

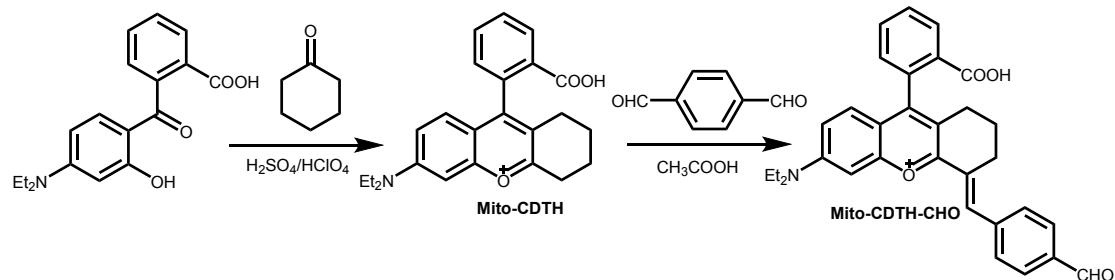
Detection limit

The detection limit is calculated by Equation 1, as shown below:

$$\text{Detection limit} = 3\sigma/\kappa \quad (1)$$

In which σ is the standard deviation of the blank measurements, by measuring the probe ($20\mu\text{M}$) of emission intensity without Na_2SO_3 and NaHSO_3 for ten times. κ is the slope of the intensity *vs* concentrations of Na_2SO_3 or NaHSO_3 .

Scheme S1. Synthesis route of probe **Mito-CDTH-CHO**



Characterization data for synthesis

Fig S1: $^1\text{H-NMR}$ spectrum of probe **Mito-CDTH-CHO** in $\text{DMSO}-d_6$

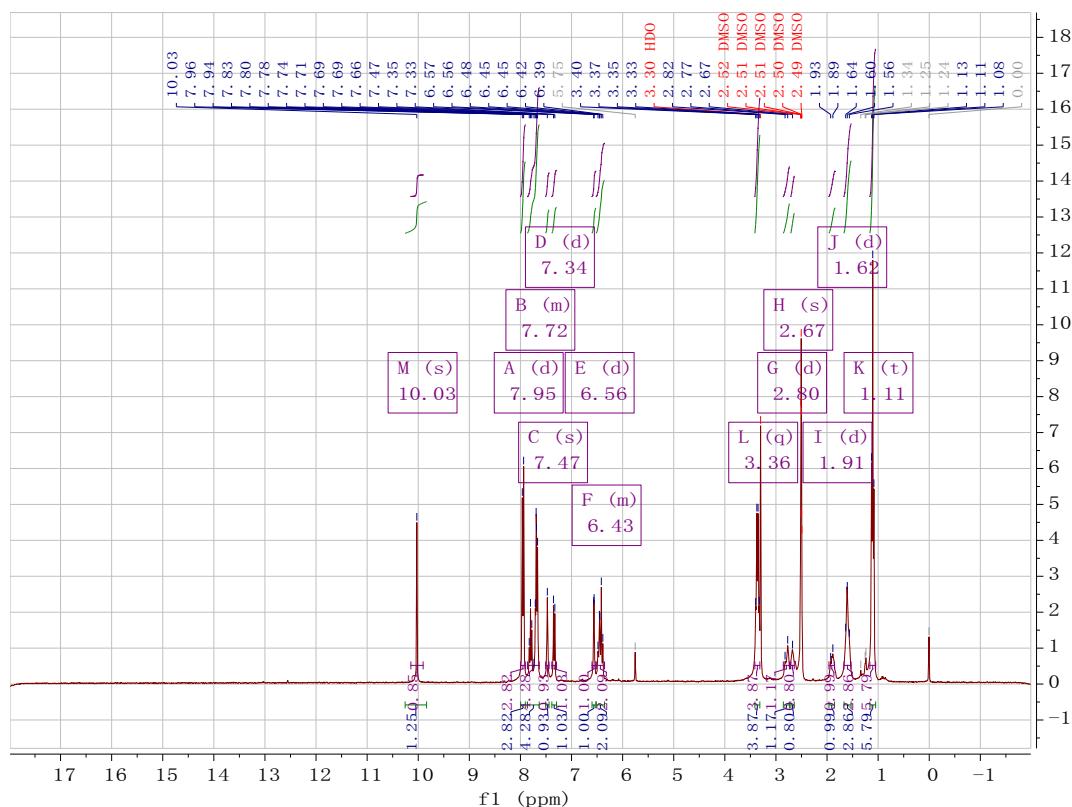


Fig S2: $^{13}\text{C-NMR}$ spectrum of probe **Mito-CDTH-CHO** in $\text{DMSO}-d_6$

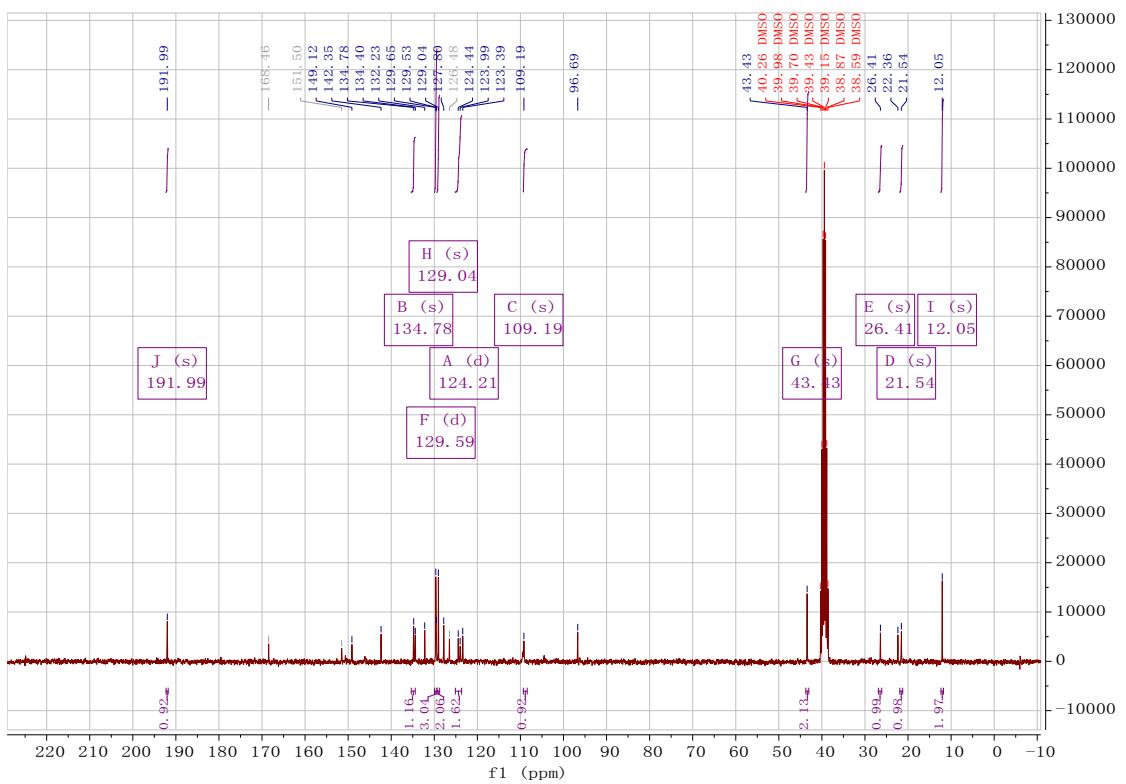


Fig S3: ESI-MS of Mito-CDTH

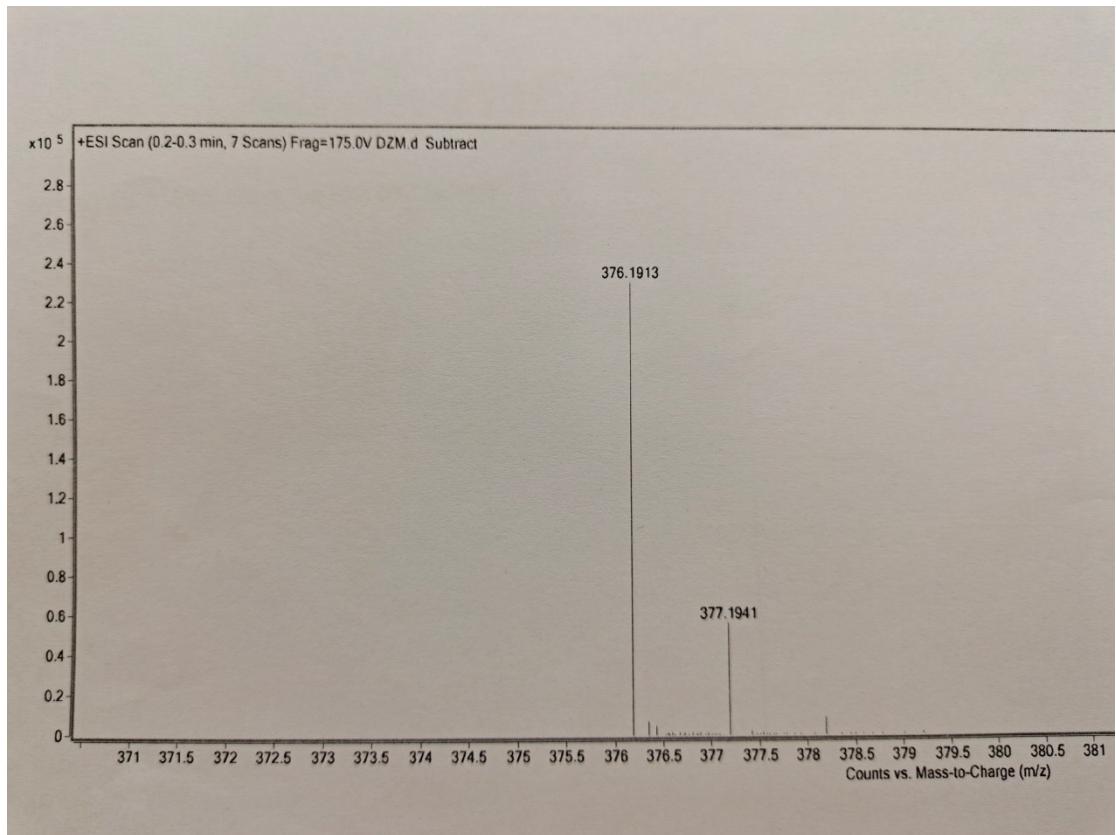


Fig S4: ESI-MS of **Mito-CDTH-CHO**

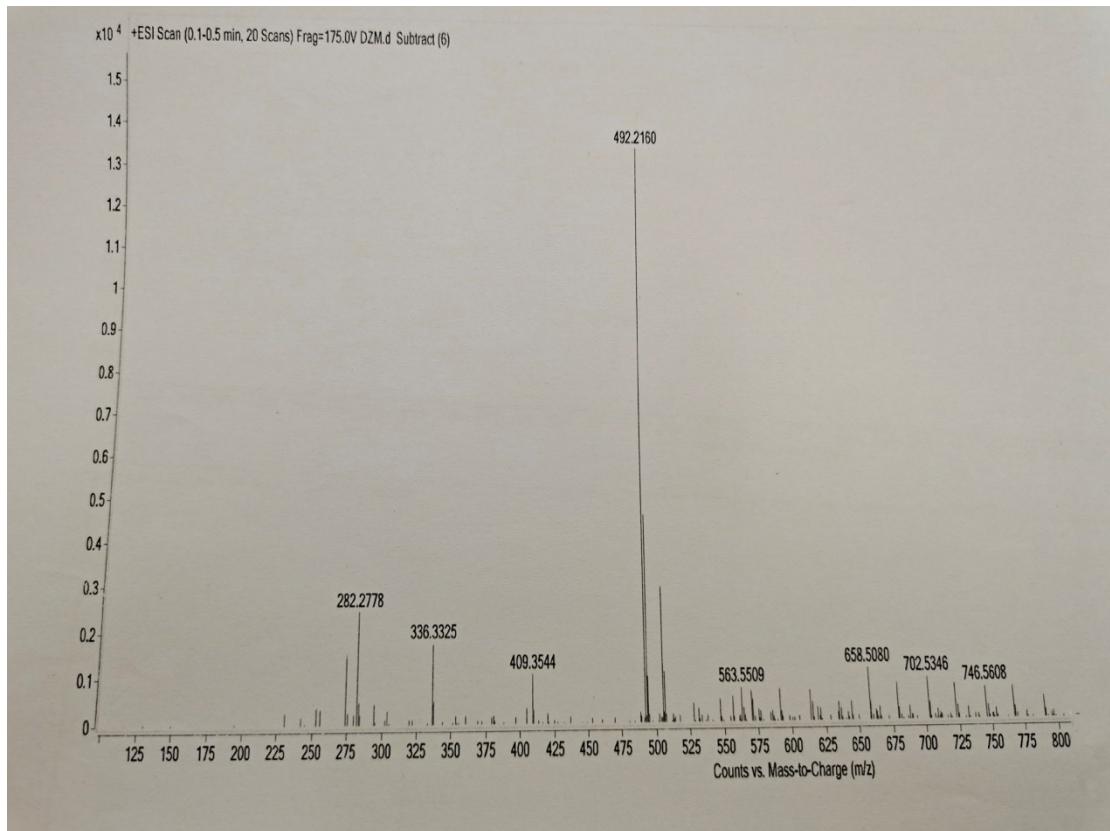


Fig S5: Fluorescence spectra changes of **Mito-CDTH-CHO** (20μM) with 50μM SO₂ derivatives in PBS buffer (containing 1% DMSO). Red: **Mito-CDTH-CHO**; Blue: NaHSO₃, λ_{ex} = 370 nm; Green: Na₂SO₃, λ_{ex} = 390 nm.

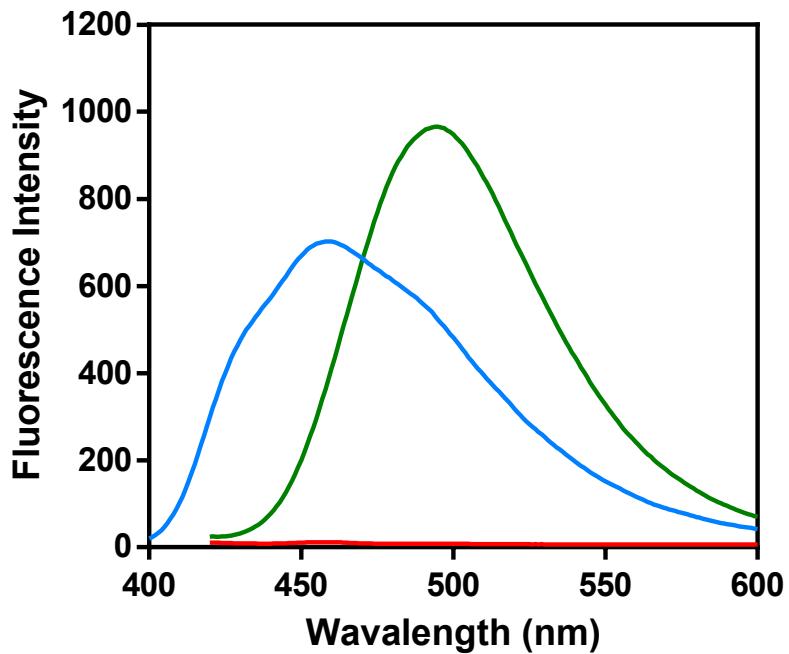


Fig S6: The fluorescence intensity of **Mito-CDTH-CHO** with Na₂SO₃ with diverse pH values.

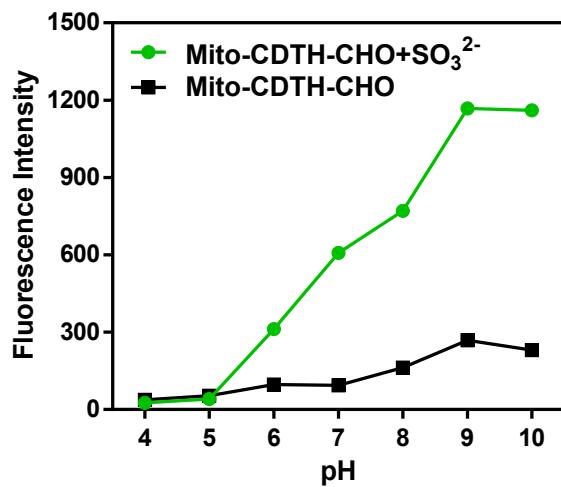
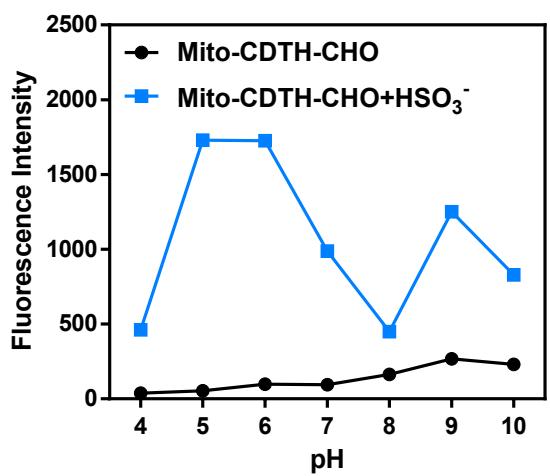


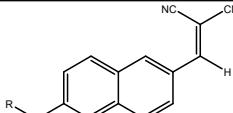
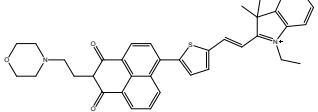
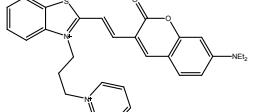
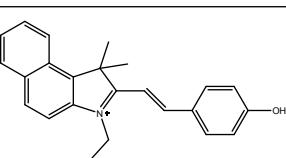
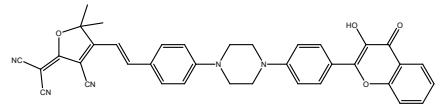
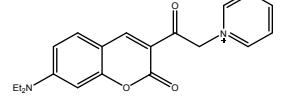
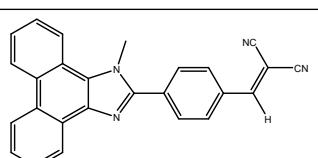
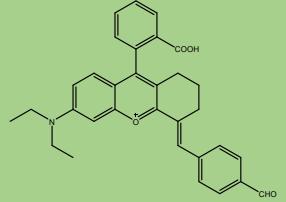
Fig S7: The fluorescence intensity of **Mito-CDTH-CHO** with NaHSO₃ with diverse pH values.



1

Table S1: A comparison of mitochondria-targeted dual-site fluorescent probes for SO₃²⁻ and HSO₃⁻

Probe	Dual-site	water solubility	LOD	Response time	Targeting mitochondria	Selectivity for SO ₃ ²⁻ and HSO ₃ ⁻
RCS ADV. 2019, 9,1147	No	DMF/PBS 3:7	62nM	2 min	No	No
Talanta. 2019, 191, 428-434	No	EtOH/PBS 4:6	26 nM	30 min	Yes	No
RCS ADV. 2019, 9, 8943	No	PBS	130nM	3 min	Yes	No
SENSOR ACTUAT B-CHEM. 2019, 284, 330-336	No	DMF/H ₂ O 1:9	17.7nM	60 s	Yes	No
SENSOR ACTUAT B-CHEM. 2019, 292,	No	DMSO/PBS	820nM	30 min	Yes	No

80-87						
 J MATER CHEM B. 2013, 00, 1-3	No	DMSO/PBS 1:9	15.5nM	50 s	Yes	No
 Anal. Chem. 2019, 91, 11946-11951	No	5% DMSO in PBS	20.7nM	200 s	No	No
 NEW J CHEM. 2012, 00, 1-3	No	DMSO/PBS	29.2μM	1 min	Yes	No
 Molecules. 2019, 24, 4011	No	DMSO/PBS	28nM	30 min	No	No
 Dyes Pigm. 2018, 151, 95-101	No	EtOH/PBS 4:6	17nM	30 min	No	No
 SENSOR ACTUAT B-CHEM. 2019, 295, 215-222	No	THF/PBS 3:1	Not mentioned	15 min	Yes	No
 Biomaterials. 2017, 183, 82-93	No	DMSO/PBS 50:50	Not mentioned	60 s	No	No
 This work	Yes	2% EtOH in PBS	100 and 80nM	Within 10 min	Yes	Yes

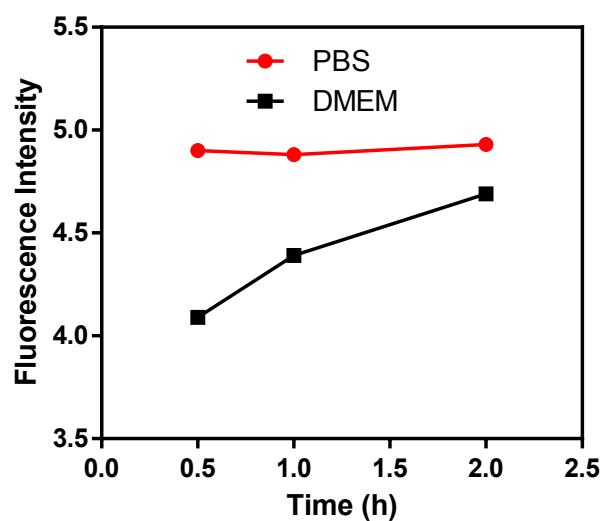


Fig. S8: The fluorescence intensity changes of Mito-CDTH-CHO without SO₂ derivatives in PBS and DMEM medium within 2 h