

## Electronic supplementary information (ESI)

for

Near-infrared fluorescence of  $\pi$ -conjugation extended benzothiazole and its application for  
biothiols imaging in living cells

Xuan Zhang,\* Jing-Yun Liu†, Wei-Wei Ma† and Meng-Lu Yang

*College of Chemistry, Chemical Engineering & Biotechnology, Donghua University, Shanghai*

*201620, China.*

*\*Corresponding Author. E-mail: xzhang@dhu.edu.cn.*

*† These authors contributed equally to this work.*

### Contents:

**Fig. S1** HOMO and LUMO orbitals of keto (K\*) conformers of **1** and **2** in the excited state.

**Fig. S2** ESI-massspectra of **4** in the presence (a) and absence (b) of Cys.

**Fig. S3**  $^1\text{H}$  NMR spectrum of **2**.

**Fig. S4**  $^{13}\text{C}$  NMR spectrum of **2**.

**Fig. S5**  $^1\text{H}$  NMR spectrum of **3**.

**Fig. S6**  $^{13}\text{C}$  NMR spectrum of **3**.

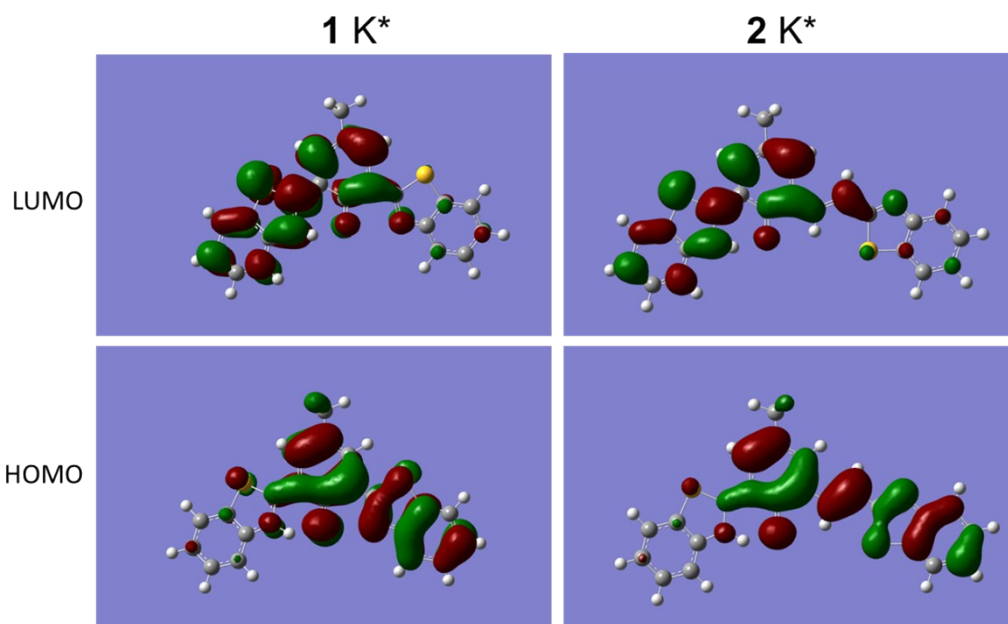
**Fig. S7**  $^1\text{H}$  NMR spectrum of **4**.

**Fig. S8**  $^{13}\text{C}$  NMR spectrum of **4**.

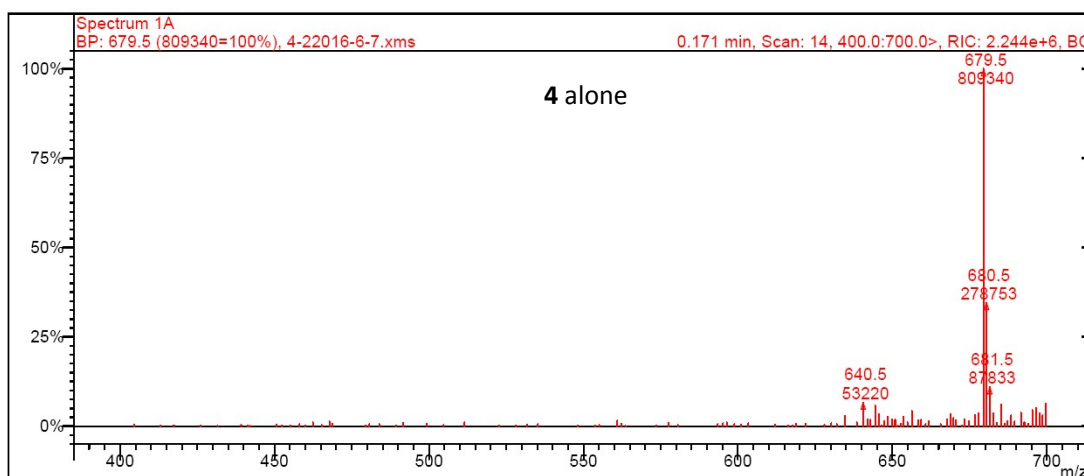
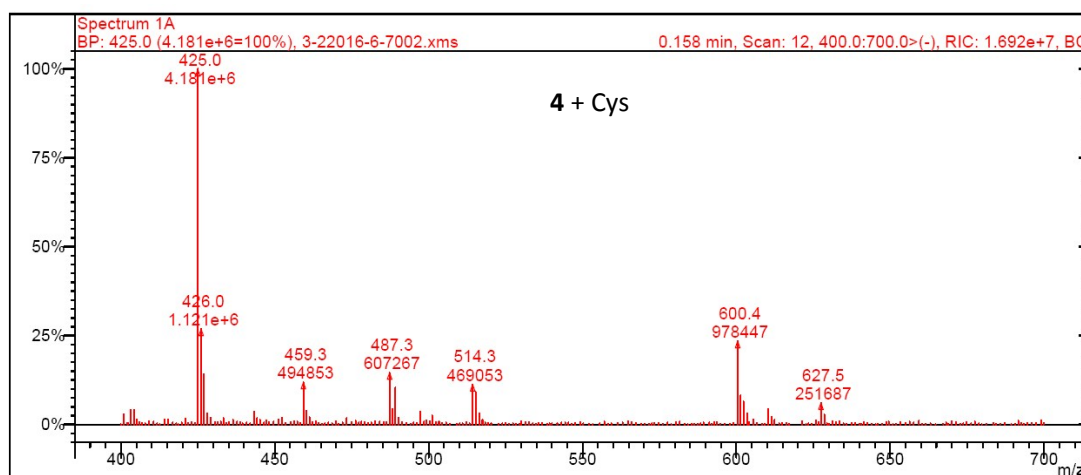
**Fig. S9** Massspectrum of **2**.

**Fig. S10** Massspectrum of **3**.

**Fig. S11** Massspectrum of **4**.



**Fig. S1** HOMO and LUMO orbitals of keto ( $K^*$ ) conformers of **1** and **2** in the excited state.



**Fig. S2** ESI-mass spectra of **4** in the presence and absence of Cys.

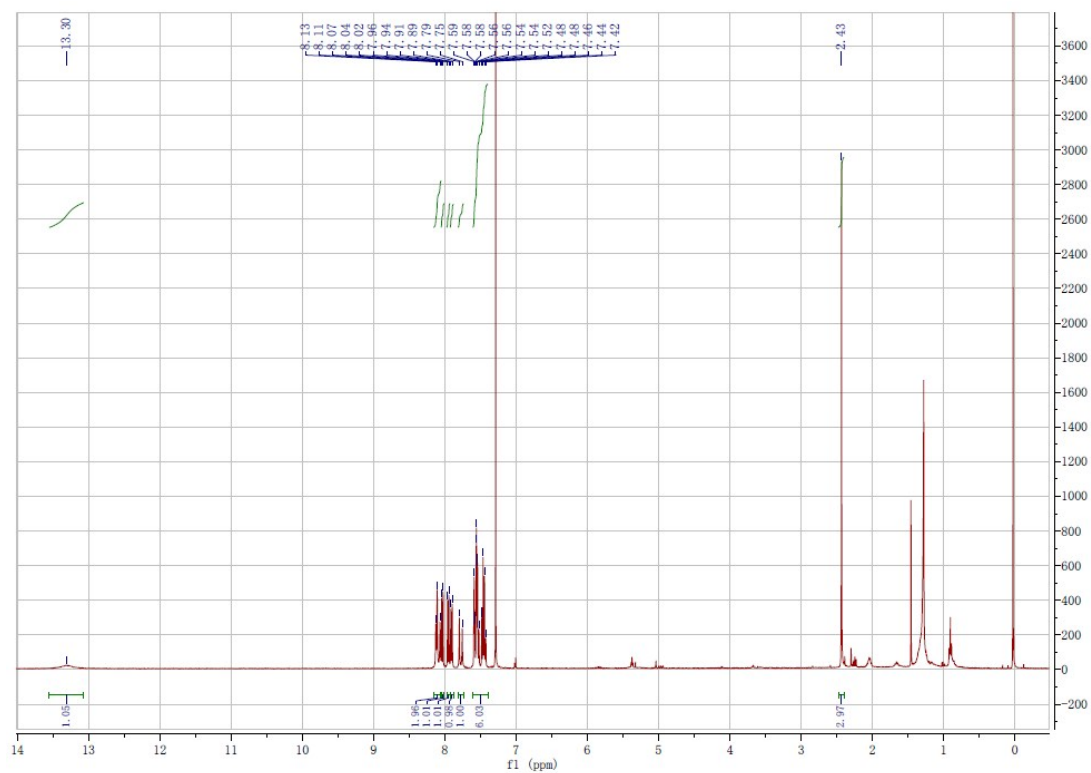


Fig. S3  $^1\text{H}$  NMR spectrum of **2**.

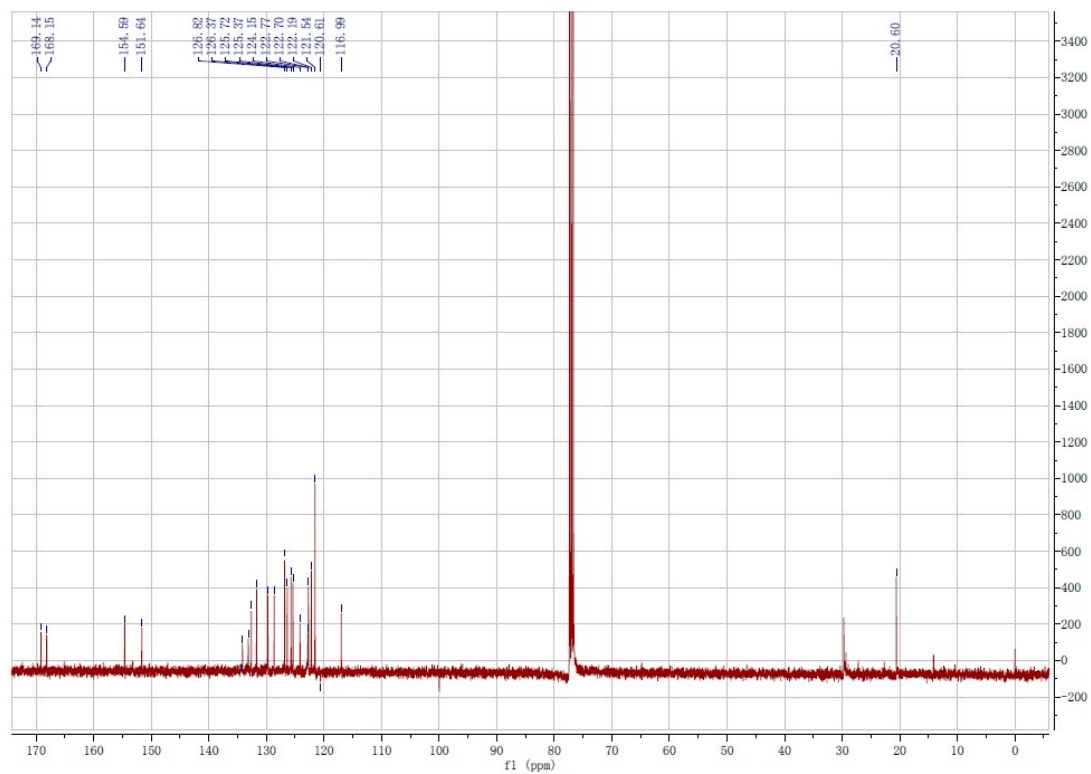


Fig. S4  $^{13}\text{C}$  NMR spectrum of **2**.

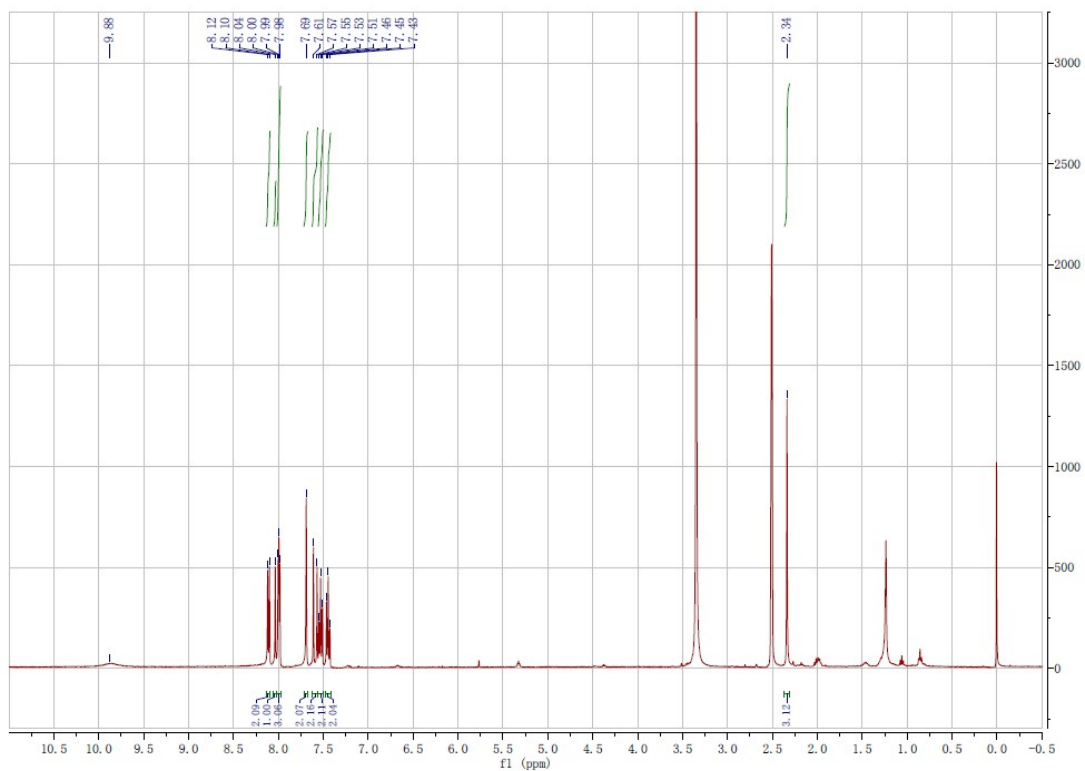


Fig. S5  $^1\text{H}$  NMR spectrum of **3**.

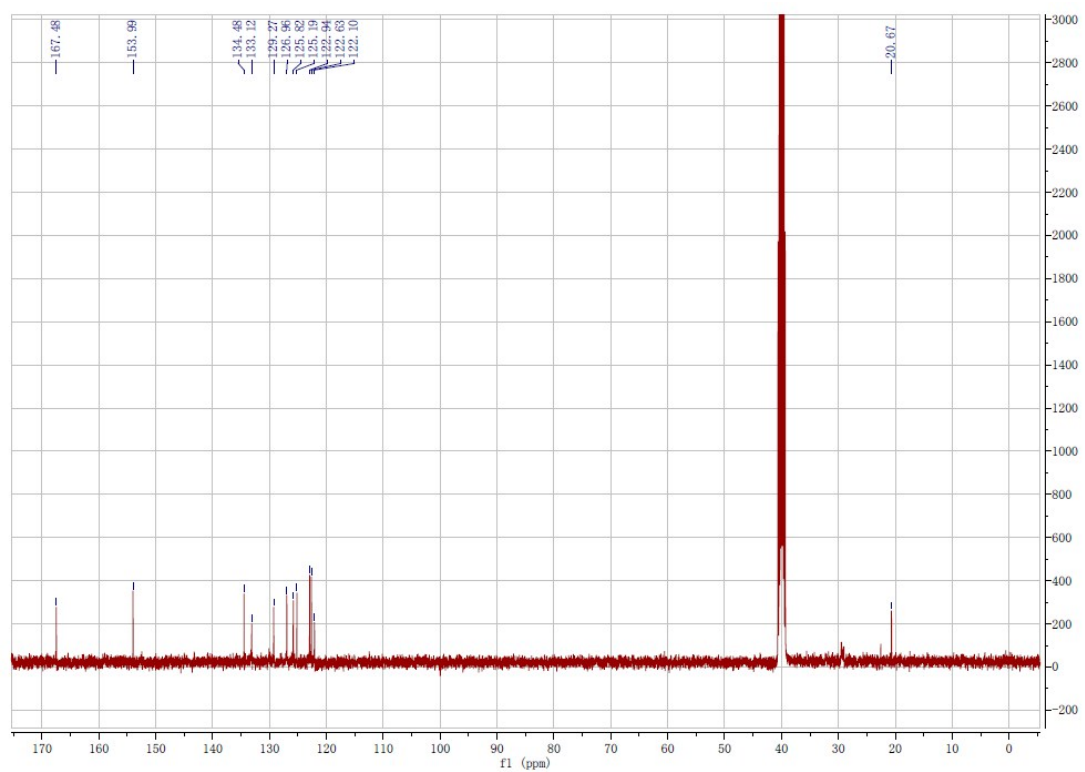


Fig. S6  $^{13}\text{C}$  NMR spectrum of **3**.

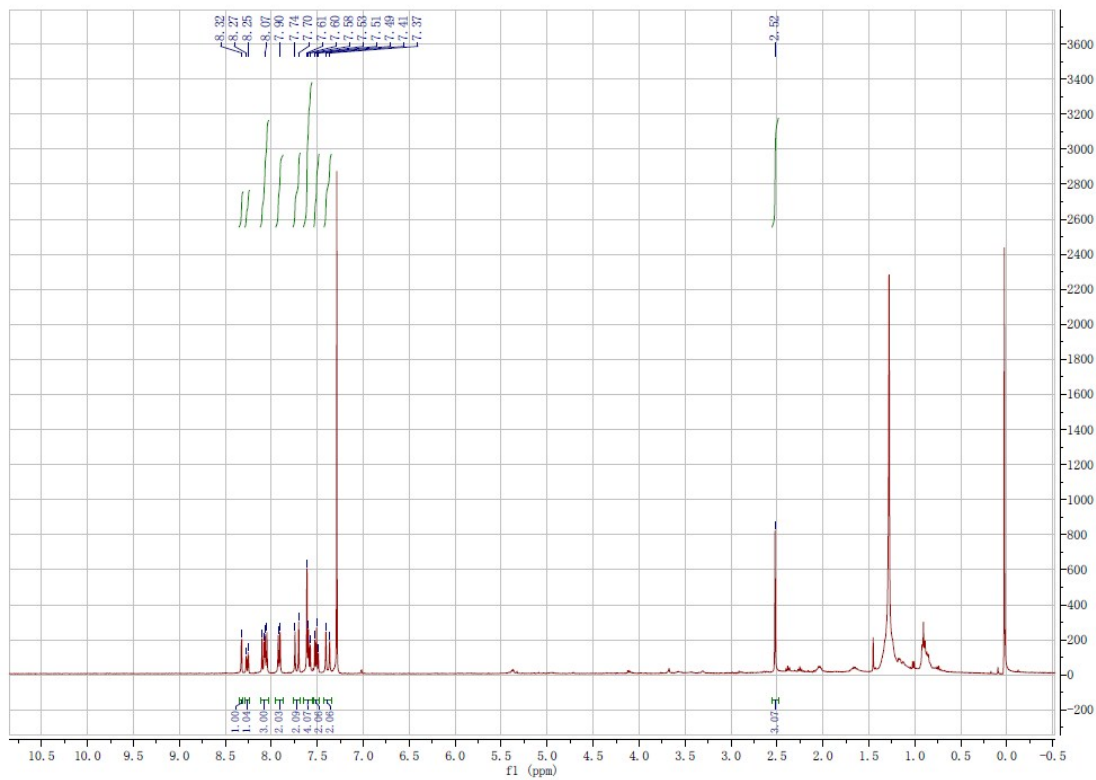


Fig. S7 <sup>1</sup>H NMR spectrum of 4.

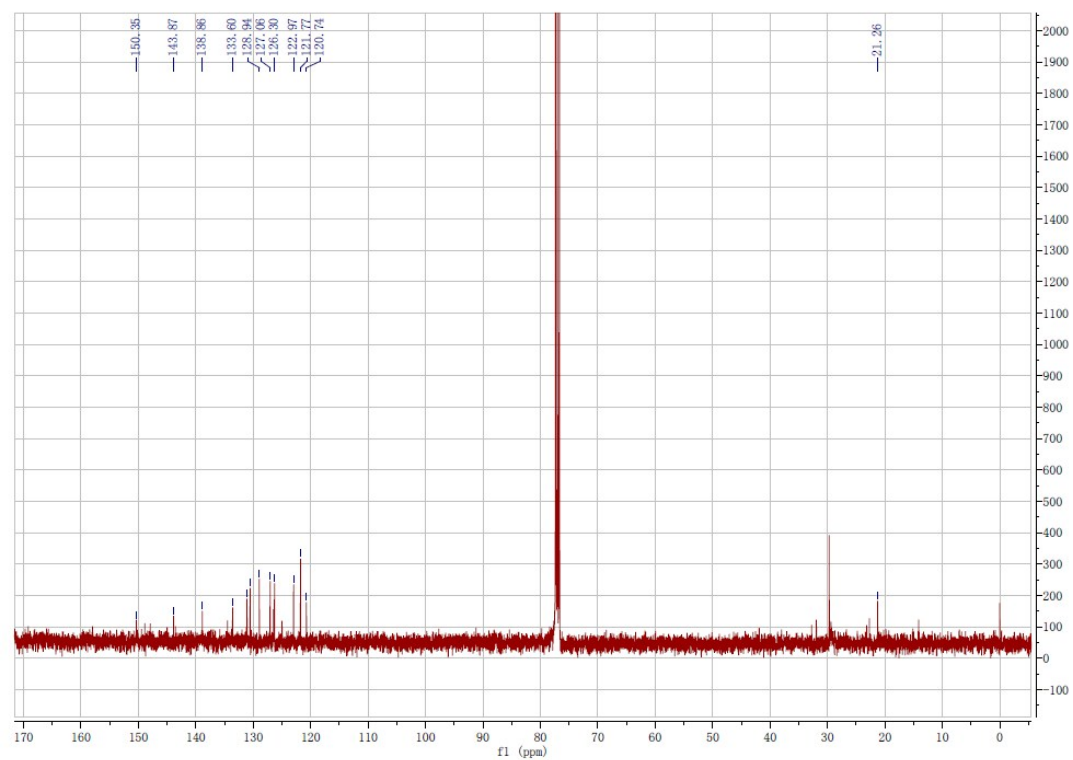


Fig. S8 <sup>13</sup>C NMR spectrum of 4.

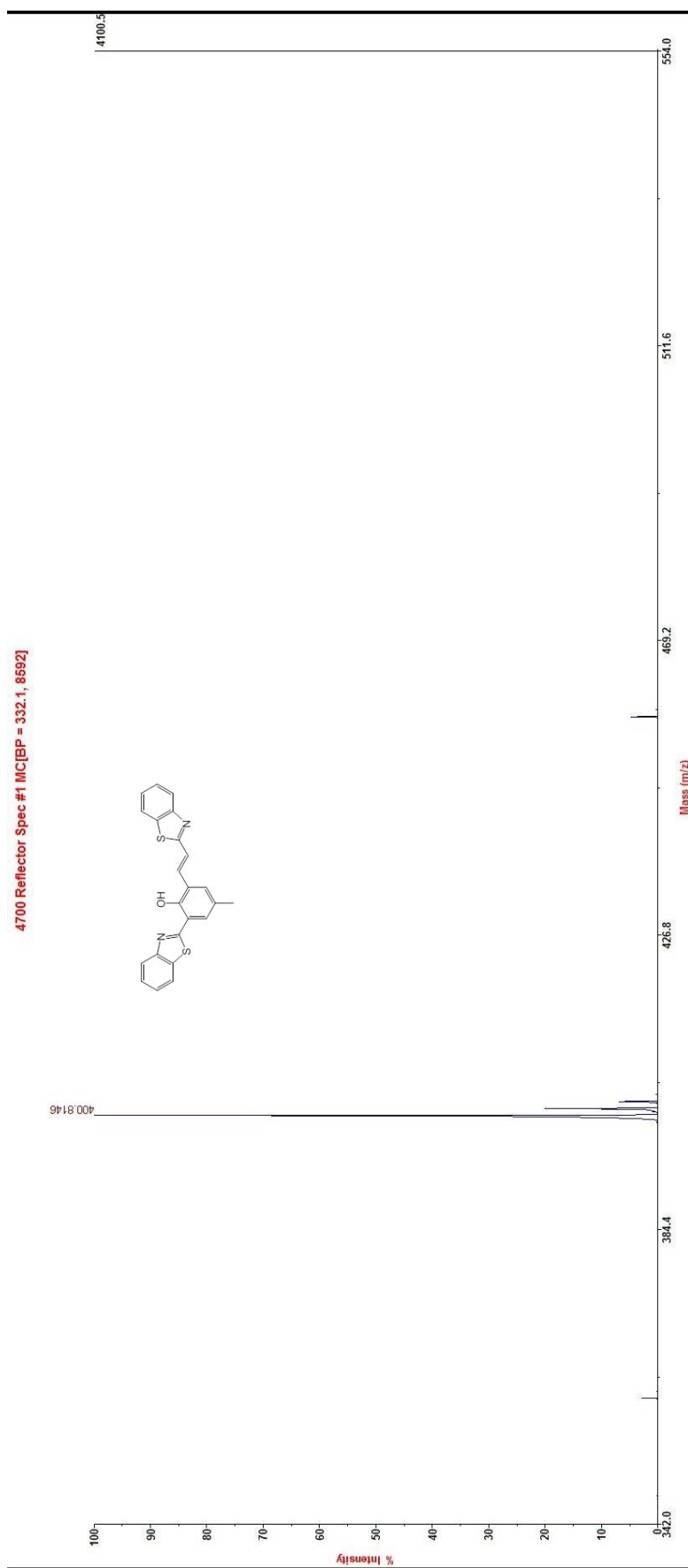


Fig. S9 Mass spectrum of 2.

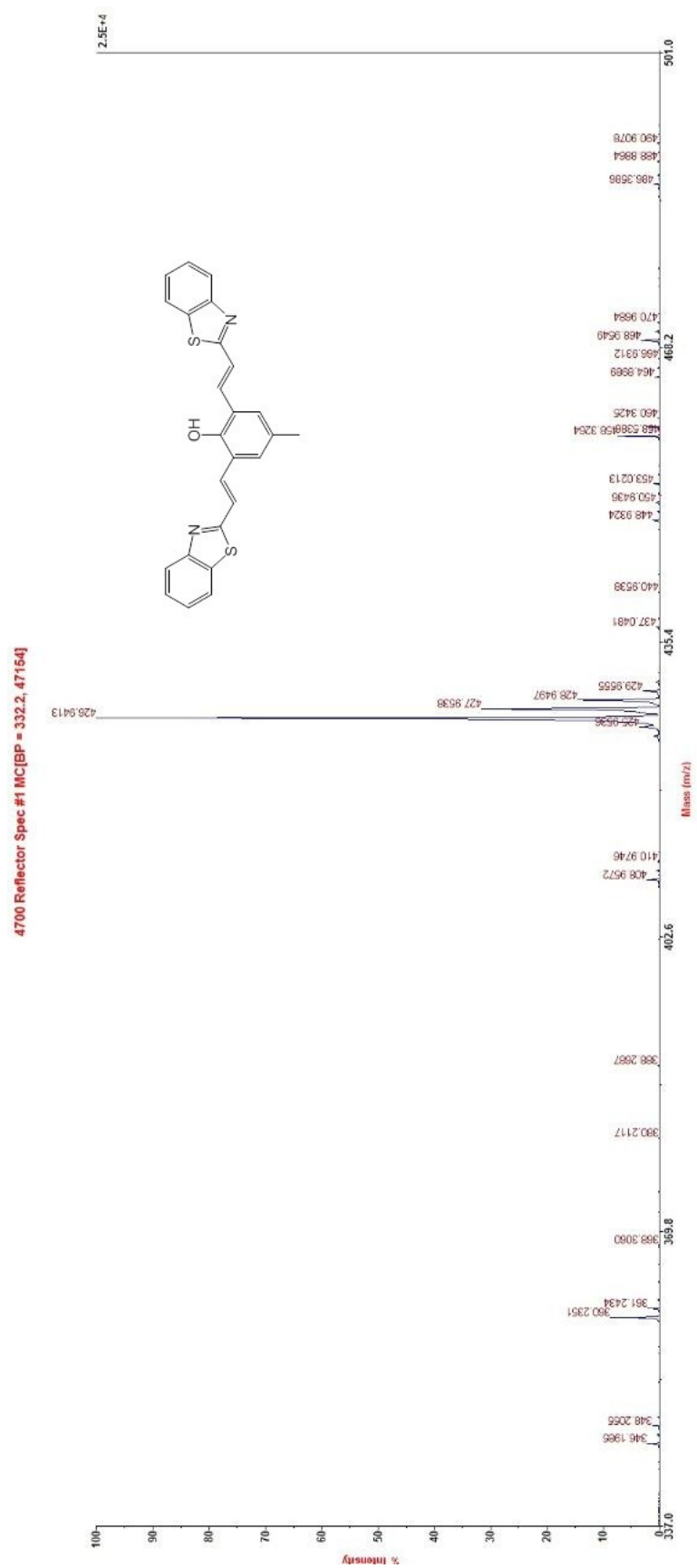


Fig. S10 Mass spectrum of 3.

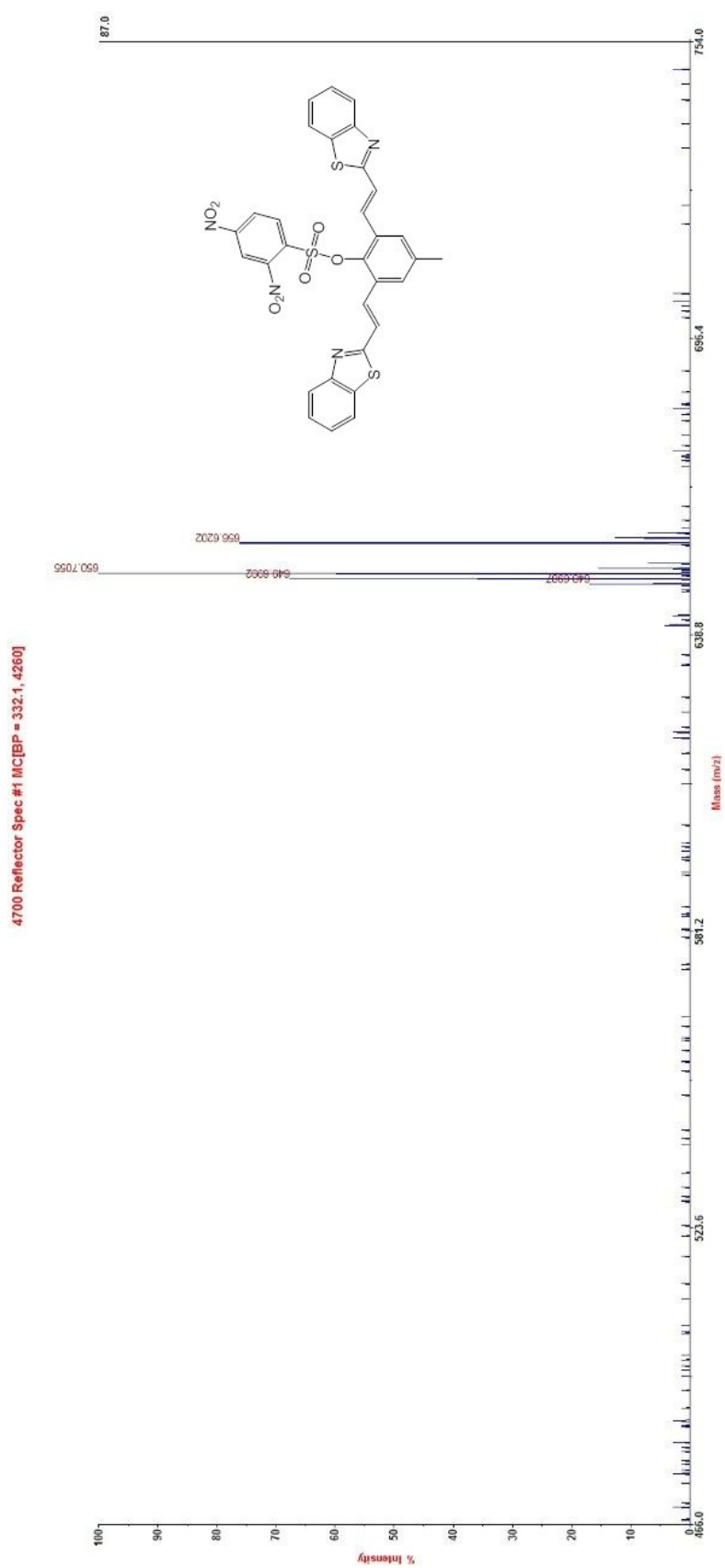


Fig. S11 Mass spectrum of 4.