

## Supporting Information

### Ratiometric fluorescence chemosensor based on Tyrosine derivatives for monitoring mercury ions in aqueous solutions

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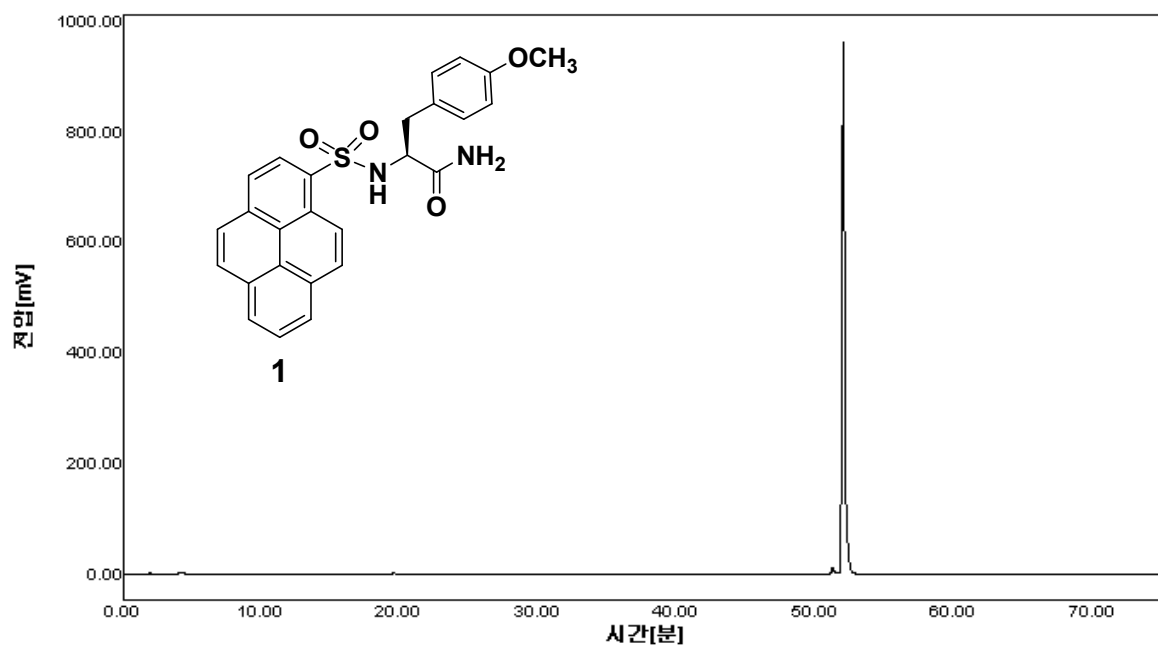
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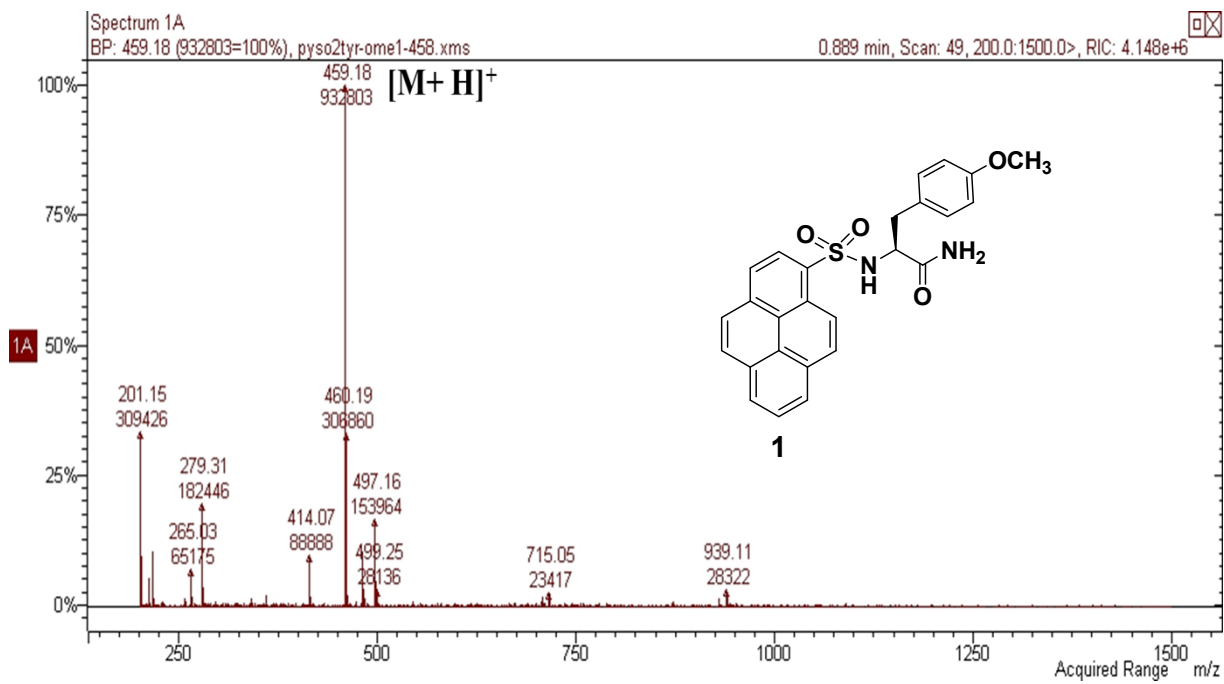
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## 1. Figures



**Fig. S1** HPLC chromatogram of compound **1**



**Fig. S2** ESI mass spectrum of **1**

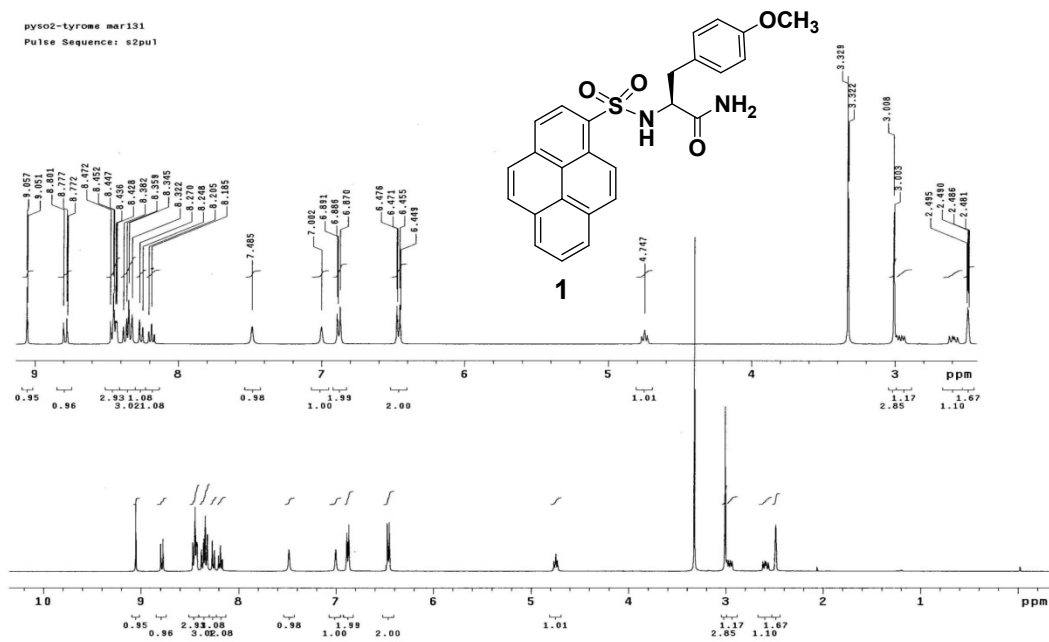


Fig. S3 <sup>1</sup>H NMR spectrum of compound 1

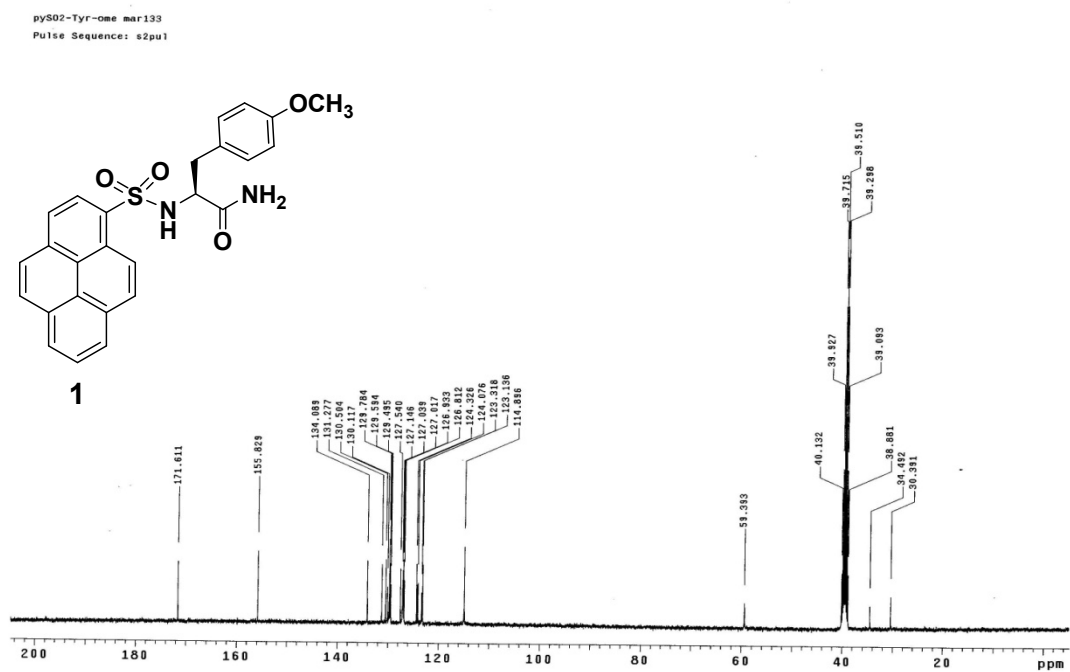


Fig. S4  $^{13}\text{C}$  NMR spectrum of compound 1

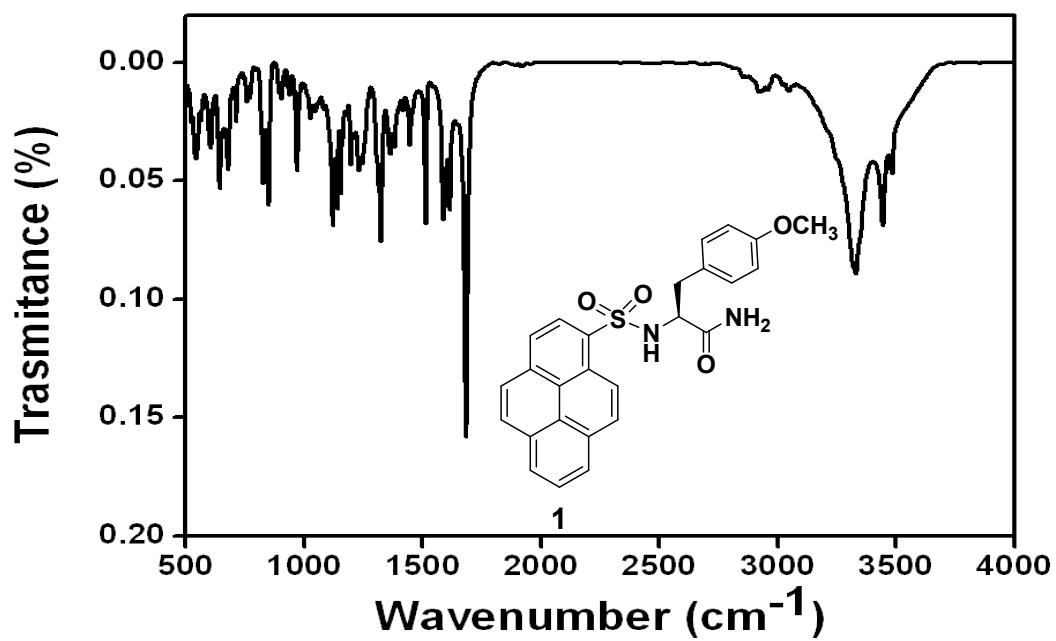


Fig. S5 IR spectrum of 1

1) PYSO2-1 *with GLY (POS)*

140407\_PYSO2-1\_001 #18-29 RT: 0.27-0.43 AV: 12 SB: 34 0.49-0.96 NL: 5.96E6  
T: + c FAB Full ms [ 199.50-800.50]

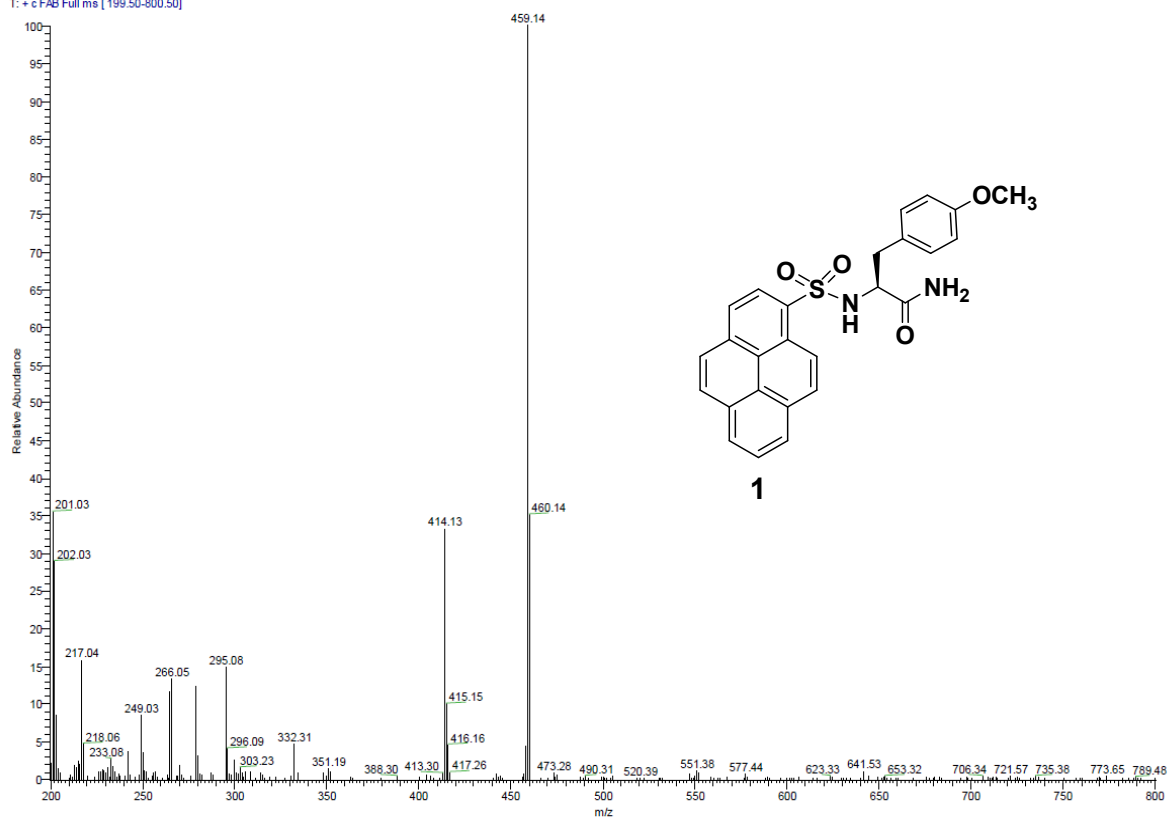
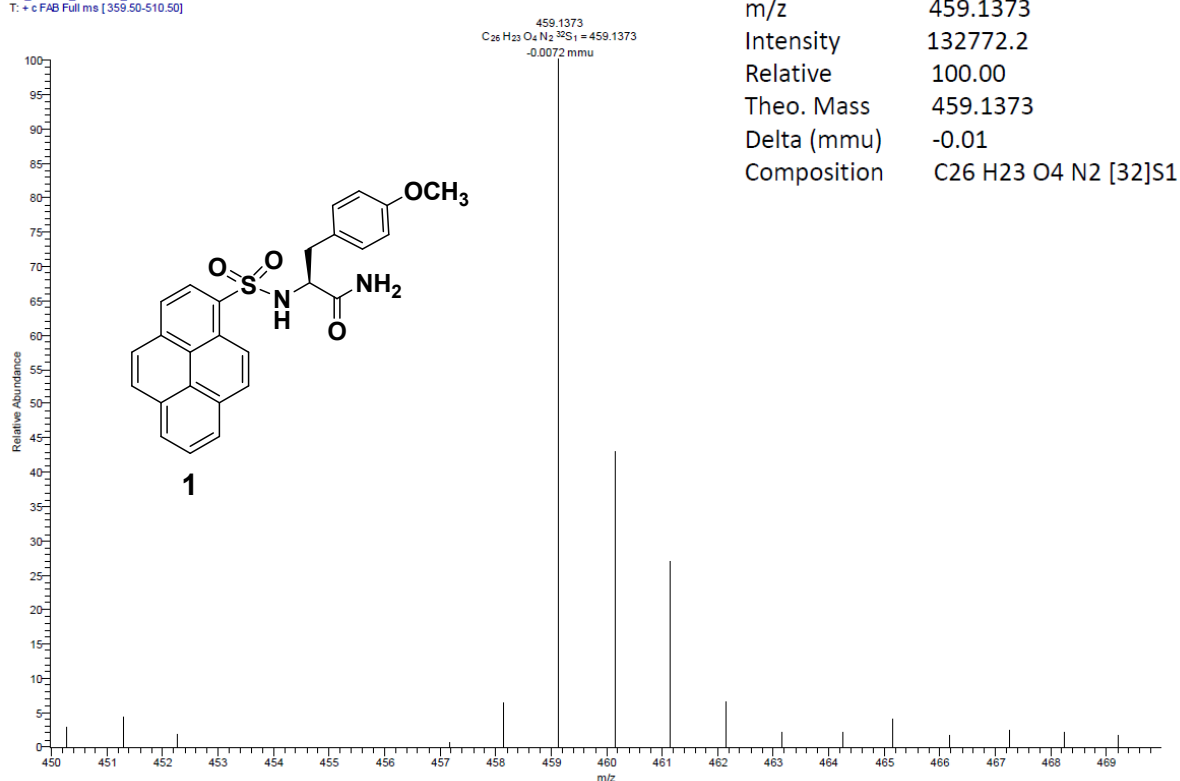


Fig. S6 HRMS-FAB mass spectrum of 1

### 1) PYSO2-1 with GLY (POS)

BG\_140414\_PYSO2-1\_002-c3 #22-38 RT: 0.36-0.62 AV: 17 SB: 39 0.76-1.38 NL: 1.33E5  
T: + c FAB Full ms [359.50-510.50]



**Fig. S7 HRMS-FAB elemental composition of 1**



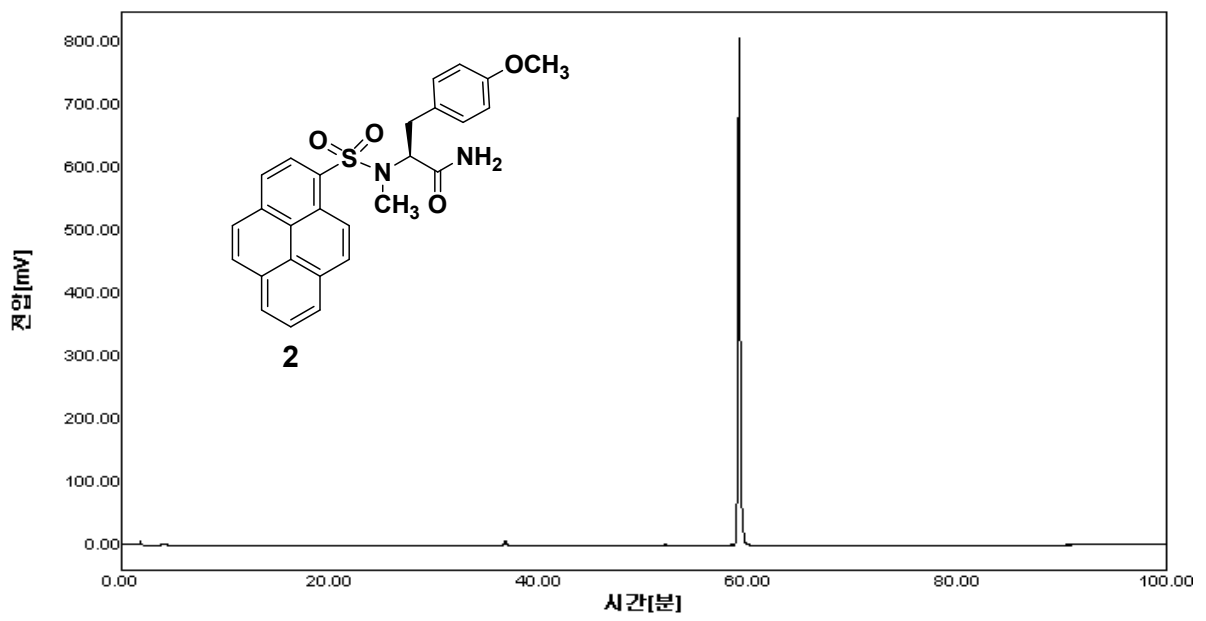
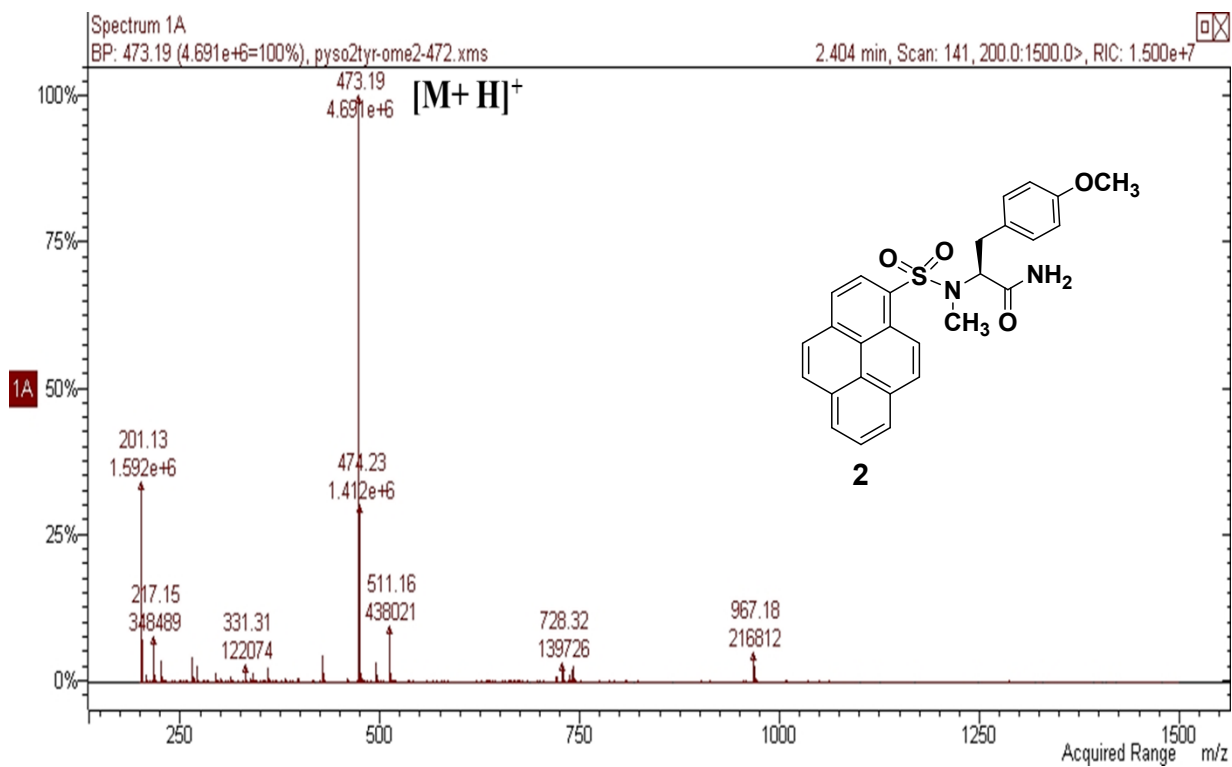


Fig. S8 HPLC chromatogram of compound 2



**Fig. S9** ESI mass spectrum of **2**

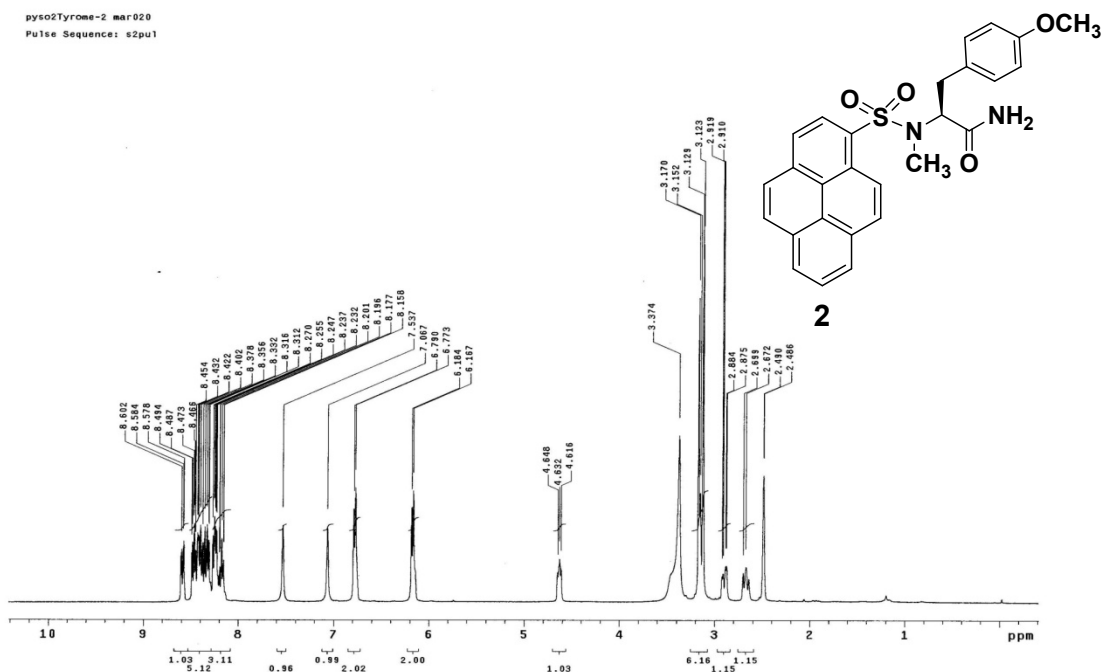


Fig. S10  $^1\text{H}$  NMR spectrum of compound 2

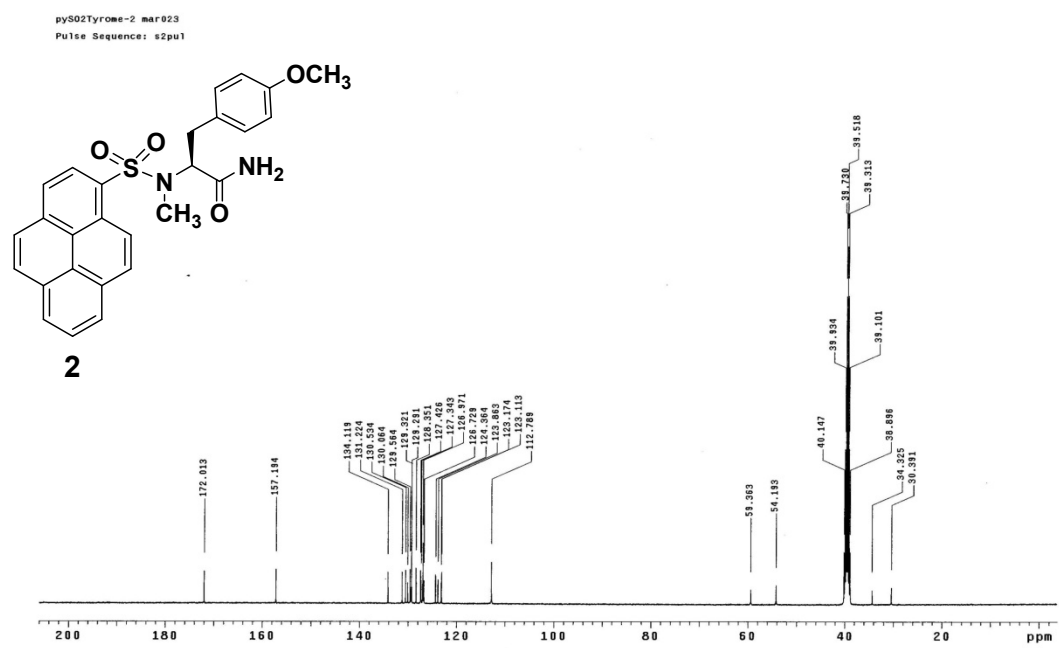


Fig. S11 <sup>13</sup>C NMR spectrum of compound 2

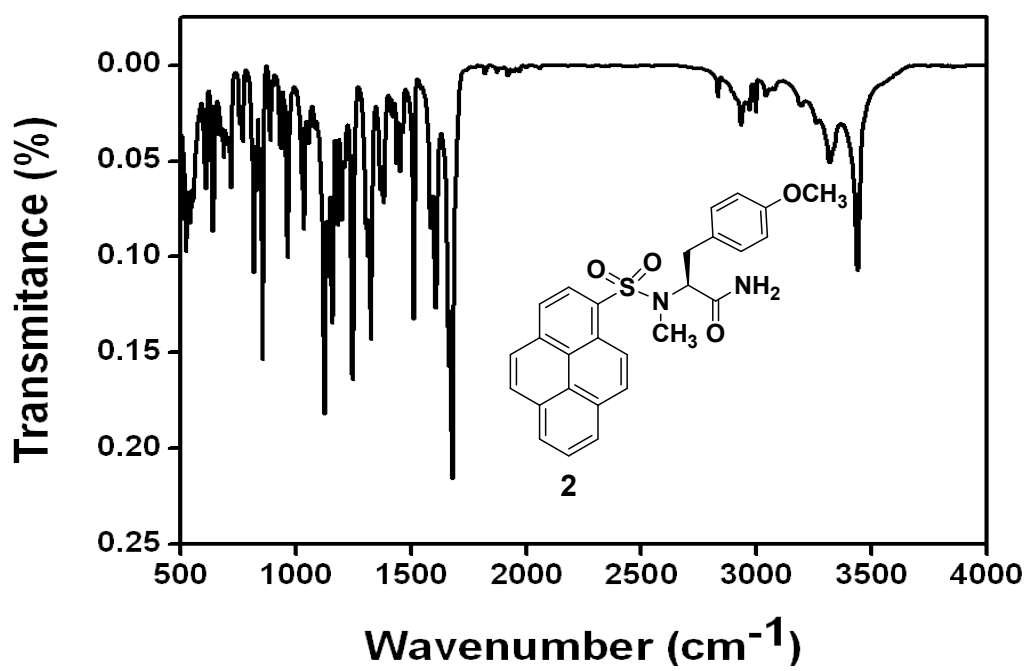


Fig. S12 IR spectrum of 2

## 2) PYSO2-2 *with GLY (POS)*

140407\_PYSO2-2\_001 #2-67 RT: 0.02-0.94 AV: 66 SB: 45 1.00-1.62 NL: 8.03E5  
T: + c FAB Full ms [ 199.50-800.50]

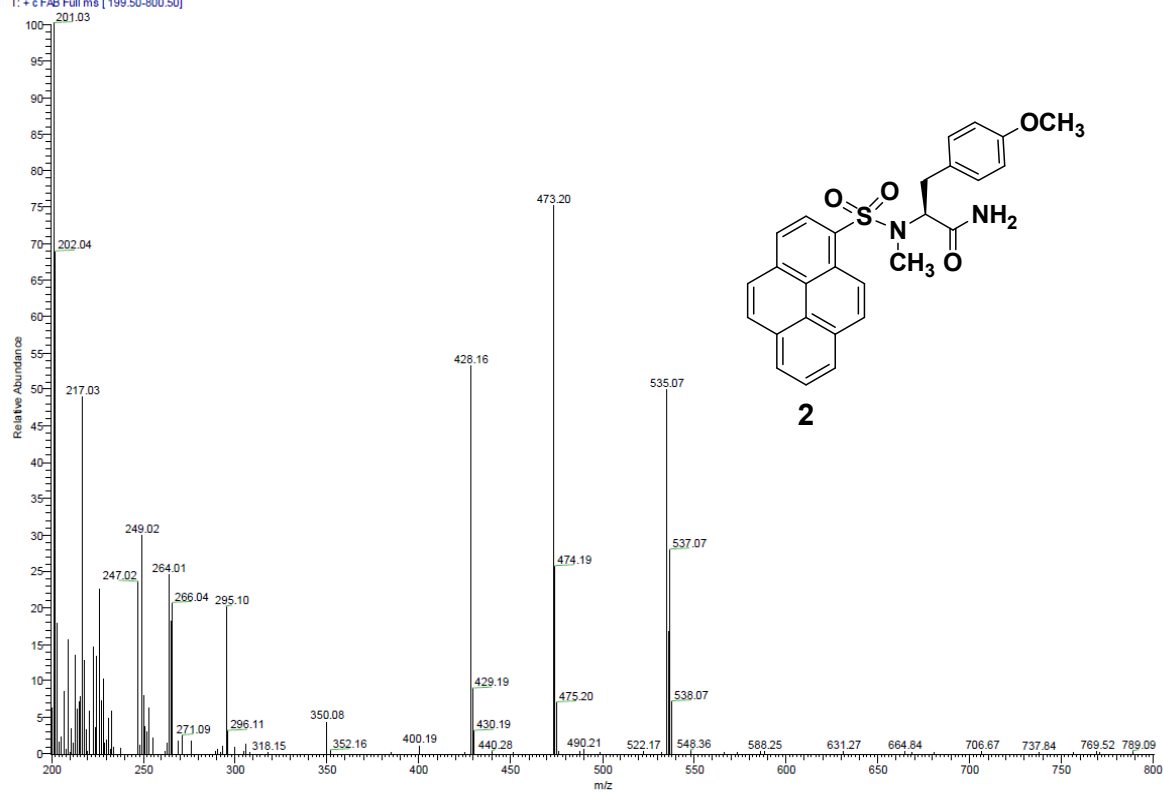


Fig. S13 HRMS-FAB mass spectrum of 2

## 2) PYSO2-2 with GLY (POS)

FIG\_140414\_PYSO2-2\_002-c2 #2 RT: 0.03 AV: 1 SB: 21 0.63-0.98 NL: 5.88E5  
T: +c FAB Full ms [404.50-555.50]

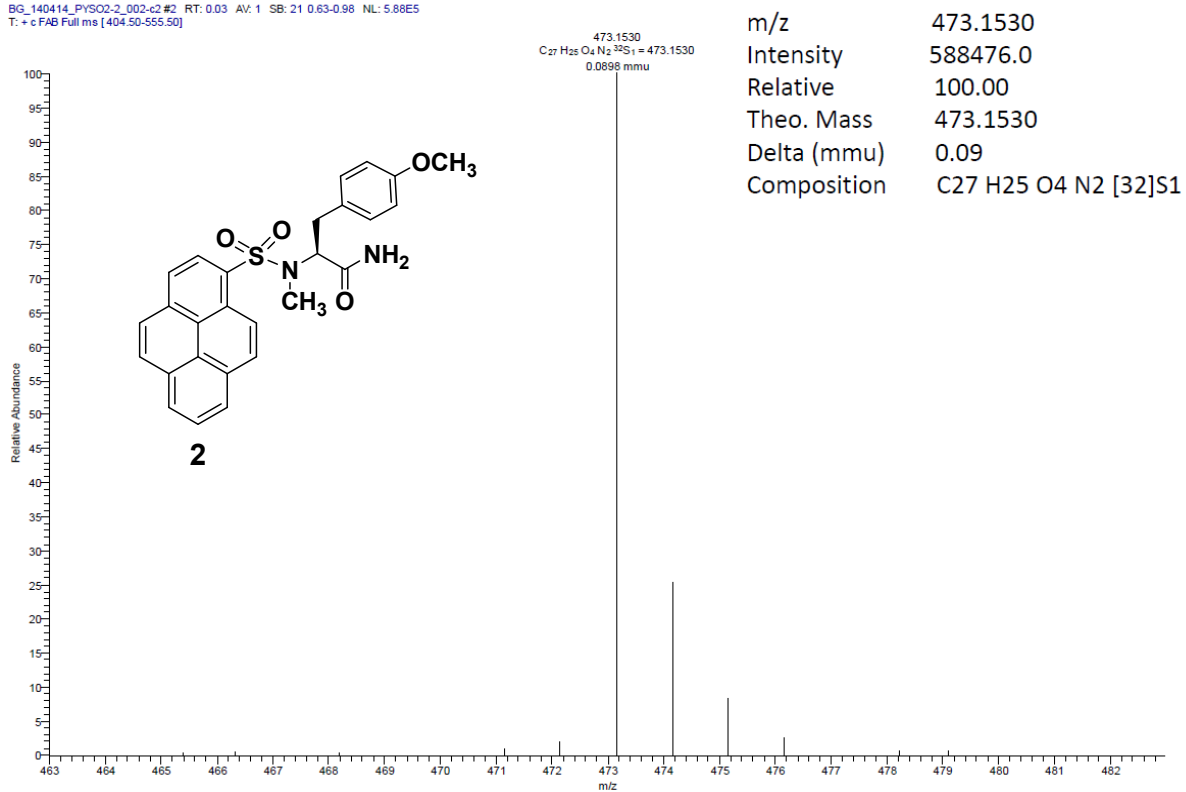
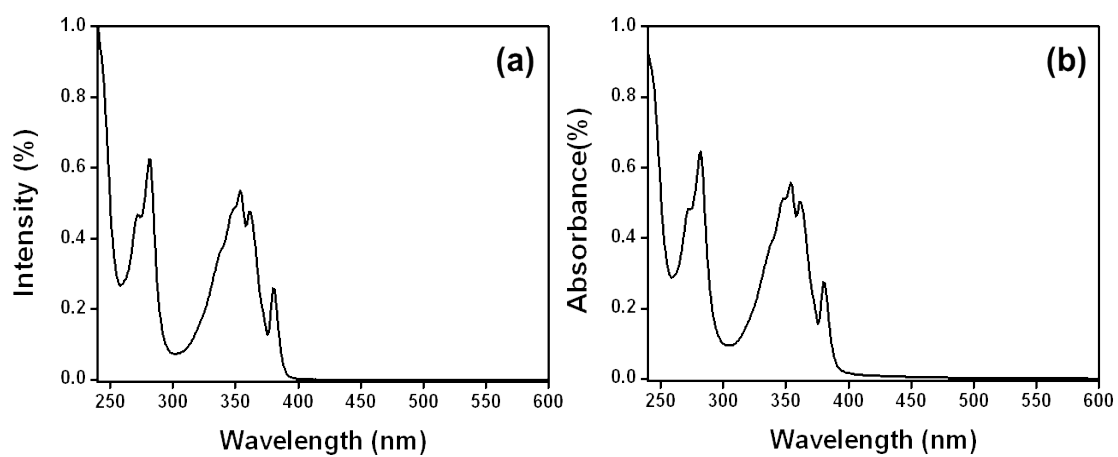
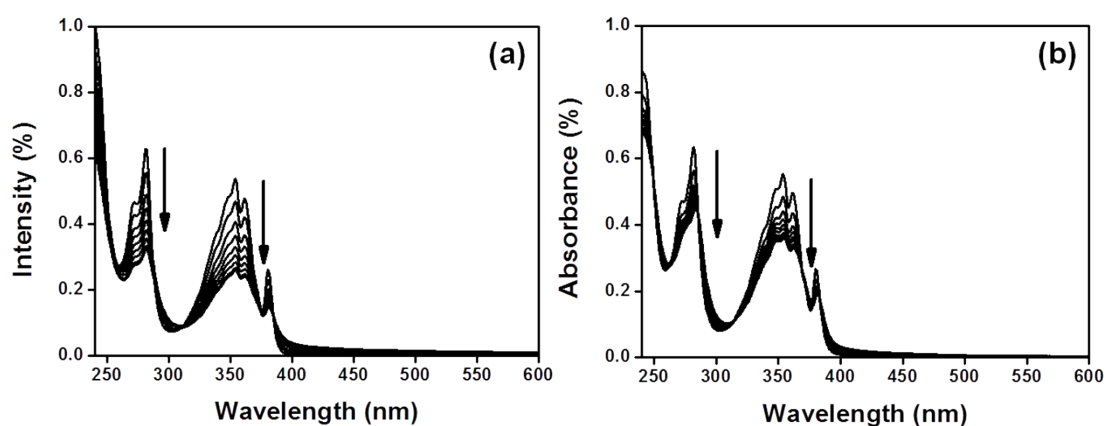


Fig. S14 HRMS-FAB elemental composition of **2**

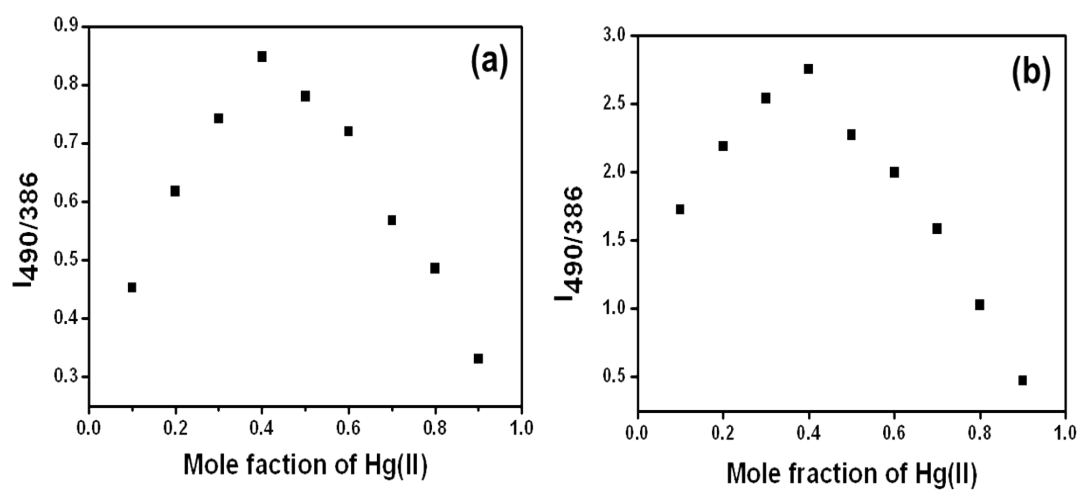


**Fig. S15** UV-Visible absorption spectra of (a) **1** (40  $\mu\text{M}$ ) and (b) **2** (40  $\mu\text{M}$ ) in aqueous solution ( $\text{H}_2\text{O}/\text{DMSO} = 95:5$ , v/v, 10 mM HEPES at pH 7.4).

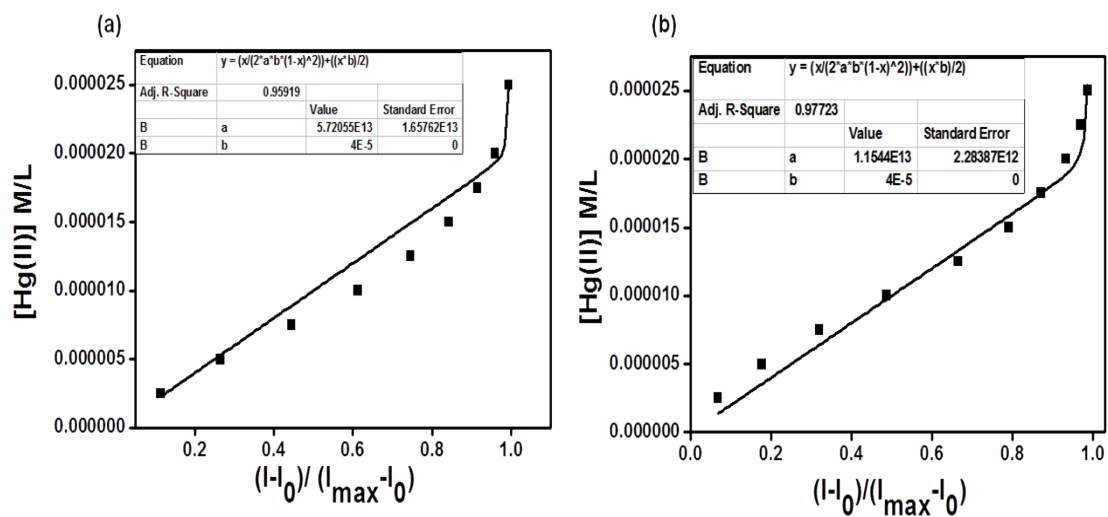




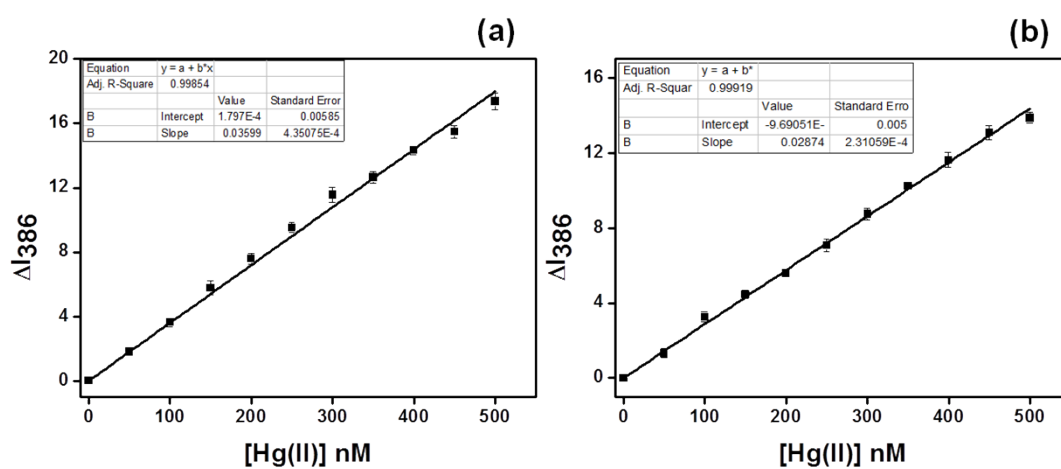
**Fig. S16** UV–Visible absorption spectra of (a) **1** (40  $\mu\text{M}$ ) upon gradual addition of Hg(II) (0, 0.125, 0.250, 0.375, 0.500, 0.625, 0.75, 0.875, 1.00 and 1.125 equiv) and (b) **2** (40  $\mu\text{M}$ ) upon gradual addition of Hg(II) (0, 0.125, 0.250, 0.375, 0.500, 0.625, 0.75, 0.875, 1.00, 1.125 and 1.25 equiv) in aqueous solution ( $\text{H}_2\text{O}/\text{DMSO}$ , 95:5, v/v, 10 mM HEPES at pH 7.4).



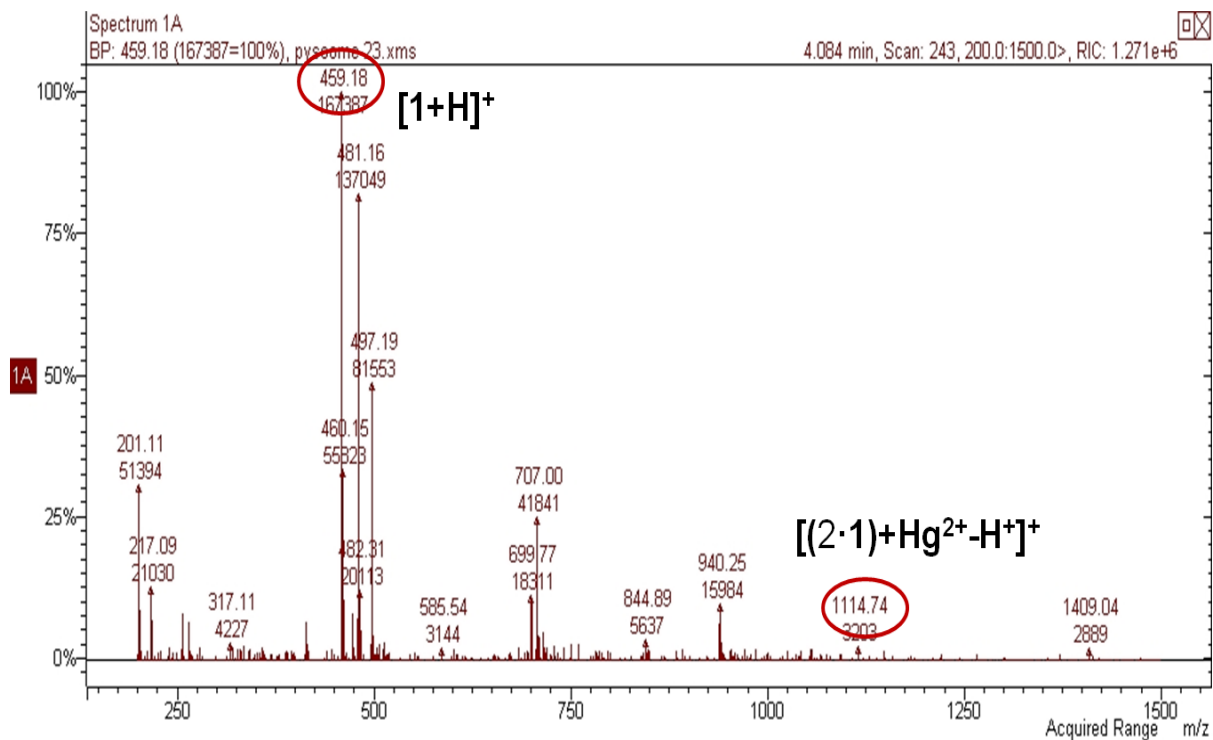
**Fig. S17 A** Job's plot analysis for (a) **1**, and (b) **2** with Hg(II).



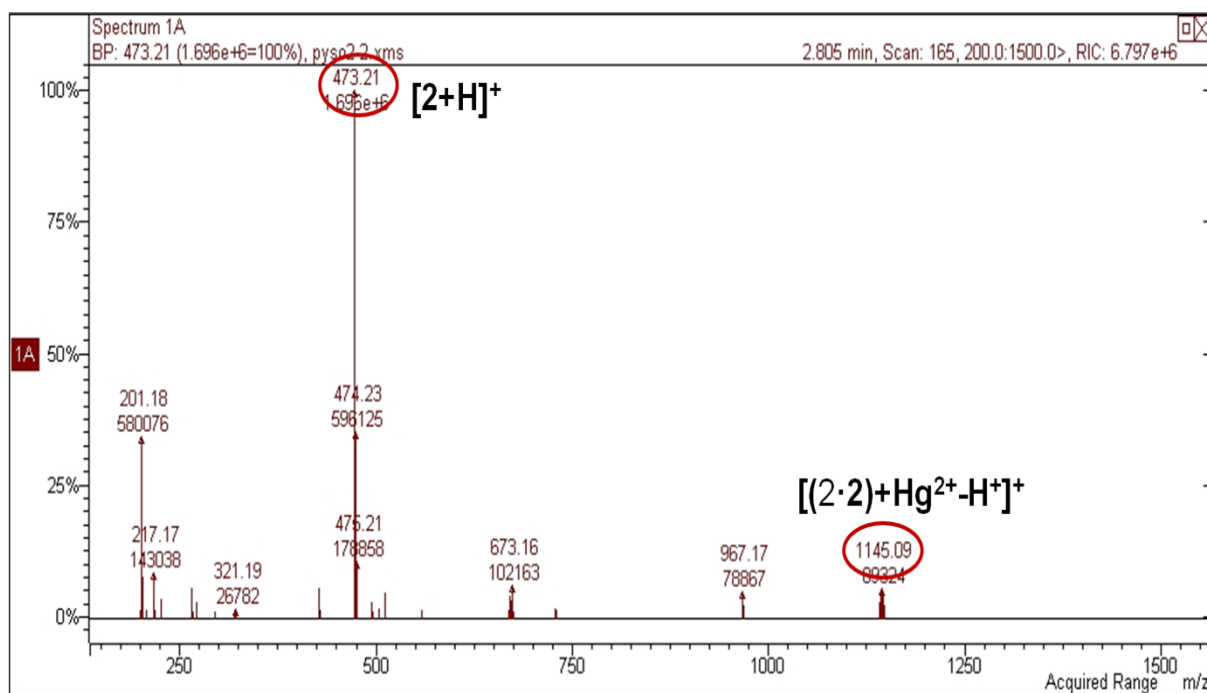
**Fig. S18** Non-linear fitting of the fluorescence intensity change of (a) **1** at 490 nm vs concentration of Hg(II) (slit 15/5) (b) **2** at 486 nm vs concentration of Hg(II) (slit 15/6) in aqueous solution (H<sub>2</sub>O/DMSO, 95:5, v/v, 10 mM HEPES at pH 7.4).



**Fig. S19** Detection limit for (a) **1** and (b) **2** with Hg(II) (Intensity change at 386 nm) in aqueous solution ( $\text{H}_2\text{O}/\text{DMSO} = 95:5$ , v/v, 10 mM HEPES at pH 7.4;  $\lambda_{\text{ex}} = 353$  nm, slit 15/6).



**Fig. S20** ESI mass spectra of **1** (500  $\mu$ M) in the presence of 1 equiv Hg(II) in aqueous solution (H<sub>2</sub>O/ACN, 7:3, v/v).



**Fig. S21** ESI mass spectra of **1** (500  $\mu$ M) in the presence of 1 equiv Hg(II) in aqueous solution (H<sub>2</sub>O/ACN, 7:3, v/v).