

## Supporting Information

### A novel fluorescent probe based on triphenylamine for detecting sulfur dioxide derivatives

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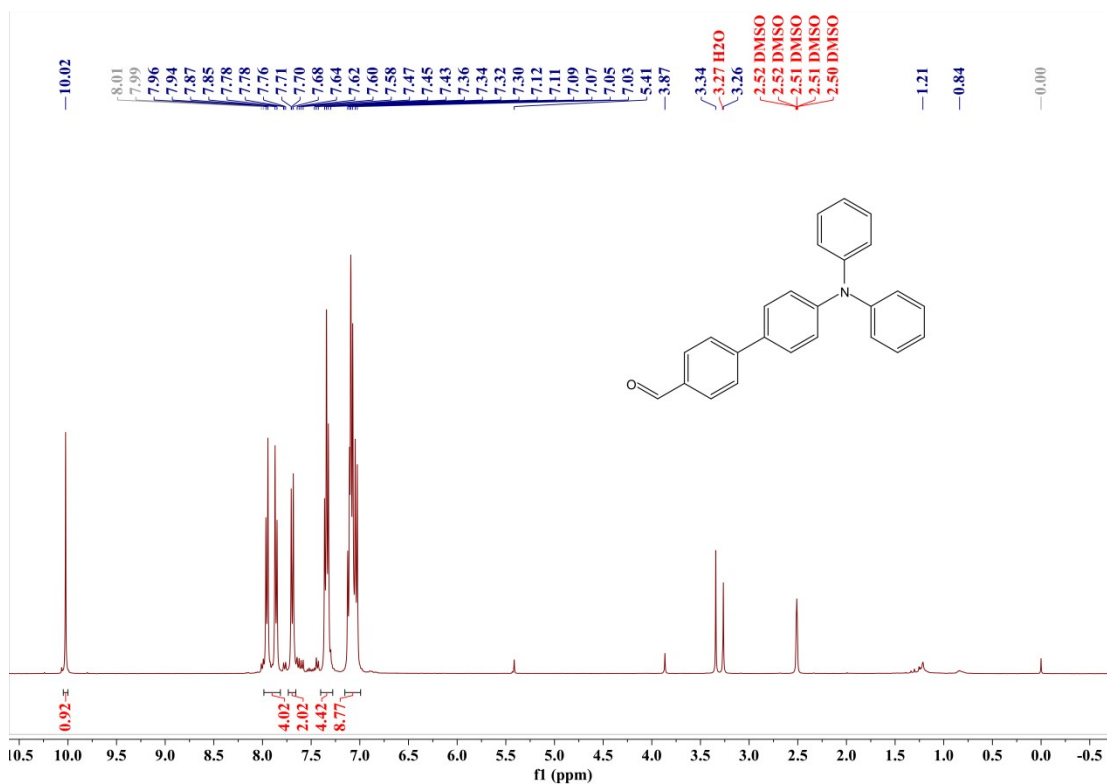


Fig. S1.  $^1\text{H NMR}$  spectrum of compound 1. (DMSO- $d_6$ , 400 MHz).

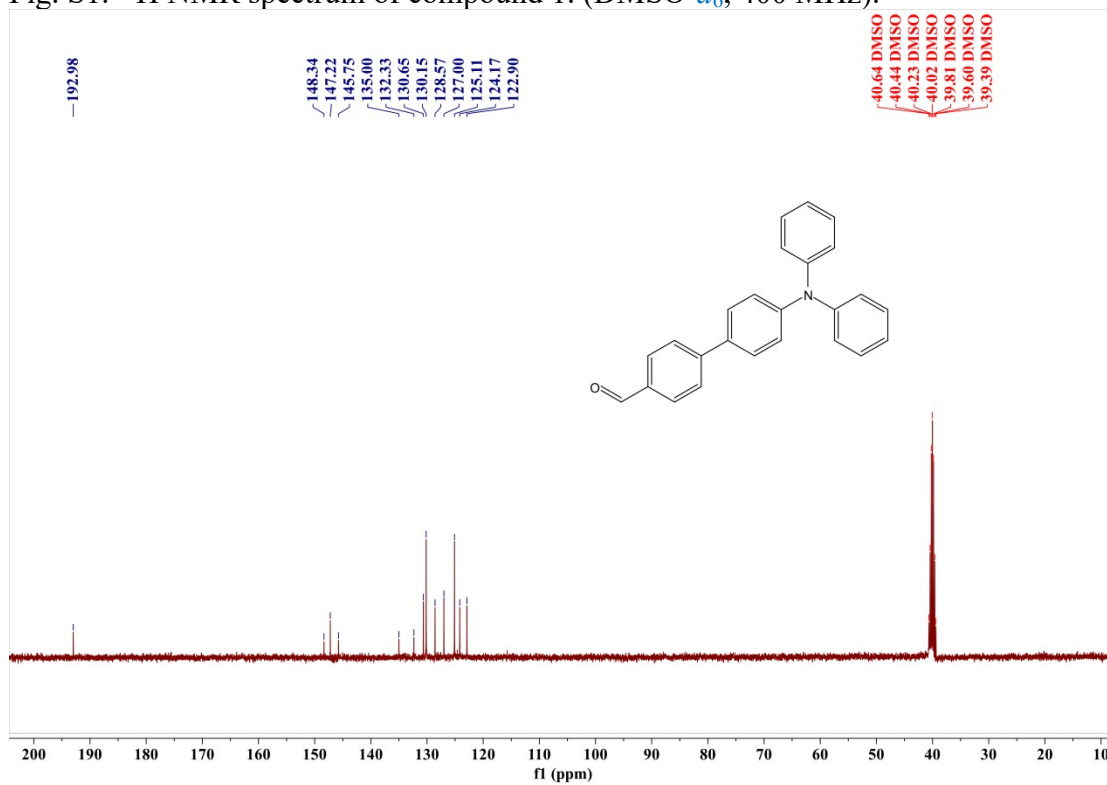


Fig. S2.  $^{13}\text{C NMR}$  spectrum of compound 1. (DMSO- $d_6$ , 101 MHz).

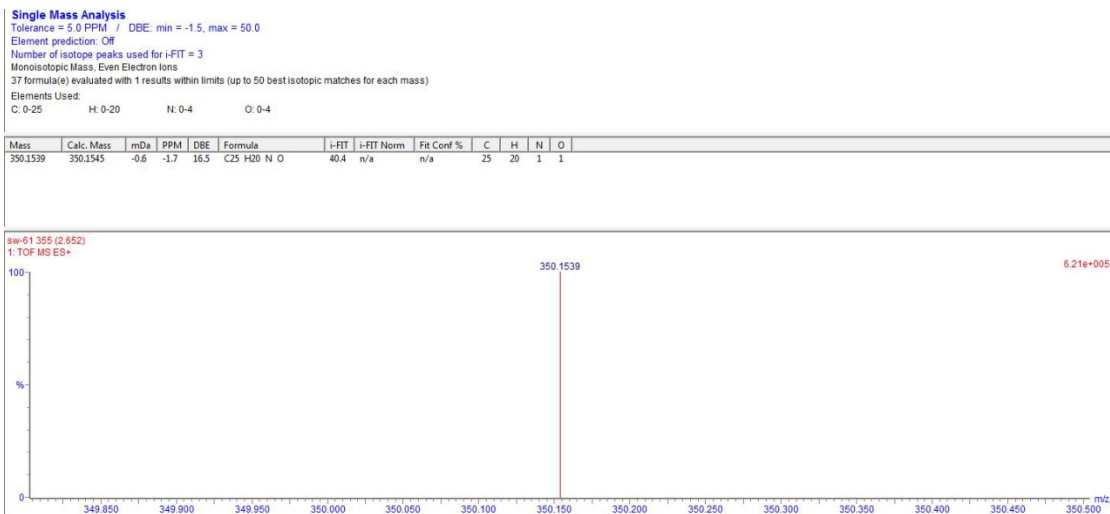


Fig. S3. HRMS of compound 1.

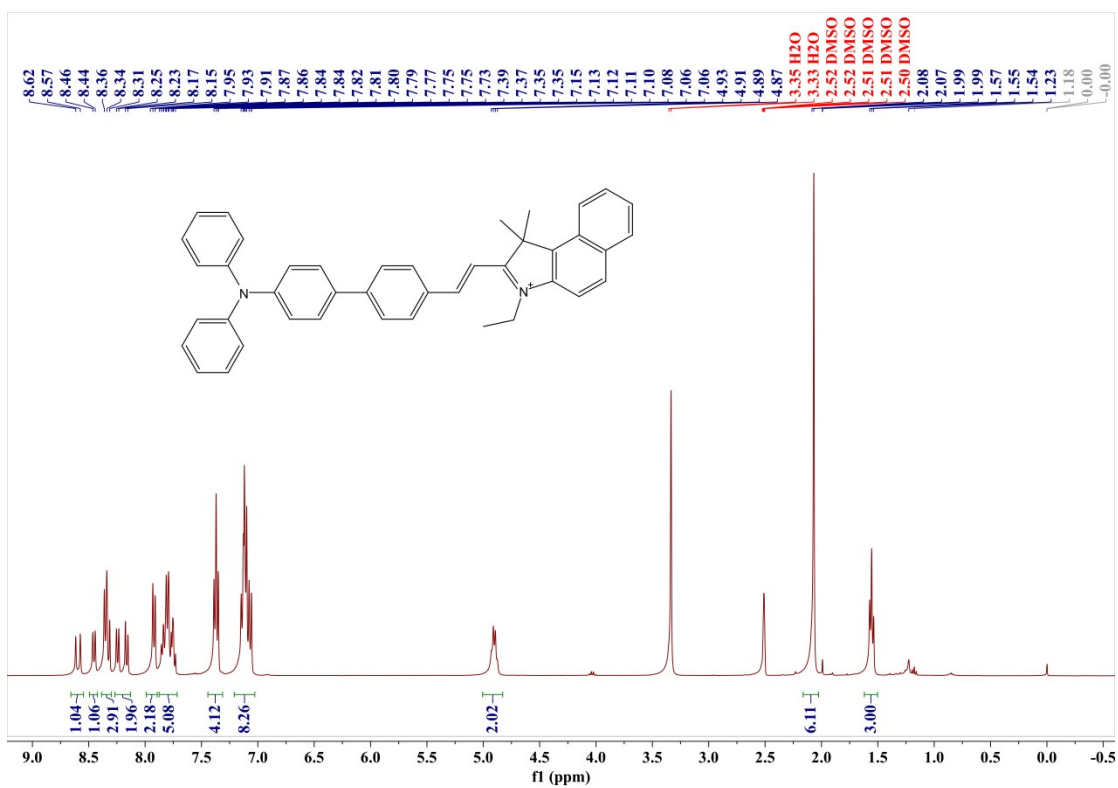


Fig. S4. <sup>1</sup>H NMR spectrum of BLT-SW (DMSO-*d*<sub>6</sub>, 400 MHz).

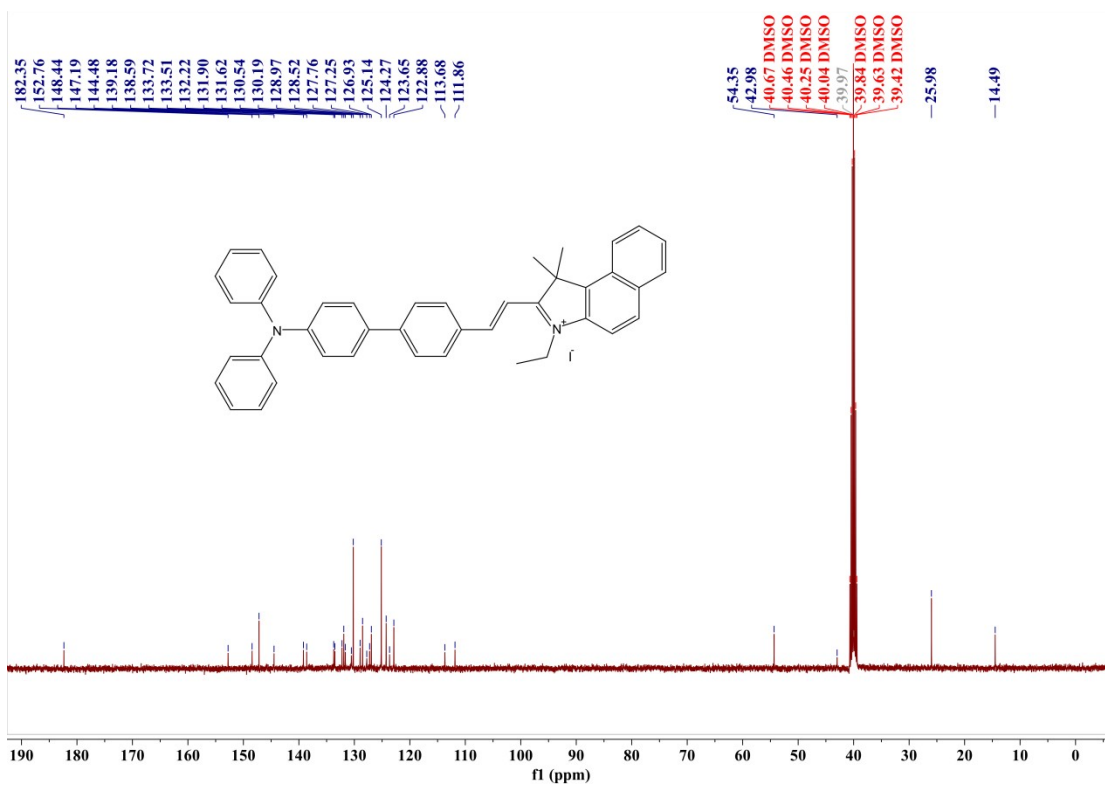


Fig. S5. <sup>13</sup>C NMR spectrum of BLT-SW (DMSO-*d*<sub>6</sub>, 101 MHz).

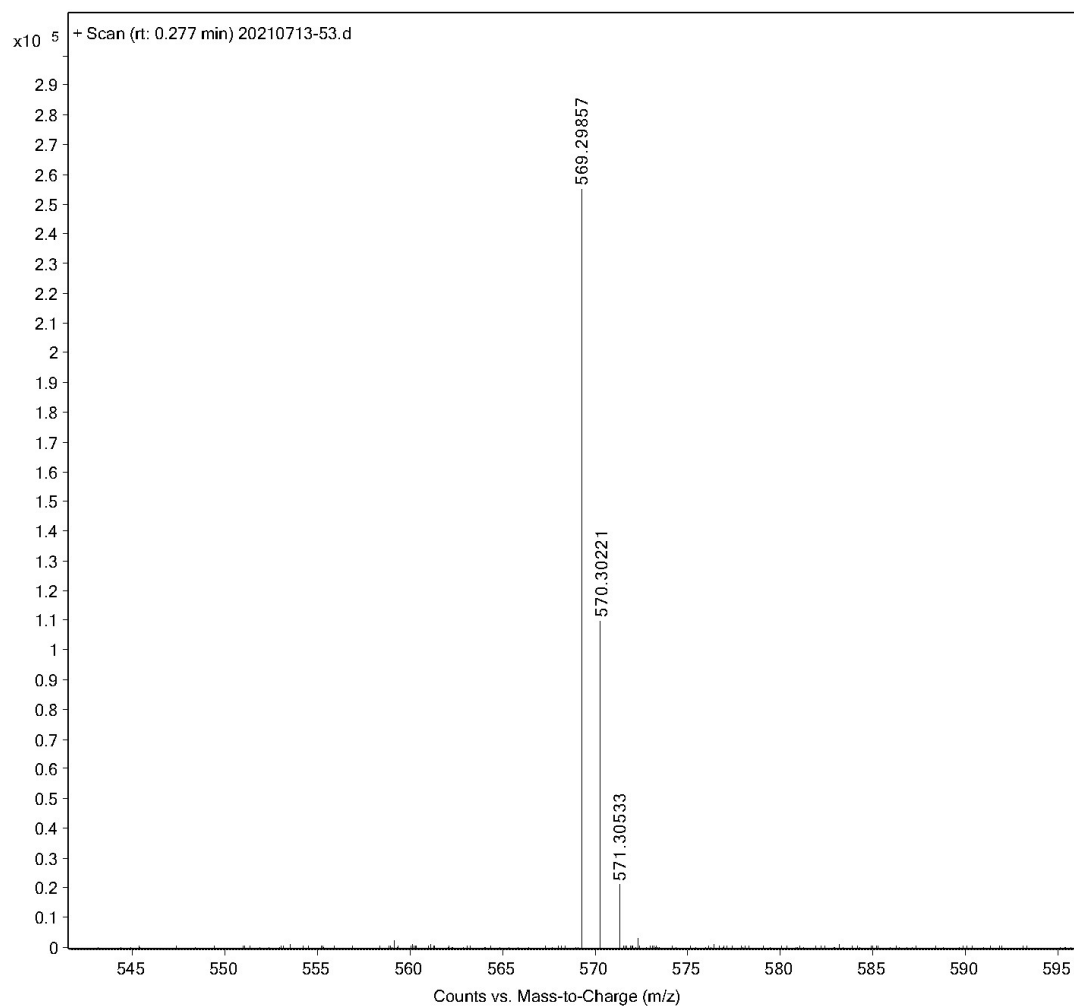


Fig. S6. HRMS of BLT-SW.

### Determination of quantum yield

Fluorescence quantum yield of probe A1-A6 and their products were determined in PBS solution (10 mM, pH = 7.4) with optically matching solutions of fluorescein ( $\Phi = 0.79$  in 0.1 M NaOH solution) as the standard and the quantum yield was calculated using the following equation:

$$\Phi_s = \Phi_r (A_r F_s / A_s F_r) (n_s^2 / n_r^2)^2$$

Where, s and r denote sample and reference, respectively. A is the absorbance. F is the relative integrated fluorescence intensity and n is the refractive index of the solvent.

Table S1. Photophysical properties of BLT-SW and it's product

Compound	Quantum yield
BLT-SW	0.019
BLT-SW+SO <sub>3</sub> <sup>2-</sup>	0.471

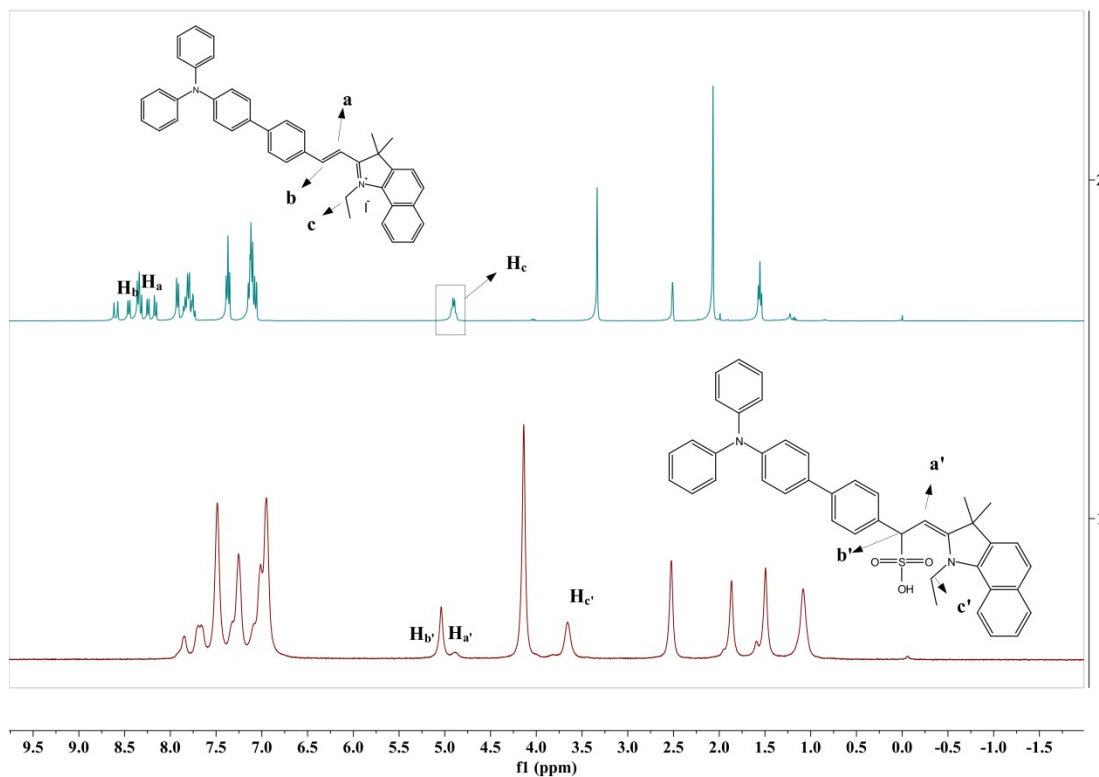


Fig. S7. <sup>1</sup>H NMR spectrum of BLT-SW + SO<sub>3</sub><sup>2-</sup> in DMSO-*d*<sub>6</sub>-D<sub>2</sub>O(4:1).

**Single Mass Analysis**

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3  
 Monoisotopic Mass, Even Electron Ions  
 9 formula(e) evaluated with 0 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:  
 C: 39-43 H: 30-39 N: 1-3 O: 1-3 S: 0-2

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S
650.2616	---												

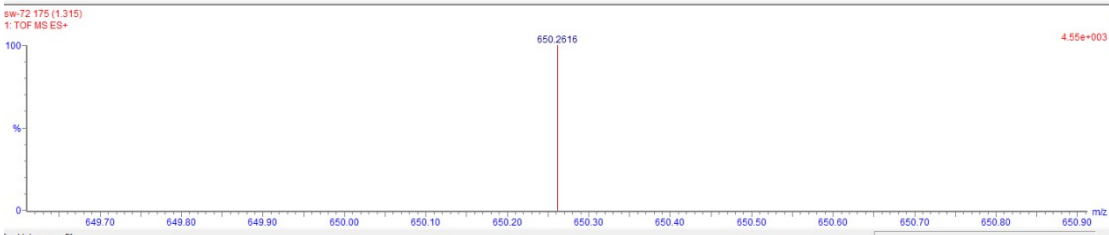


Fig. S8. HRMS of BLT-SW+SO<sub>3</sub><sup>2-</sup>.

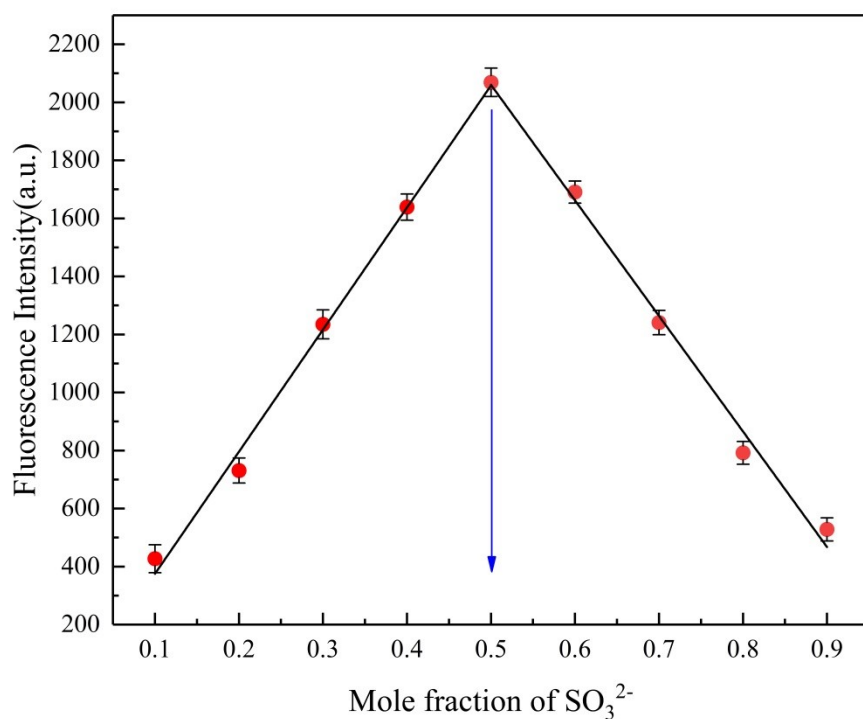


Fig. S9. Fluorescence Job's plot for the determination of stoichiometry between BLT-SW and SO<sub>3</sub><sup>2-</sup> in PBS-DMSO (10 mM, pH = 7.4, 1% DMSO), the total concentration of [BLT-SW] + [SO<sub>3</sub><sup>2-</sup>] = 40μM.

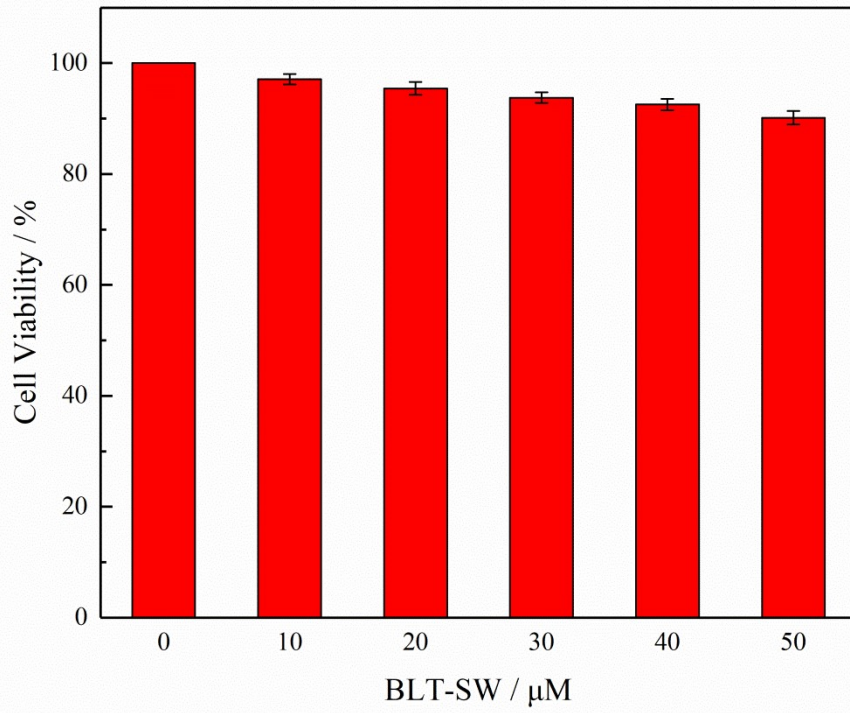
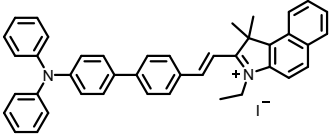
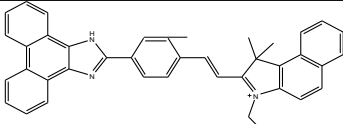
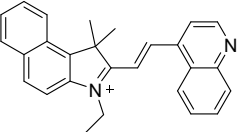
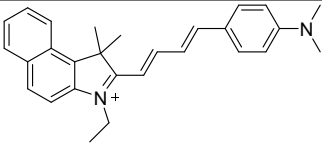
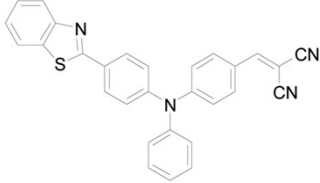


Fig. S10. MTT assay of HepG-2 cells with BLT-SW at different concentration (0-50  $\mu\text{M}$ ) for 24 hours.



Table S2: Comparison of the characteristics with reported sensors for SO<sub>2</sub> derivatives

Probe	water solubility	Response time	LOD (M)	Cell imaging	test strips	Actual sample testing
 <p>This work</p>	1% DMSO in PBS	5 min	$2.75 \times 10^{-6}$	Yes	Yes	Yes
 <p>Talanta. 2019, 191, 428-434</p>	EtOH/PBS 4:6	30 min	$2.6 \times 10^{-8}$	Yes	No	No
 <p>J. Mater. Chem. B, 2017,5, 3862-3869</p>	/	15 S	$2.2 \times 10^{-8}$	Yes	No	No
 <p>Chem. Commun., 2016,52, 10381-10384</p>	100% aqueous	140 S	$1.06 \times 10^{-7}$ M	Yes	No	No
 <p>Anal. Methods, 2021, 13, 3667</p>	DMF/Tris (v/v = 1 : 1)	3 min	$3.19 \times 10^{-8}$	Yes	No	No