Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

A near-infrared and mitochondria-targeted fluorescence probe for ratiometric monitoring of sulfur dioxide derivatives in living cells

Ye-Hao Yan[a], Xiao-Ying He[b], Jun-Ying Miao[b], Bao-Xiang Zhao[a]*

[a] *Institute of Organic Chemistry, School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, P.R. China*

[b] *Shandong Provincial Key Laboratory of Animal Cells and Developmental Biology, School of Life Science, Shandong University, Qingdao 266237, P.R. China*

1. Energy transfer efficiency was obtained based on the following equality:

$$E = 1 - F_{DA}/F_D$$

In this equation, E represents the FRET energy transfer efficiency in probe **SNB**. F_{DA} represents fluorescence intensity of donor moiety in probe **SNB**. F_D represents fluorescence intensity of the donor alone.

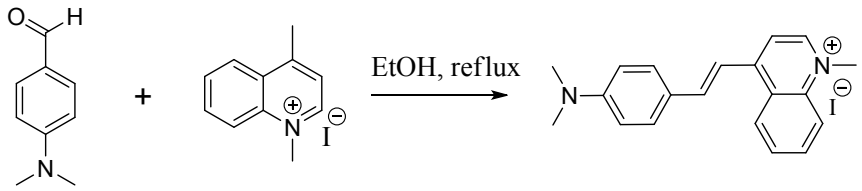
2. Detection limit calculation:

$$L_{OD} = 3\sigma/k$$

Where, σ represents the standard deviation of the blank solutions without the addition of sulfur dioxide derivatives, and k represents the slope of titration linear relationship.

Scheme S1 Synthesis route of the acceptor.

Fig. S1-4 The ^{1}H NMR, ^{13}C NMR, IR and MS spectra of probe **SNB**.



Scheme S1 Synthesis route of the acceptor

The acceptor of probe **SNB** was prepared according to previous report [S1]. *p*-Dimethylaminobenzaldehyde (178.4 mg) and 1,4-dimethylquinolin-1-ium iodide (286.3 mg) were dissolved into EtOH (20.00 mL) under the catalysis of piperdine (0.50 mL) and kept refluxing 6 h. Then, the mixture was purified by column chromatography (DCM : MeOH = 15:1) to give the acceptor in 62% yield.

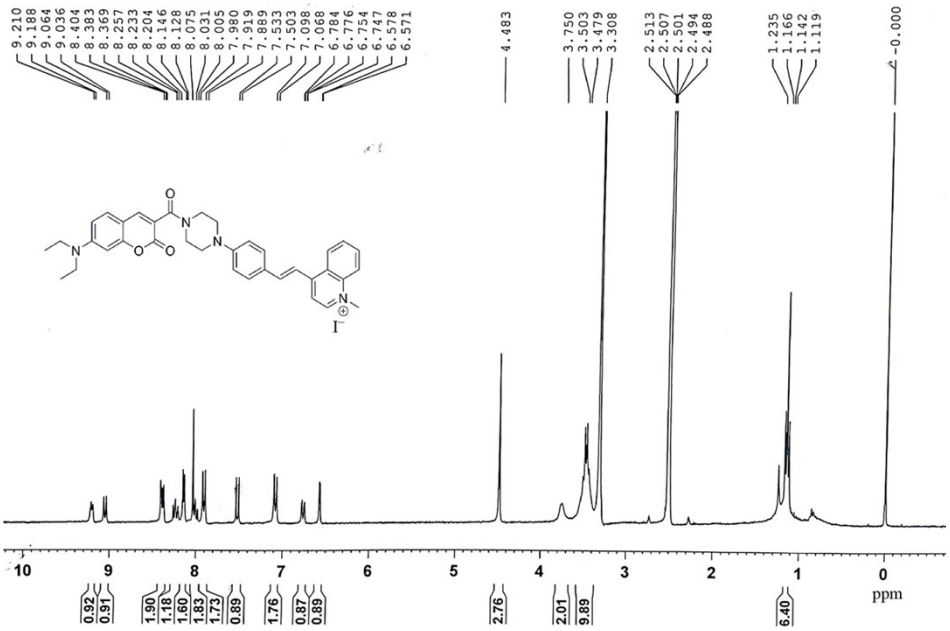


Fig. S1 The ^{1}H NMR spectrum of probe **SNB**.

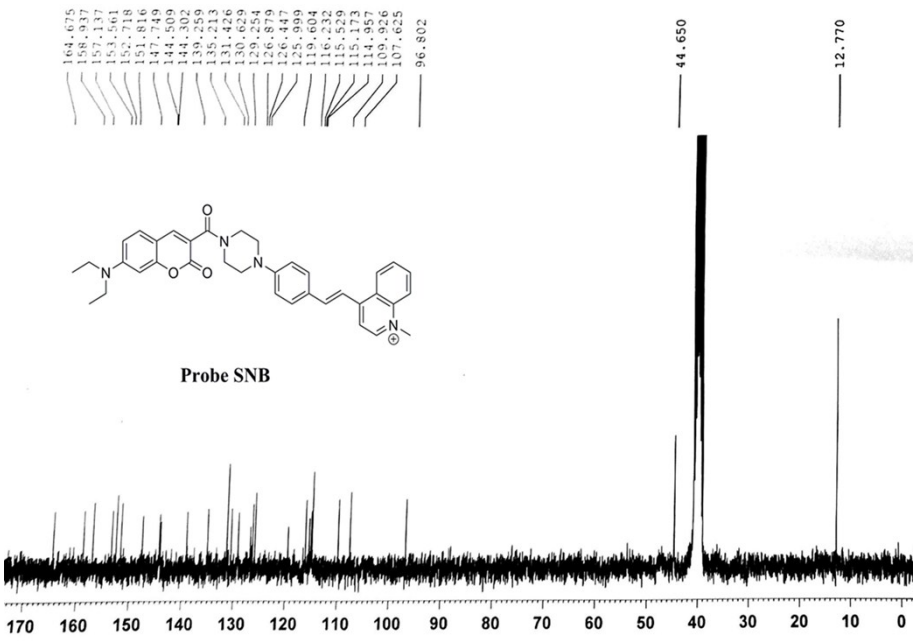


Fig. S2 The ^{13}C NMR spectrum of probe **SNB**.

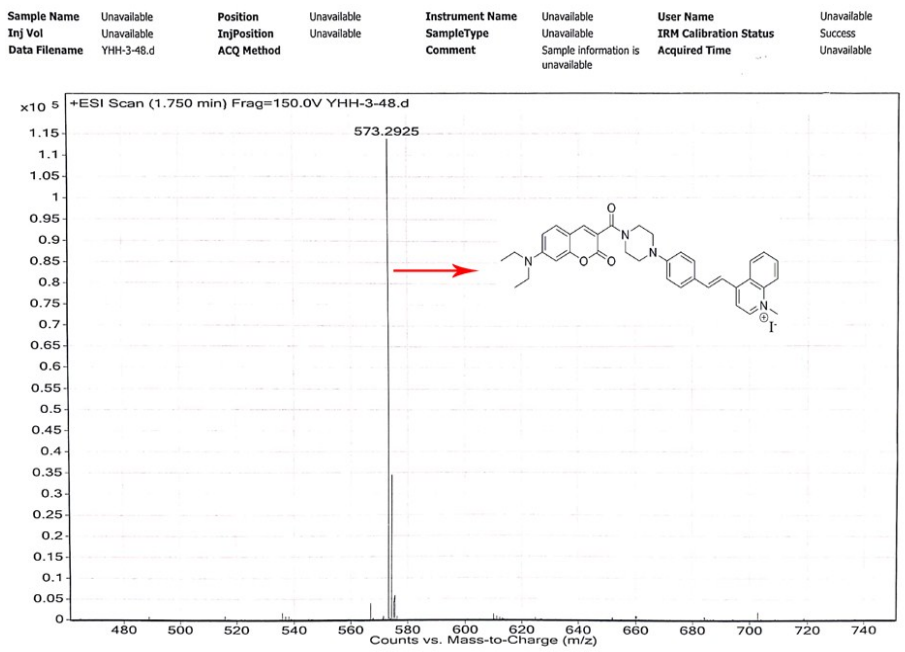


Fig. S3 The MS spectrum of probe **SNB**.

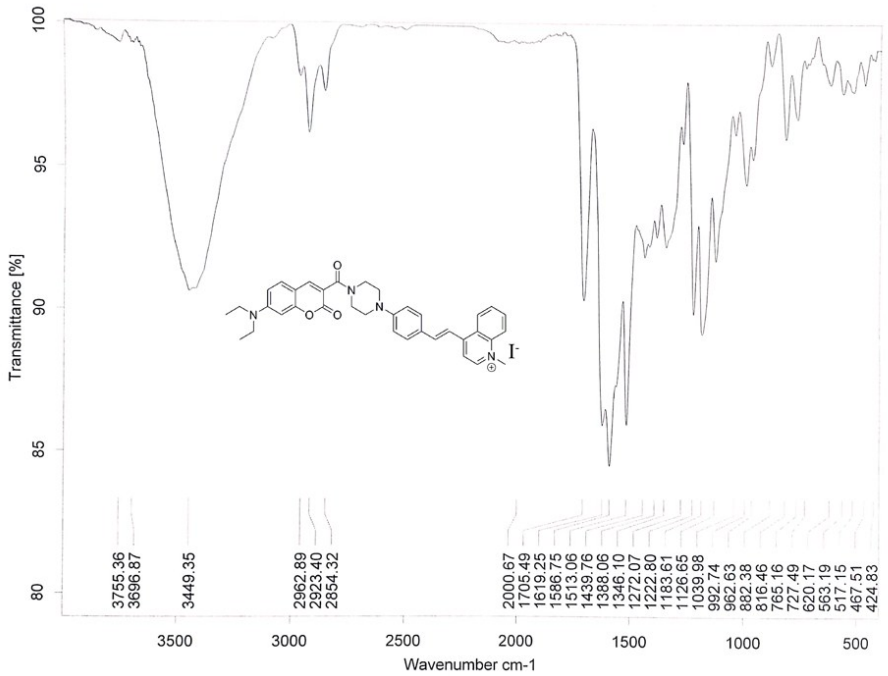


Fig. S4 The IR spectrum of probe **SNB**.

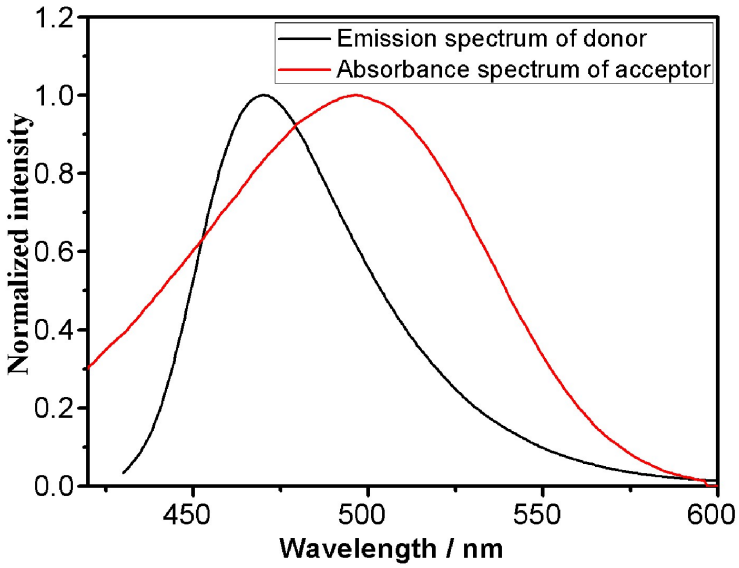


Fig. S5 The overlap between the emission band of the donor and the absorbance band of the acceptor. (5 μM; Fluorescence spectra: λ_{ex} = 420 nm, speed: 1200 nm/s)

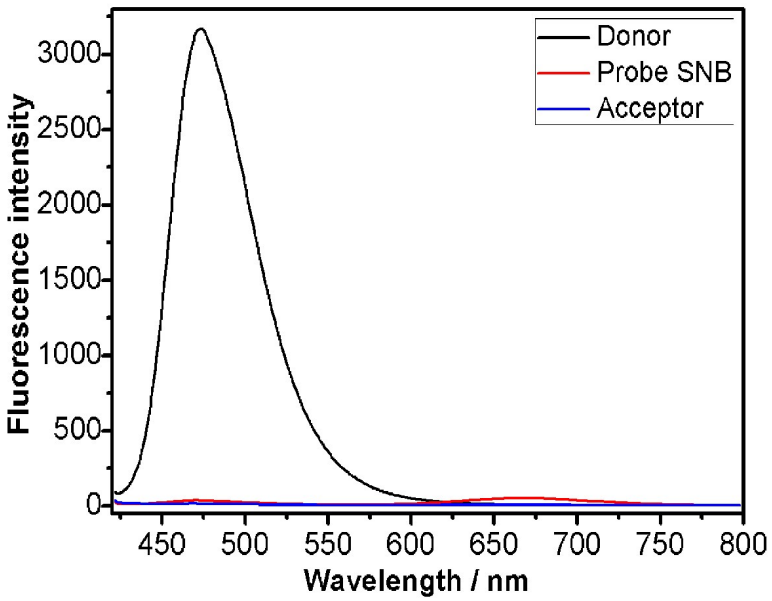


Fig. S6 The energy transfer efficiency. (5 μM, λ_{ex} = 420 nm, speed: 1200 nm/s, slit: 5/5)

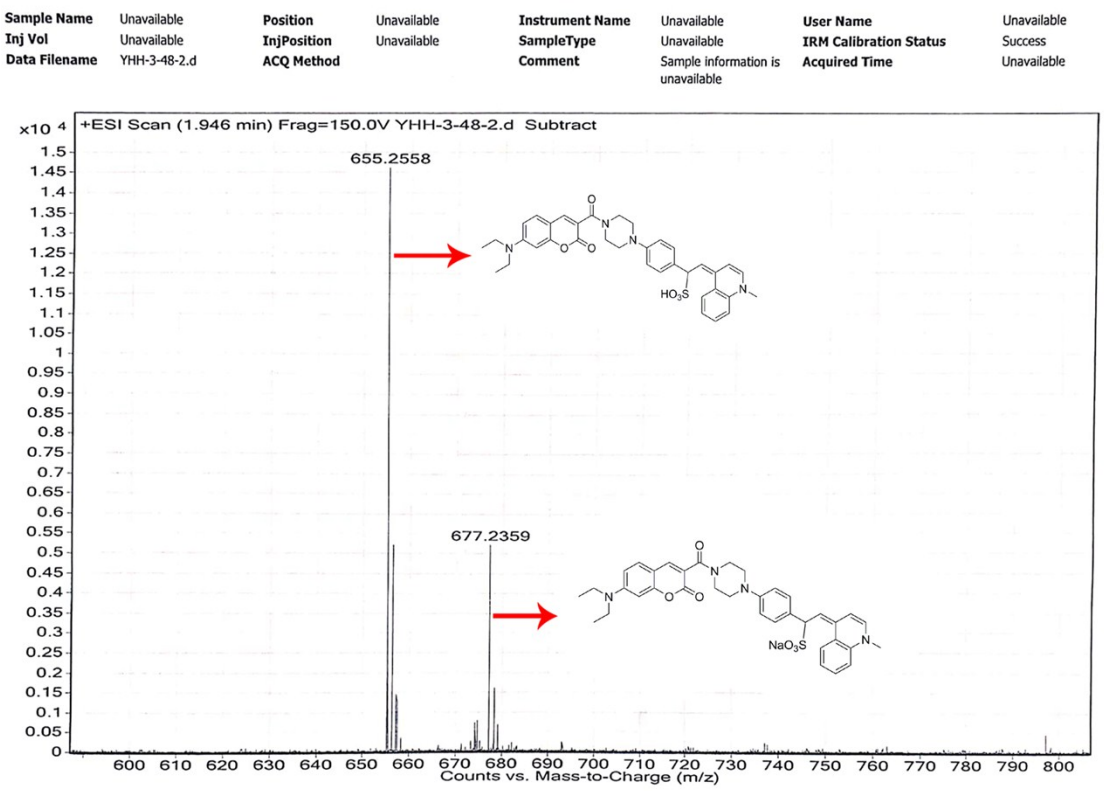


Fig. S7 MS of the mixture of **SNB** and HSO_3^-/SO_3^{2-} (DMSO/water mixed solution).

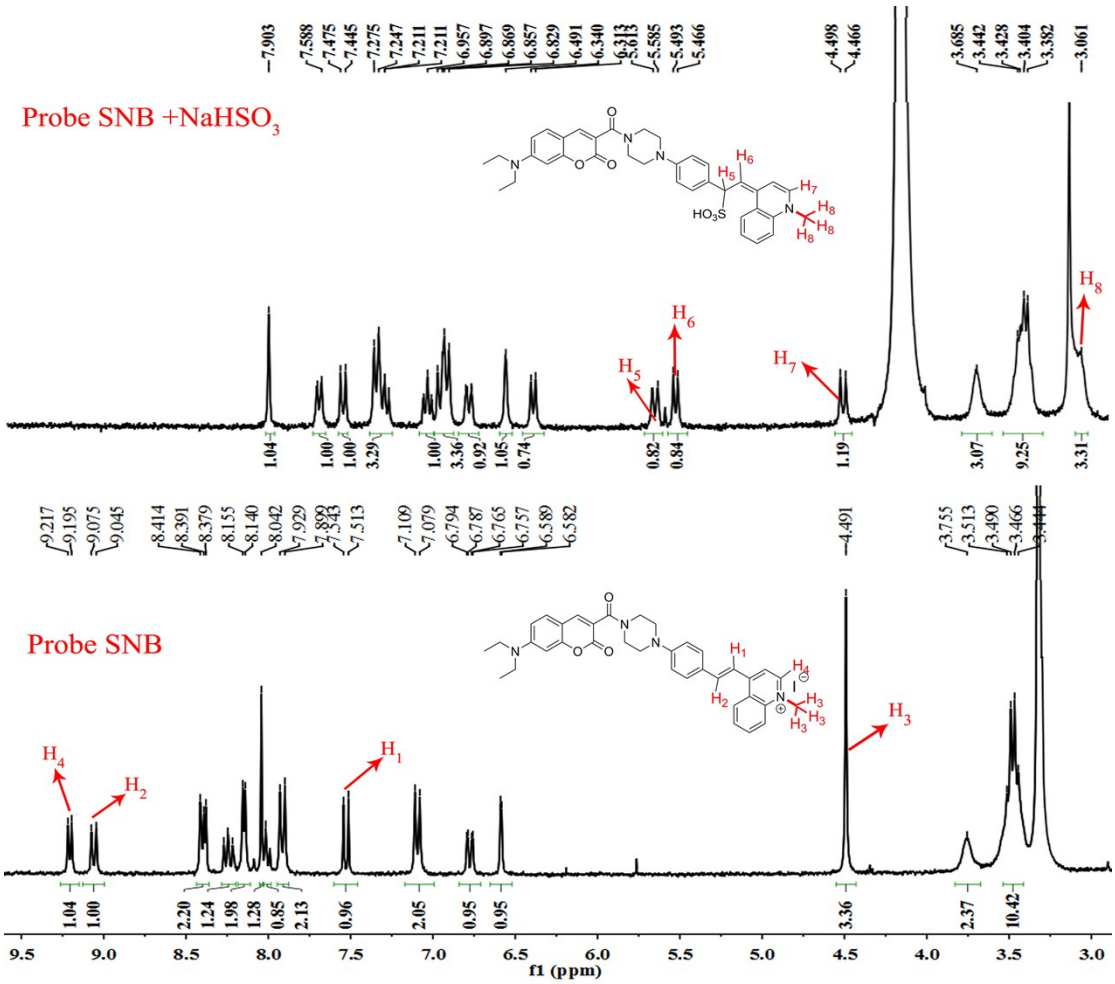


Fig. S8 The ^{1}H NMR of the mixture of **SNB** and HSO_3^-/SO_3^{2-} (DMSO-d_6 and D_2O mixed solution).

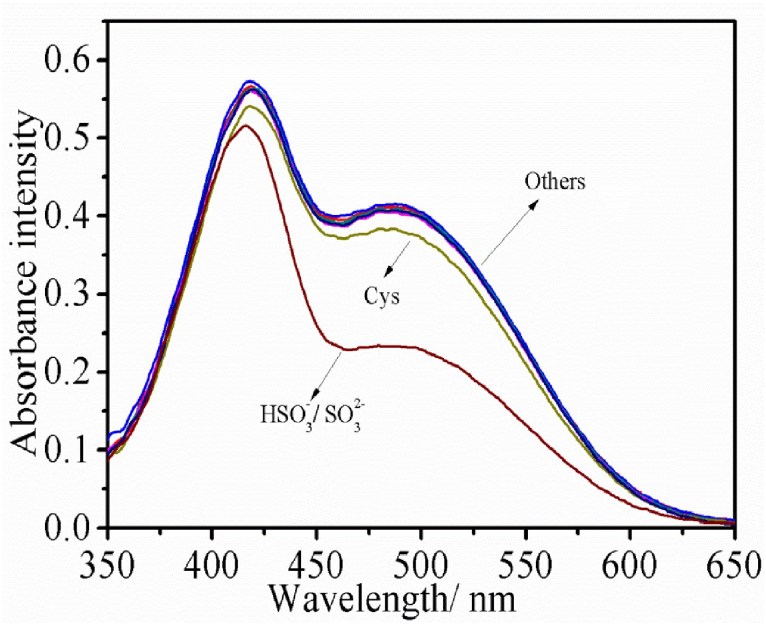


Fig. S9 Selectivity of **SNB** toward HSO_3^-/SO_3^{2-} by UV-Vis spectra.

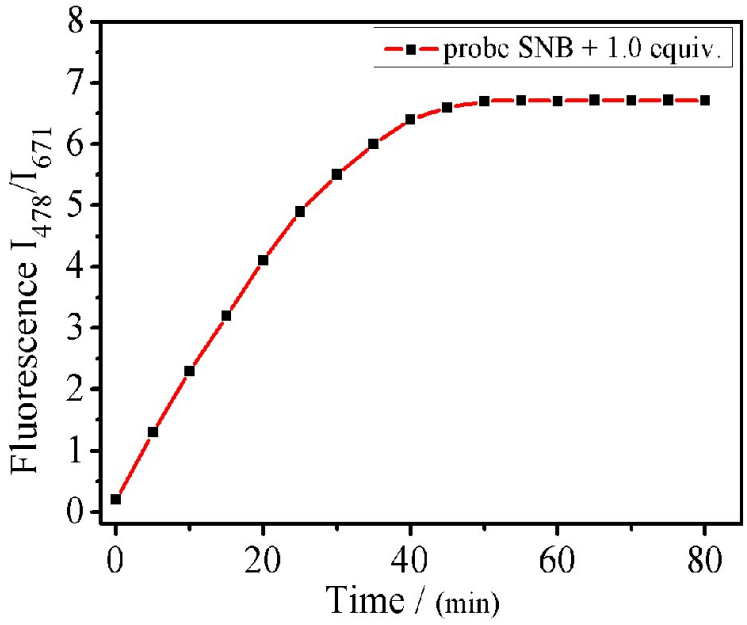


Fig. S10 The time dependent of the **SNB** response to HSO_3^-/SO_3^{2-}. (5 μM, λ_{ex} = 420 nm, speed: 1200 nm/s, slit: 5/5)

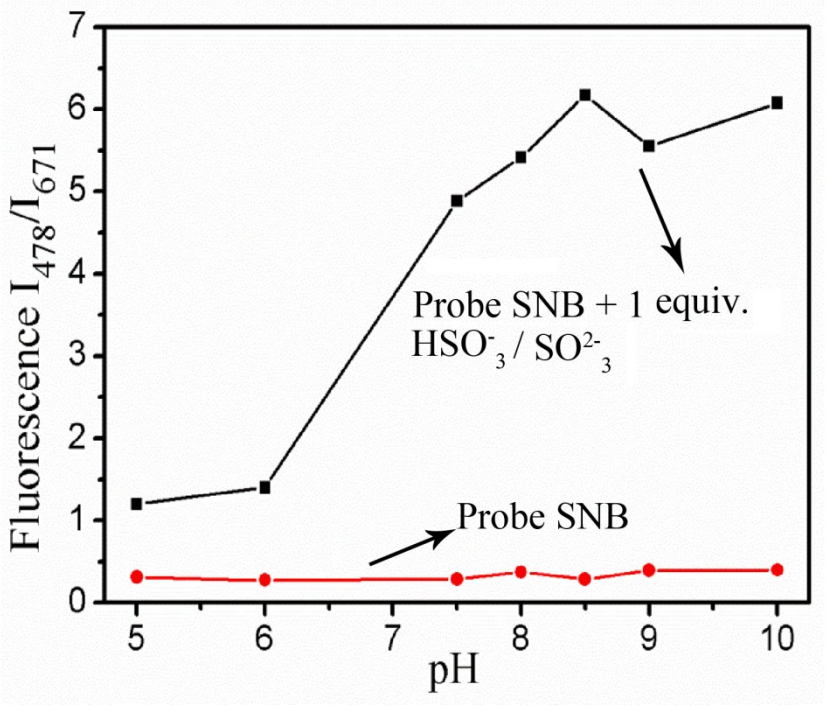


Fig. S11 The pH dependence of the **SNB** for the detection of HSO_3^-/SO_3^{2-}.

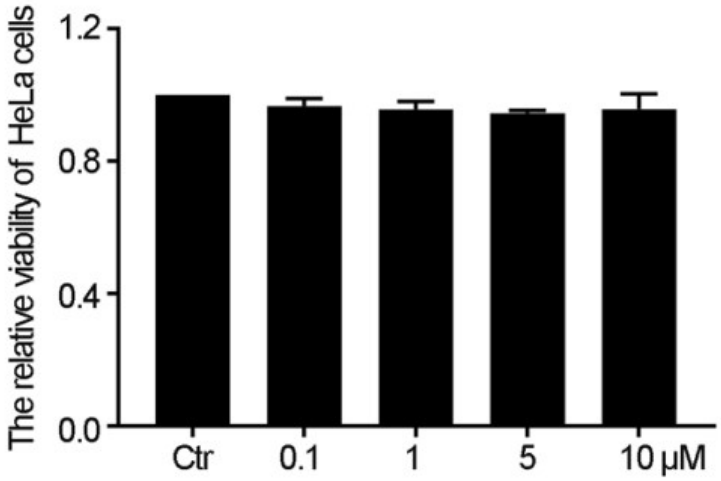


Fig. S12 The toxicity analysis of **SNB** for HeLa cells. Hela cells were cultivated with Dulbecco's modified Eagle's medium (DMEM) which contains supplement of 10% FBS (Fetal Bovine Serum) in the carbon dioxide incubator with an atmosphere of 5% CO_2 and 95% air at 37 ℃. HeLa cells were placed to a 96-well plate in the concentration of 40000 per mL for 24 h, and then incubated with probe **SNB** (0, 0.1, 1, 5 and 10 μM) for 6 h, respectively. After that SRB assay was conducted to measure the viability of cells.

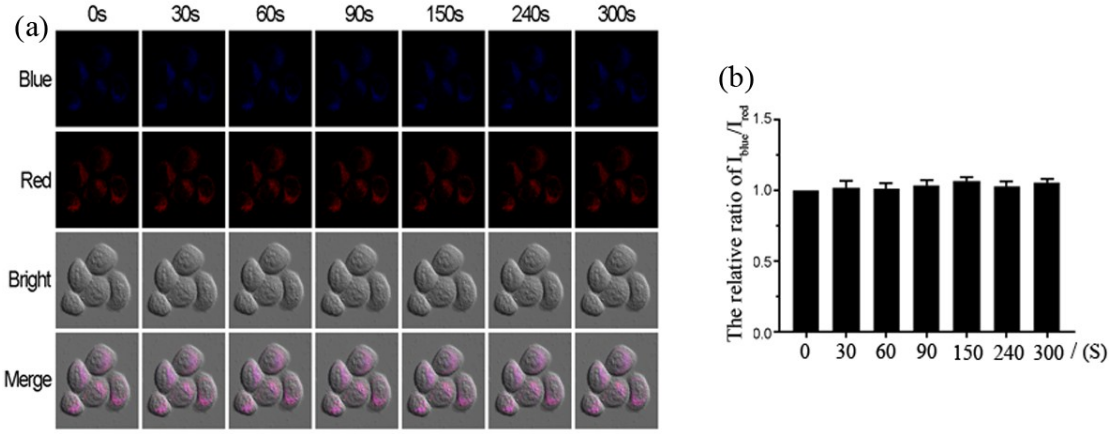


Fig. S13 The photo-stability analysis of **SNB** in bioimaging. HeLa cells were pre-treated with **SNB** (1 μM) for 1 h. First line: fluorescence images at the blue channel (450-610 nm); Second line: fluorescence images at the red channel (610-700 nm); Third line: images at bright field; Forth line: merged images of the first and second lines. (λ_{ex} = 405 nm)

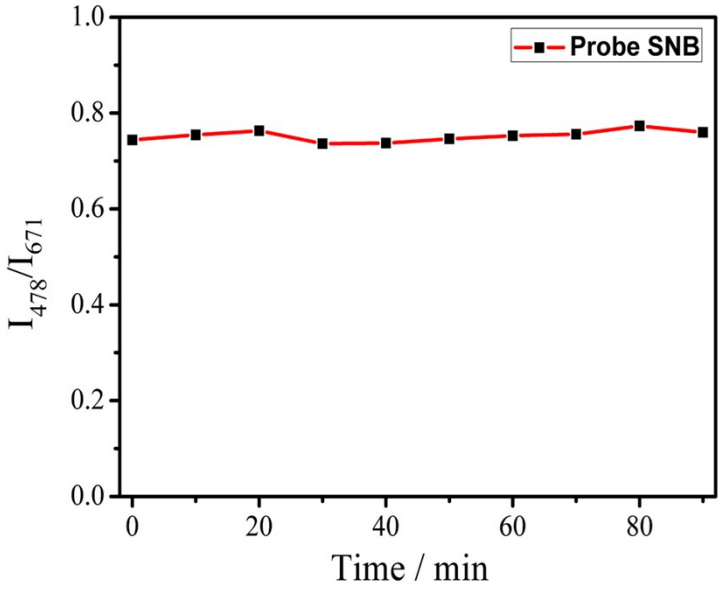


Fig. S14 The photo-stability analysis of **SNB** in daylight.

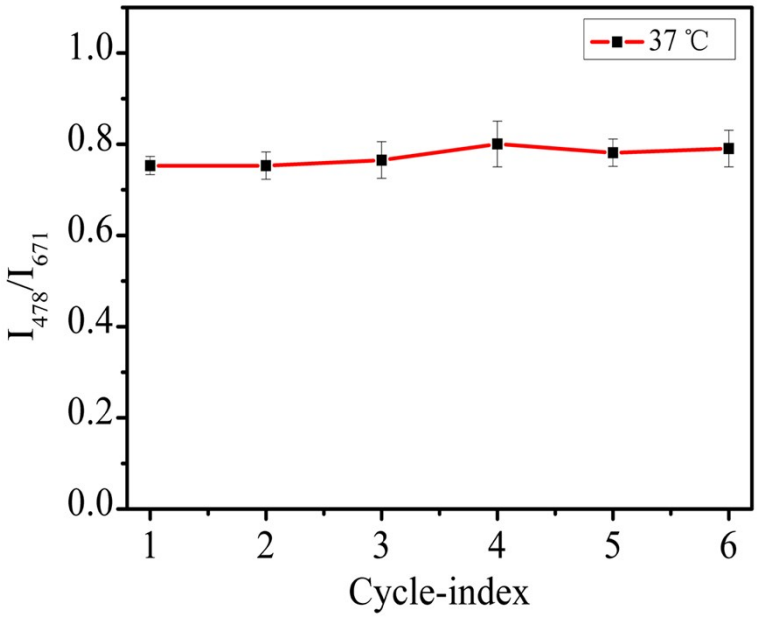
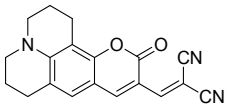
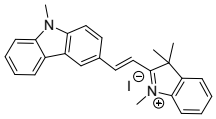
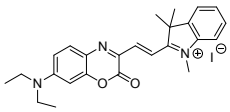
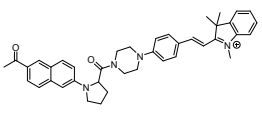
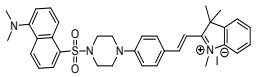
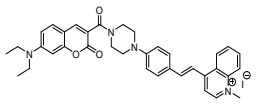


Fig. S15 The thermostability analysis of **SNB** in temperature cycle experimental. Firstly, the fluorescence spectra of probe **SNB** were recorded at 37 °C, then heated to 60 °C and cold down 37 °C to measure fluorescence, 5 times cycles.

Table S1 The comparison of probe **SNB** with other probes

Probe	**Response ions**	**Ratiometric**	**Detection limit**	**Targeted subcellar**	**Ref.**
	HSO_3^-	No	0.87 μM	No	S2
	HSO_3^-	Yes	0.15 μM	Mitochondria	S3
	HSO_3^-	Yes	87 nM	No	S4
	HSO_3^-/SO_3^{2-}	Yes	0.24 μM	No	S5

	HSO_3^-/SO_3^{2-}	Yes	0.1 μM	Mitochondria	S6
 **SNB**	HSO_3^-/SO_3^{2-}	Yes	17 nM	Mitochondria	This work

Reference

[1] Y. Li, D. Xu, S.L. Ho, H.W. Li, R. Yang and M.S. Wong, *Biomaterials* 2016, **94**, 84-92.

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