Supporting Information

A highly selective fluorescence-enhanced probe for the rapid detection of SO_2 derivatives and its bio-imaging in living cells

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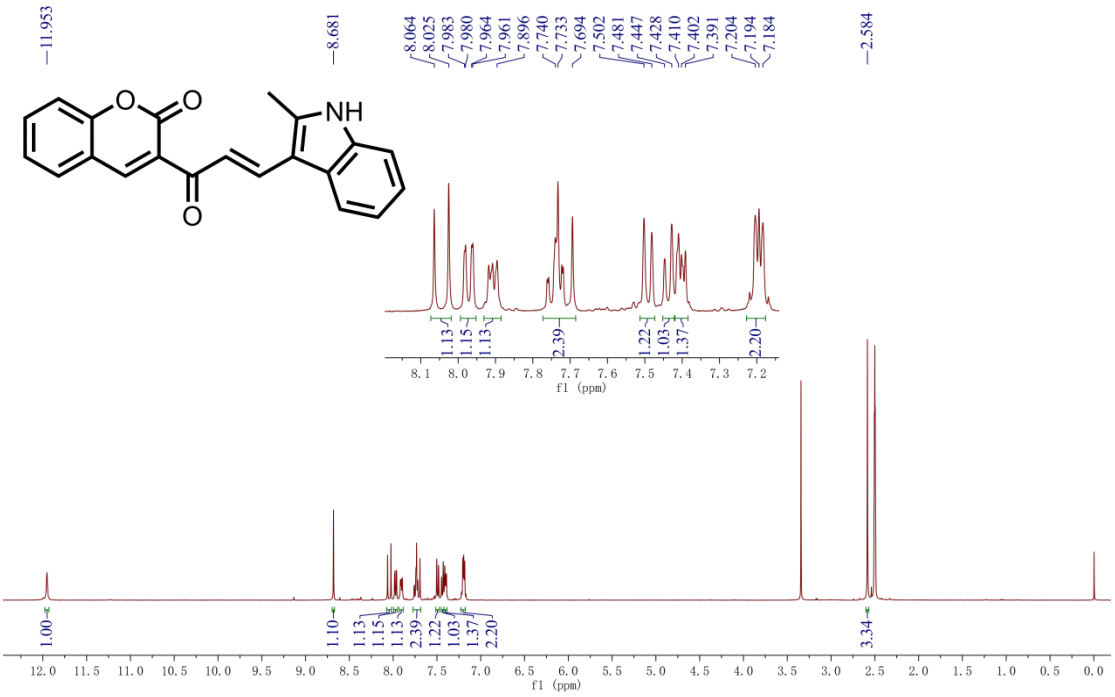

Fig. S1 ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **CISD**

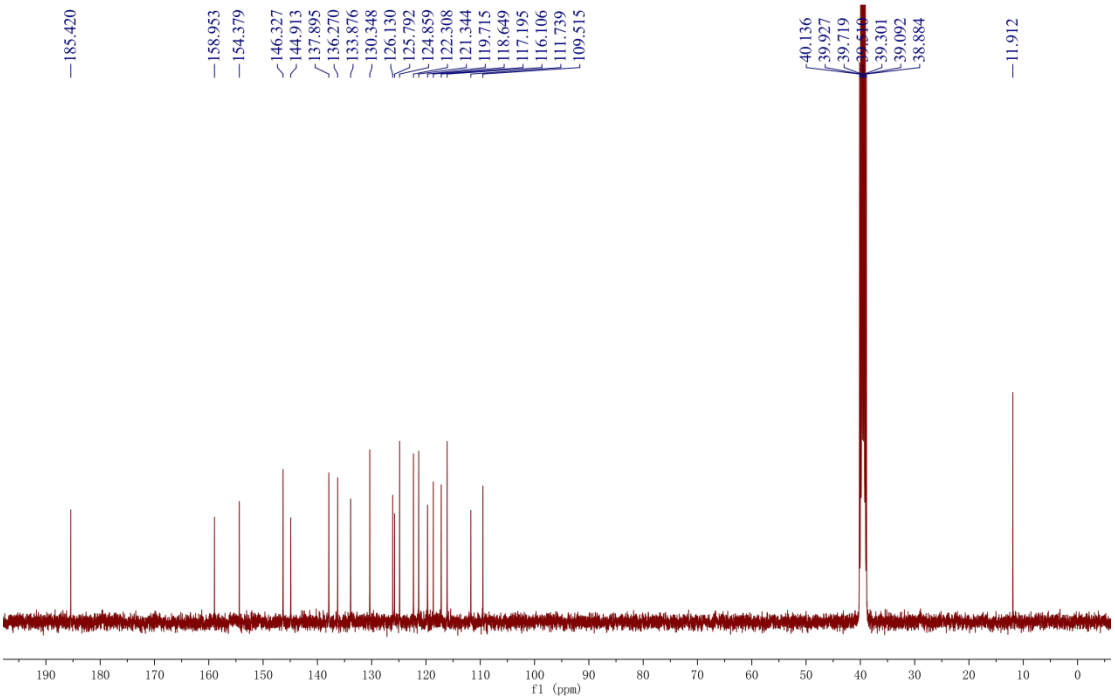

Fig. S2 ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **CISD**

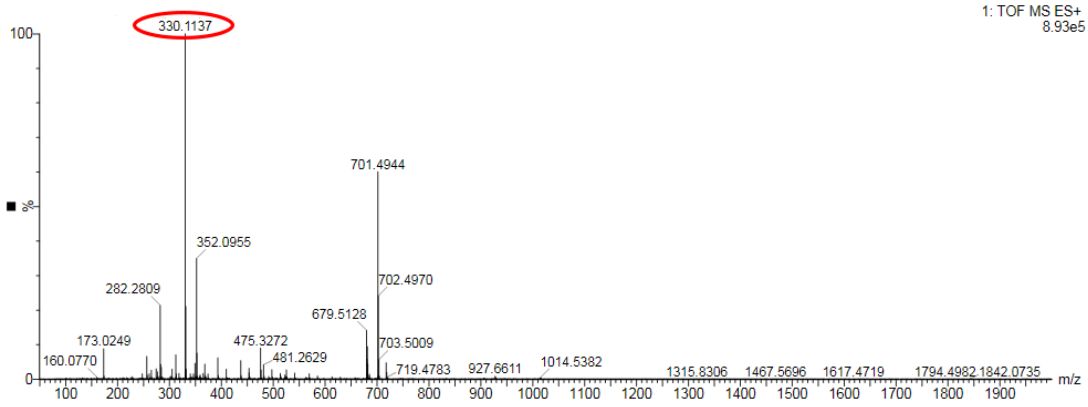

Fig. S3 HRMS spectrum of **CISD**

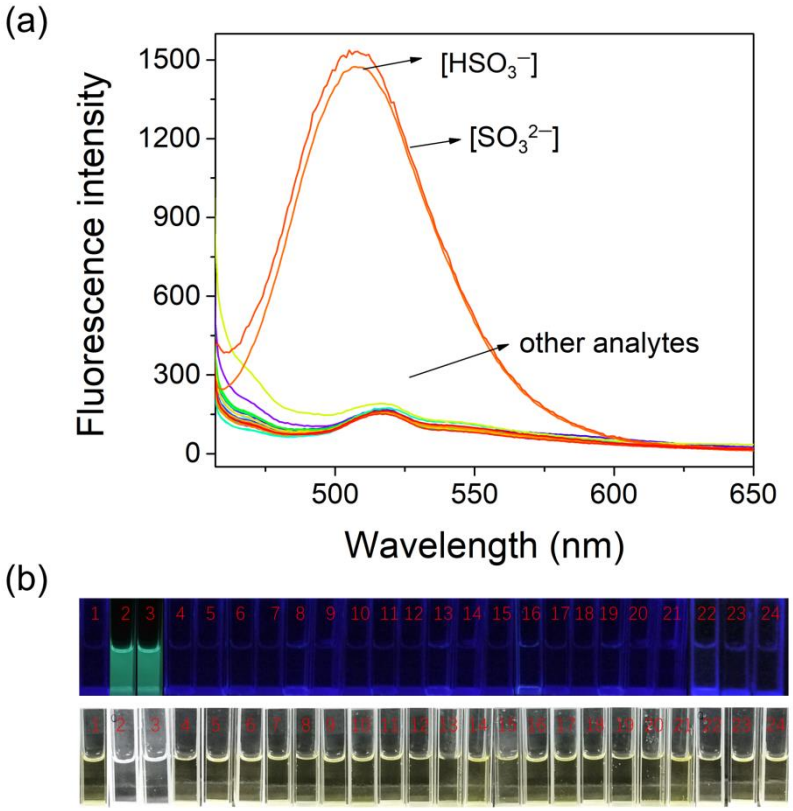

Fig. S4 (a) Fluorescence spectra of **CISD** (10 μM) in the presence of 260 μM of various test analytes in DMSO/PBS buffer solution (v/v = 3/7, pH 7.4). Analytes include 1 to 24: 1. None, 2. HSO_3^-, 3. SO_3^{2-}, 4. F^-, 5. Cl^-, 6. Br^-, 7. I^-, 8. NO_3^-, 9. AcO^-, 10. Ca^{2+}, 11. Zn^{2+}, 12. Fe^{3+}, 13. Al^{3+}, 14. $H_2PO_4^-$, 15. HPO_4^{2-}, 16. $S_2O_3^{2-}$, 17. HS^-, 18. SO_4^{2-}, 19. HCO_3^-, 20. Hcy, 21. H_2O_2, 22. ClO^-, 23. Cys, 24. GSH. (b) The fluorescence (top) and color images (bottom) of **CISD** in the presence of above analytes in DMSO/PBS solution (v/v = 3/7, pH 7.4).

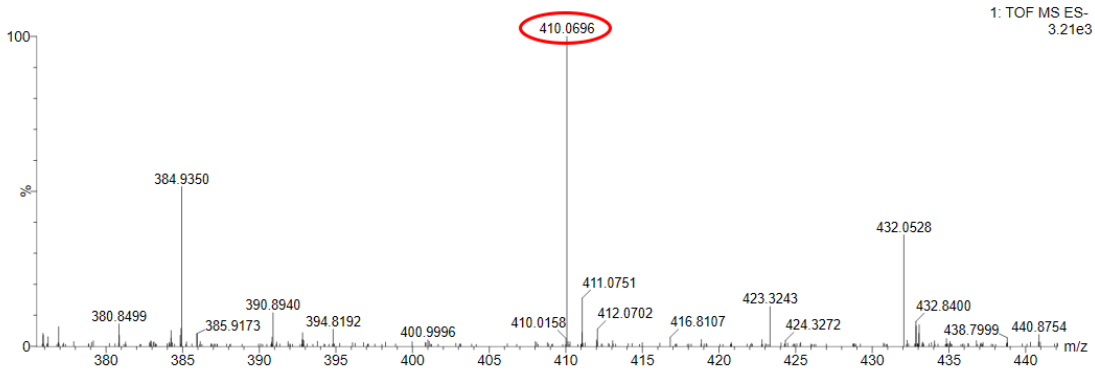

Fig. S5 HRMS spectrum of **CISD** in the presence of excess HSO_3^-

Table S1 Crystal data and structure refinement for **CISD**

Identification code	**CISD**
Empirical formula	$C_{21}H_{15}NO_3$
Formula weight (g/mol)	329.34
Temperature (K)	293(2)
Crystal system	monoclinic
Space group	*P* 2_1/c
a (Å)	6.2785(15)
b (Å)	27.412(5)
c (Å)	9.516(3)
α (°)	90
β (°)	102.93(3)
γ (°)	90
Volume ($Å^3$)	1596.1(6)
Z	4
ρ_{calc} ($g \cdot cm^{-3}$)	1.371
μ (mm^{-1})	0.092
F (000)	688.0
Crystal size/mm^3	0.220 × 0.200 × 0.180
Radiation	MoKα (λ = 0.71073 Å)
2θ range for data collection (°)	5.304 to 49.978
Index ranges	$-2 \le h \le 7$, $-31 \le k \le 32$, $-11 \le l \le 11$
Reflections collected	5102
Independent reflections	2816 [R_{int} = 0.0480, R_σ = 0.0949]
Data/restraints/parameters	2816/0/227
Goodness-of-fit on F^2	0.956
Final R indexes [I>=2σ(I)]	R_1 = 0.0636, ωR_2 = 0.1432
Final R indexes [all data]	R_1 = 0.1474, ωR_2 = 0.1835
Largest diff. peak/hole (eA^{-3})	0.19/-0.23

Table S2 Bond Lengths (Å) for **CISD**

Atom	Length/Å	Atom	Length/Å
C1-C2	1.361(6)	C10-C11	1.458(4)
C1-C6	1.371(5)	C11-C12	1.344(4)
C1-O1	1.378(4)	C12-C13	1.428(4)
C2-C3	1.383(6)	C13-C14	1.400(4)
C3-C4	1.350(6)	C13-C16	1.445(4)
C4-C5	1.365(5)	C14-N1	1.357(4)
C5-C6	1.397(4)	C14-C15	1.487(4)
C6-C7	1.425(5)	C16-C17	1.404(4)
C7-C8	1.362(4)	C16-C21	1.409(4)
C8-C9	1.451(5)	C17-C18	1.378(4)
C8-C10	1.506(5)	C17-N1	1.384(4)
C9-O2	1.221(4)	C18-C19	1.385(5)
C9-O1	1.384(4)	C19-C20	1.398(5)
C10-O3	1.224(4)	C20-C21	1.375(4)

Table S3 Bond angles (˚) for **CISD**

Atom	Angle/˚	Atom	Angle/˚
C2-C1-C6	121.6(4)	C12-C11-C10	120.2(3)
C2-C1-O1	117.9(4)	C11-C12-C13	129.2(3)
C6-C1-O1	120.5(3)	C14-C13-C12	123.0(3)
C1-C2-C3	118.9(4)	C14-C13-C16	106.3(3)
C4-C3-C2	120.6(4)	C12-C13-C16	130.7(3)
C3-C4-C5	120.8(4)	N1-C14-C13	109.2(3)
C4-C5-C6	119.6(4)	N1-C14-C15	120.5(3)
C1-C6-C5	118.6(4)	C13-C14-C15	130.3(3)
C1-C6-C7	117.4(3)	C17-C16-C21	118.1(3)
C5-C6-C7	124.0(4)	C17-C16-C13	106.8(3)
C8-C7-C6	123.2(3)	C21-C16-C13	135.1(3)
C7-C8-C9	118.4(3)	C18-C17-N1	128.6(3)
C7-C8-C10	117.3(3)	C18-C17-C16	123.6(3)
C9-C8-C10	124.2(3)	N1-C17-C16	107.8(3)
O2-C9-O1	114.8(3)	C17-C18-C19	117.1(3)
O2-C9-C8	128.1(3)	C18-C19-C20	120.8(3)
O1-C9-C8	117.0(3)	C21-C20-C19	121.7(4)
O3-C10-C11	122.2(3)	C20-C21-C16	118.7(3)
O3-C10-C8	116.7(3)	C14-N1-C17	109.9(3)
C11-C10-C8	121.0(3)	C1-O1-C9	123.3(3)