

## Supporting Information

### **A chemosensor with paddle structure based on BODIPY chromophore for sequential recognition of Cu<sup>2+</sup> and HSO<sub>3</sub><sup>-</sup>**

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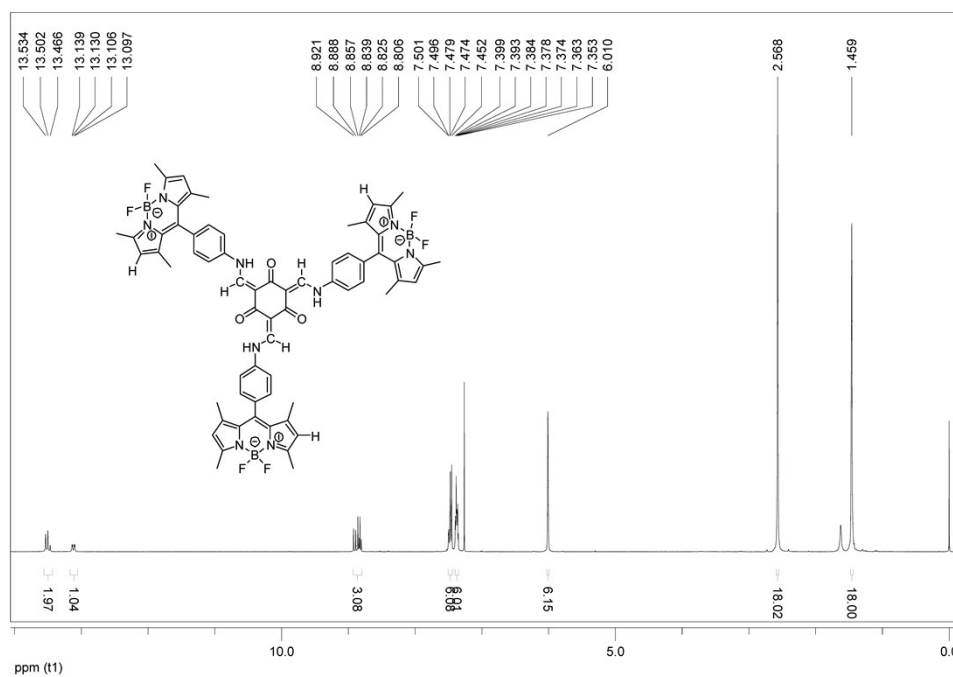
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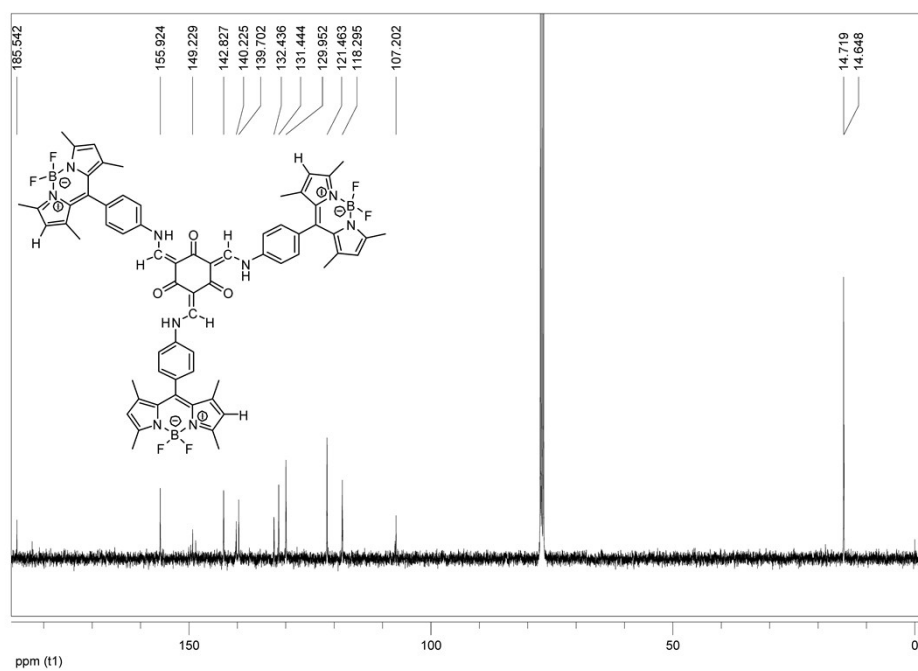
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## 1. $^1\text{H}$ NMR spectra of sensor **ML**



**Fig.S1.**  $^1\text{H}$  NMR spectra of sensor **ML**

## 2. $^{13}\text{C}$ NMR spectra of sensor **ML**



**Fig.S2.**  $^{13}\text{C}$  NMR spectra of sensor **ML**

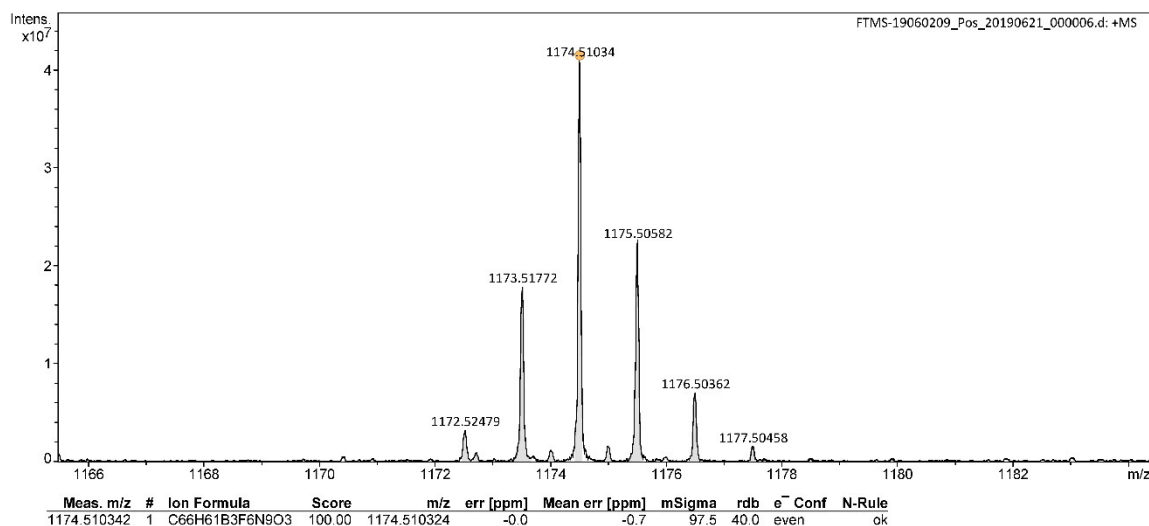
### 3. ESI-MS spectra of sensor ML

#### Peking University Mass Spectrometry Sample Analysis Report

##### Analysis Info

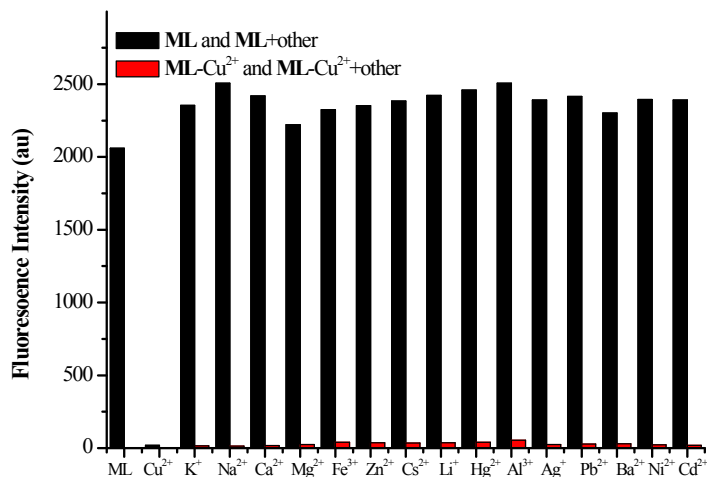
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 Sample BODIPY  
 Comment

Acquisition Date 6/21/2019 2:36:33 PM  
 Instrument Bruker Solarix XR FTMS  
 Operator Peking University



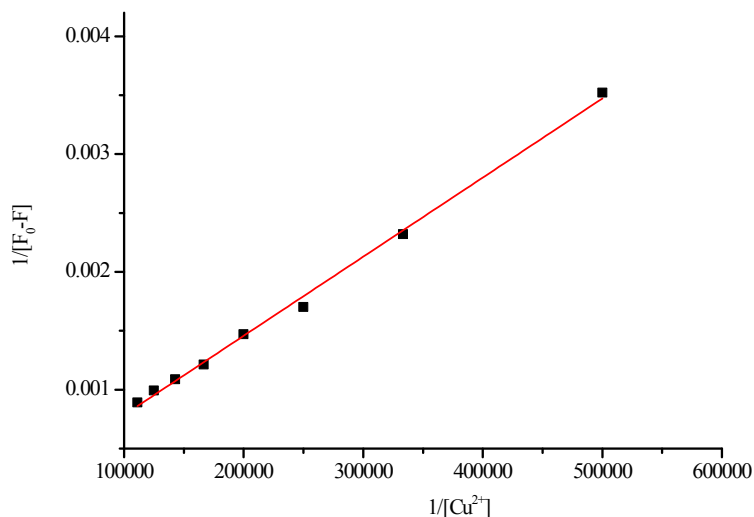
**Fig.S3.** ESI-MS spectra of sensor ML

### 4. Fluorescence intensity of sensor ML towards Cu<sup>2+</sup> -selective sensor



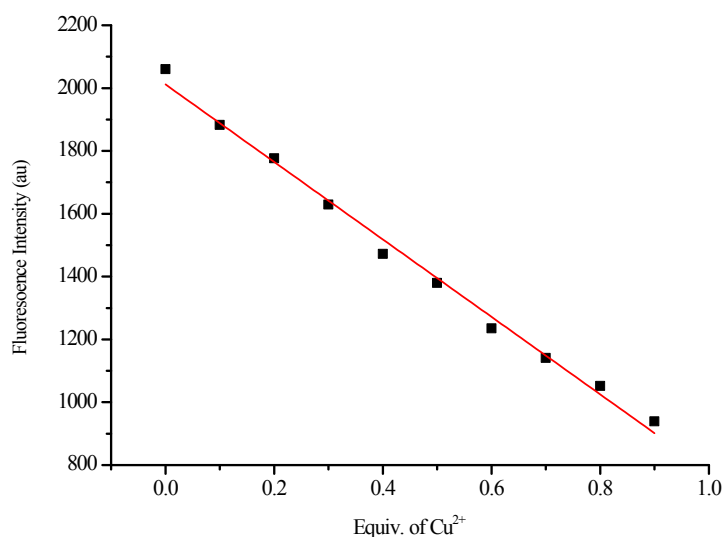
**Fig. S4.** Fluorescence intensity of sensor ML (5 μM) with selected cations (10 equiv.) in the absence (black bars) or presence (red bars) of Cu<sup>2+</sup> (10 equiv.).

## 5. Calculation of binding constant $K_a$



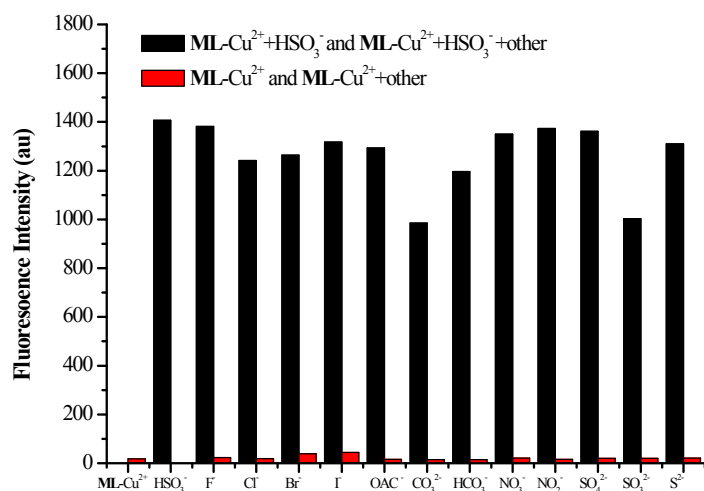
**Fig. S5.** The Benesi-Hilderbrand plot of sensor **ML** with  $Cu^{2+}$ . Linear Equation:  $Y=6.72 \times 10^{-9}X + 1.14 \times 10^{-4}$ ,  $R^2=0.99675$ ,  $K=1.70 \times 10^4 M^{-1}$ .

## 6. Determination of detection Limit of $Cu^{2+}$



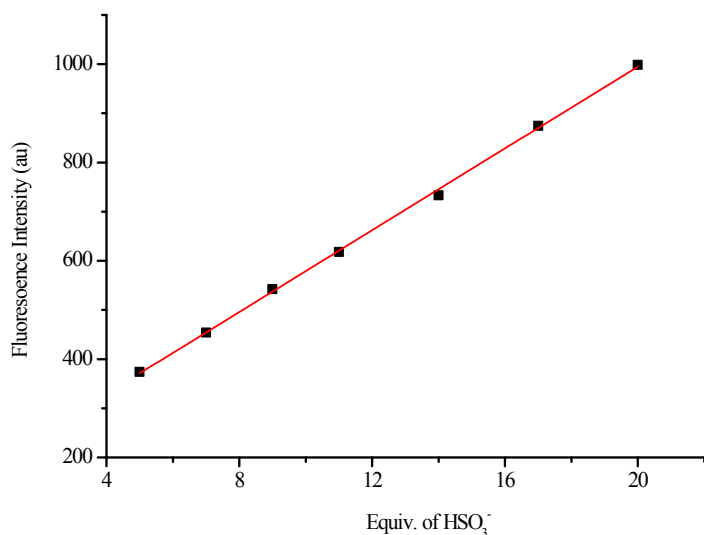
**Fig. S6.** Plot of the intensity at 475 nm for a mixture of sensor **ML** and  $Cu^{2+}$  in  $CH_3OH/H_2O$  (99:1 v/v) system in the range 0~0.9 equiv. Linear Equation:  $Y=-1.23 \times 10^8 X + 2012$ ,  $R^2=0.99239$ . The calculated detection limit of sensor **ML** is 0.36  $\mu M$ .

## 7. Fluorescence intensity of $\text{ML-Cu}^{2+}$ towards $\text{HSO}_3^-$ -selective sensor



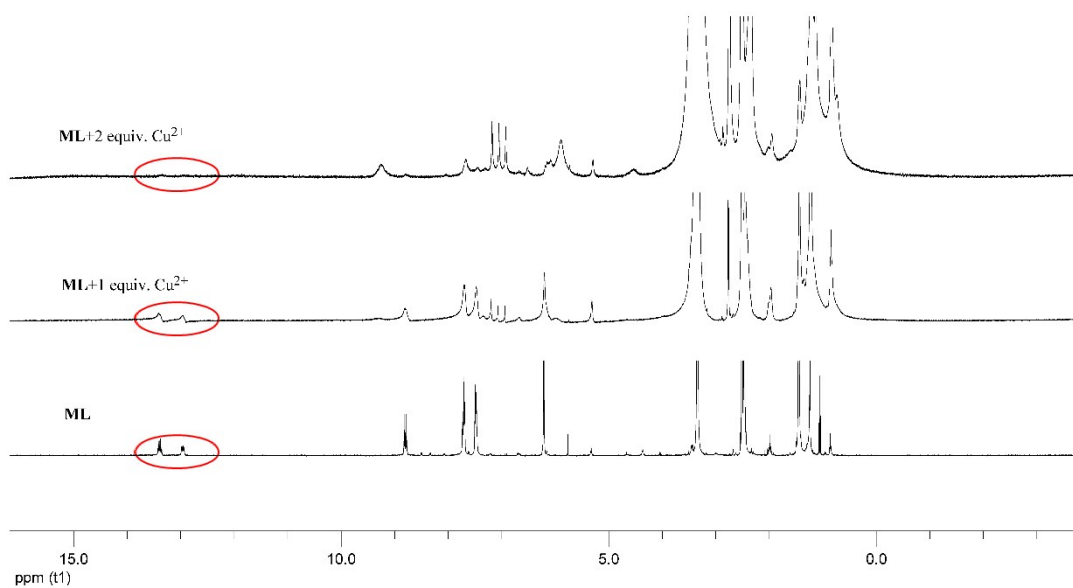
**Fig. S7.** Fluorescence intensity of  $\text{ML-Cu}^{2+}$  (5  $\mu\text{M}$ ) with selected anions (10 equiv.) in the absence (red bars) or presence (black bars) of  $\text{HSO}_3^-$  (10 equiv.).

## 8. Determination of detection Limit of $\text{HSO}_3^-$



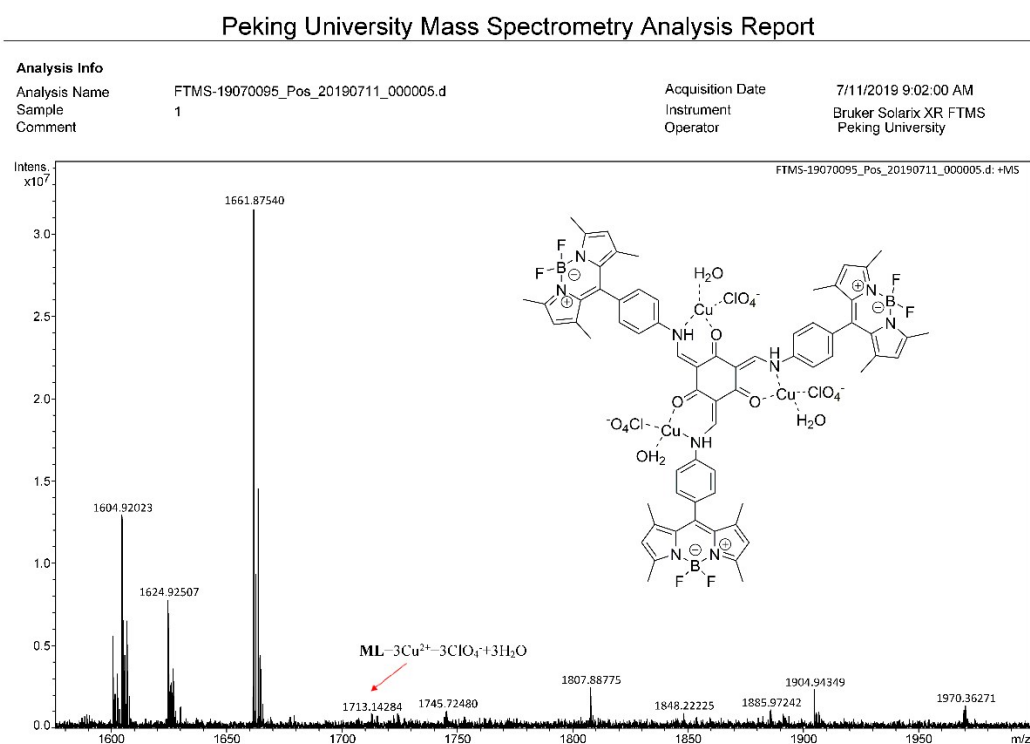
**Fig. S8.** Plot of the intensity at 475 nm for a mixture of  $\text{ML-Cu}^{2+}$  and  $\text{HSO}_3^-$  in  $\text{CH}_3\text{OH}/\text{H}_2\text{O}$  (99:1 v/v) system in the range 5.0~20 equiv. Linear Equation:  $Y=4.59 \times 10^6 X + 163.20$ ,  $R^2=0.99911$ . The detection limit of  $\text{ML-Cu}^{2+}$  is 1.4  $\mu\text{M}$ .

## 9. $^1\text{H}$ NMR titration spectra of sensor **ML** to $\text{Cu}^{2+}$



**Fig. S9.**  $^1\text{H}$  NMR titration spectra of sensor **ML** upon addition of 1 equiv.  $\text{Cu}^{2+}$  and 2 equiv.  $\text{Cu}^{2+}$  in  $\text{DMSO}-d_6$  solution.

## 10. ESI-MS spectra of **ML**- $\text{Cu}^{2+}$



**Fig. S10.** ESI-MS spectra of **ML**- $\text{Cu}^{2+}$