

A mitochondria-targetable fluorescent probe for detection of bisulfite in living cells

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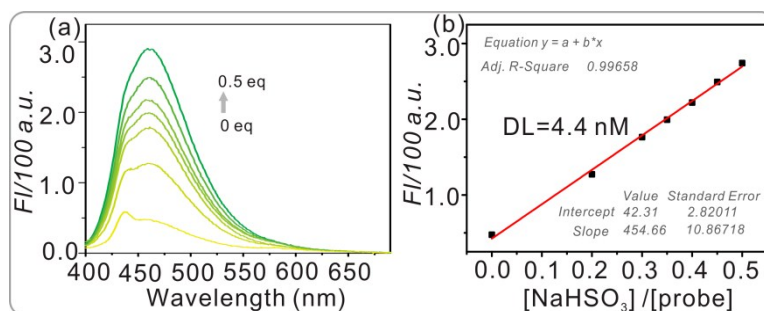


Fig. S1 Detection limit test of probe **3** (1 μM) toward different NaHSO_3 concentration in PBS buffer. (a) Emission spectra ($\lambda_{\text{ex}} = 380$ nm, slit width: 5 nm/10 nm). (b) Plot of the fluorescence intensity upon addition of NaHSO_3 (0–0.5 eq.).

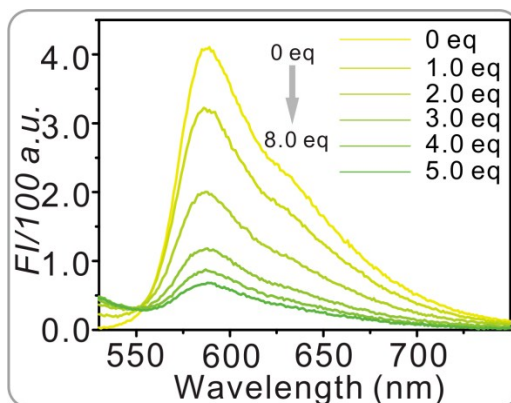


Fig. S2 Emission titration of probe **3** (10 μM) toward NaHSO_3 (0–5.0 eq.) in PBS buffer (20 mM, pH=7.4) containing 10% DMSO. ($\lambda_{\text{ex}} = 514$ nm, slit: 5 nm/5 nm)

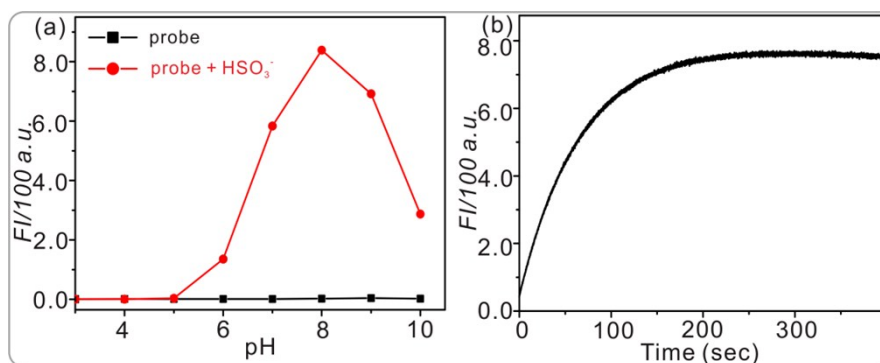


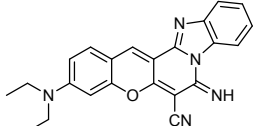
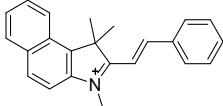
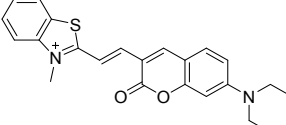
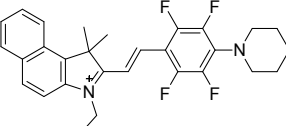
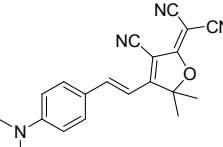
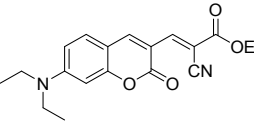
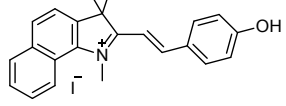
Fig. S3 The pH-dependent and time responses of probe **3** (10 μM) to HSO_3^- (4.0 eq.) in PBS buffer. (a) pH-dependent response for free probe and probe + NaHSO_3 ; (b) time response. All data represent the fluorescence intensity at 460 nm ($\lambda_{\text{ex}} = 380$ nm, slit: 3 nm/3 nm).

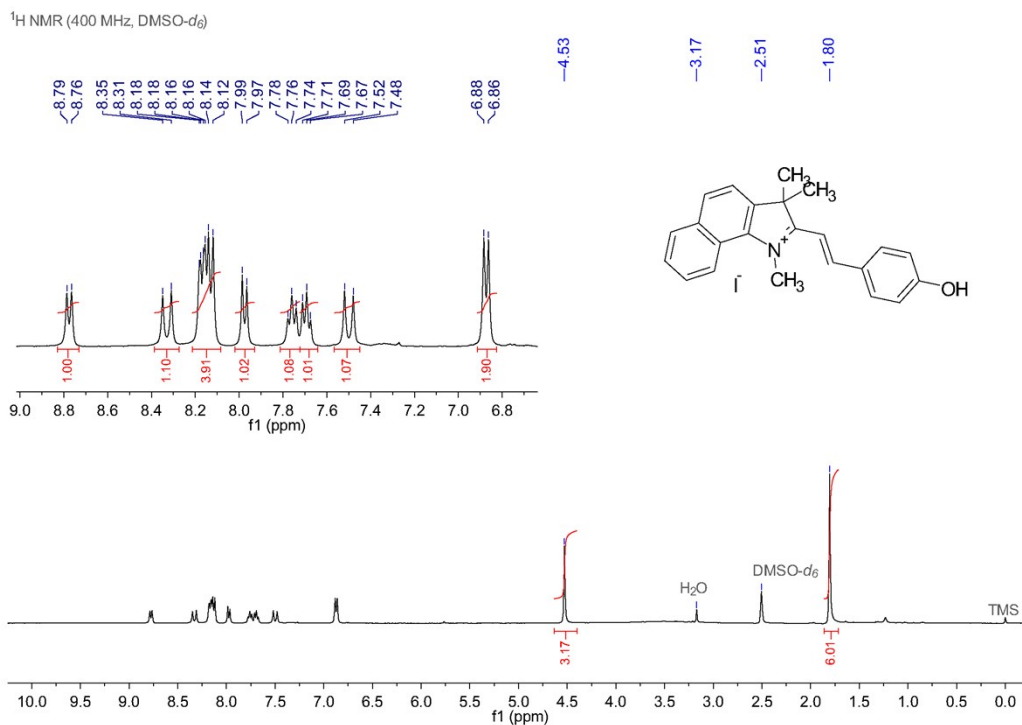
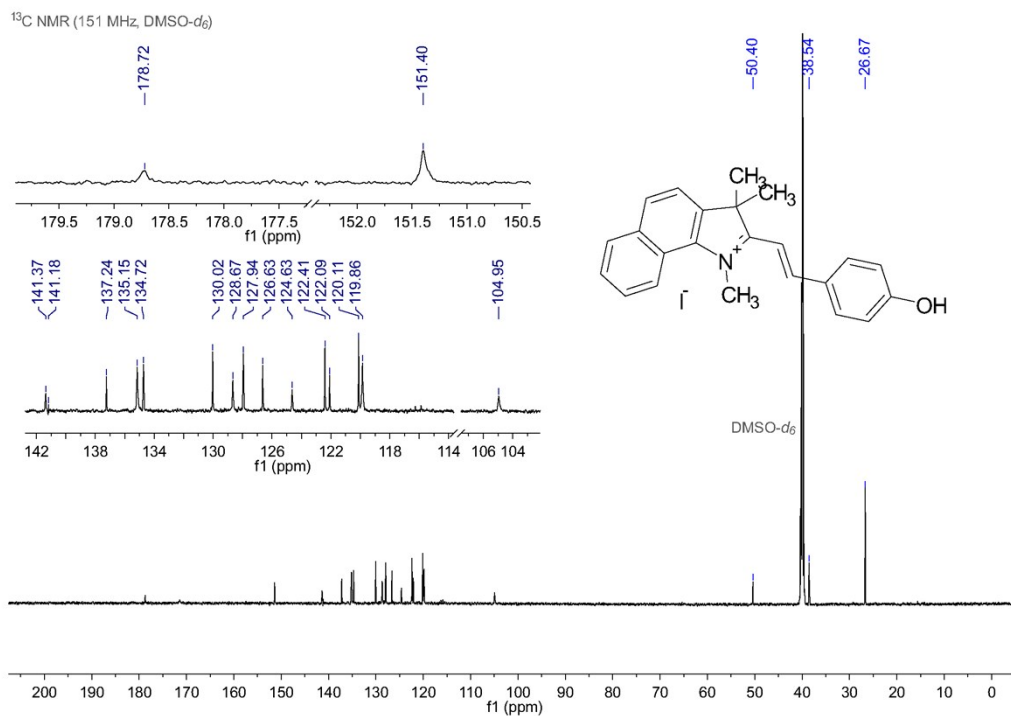
Table S1. Optical properties of probe **3**

probe	pH	$\lambda_{\text{Abs, max}}$ (nm)	$\lambda_{\text{Em, max}}$ (nm)	Stokes Shift (nm)	ϵ ($10^4 \text{ M}^{-1}\cdot\text{cm}^{-1}$)	ϕ
3	7.4	528	586	58	5.40	0.01 ^a
3 + HSO_3^-	7.4	352	460	108	1.01	0.76 ^b

^a Quantum yield of Rhodamine B ($\Phi_s = 0.69$ in ethyl alcohol solution) and ^bQuinine Sulfate ($\Phi_s = 0.546$ in 0.5 M H_2SO_4) were used as the reference compounds in quantum yield measurements

Table S2. Comparison with other skeletons based on C=C double bond for HSO_3^- detection.

Probe	$\lambda_{\text{abs,max}}/\lambda_{\text{em,max}}$ (nm)	Detection limit	Selectivity	Bioimaging	Reference
	340/575	1.76 μM	Interference for biothiols	No	1
	400/465	97 nM	Interference for H_2S and biothiols	No	2
	445/633	0.38 μM	No interference	Yes	3
	470/592	3.0 nM	Interference for H_2S and NaCN	Yes	4
	560/643	0.1 μM	Interference for H_2S and NaCN	Yes	5
	446/575	21 nM	Interference for H_2S	Yes	6
	380/460	4.4 nM	No interference	Yes	This work

Fig. S4 ¹H-NMR spectrum of compound **3**.Fig. S5 ¹³C-NMR spectrum of compound **3**.

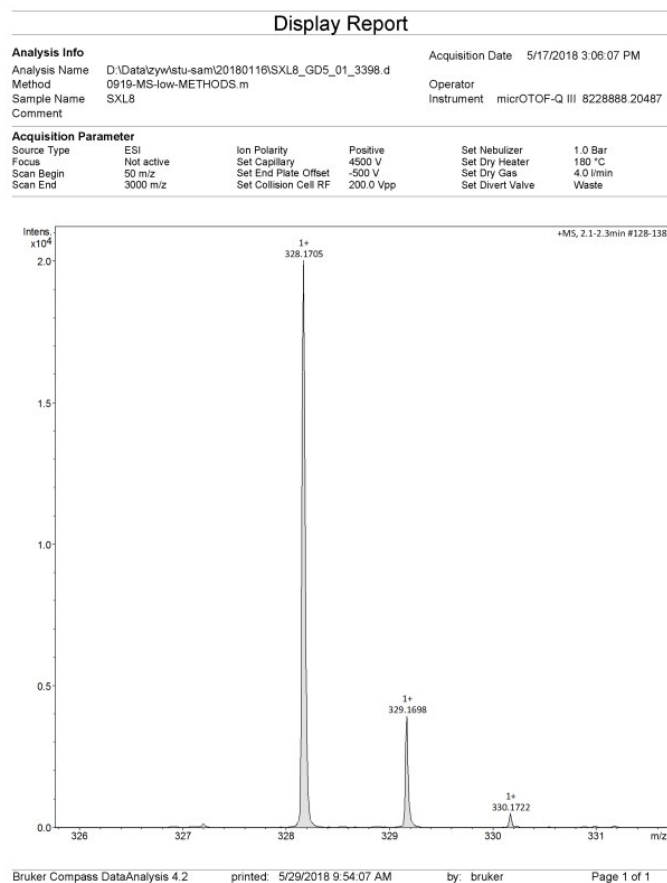


Fig. S6 HRMS(ESI⁺) of compound **3**.

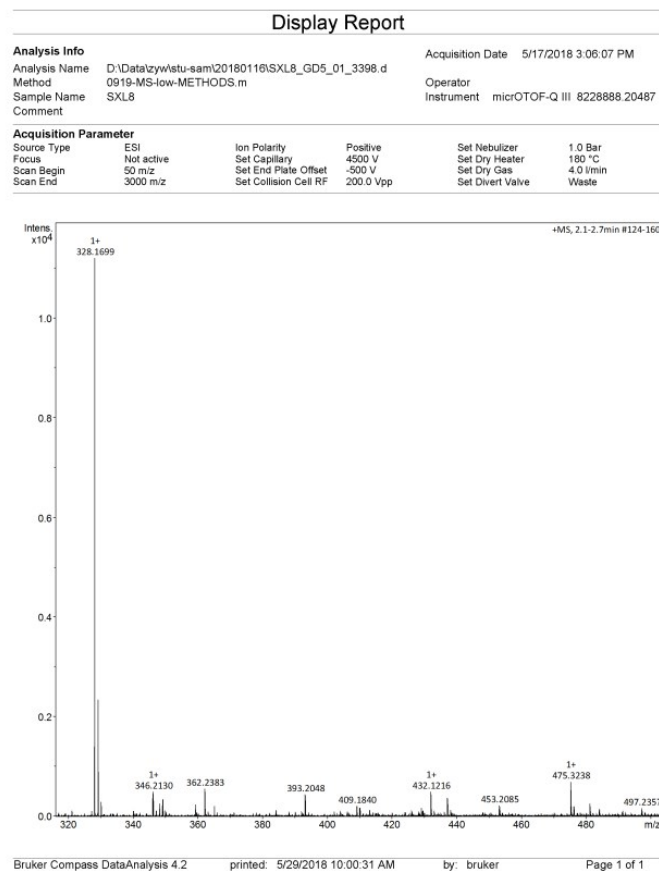


Fig. S7 HRMS(ESI⁺) of compound **3** +NaHSO₃.

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