Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting information

Contents:

1. Materials and instruments

All chemicals from Aladdin were used without further purification. In this experiment, the absorption and fluorescence spectra were measured using a UV-2450 ultraviolet spectrophotometer (Shimadzu, Japan) and F-7000 fluorescence spectrophotometer (Hitachi, Japan), respectively. ^{1}H NMR and ^{13}C NMR spectra were obtained by a Bruker AVANCE-600 MHz and 150 MHz NMR spectrometer, respectively (Bruker, Billerica, MA). A Thermo Scientific Q Exactive LC-MS/MS system was used for HRMS spectra. Cell imaging and zebrafish imaging experiments relied on a ZEISS LSM 880 confocal laser scanning microscope.

2.1 HeLa cell culture and imaging

HeLa cells were cultured in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% FBS and 0.25% trypsin at 37 °C and 5% CO_2. The cells were incubated on plates and allowed to grow for 24 h. Before the experiment, HeLa cells were washed three times with PBS (pH=7.4). First, the cells were incubated with **NIR-BN** (10 μM) for 15 min to observe the phenomenon, and then SO_3^{2-} (50 μM) was added and incubated for another 15 min. Secondly, the cells were incubated with GSH (500 μM) and $Na_2S_2O_3$ (250 μM) for 1h, and then incubated with **NIR-BN** (10 μM) for 15 min. The fluorescence images of HeLa cells were obtained at the emission ranges of 650-710 nm (λ_{ex} = 561 nm).

2.2 Zebrafish culture and imaging

The zebrafish used in the experiment were purchased from Shanghai Feixi Biological Technology Co., Ltd. One group of zebrafish was cultured with 20 μM **NIR-BN** for 30 min. The other group was treated with 20 μM **NIR-BN** for 30 min, and then co-incubated with 100 μM SO_3^{2-} for further 30 min. The fluorescence images of zebrafish were obtained at the emission ranges of

650-710 nm (λ_{ex} = 561 nm).

2. Supplementary figures

Fig. S1 ^{1}H-NMR spectrum of probe **NIR-BN** in DMSO-d_6

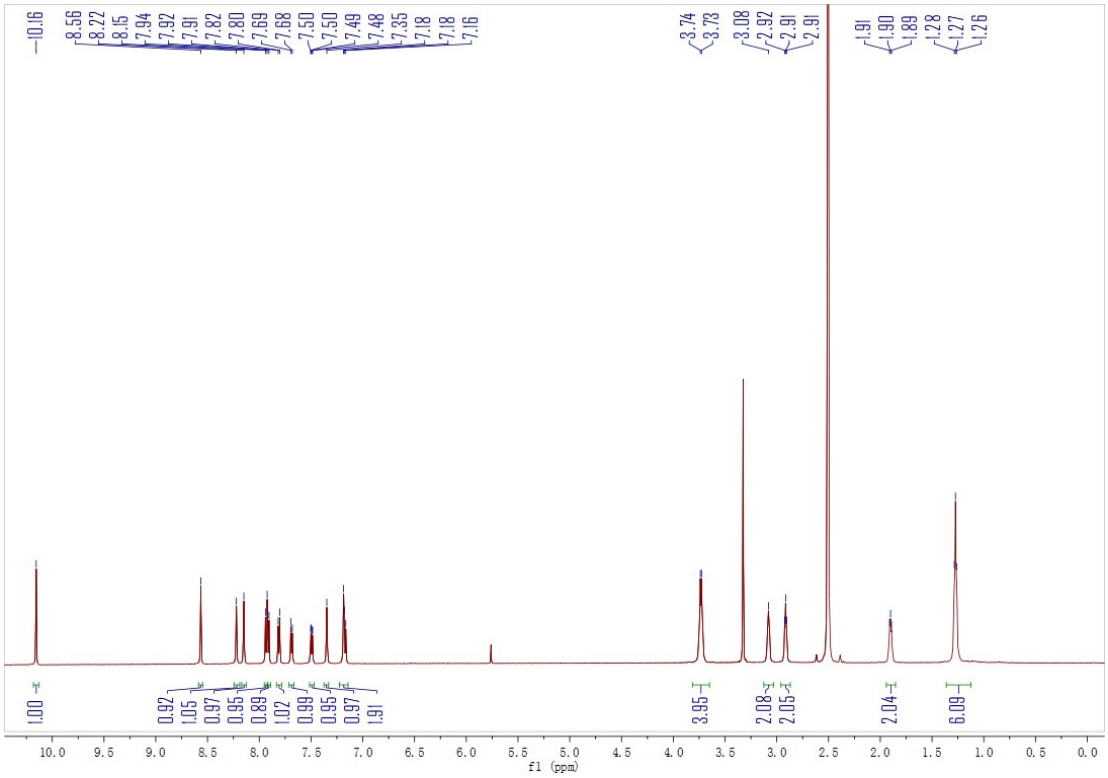

Fig. S2 ^{13}C-NMR spectrum of probe **NIR-BN** in DMSO-d_6

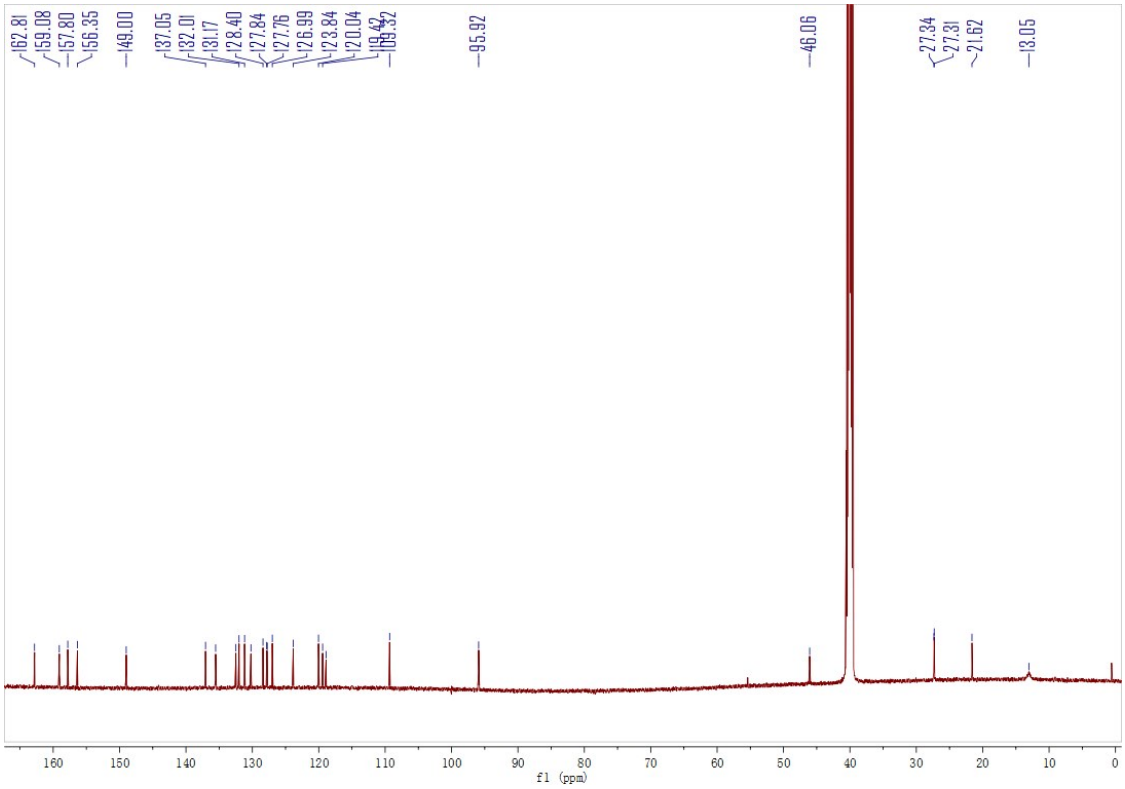

Fig. S3 HRMS spectrum of **NIR-BN**

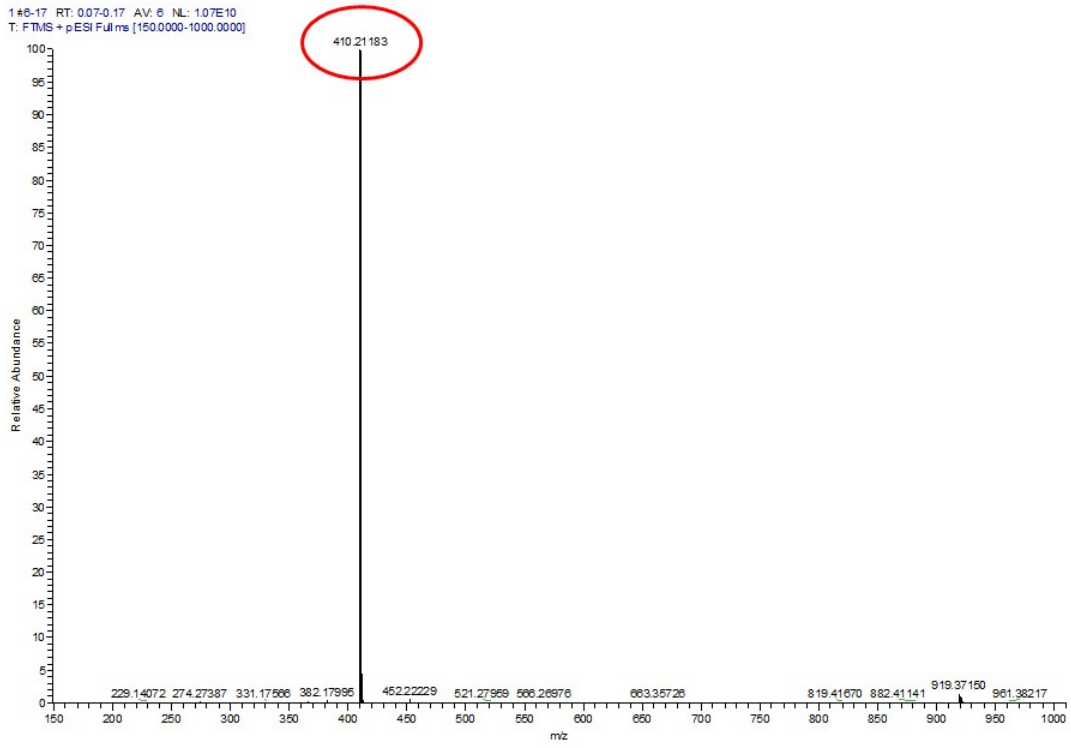

Fig. S4 The specificity of **NIR-BN**-SO_3^{2-} for the reversible reaction of HCHO (60 μM) in CH_3CN/PBS (v/v, 2/8, pH= 7.4). (1) Probe **NIR-BN**, (2) HCHO, (3) Fe^{2+}, (4) Cu^{2+}, (5) H_2O_2, (6)

ClO^-, (7) Al^{3+}, (8) MnO_4^-, (9) CH_3COO^-, (10) NO_3^{2-}, (11) NO_2^-, (12) K^+.

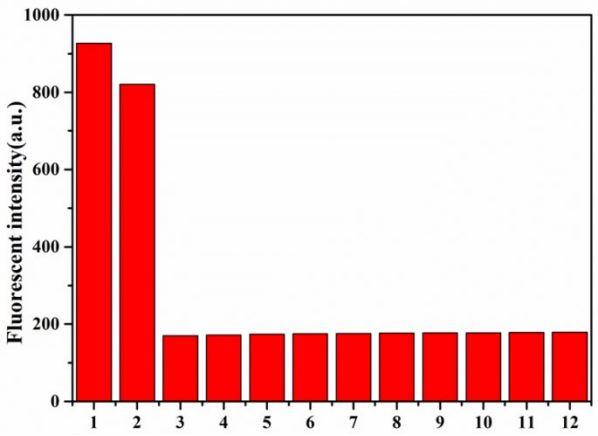

Fig. S5 (a) The selectivity of **NIR-BN** for SO_3^{2-}. (b)Fluorescence intensity of **NIR-BN** (20 μM) toward 100 μM SO_3^{2-} in the presence of 100 μM interfering species each in CH_3CN/PBS (v/v, 2/8, pH= 7.4). (1)probe **NIR-BN**, (2)SO_4^{2-}, (3)$S_2O_3^{2-}$, (4) HS^-, (5)Cys, (6)Hcy, (7)GSH, (8)Cl^-, (9)Br^-, (10)CO_3^{2-}, (11)NO_2^-, (12)CH_3COO^-, (13)NO_3^{2-},(14)H_2O_2, (15)ClO^-, (16)SO_3^{2-}.

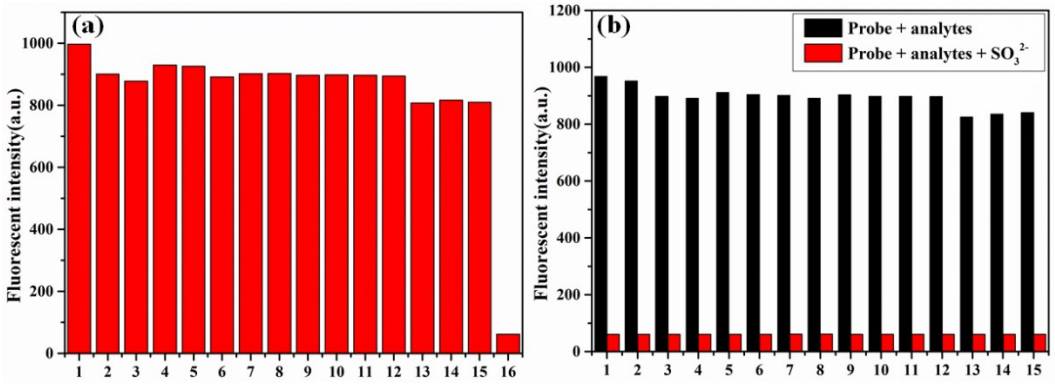

Fig. S6 Fluorescence intensity of the **NIR-BN** (20 μM) at different pH values in the absence or presence of SO_3^{2-} (20 μM) in CH_3CN/PBS (v/v, 2/8, pH= 7.4).

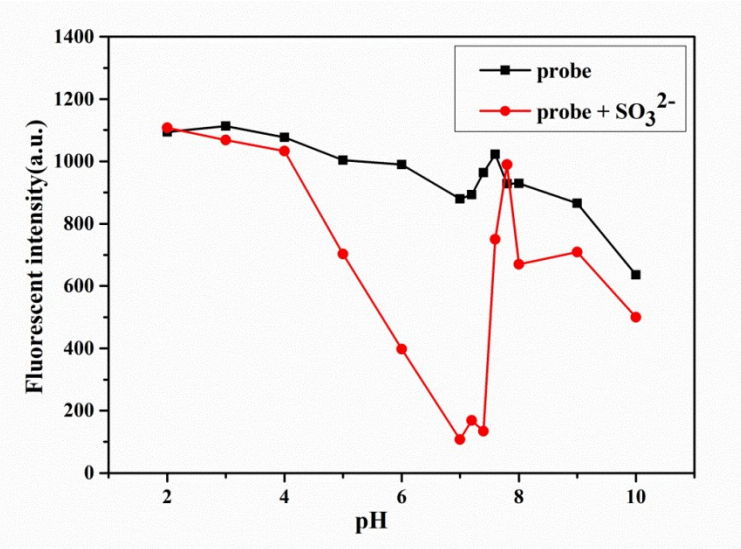

Fig. S7 The reaction time of **NIR-BN** (20 μM) for SO_3^{2-} (20 μM)

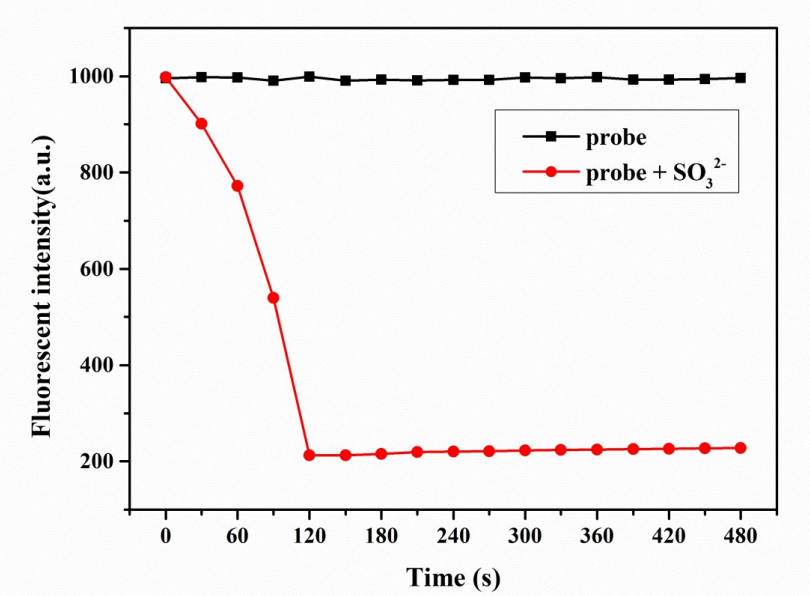

Fig. S8 HRMS spectra of **NIR-BN**-SO_3^{2-}

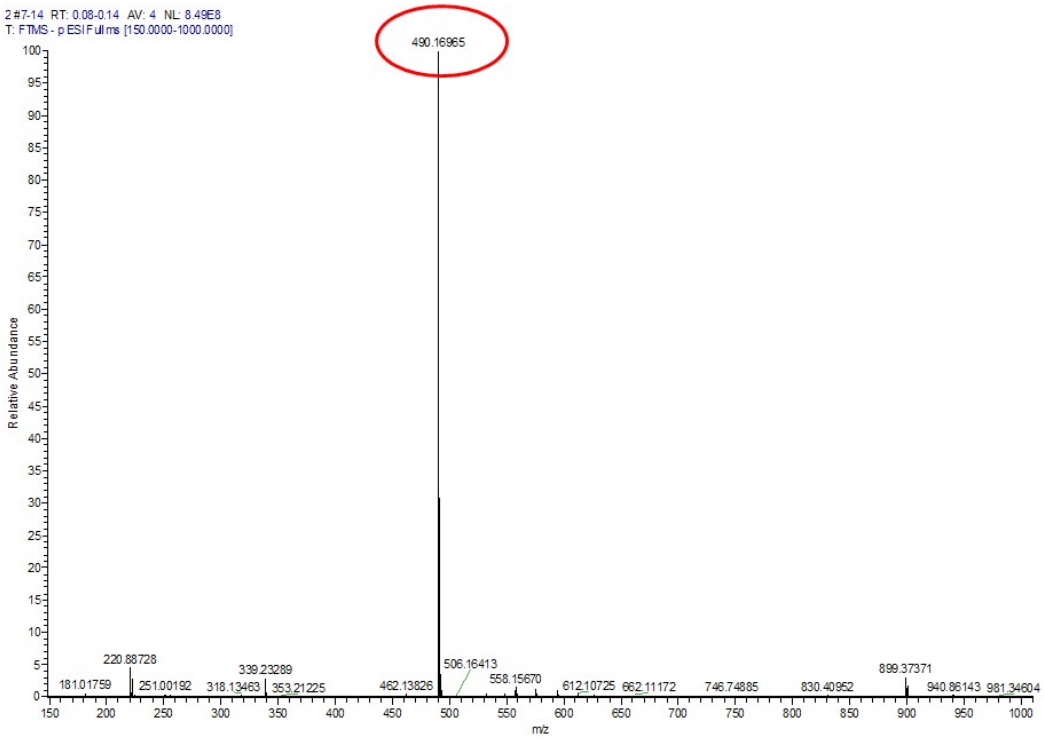

Table S1. Comparison of **NIR-BN** and other probes for SO_3^{2-} detection

Refs.	Targeting mitochondria	$\lambda_{ex}/\lambda_{em}$ (nm)	Food application	Living cell imaging	Detection limit	Time
1	Yes	380/470,578	No	endogenous, exogenous	40 nM	2 min
2	No	360/430,520	Yes	exogenous	79.2 nM	60 s

3	No	405/485,565	No	endogenous, exogenous	20 μM	1 min
4	No	404/467,587	No	endogenous, exogenous	0.21μM	2 min
5	Yes	405,561/534,634	No	exogenous	0.047μM	8 min
6	Yes	420/494,579	No	exogenous	299 nM	5 min
This work	Yes	580/680	Yes	endogenous, exogenous	0.17 μM	2 min

Notes and references

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