

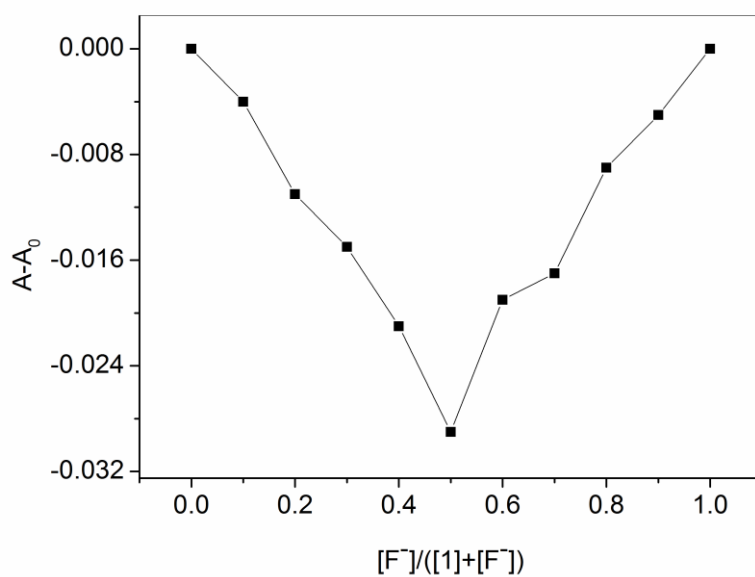
## Electronic Supplementary Information

### **A BODIPY derivative as highly selective "Off-On" fluorescent chemosensor for hydrogen sulfate anion**

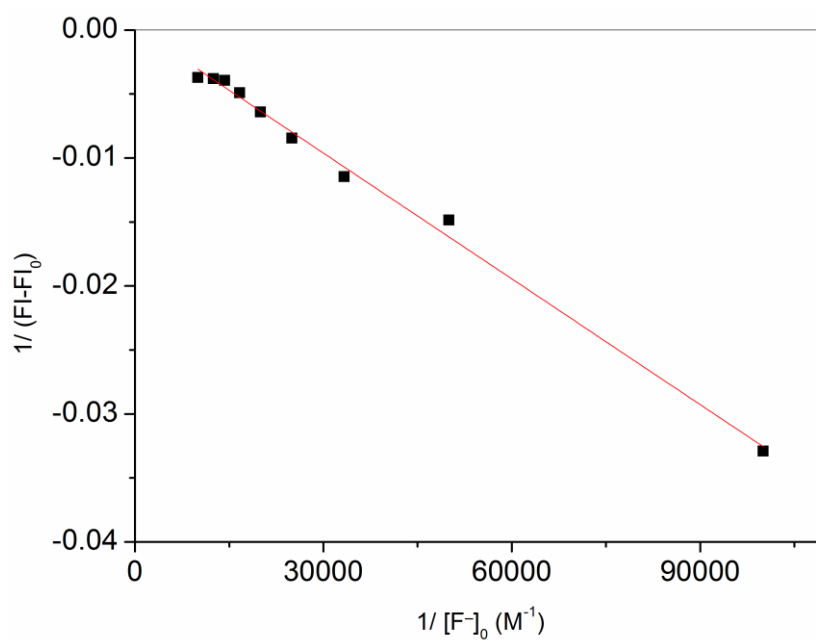
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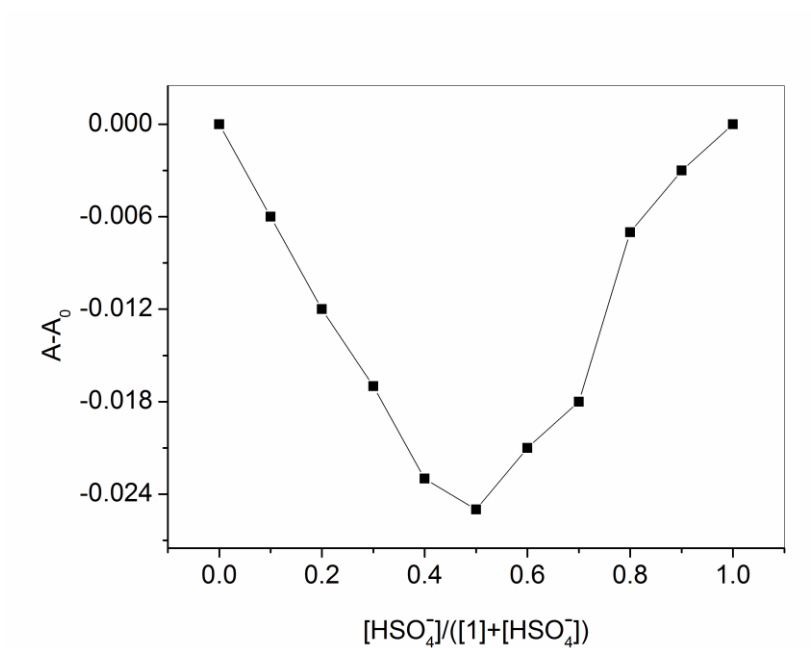
<sup>b</sup> *Graduate School of the Chinese Academy of Sciences, Beijing 100039, P. R. China.*



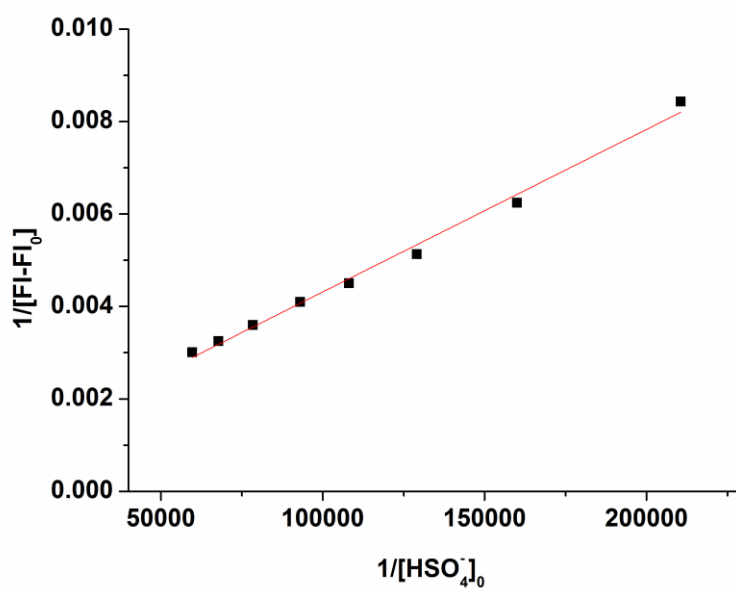
**Fig. S1.** Job's plot for a 1:1 complex of **1** and  $F^-$ , where the difference in absorbance intensity at 324 nm



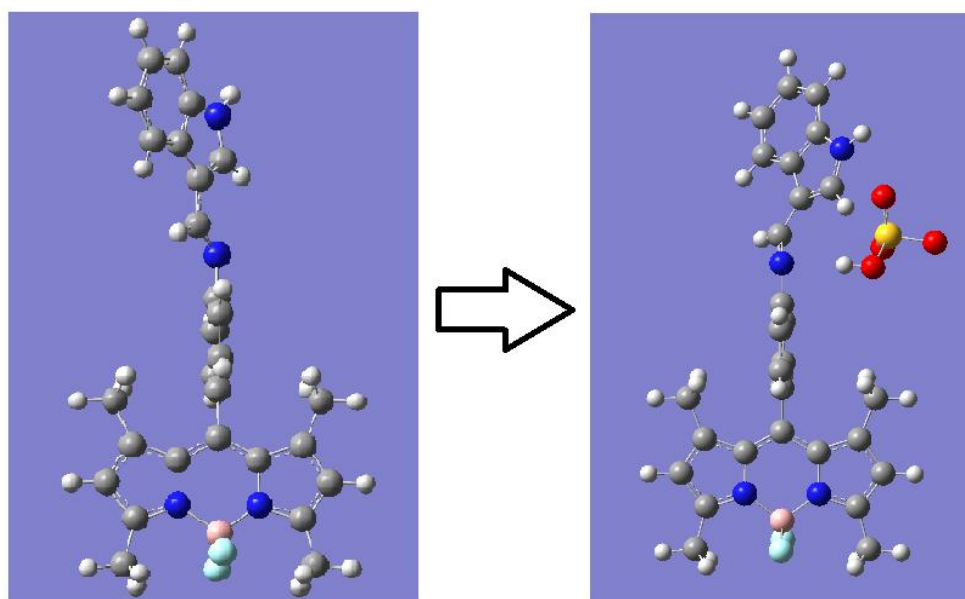
**Fig. S2** Benesi-Hildebrand plot assuming 1:1 stoichiometry for association between receptor **1** and  $F^-$ .



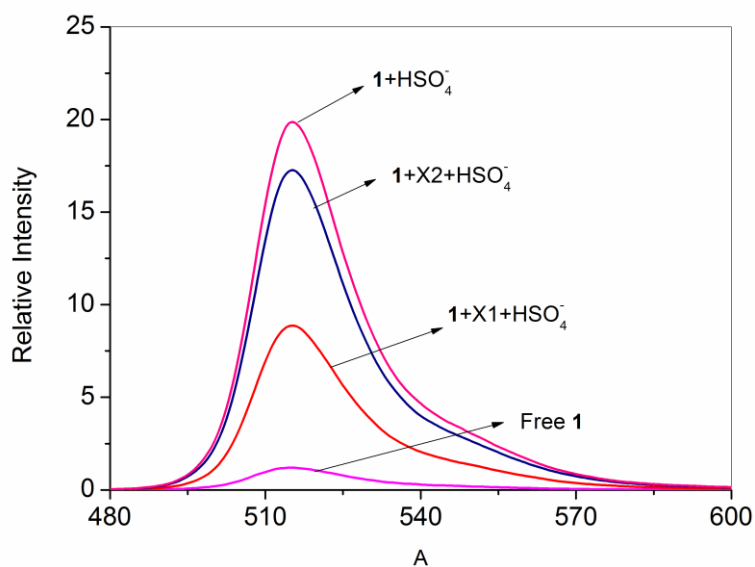
**Fig. S3.** Job's plot for a 1:1 complex of **1** and  $\text{HSO}_4^-$ , where the difference in absorbance intensity at 324 nm.



**Fig. S4.** Benesi-Hildebrand plot assuming 1:1 stoichiometry for association between receptor **1** and  $\text{HSO}_4^-$ .



**Fig. S5.** Optimized structure of sensor 1 and 1+HSO<sub>4</sub><sup>-</sup> complex calculated on the DFT level by B3LYP method with the 6-31G\*\*basis set.



**Fig. S6.** Fluorescence spectra of **1** (5.0 μM) in CH<sub>3</sub>CN in the presence of HSO<sub>4</sub><sup>-</sup> (50 equiv.) and other anions (X1= F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, AcO<sup>-</sup>, ClO<sub>4</sub><sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>; X2= Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, AcO<sup>-</sup>, ClO<sub>4</sub><sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>)

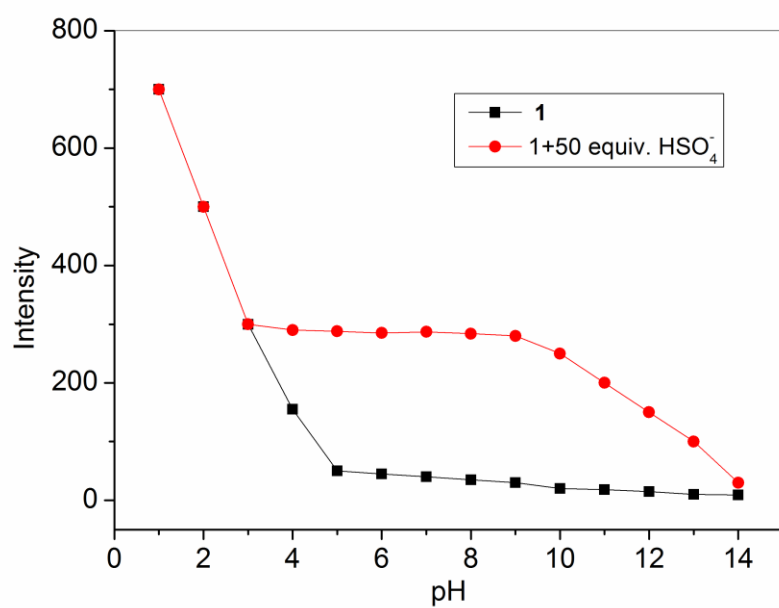


Fig. S7 Fluorescent intensity at 512 nm of sensor **1** and **1**+30 equiv. of HSO<sub>4</sub><sup>-</sup> in CH<sub>3</sub>CN/H<sub>2</sub>O (v:v, 1:1) solution with different pH condition.

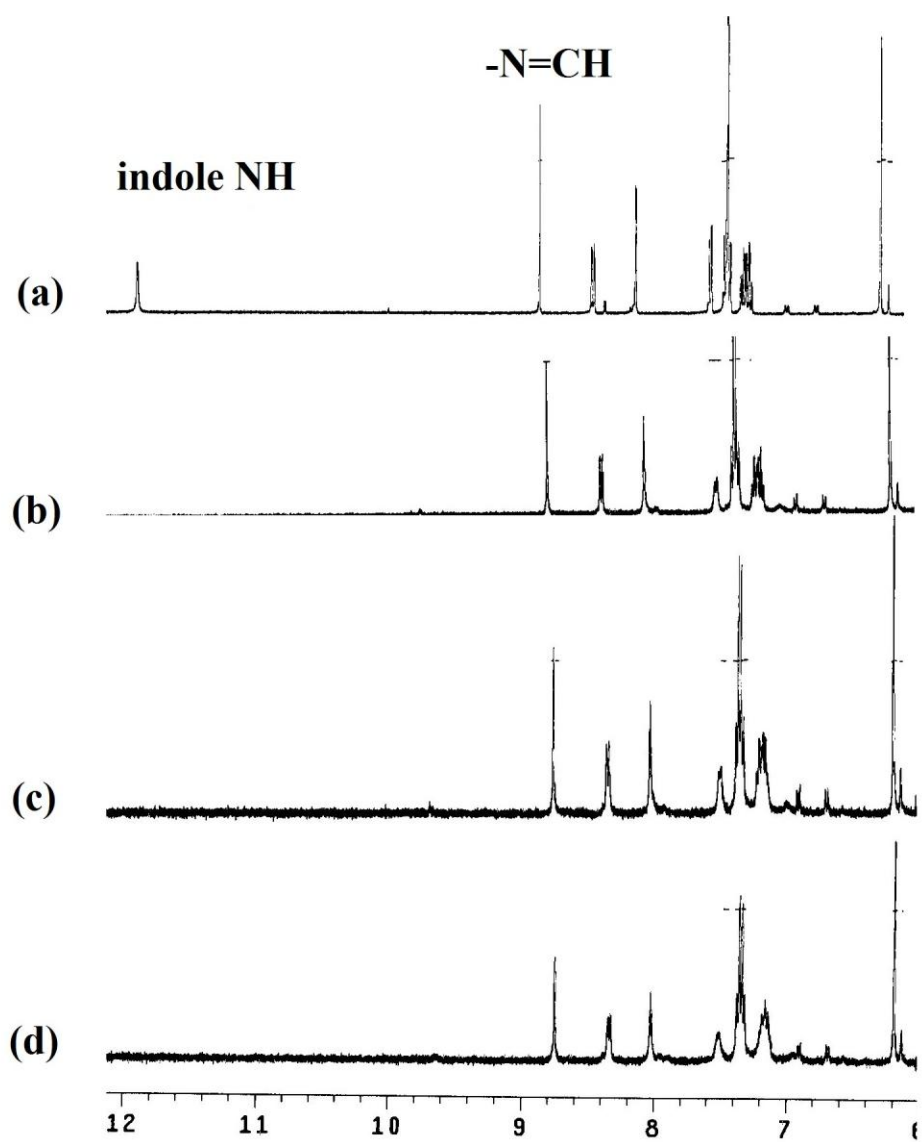


Fig. S8 Partial  $^1\text{H}$  NMR spectra of receptor **1** on addition of  $\text{F}^-$  (TBA salts) in  $\text{DMSO}-d_6$ : (a) 0 equiv.  $\text{F}^-$ ; (b) 0.5 equiv.  $\text{F}^-$ ; (c) 1 equiv.  $\text{F}^-$ ; (d) 3 equiv.  $\text{F}^-$ .

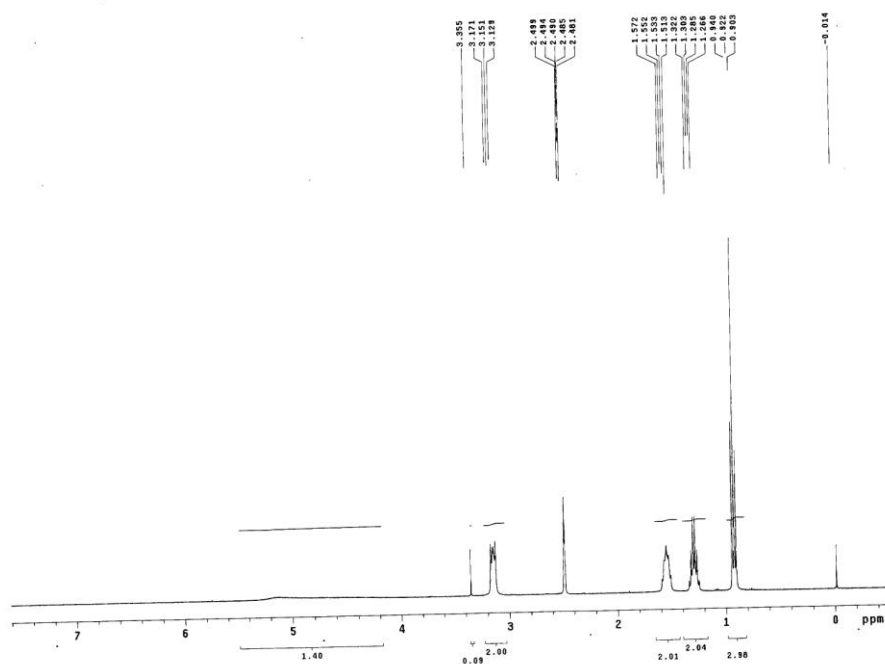


Fig. S9  $^1\text{H}$ NMR spectrum of TBAHSO<sub>4</sub> in DMSO-*d*<sub>6</sub> solvent

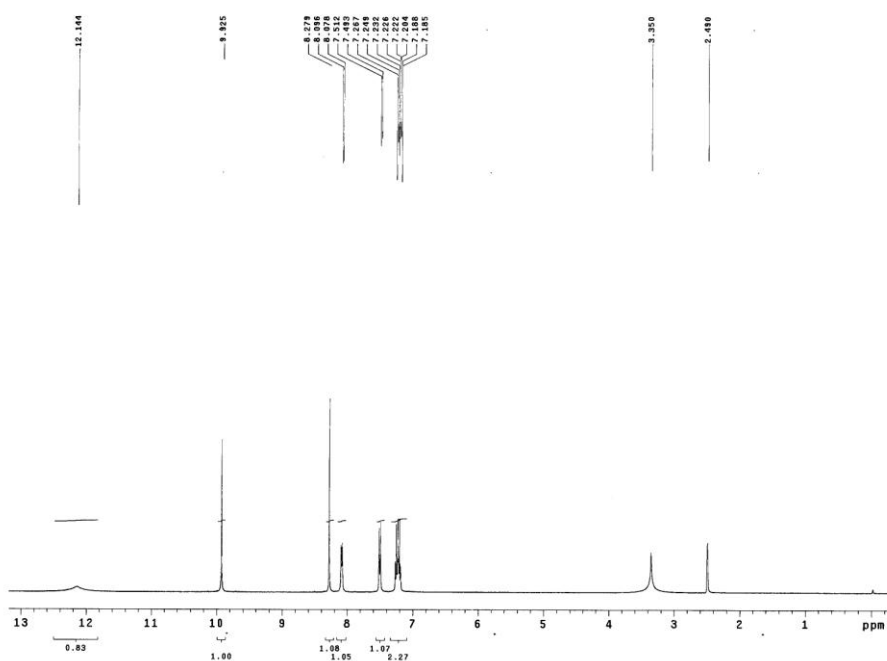
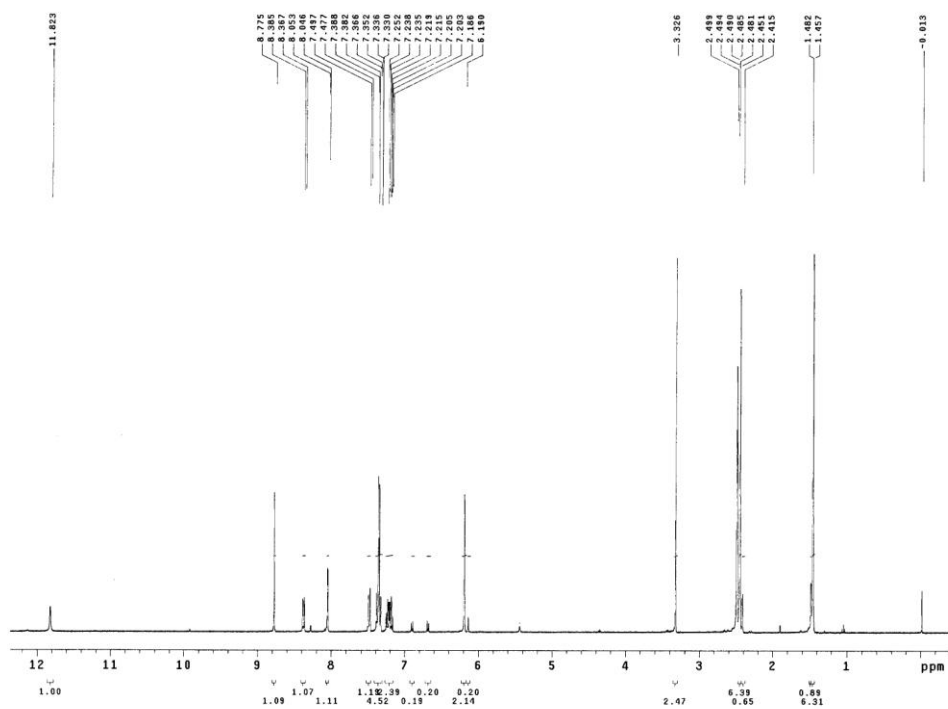
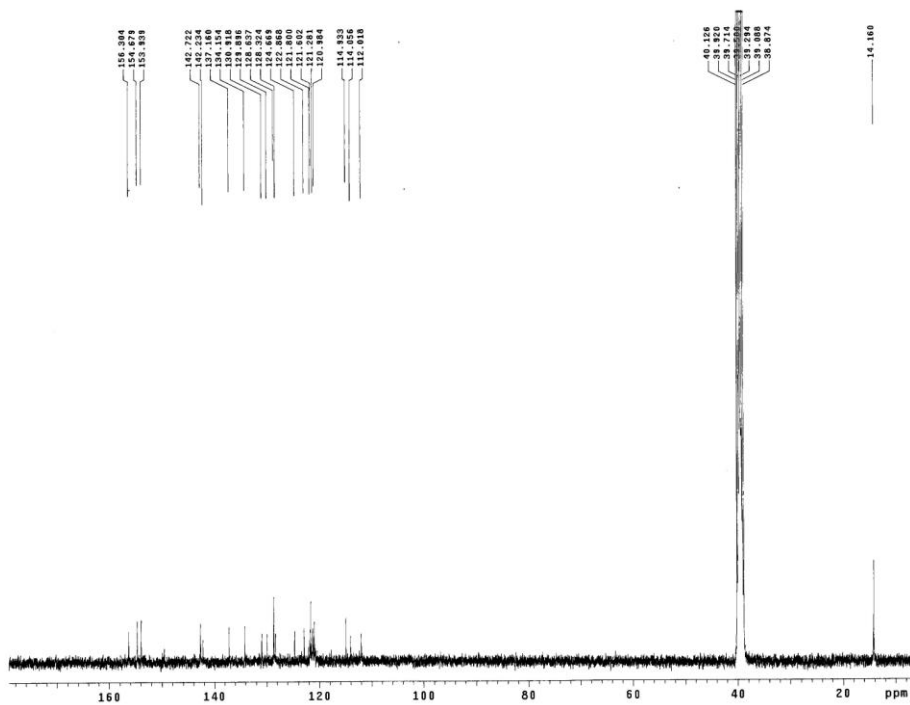


Fig. S10  $^1\text{H}$ NMR spectrum of Indole-3-carbaldehyde in DMSO-*d*<sub>6</sub> solvent

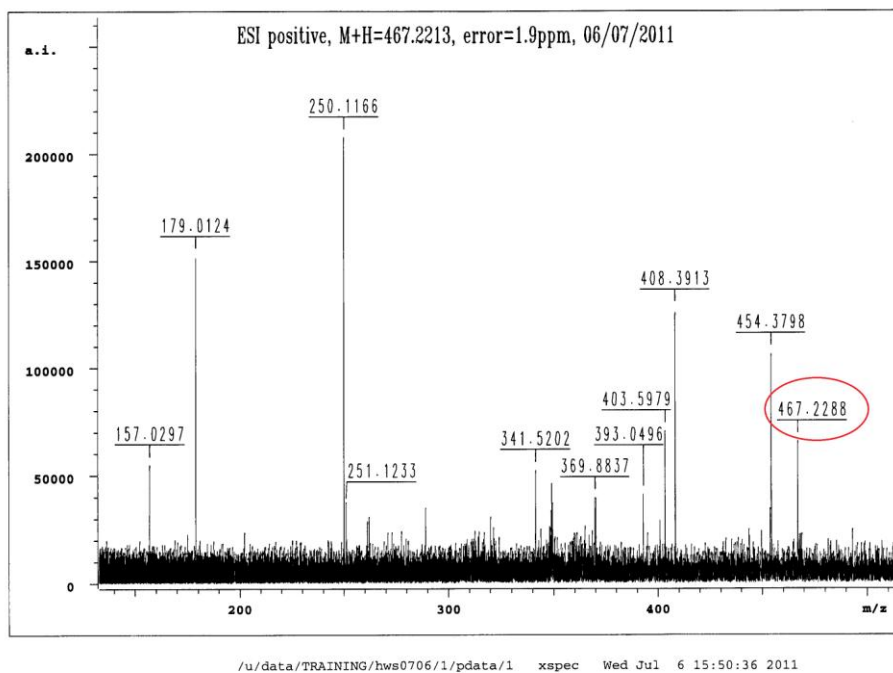


<sup>1</sup>H NMR spectrum of receptor **1** in DMSO-*d*<sub>6</sub> solvent



<sup>13</sup>C NMR spectrum of receptor **1** in DMSO-*d*<sub>6</sub> solvent





HR MS spectrum of receptor 1