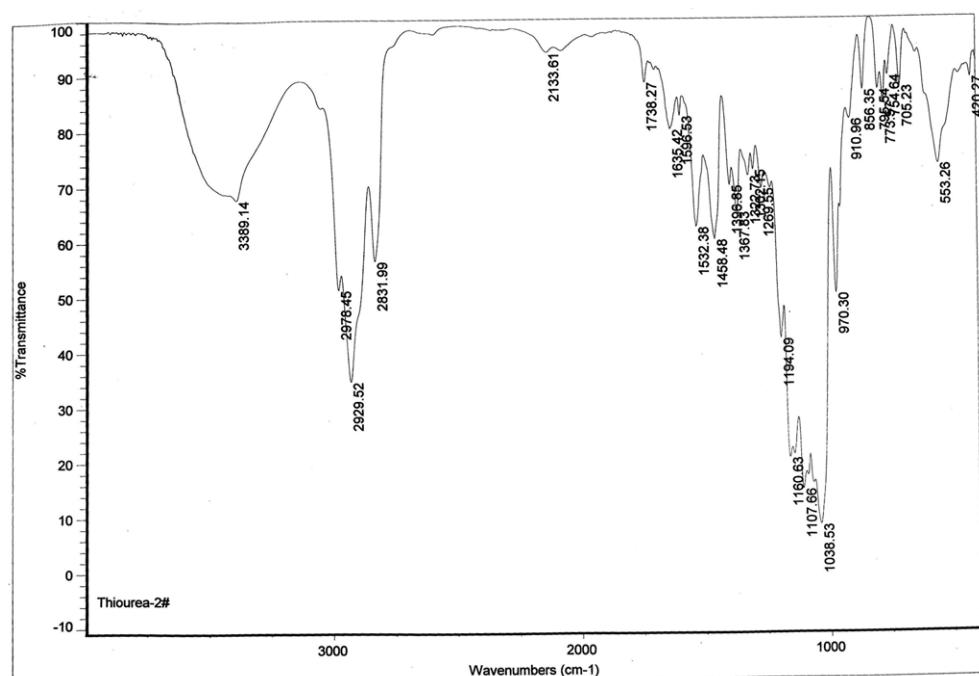


Figure S3. FT-IR spectrum of 1.

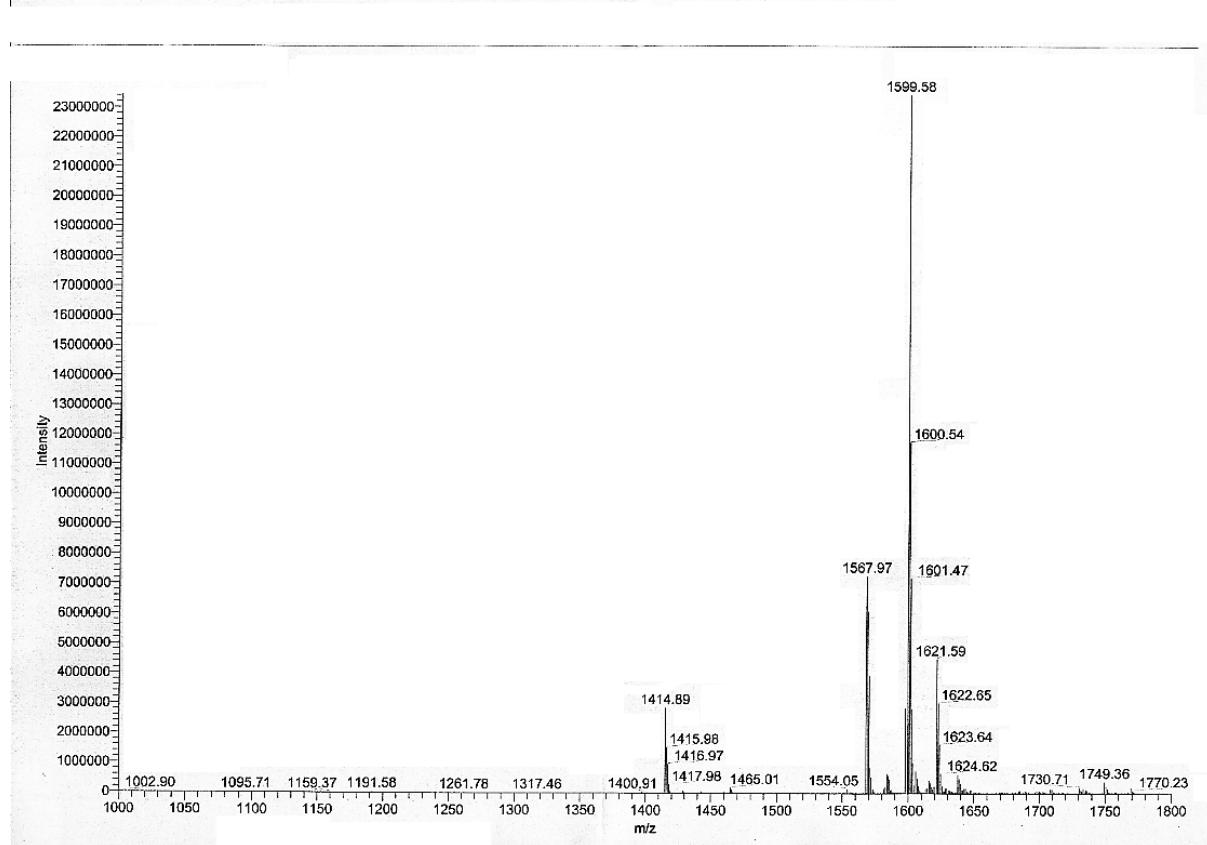
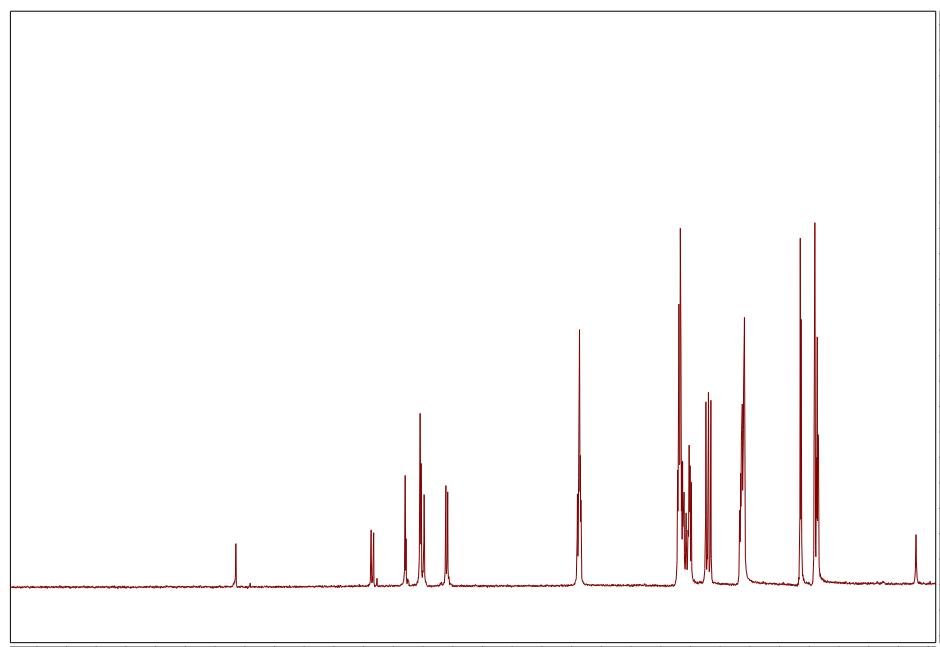
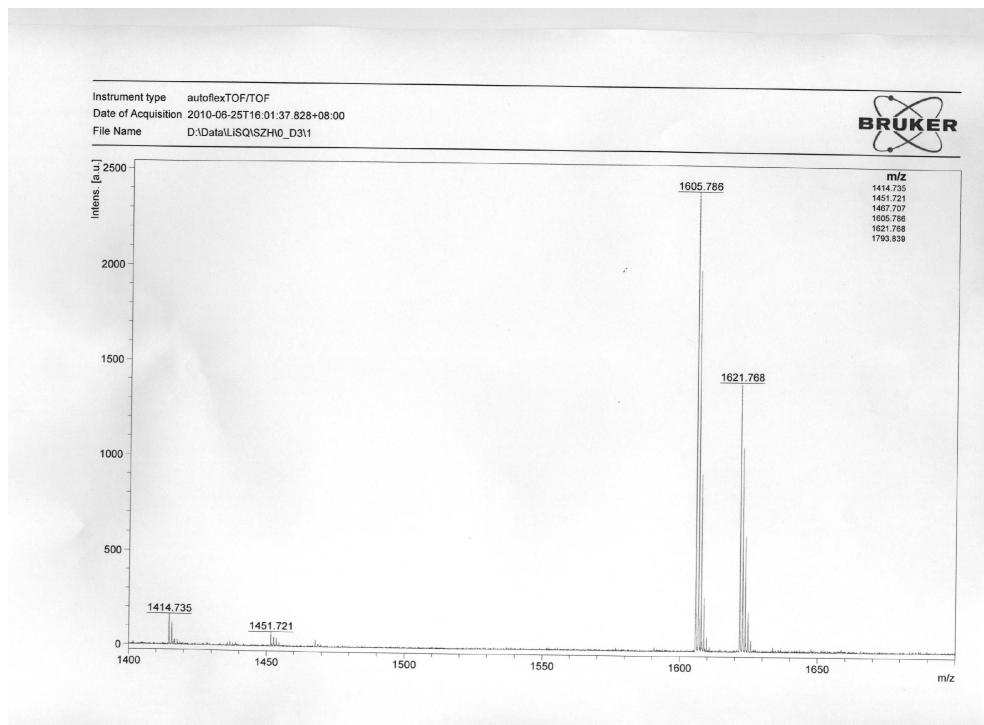


Figure S4. ESI-MS of 1.

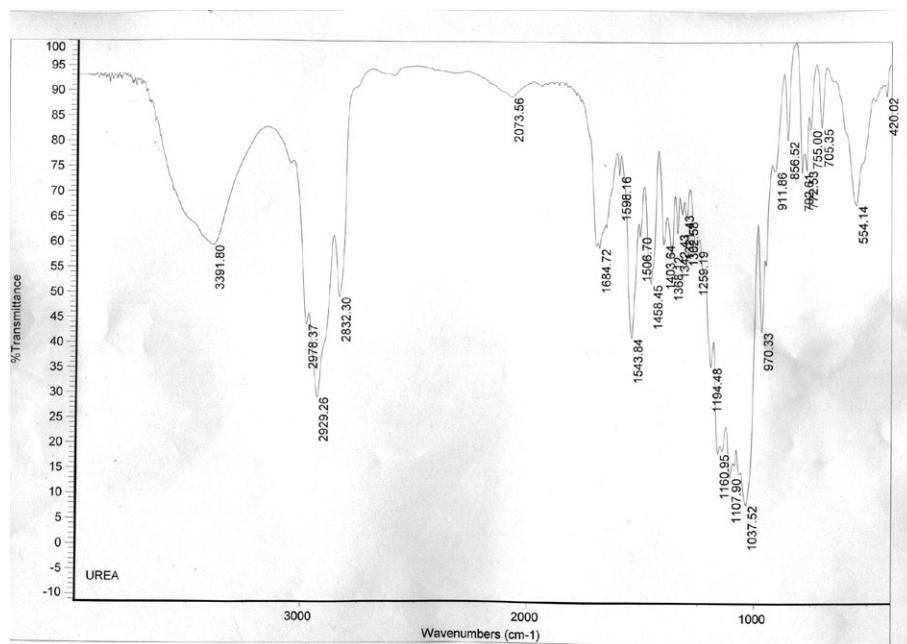
**Figure S5.**  $^1\text{H}$  NMR spectrum (400 MHz) of **2** in  $\text{D}_2\text{O}$ .



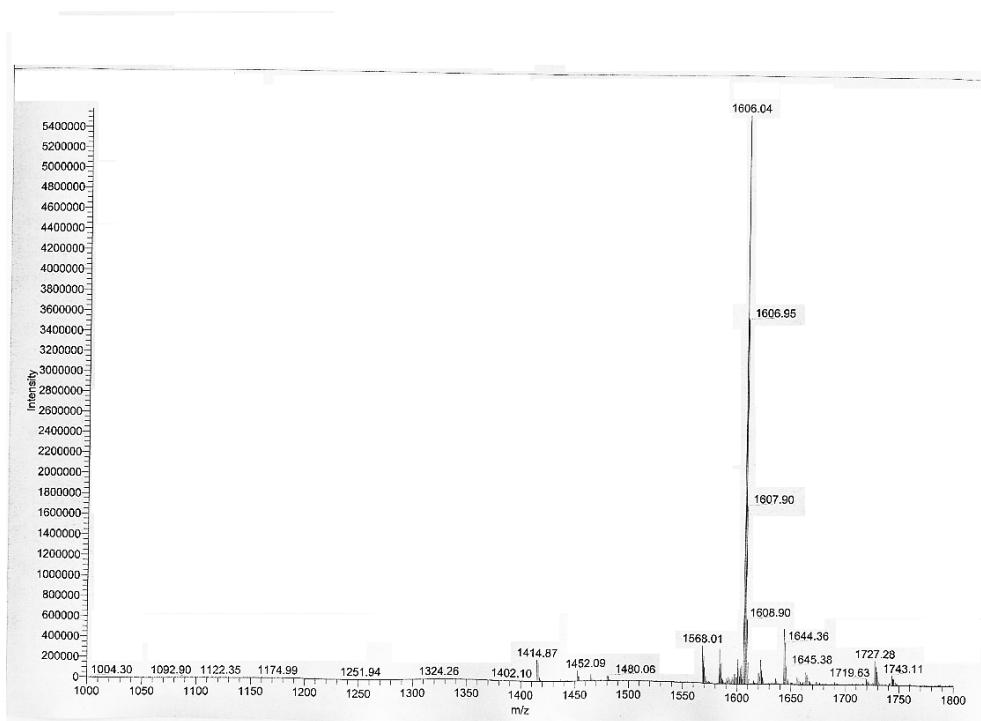
**Figure S6.**  $^{13}\text{C}$  NMR spectrum (75 MHz) of **2** in  $\text{CDCl}_3$ .



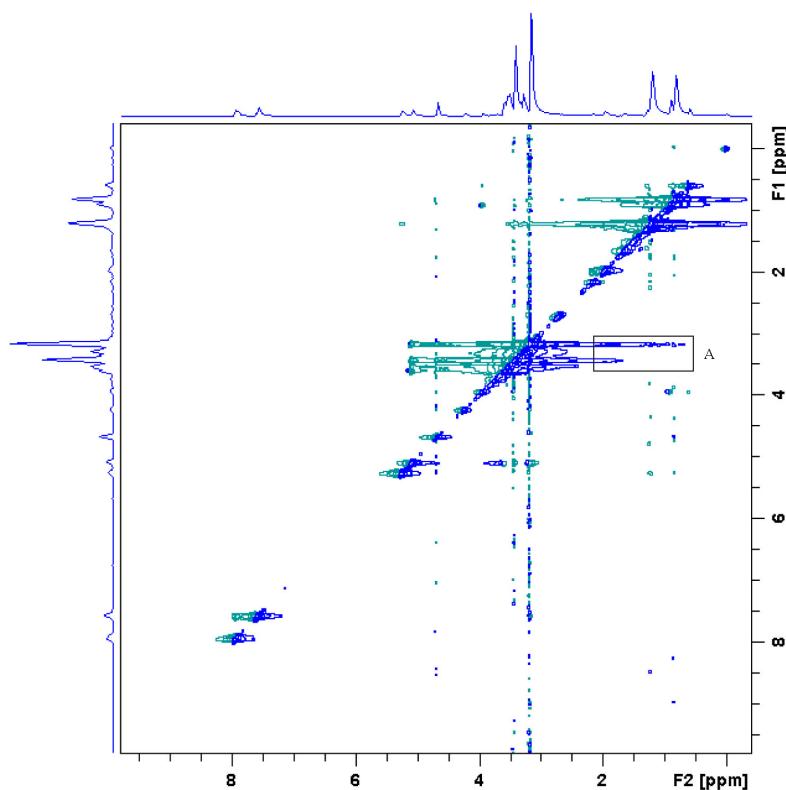
**Figure S7.** HRMS (MALDI-TOF) of **2**.



**Figure S8.** FT-IR spectrum of **2**.

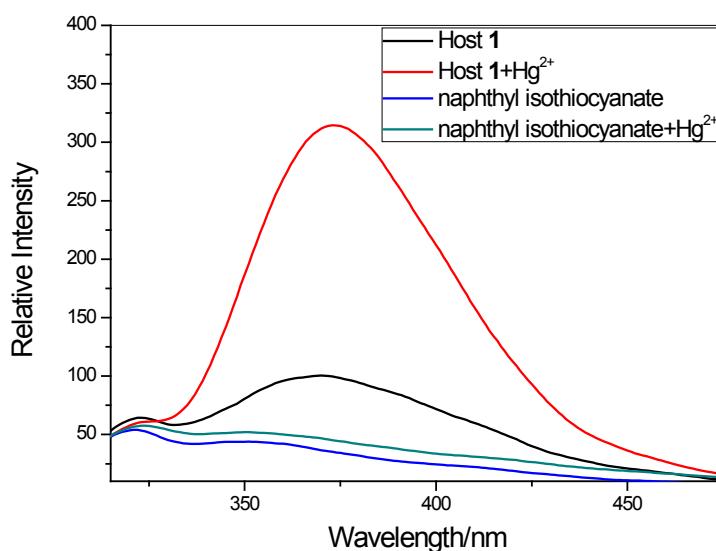


**Figure S9.** ESI-mass spectrum of **1** after the addition of  $\text{Hg}^{2+}$  ion.

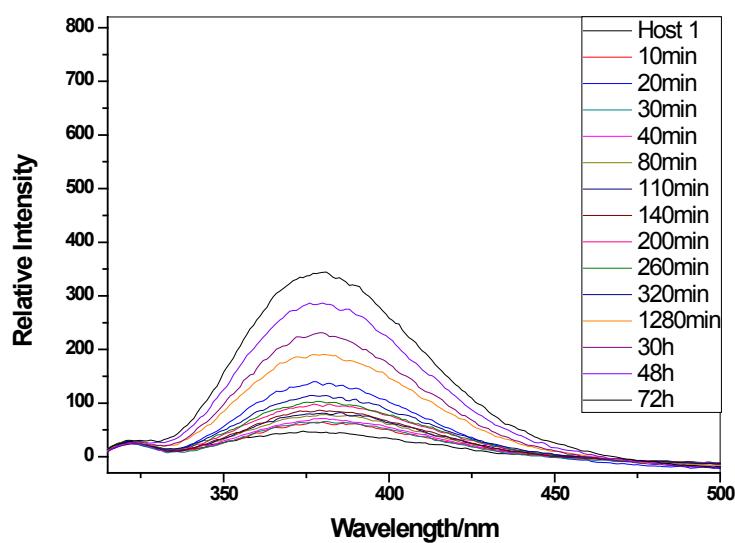


**Figure S10.** ROESY spectrum of **1** in the presence of liposome, where the peaks A were assigned to the NOE correlations between the cholesterol or lecithin protons in liposome and

the interior protons (H3/H5/H6) of PMCD.



**Figure S11.** Fluorescence spectra of **1** and free 1-naphthyl isothiocyanate (5  $\mu$ M in  $\text{H}_2\text{O}/\text{MeCN}$ ) with and without the addition of  $\text{Hg}^{2+}$  (200 equiv).



**Figure S12.** Fluorescence spectra of **1** (5  $\mu$ M in  $\text{H}_2\text{O}$ ) with the addition of  $\text{Ag}^+$  (200 equiv) within 72h.