

Supporting Information

Pillar[5]arene-based fluorescent polymer for selective detection and removal of mercury ions

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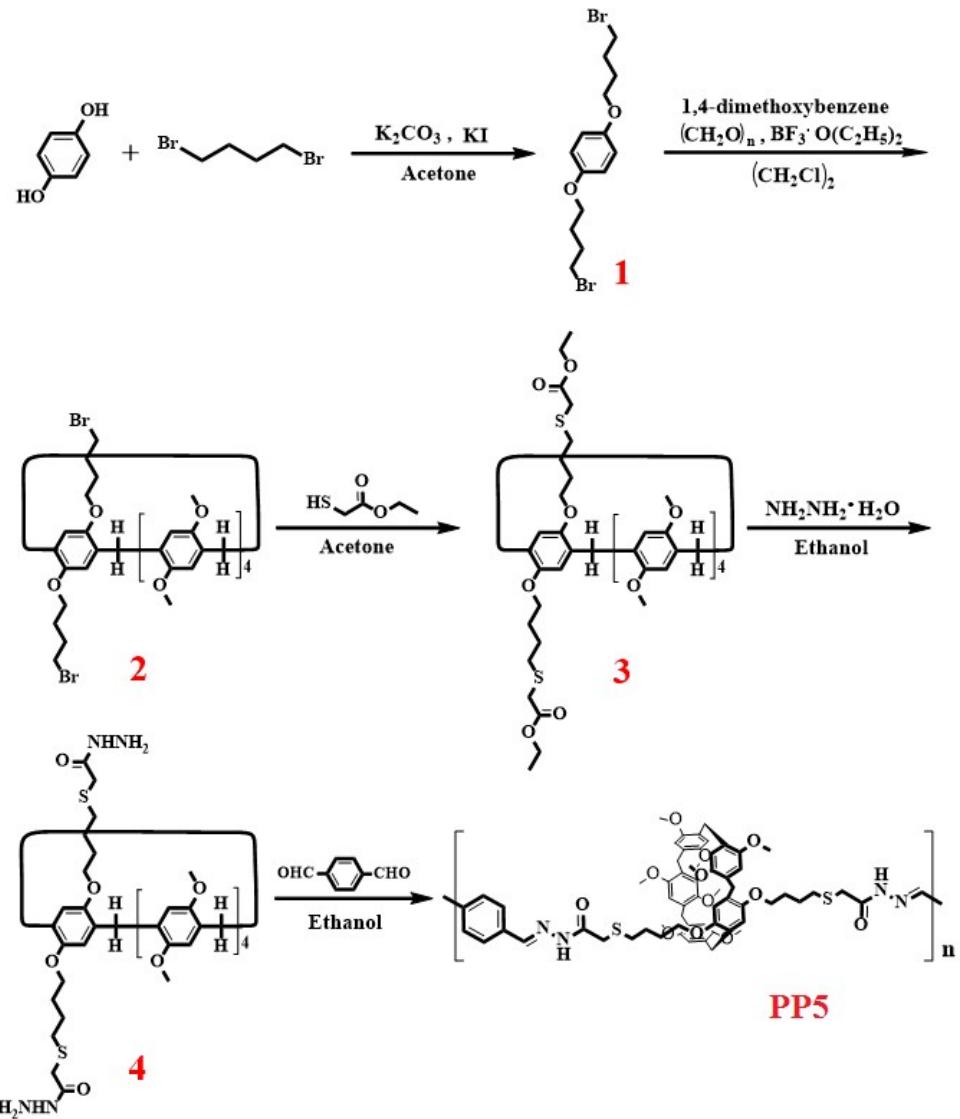
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1. Synthesis of polymer PP5



Scheme S1 Synthesis of polymer PP5.

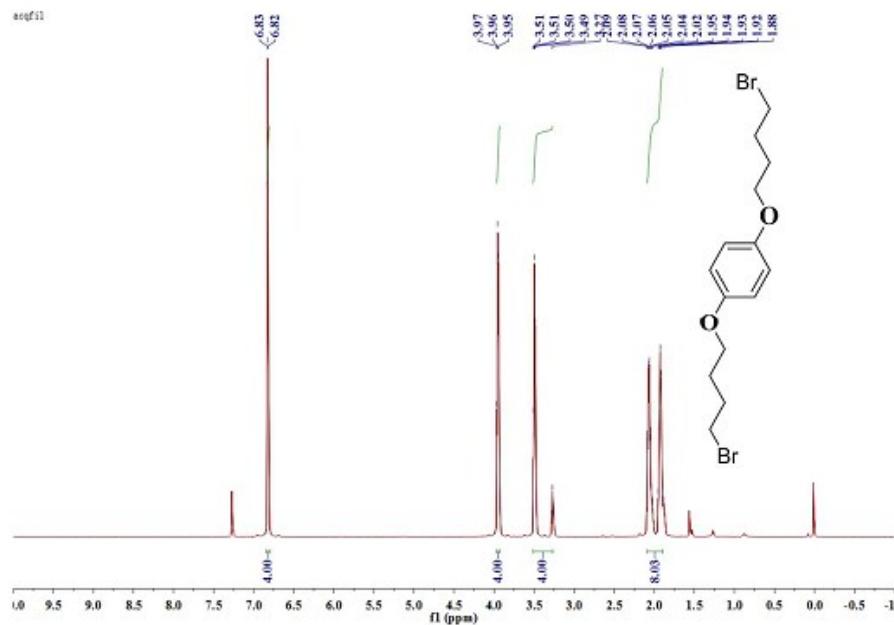


Fig. S1 ^1H NMR spectra (600 MHz, CDCl_3) of 1,4-bis (4-bromobutoxyl) benzene **1**.

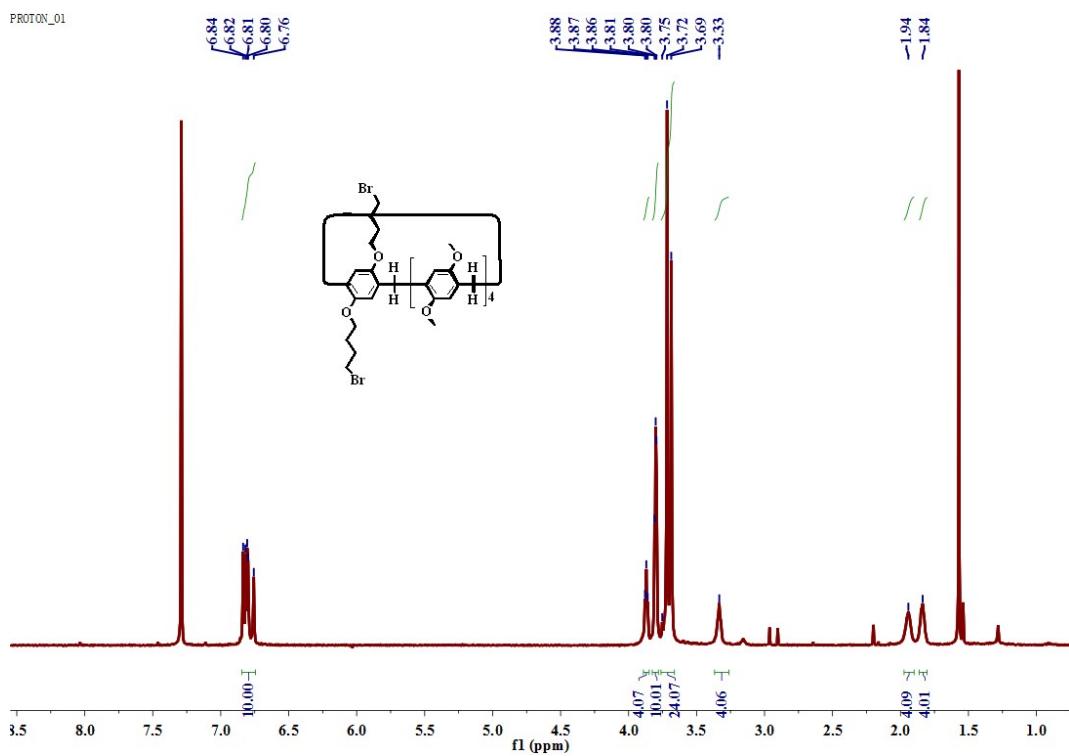


Fig. S2 ^1H NMR spectra(600 MHz, CDCl_3) of a copillar[5]arene **2**.

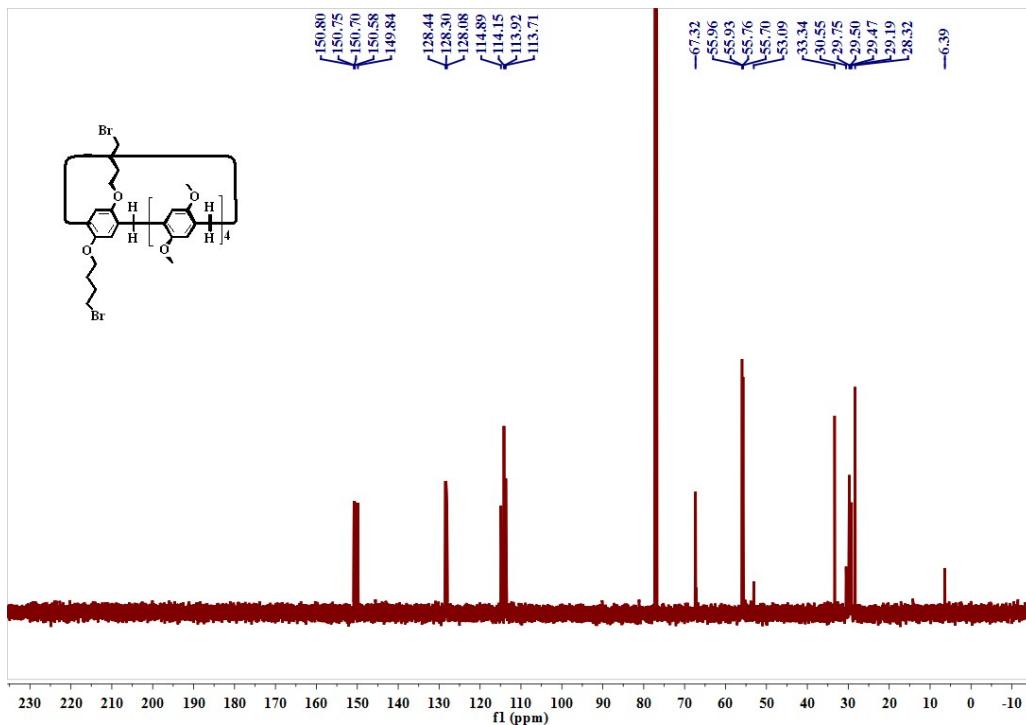


Fig. S3 ^{13}C NMR spectra(151 MHz, CDCl_3) of a copillar[5]arene **2**.

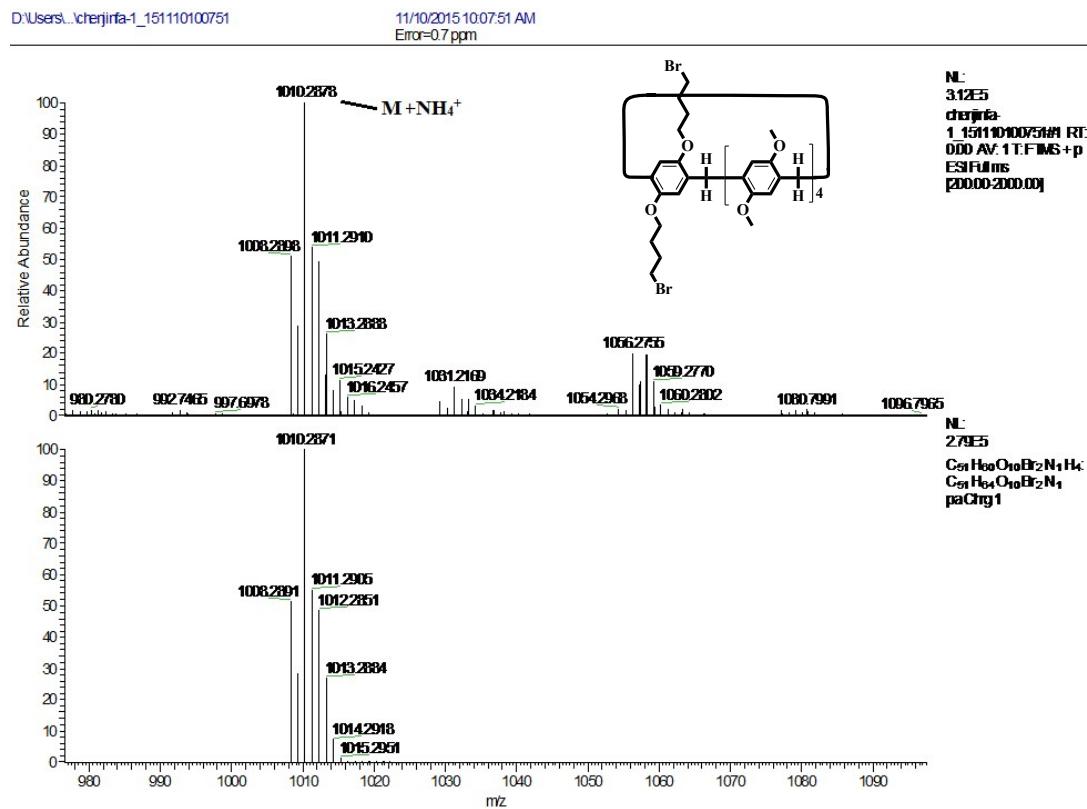


Fig. S4 High resolution mass data of a copillar[5]arene **2**.

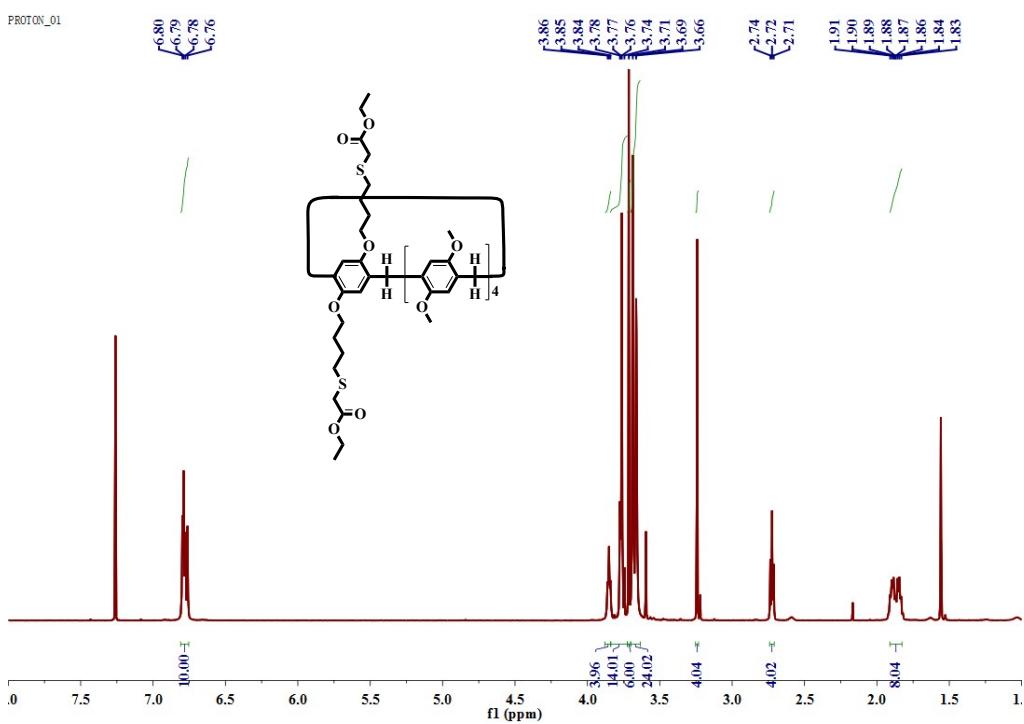


Fig. S5 ^1H NMR spectra (600 MHz, CDCl_3) of functionalized pillar[5]arene 3.

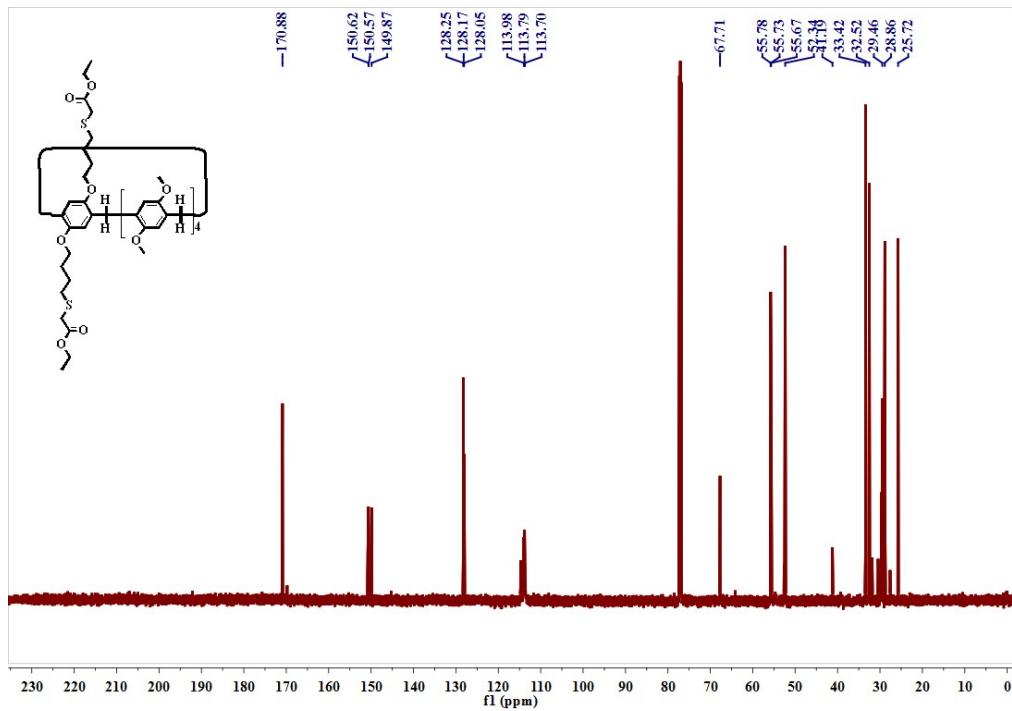


Fig. S6 ^{13}C NMR spectra (151 MHz, CDCl_3) of functionalized pillar[5]arene 3.

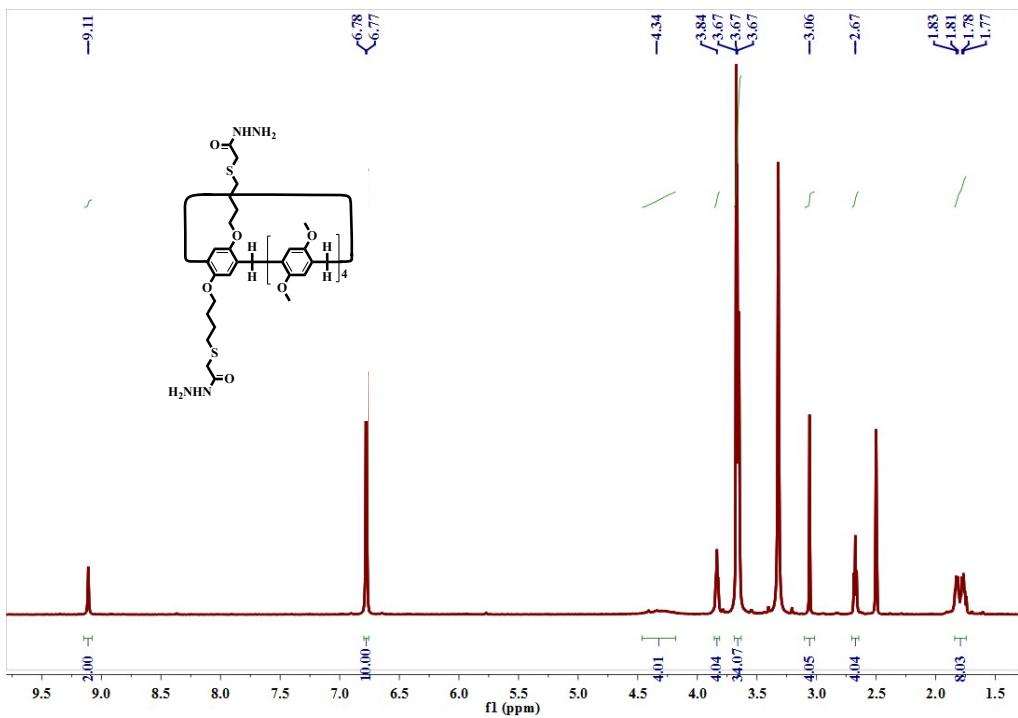


Fig. S7 ^1H NMR spectra (600 MHz, CDCl_3) of pillar[5]arene **4**.

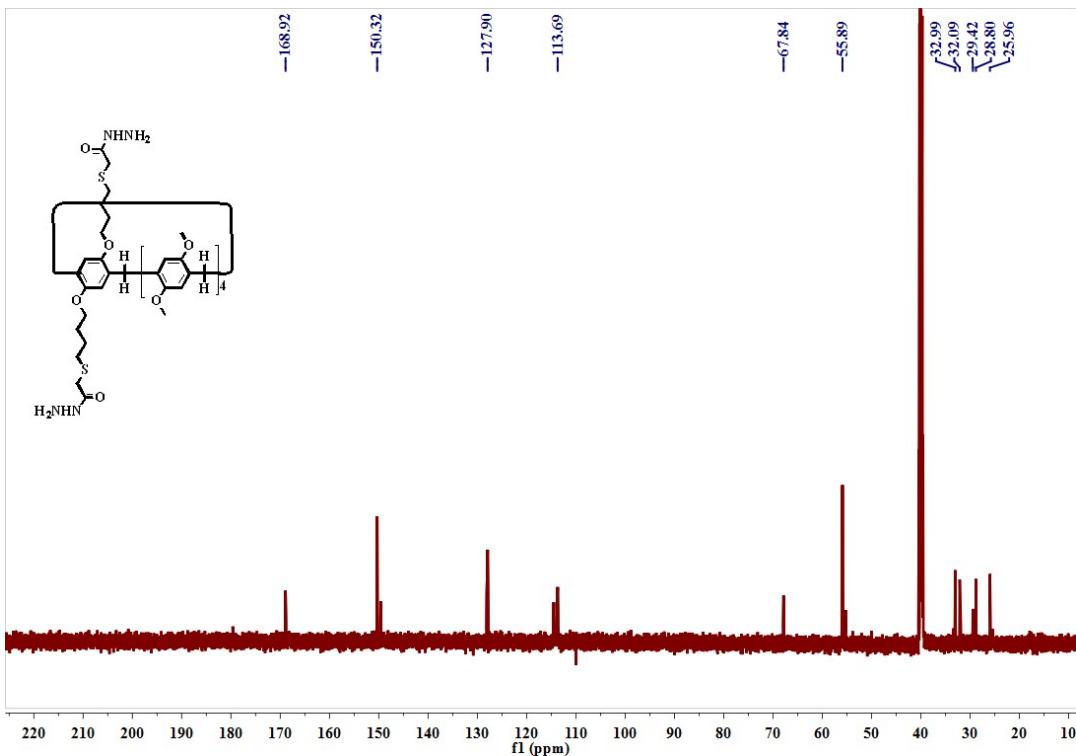


Fig. S8 ^{13}C NMR spectra (151 MHz, CDCl_3) of pillar[5]arene **4**.

Generic Display Report

Analysis Info

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Sample Name CHENJINFA160427_3
Comment

Acquisition Date 4/27/2016 5:28:17 PM

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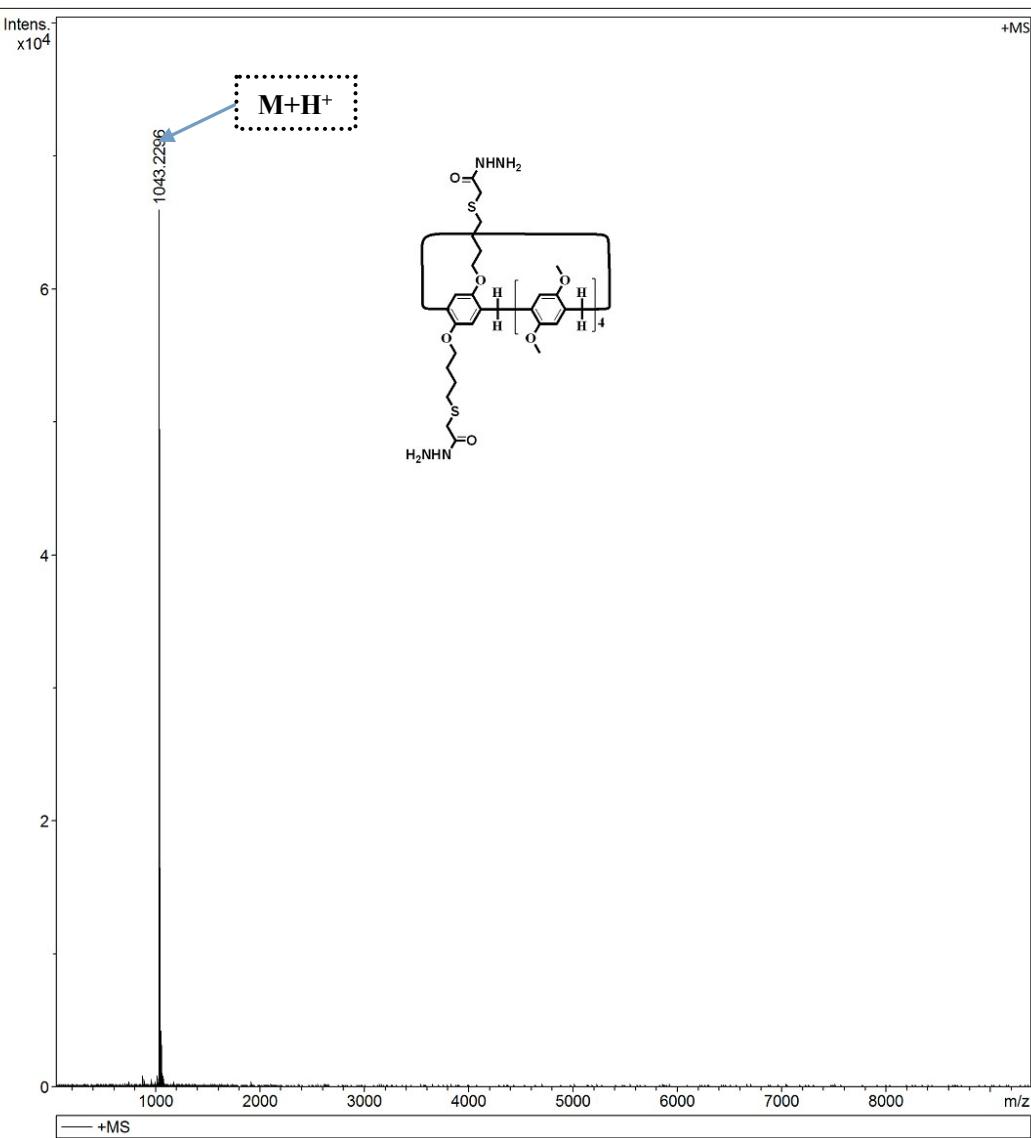


Fig. S9 High resolution mass data of pillar[5]arene 4.

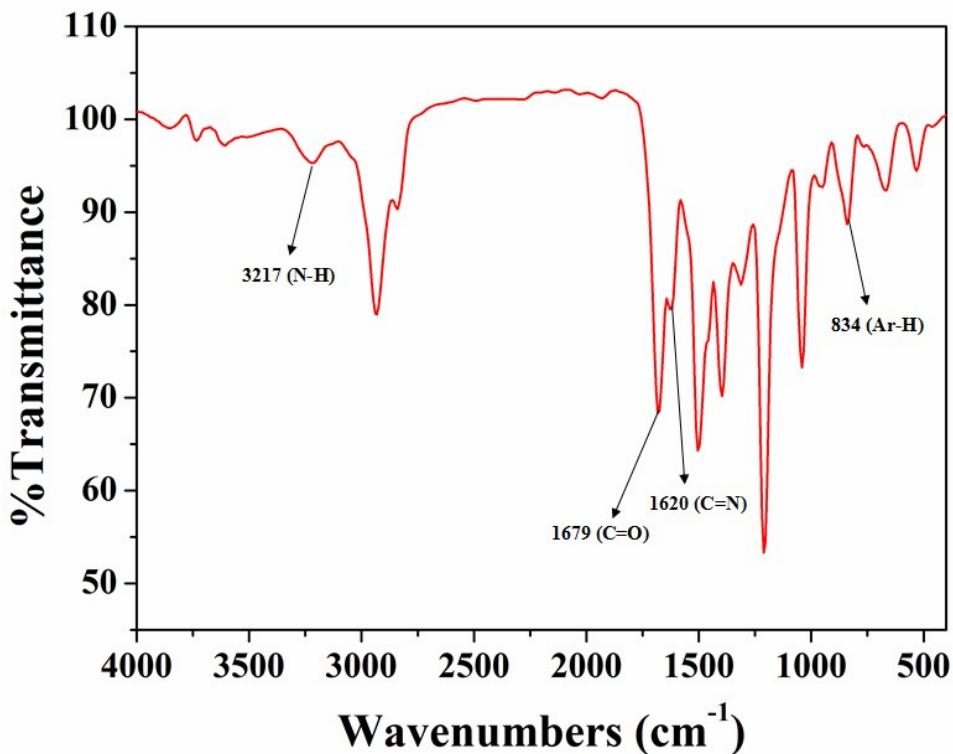
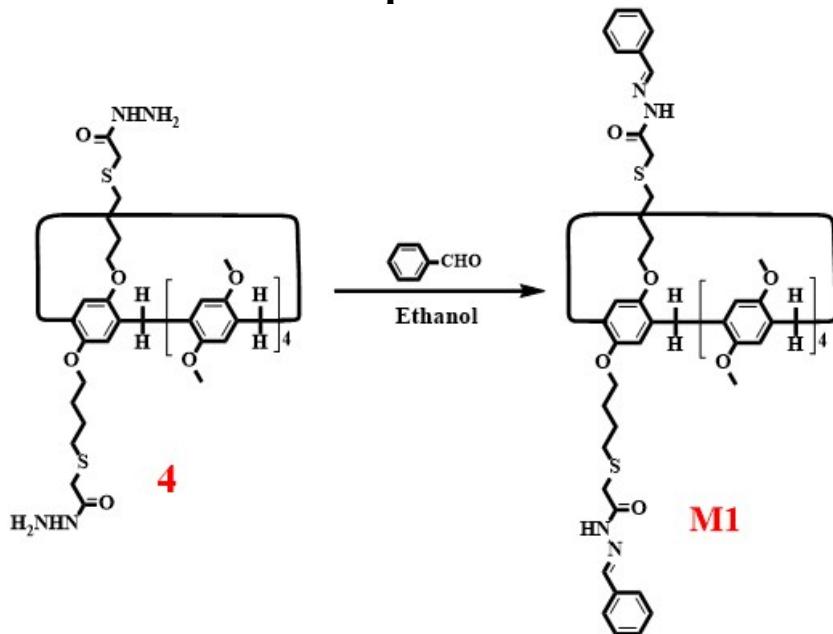


Fig. S10 FT-IR spectra of polymer **PP5**. The $\nu_{\text{C}=\text{N}}$ band at 1620 cm^{-1} was found, implying that polymer **PP5** was synthesized.

2. Synthesis of the model compound M1



Scheme S2 Synthesis of the model compound **M1**.

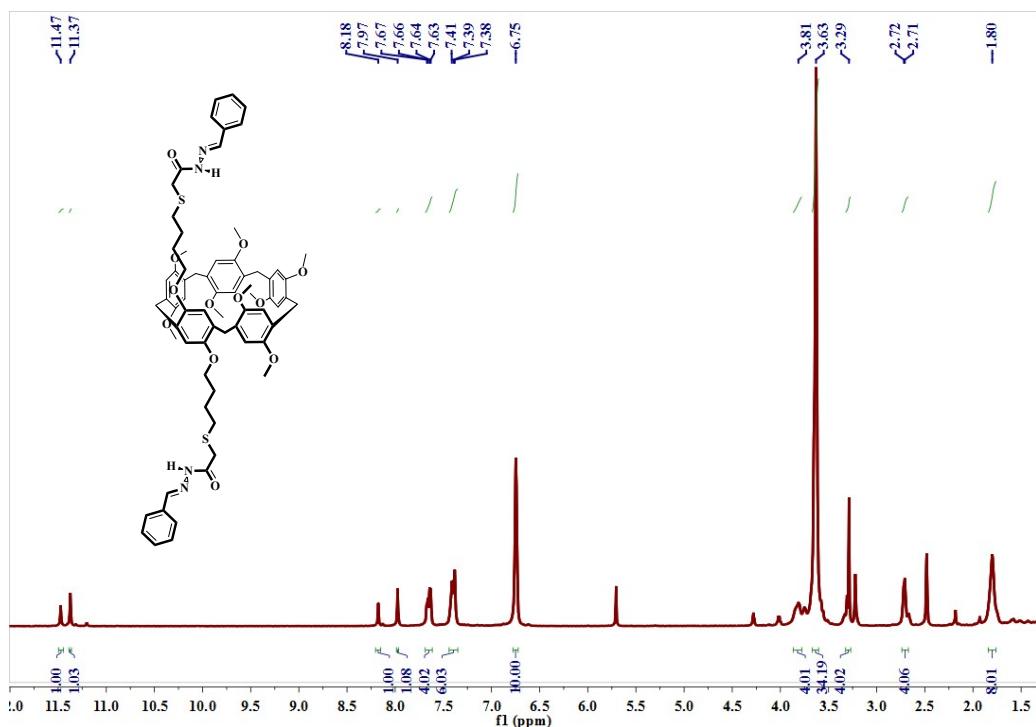


Fig. S11 ^1H NMR spectra (600 MHz, $\text{DMSO}-d_6$) of the model compound **M1**.

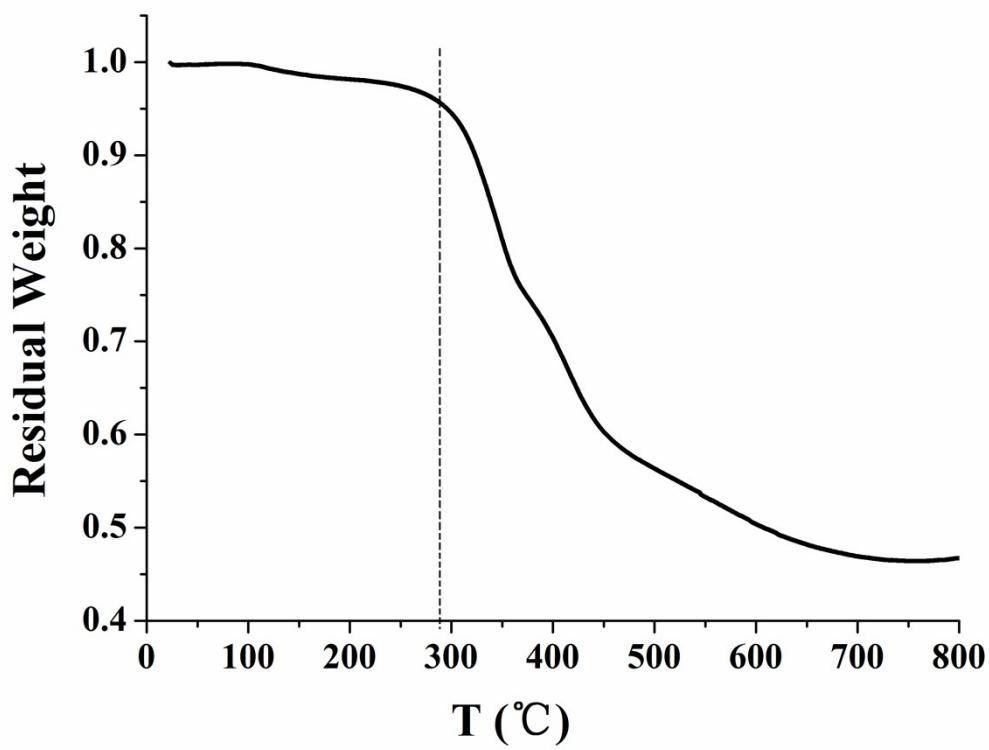


Fig. S12 TGA data for **PP5**.

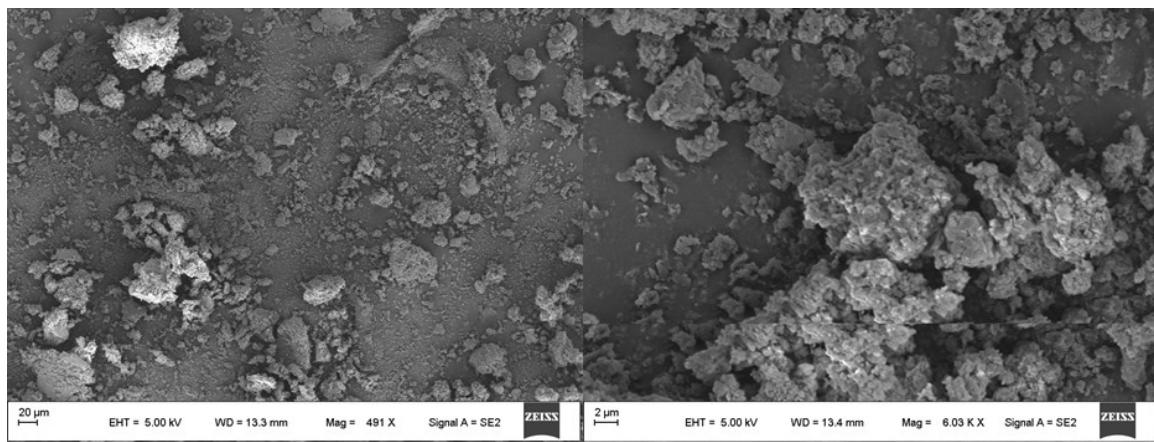


Fig. S13 SEM images of polymer **PP5**.

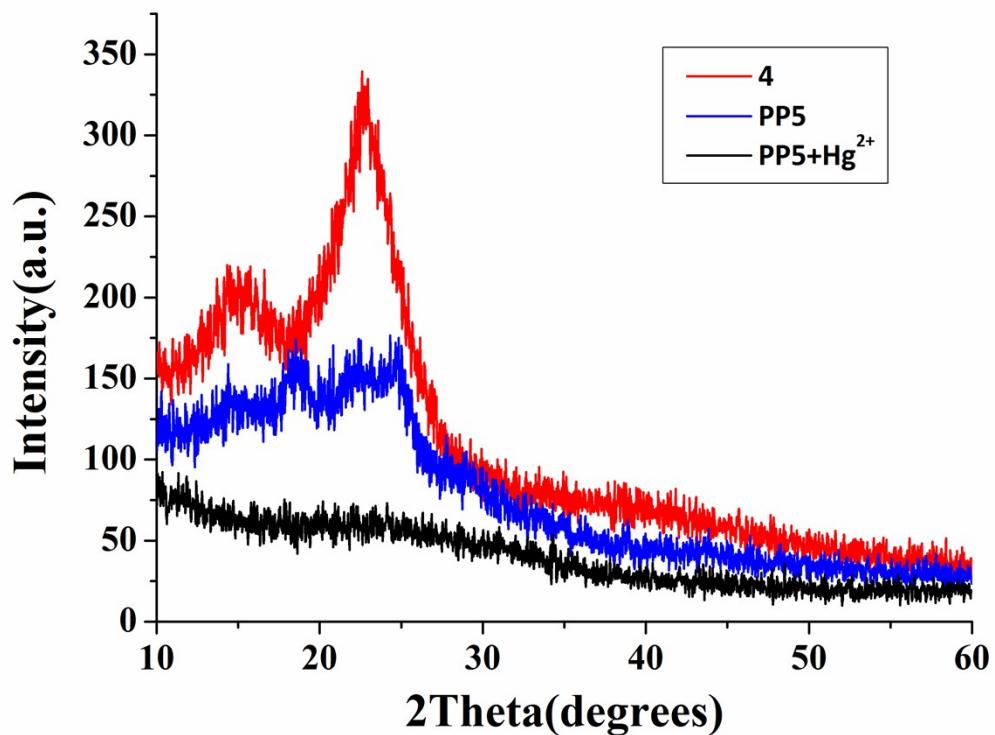


Fig. S14 XRD patterns of compound **4** (red), **PP5** (blue), and **PP5+Hg²⁺** (black).

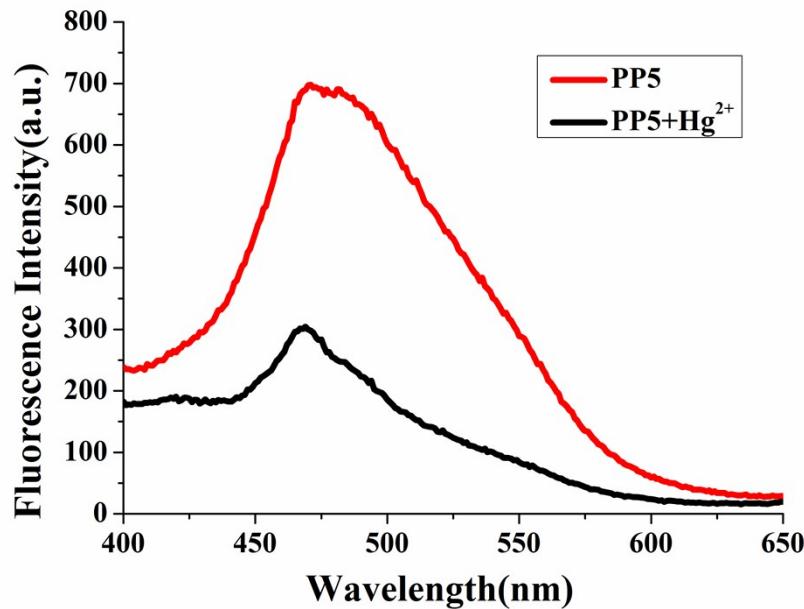


Fig. S15 Fluorescence spectral response of **PP5** ($[RU]=4\times10^{-5}$ M) in DMSO/H₂O (1 : 1, v/v) upon addition of 10 equiv. of Hg²⁺ ($\lambda_{ex} = 340$ nm).

Determination of the detection limit

We use the 3δ way to figure out the detection limit. The process of the analysis as follows.

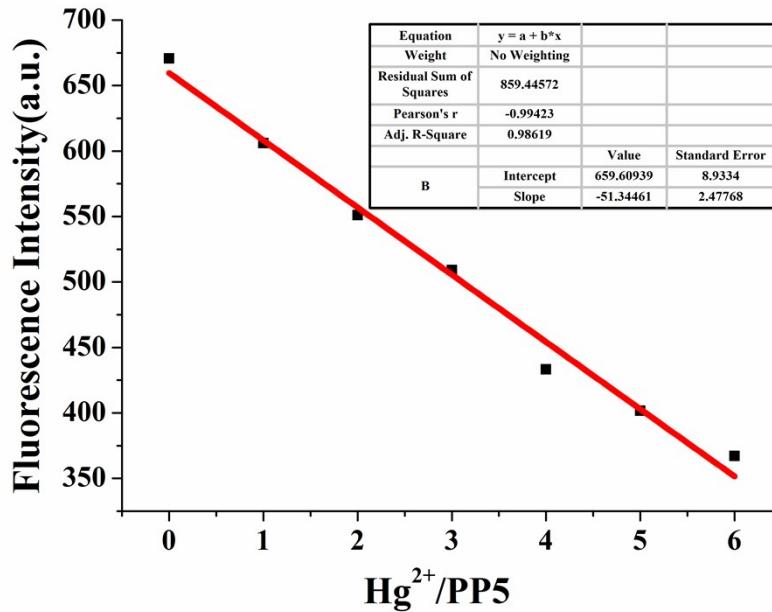


Fig. S16 The photograph of the linear range.

Linear Equation: Y=-51.34461X+659.60936 R²=0.98619

$$S=51.34461 \times 10^6$$

$$\delta = \sqrt{\frac{\sum_{i=1}^n (X_i - \bar{X})^2}{n-1}} = 13.9 (n=20)$$

K=3

LOD = K × δ/S = 8.12 × 10⁻⁷ M

Table S1 The adsorption experiment data of polymer (**PP5**) to Hg²⁺.

	Adsorbent dose (M)	Hg ²⁺ initial concentration (M)	Hg ²⁺ residual concentration (M)	Adsorption capacity (mg/g)	Absorbing rate (%)
Sample 1	1×10 ⁻⁶	1×10 ⁻⁶	3.49×10 ⁻⁷	114	65.1%
Sample 2	1×10 ⁻⁵	1×10 ⁻⁵	4.25×10 ⁻⁶	101	57.5%
Sample 3	1×10 ⁻⁵	1×10 ⁻⁵	3.75×10 ⁻⁶	110	62.5%

1) The adsorption capacity: $Q = \frac{M_i(C_0 - C)}{C_H M_H}$; (M_i: the molar mass of mercury ions; C₀:

Hg²⁺ initial concentration; C: Hg²⁺ residual concentration; C_H: the molar mass of the adsorbent; M_H: the molar mass of adsorbent)

2) The adsorption rate: $q = \frac{C_0 - C}{C_0} \times 100\%$.

The average adsorption capacity: $\bar{Q} = \frac{Q_1 + Q_2 + Q_3}{3} = \frac{114 + 101 + 110}{3} = 108$ mg/g.

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