## **Electronic Supplementary Information**

## A rapid cell-permeating turn-on probe for sensitive and selective detection of sulfite in living cells

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| Sı | Ipplementary figures and tables2   |
|----|--|
|    | Figure S1. The absorption spectrum of NJUXJ-1 and the detecting system in PBS buffer2  |
|    | Figure S2. The fluorescence intensity changes at 483 nm in various pH environments2  |
|    | Figure S3. Fluorescence intensity of the detecting system with incubation time3  |
|    | Figure S4. The fluorensnece response of NJUXJ-1 towards SO <sub>3</sub> <sup>2-</sup> compared with various amino acids  |
|    | Figure S5. The fluorensnece response of <b>NJUXJ-1</b> towards SO <sub>3</sub> <sup>2-</sup> compared with various metallic ions                               |
|    | Figure S6. The fluorensnece response of NJUXJ-1 compared with reactive nitrogen and oxygen species   |
|    | Figure S7. The physiological selectivity and interference experiments of NJUXJ-1 towards SO <sub>3</sub> <sup>2-</sup> compared with sulfur-containing species |
|    | Figure S8. The analysis of the pseudo color values5  |
|    | Figure S9. Confocal fluorescence images of NJUXJ-1 in HeLa cells incubated with different concentrations of $SO_3^{2^-}$                                       |
|    | Figure S10. Cell viability with different concentrations of NJUXJ-17   |
|    | Figure S11. <sup>1</sup> H NMR of compound <b>NJUXJ-1</b> 7  |
|    | Figure S12. <sup>13</sup> C NMR of compound NJUXJ-18   |
|    | Figure S13. HR-MS spectrum of NJUXJ-1, NJUXJ-1-Prod and the mixture of NJUXJ-1 with $Na_2SO_3$ in PBS buffer   |
|    | Table S1. Comparison of NJUXJ-1 and recent sulfite probes  |



**Figure S1.** The absorption spectrum of **NJUXJ-1** (10  $\mu$ M) and the detecting system (**NJUXJ-1**: 10  $\mu$ M and SO<sub>3</sub><sup>2-</sup> 100  $\mu$ M) in PBS buffer (pH 7.4, 10 mM, 5% DMSO, v/v) at 37 °C.



**Figure S2.** The fluorescence intensity changes at 483 nm in various pH environments (Red: NJUXJ-1+SO<sub>3</sub><sup>2-</sup>; Black: NJUXJ-1).



**Figure S3.** Fluorescence intensity of the detecting system with incubation time. a) Fluorescence spectrum and b) scattered diagram of fluorescence intensity at 483 nm. Time range: 0 - 12 h. The Fluorescence intensity sharply rose to over half the max in 1 min, then stepwisely increased and reached the max with in 50 min.



**Figure S4.** The fluorensence response of **NJUXJ-1** (10  $\mu$ M) towards SO<sub>3</sub><sup>2-</sup> compared with various amino acids. a) The fluorescence spectrum and b) the relative fluorescence changes at 483 nm. The concentration of SO<sub>3</sub><sup>2-</sup> was 100  $\mu$ M and of all other analytes were 1 mM.



**Figure S5.** The fluorensence response of **NJUXJ-1** (10  $\mu$ M) towards SO<sub>3</sub><sup>2-</sup> compared with various metallic ions. a) The fluorescence spectrum and b) the relative fluorescence changes at 483 nm. The concentration of SO<sub>3</sub><sup>2-</sup> was 100  $\mu$ M and of all other analytes were 1 mM.



**Figure S6.** The relative fluorescence changes at 483 nm of **NJUXJ-1** (10  $\mu$ M) towards SO<sub>3</sub><sup>2-</sup> compared with reactive nitrogen and oxygen species. The concentration of all analytes were 100  $\mu$ M.



**Figure S7.** The physiological selectivity and interference experiments of **NJUXJ-1** (10  $\mu$ M) towards SO<sub>3</sub><sup>2-</sup> (100  $\mu$ M) compared with sulfur-containing species. a) The fluorescence spectrum and b) the relative fluorescence changes at 483 nm. Physiological concentrations of S<sup>2-</sup> (100  $\mu$ M), Cys (100  $\mu$ M), Hcy (1000  $\mu$ M) and GSH (1000  $\mu$ M) were used separately and along with sulfite. Higher level of GSH (10 mM) was also used.



**Figure S8.** The analysis of the pseudo color values supported the adequacy of 2-min incubation. Blue: The pseudo values of the original imaged groups in cell-permeating evaluation; Red: The restored pseudo color values of the groups after centrifugation, resuspending, ultrasonication and conversion.



**Figure S9.** Confocal fluorescence images of **NJUXJ-1** in HeLa cells incubated with different concentrations of  $SO_3^{2-}$  (50  $\mu$ M, 100  $\mu$ M and 150  $\mu$ M). HeLa cells were incubated with **NJUXJ-1** (10  $\mu$ M) at 37 °C for 2 min. Further incubation with different concentrations of  $SO_3^{2-}$  for 30 min were conducted with the same conditions. Fluorescence imaging of HeLa cells was performed from green channel ( $\lambda_{ex}$  = 364 nm,  $\lambda_{ex}$  = 425 - 475 nm). Scale bar: 75  $\mu$ m. As concentrations of  $SO_3^{2-}$  increased, the fluorescence signals enhanced in HeLa cells.



**Figure S10.** Cell viability of HeLa (human cancer cell line), HEK293T (human embryonic kidney cell line), A549 (human alveolar epithelial cell line) and LO<sub>2</sub> (human embryonic liver cell line) with different concentrations of **NJUXJ-1**.



**Figure S11.** <sup>1</sup>H NMR of compound **NJUXJ-1** (600 MHz, in DMSO- $d_6$ ).



Figure S12. <sup>13</sup>C NMR of compound NJUXJ-1 (150 MHz, in DMSO- $d_6$ ).



**Figure S13.** HR-MS spectrum of **NJUXJ-1, NJUXJ-1-Prod** and the mixture of **NJUXJ-1** with Na<sub>2</sub>SO<sub>3</sub> in PBS buffer (pH 7.4).

| Probe   | Total Imaging | Limit of  | Toxicity | Time of Cell- | Biological   | Selectivity            |
|---------|---------------|-----------|----------|---------------|--------------|------------------------|
|         | Time          | Detection |          | permeating    | Imaging      |                        |
|         |               |           |          | Protocol      |              |                        |
| NJUXJ-1 | 32 min        | 13.0 nM   | Low      | 2 min         | exogenous &  | high                   |
|         |               |           |          |               | endogenous   |                        |
| Ref 44  | 50 min        | 8.8 nM    | Low      | 30 min        | exogenous    | high                   |
| Ref 45  | 1 h           | 3.8 µM    | NG       | 30 min        | exogenous    | high                   |
| Ref 46  | in vitro      | 200 nM    | NG       | NG            | in vitro     | except GSH             |
| Ref 47  | 1 h           | 0.27 nM   | Low      | 30 min        | exogenous &  | except donor           |
|         |               |           |          |               | endogenous   |                        |
| Ref 48  | 1 h           | 10 nM     | NG       | 30 min        | exogenous &  | high                   |
|         |               |           |          |               | endogenous   |                        |
| Ref 49  | 1 h           | 0.23 μM   | NG       | 30 min        | exogenous    | high                   |
| Ref 53  | 1 h           | 1.74 μM   | Low      | 30 min        | exogenous    | high                   |
| Ref 56  | 1 h           | 89 nM     | NG       | 30 min        | exogenous    | high                   |
| Ref 57  | 50 min        | 0.1 μM    | Low      | 30 min        | exogenous    | high                   |
| Ref 58  | 1 h           | 0.39 μM   | NG       | 30 min        | brain tissue | high                   |
|         |               |           |          |               | & zebrafish  |                        |
| Ref 60  | 30 min        | 0.15 μM   | Low      | 15 min        | exogenous    | high                   |
| Ref 61  | 65 min        | 1.8 µM    | NG       | 20 min        | exogenous    | not good               |
| Ref 62  | 20 min        | 22 nM     | NG       | 10 min        | exogenous    | high                   |
| Ref 63  | 40 min        | 3.0 nM    | NG       | 30 min        | exogenous    | except SH <sup>-</sup> |
| Ref 64  | 1 h           | 28 nM     | NG       | 30 min        | exogenous    | high                   |

| Table S1. Compa | arison of NJUXJ-1 | and recent | sulfite probes. |
|-----------------|-------------------|------------|-----------------|
|-----------------|-------------------|------------|-----------------|

NG means Not Given.