

Supplementary Material

An A- π -A' structural ratiometric fluorescent probe based on benzo [e] indolium for bisulfite and its application in sugar samples and Living cells

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1. Characterization of Probe 1.

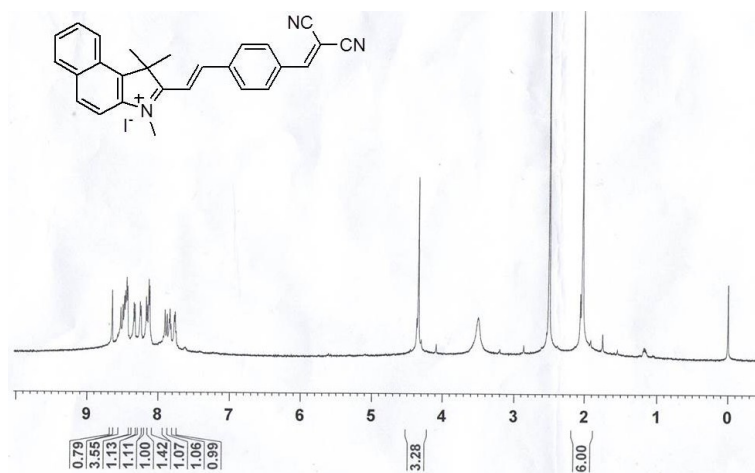


Fig. S1. ^1H NMR spectrum of probe 1 in $\text{DMSO}-d_6$.

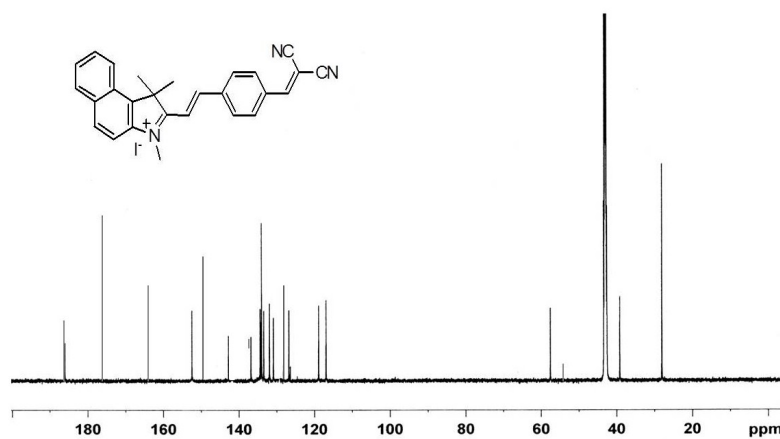


Fig. S2. ^{13}C NMR spectrum of probe 1 in $\text{DMSO}-d_6$.

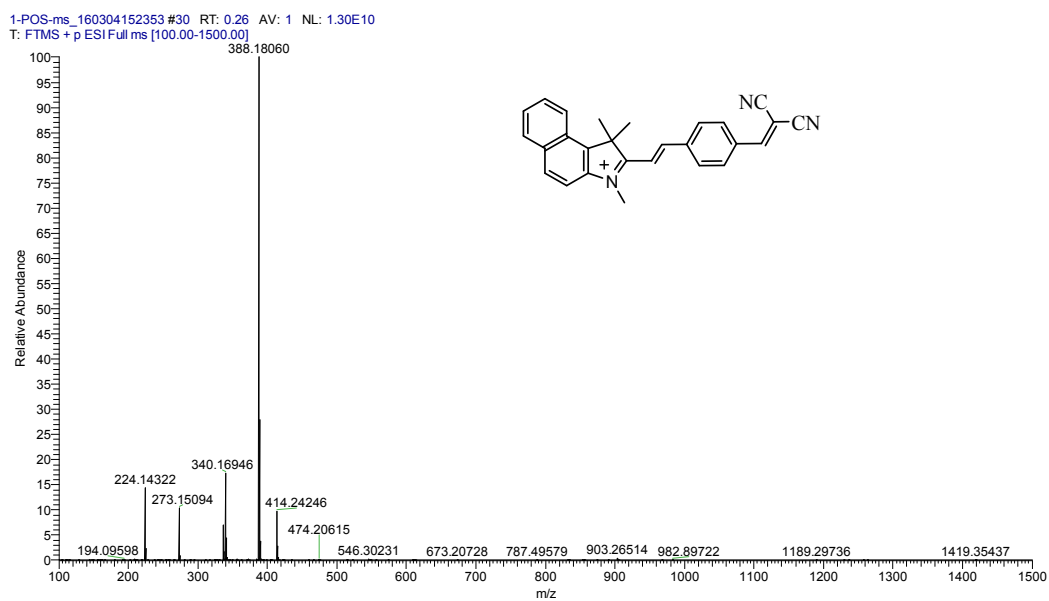


Fig. S3. ESIMS spectrum of probe 1.

2. pH effection.

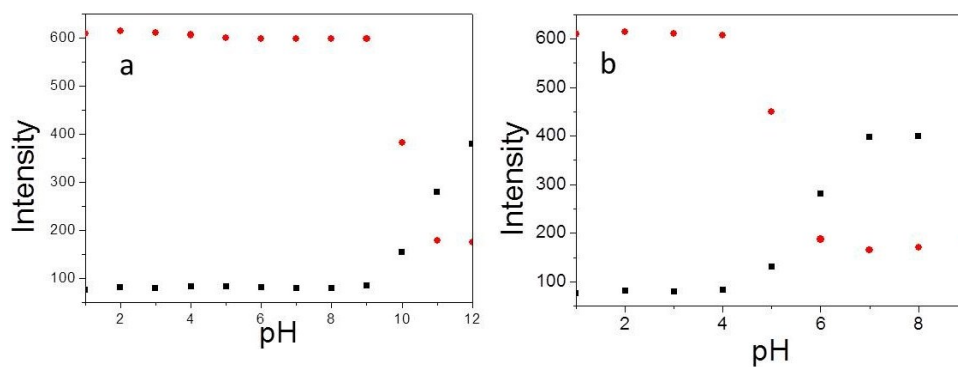


Fig. S4. Fluorescent intensity of probe **1** (10 μM) in the absence (a) and presence (b) of HSO₃⁻ under various pH values. Black squares: emission intensity at 466 nm; and red dots: emission intensity at 578 nm. $\lambda_{\text{ex}} = 400$ nm. Slits: 5 nm/ 5 nm.

3. Fluorescent ratio change.

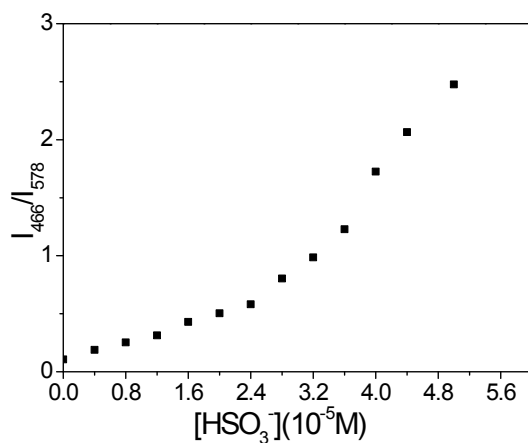


Fig. S5. Fluorescent intensity ratio (I_{466}/I_{578}) in PBS buffer (pH 7.4, 10mM) as a function of HSO₃⁻ concentration. $\lambda_{\text{ex}} = 400$ nm. Slits: 5 nm/ 5 nm.

4. Detection Limit.

The detection limit was calculated with the equation: $\text{detection limit} = 3\sigma_{\text{bi}}/m$, where σ_{bi} is the standard deviation of blank measurements, m is the slope between intensity versus sample concentration. To determine the S/N ratio, the emission intensity of **1** without HSO_3^- was measured by 10 times and the standard deviation of blank measurements was determined. The linear fitting formula was: $Y = 0.01911X + 0.10643$.

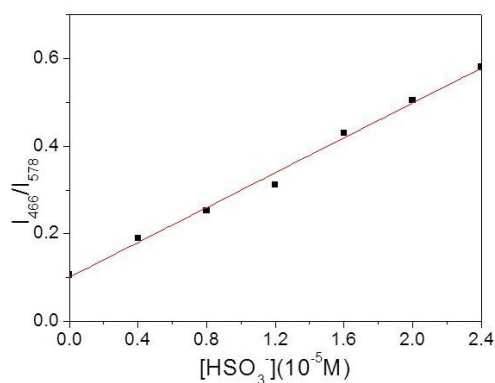


Fig. S6. The linear relation for concentration of HSO_3^- in the range of 0-24 μM .

5. Selectivity of probe **1**.

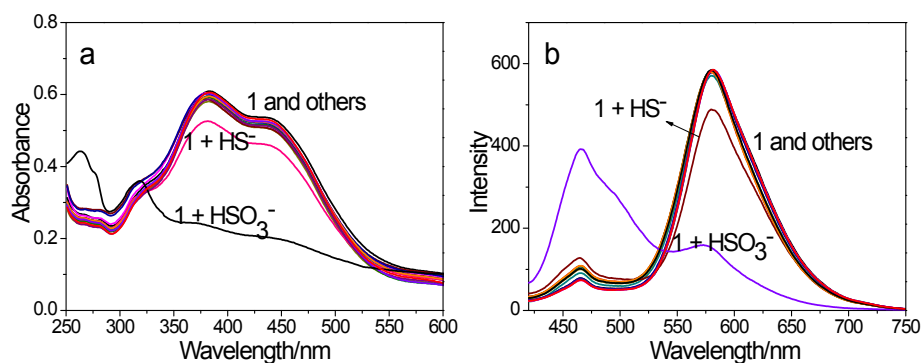


Fig. S7. Spectral of probe **1** treated with different analysts.

6. Fluorescent spectrum of probe 1 in competition experiment.

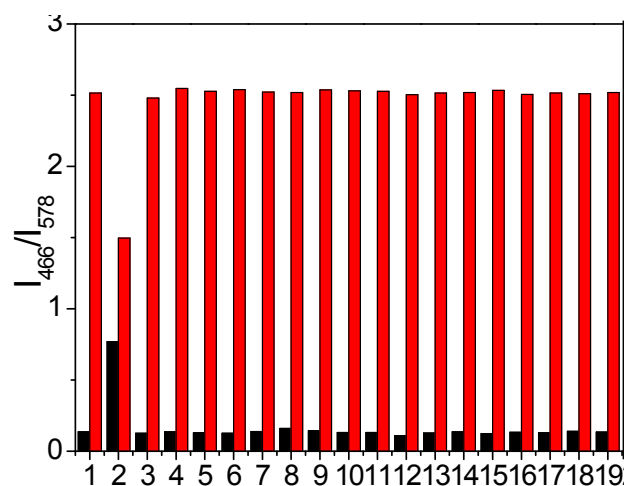


Fig. S8. Ratiometric changes of probe 1 (20 μM) in the presence of the competing species followed by HSO₃⁻. 1: probe 1 + HSO₃⁻; 2–19: HS⁻, F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, ClO₄⁻, NO₃⁻, N₃⁻, SO₄²⁻, HSO₄⁻, SCN⁻, PO₄³⁻, HPO₄²⁻, H₂PO₄⁻, Cys, Hcy and GSH (anions: 60 μM ; Cys and Hcy: 200 μM ; GSH: 10 mM). $\lambda_{\text{ex}} = 400$ nm. Slits: 5 nm/ 5 nm.

7. ESIMS spectrum of the adduct.

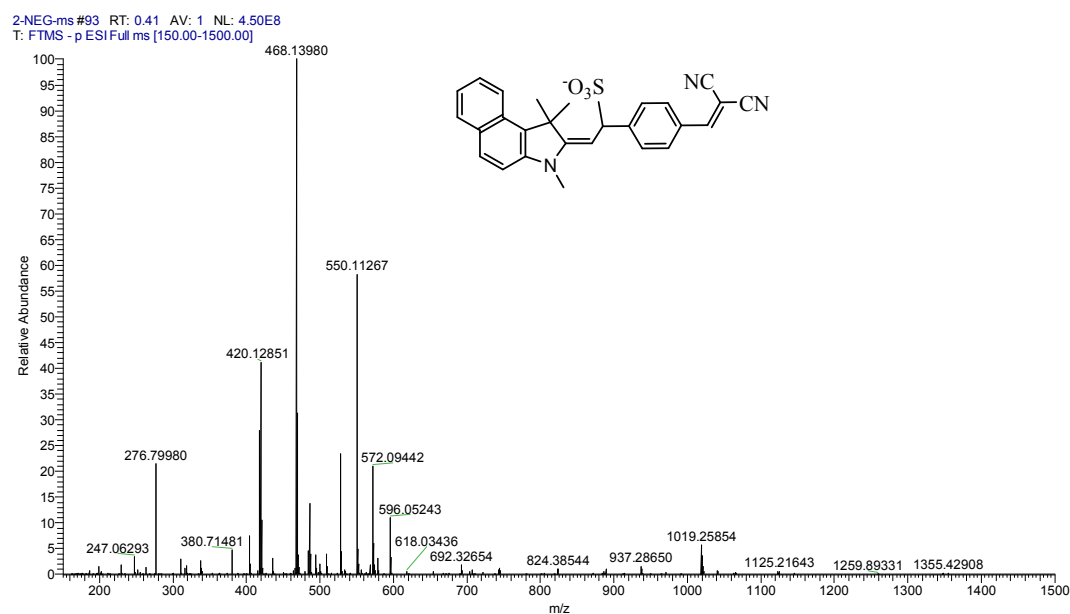


Fig. S9. ESIMS spectrum of [M-SO₃]⁻. Calc.: 468.1387, found: 468.1398.

8. Paper test



Fig. S10. Color changes of test paper with different species. 1: probe **1** alone; 2–20: probe **1** + HSO_3^- , HS^- , F^- , Cl^- , Br^- , I^- , AcO^- , ClO_4^- , NO_3^- , N_3^- , SO_4^{2-} , HSO_4^- , SCN^- , PO_4^{3-} , HPO_4^{2-} , H_2PO_4^- , Cys, Hcy and GSH.

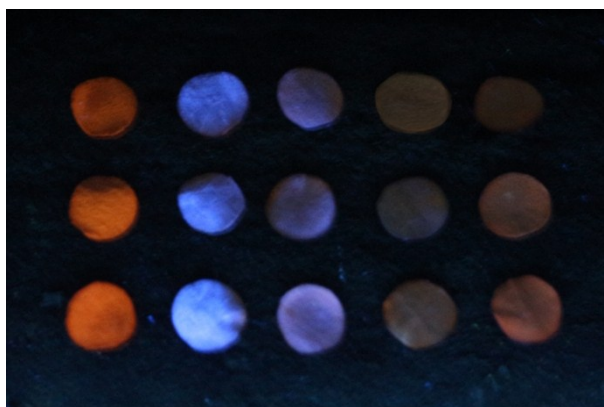


Fig. S11. Paper test for sugar samples. Top: Granulated sugar, middle: Soft sugar, and bottom: Crystal sugar. The order from left to right are: probe **1** only, concentration of sugar of 1g/10ml, 0.7g/10ml, 0.4g/10ml, and 0.1g/10ml.

9. MTT assay

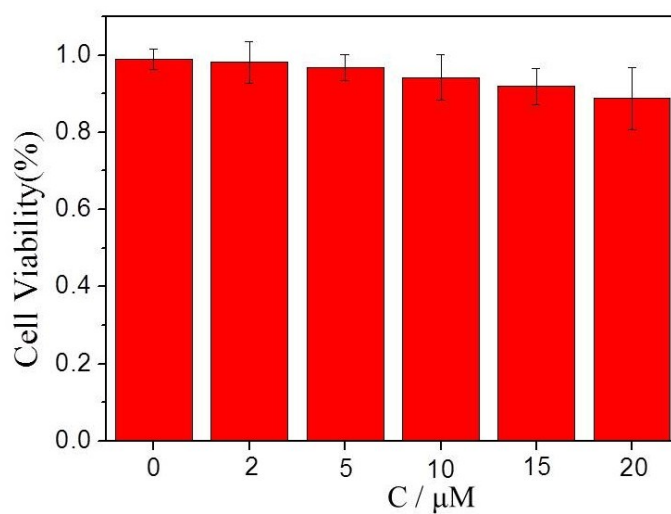


Fig. S12. Percentage of viable cells after treatment with various concentration of probe **1** after 12 hours.