Supporting information

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 μ M) toward different NaHSO ₃ concentration in PBS buffer. (a) Emission spectra (λ ex = 380 width: 5 nm/10 nm). (b) Plot of the fluorescence intensity upon addition of NaHSO ₃ (0–0.5 eq.).) nm, slit S2
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Fig. S1 Detection limit test of probe **3** (1 μ M) toward different NaHSO₃ concentration in PBS buffer. (a) Emission spectra (λ_{ex} = 380 nm, slit width: 5 nm/10 nm). (b) Plot of the fluorescence intensity upon addition of NaHSO₃ (0–0.5 eq.).



Fig. S2 Emission titration of probe 3 (10 μ M) toward NaHSO₃ (0–5.0 eq.) in PBS buffer (20 mM, pH=7.4) containing 10% DMSO. (λ_{ex} = 514 nm, slit: 5 nm/5 nm)



Fig. S3 The pH-dependent and time responses of probe **3** (10 μ M) to HSO₃⁻ (4.0 eq.) in PBS buffer. (a) pH-dependent² response for free probe and probe + NaHSO₃; (b) time response. All data represent the fluorescence intensity at 460 nm (λ_{ex} = 380 nm, slit: 3 nm/3 nm).

Table S1. Optical properties of probe 3							
	probe	pН	λ $_{\text{Abs, max}}$	$\lambda_{\mbox{ Em, max}}$	Stokes Shift	ε (10⁴ M⁻¹⋅cm⁻¹)	Φ
	·		(nm)	(nm)	(nm)		
	3	7.4	528	586	58	5.40	0.01 ª
	3 + HSO ₃ ⁻	7.4	352	460	108	1.01	0.76 ^ь

^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 H₂SO₄) were used as the reference compounds in quantum yield measurements

Probe	$\lambda_{abs,max}/P_{\lambda_{em,max}}$	Detection limit	Selectivity	Bioimaging	Reference
	(nm)				
N	340/575	1.76 μM	Interference for	No	1
			biothiols		
	400/465	97 nM	Interference for	No	2
			H_2S and		
N N			biothiols		
	445/633	0.38 μM	No interference	Yes	3
N O O N					
F, F	470/592	3.0 nM	Interference for	Yes	4
			$\rm H_2S$ and NaCN		
NC.	560/643	0 1 uM	Interference for	Yes	5
NC	500/045		H ₂ S and NaCN	103	5
N					
Ч О Ш	446/575	21 nM	Interference for	Yes	6
N OCO CN			H_2S		
Ň ×	380/460	4.4 nM	No interference	Yes	This work



Fig. S4 ¹H-NMR spectrum of compound 3.





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equisition Par urce Type cus an Begin an End	ESI Not active 50 m/z 3000 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Collision Cell RF	Positive 4500 V -500 V 200.0 Vpp	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve	1.0 Bar 180 °C 4.0 l/min Waste			
ntens, x10 ⁴ 2.0-		1+ 328.1705			+M5, 2.1-2.3min #128-13i			
1.5-								
1.0-								
0.5			1+ 329.169	28				
0.0 326	327	328	329	1* 330.1722 人 330	331 mi			

Fig. S6 HRMS(ESI*) of compound 3.



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

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