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# Supporting information

## A novel fluorescent probe for imaging endogenous hydrogen sulfide via CSE enzymatic pathway

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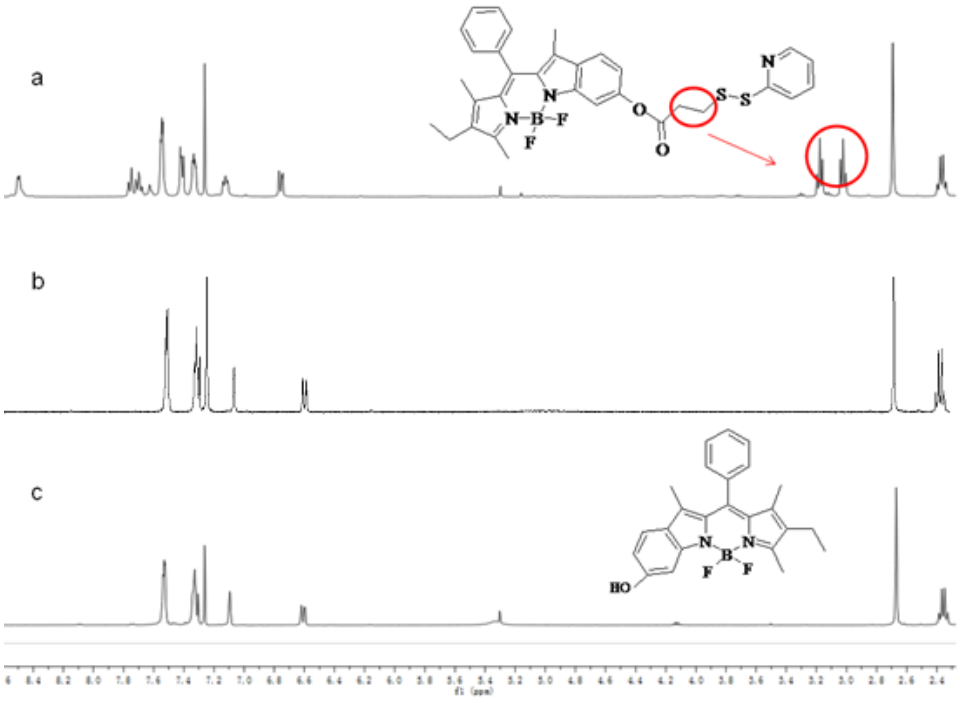
### Materials and instruments

All chemicals for synthesis were purchased from commercial suppliers and were used without further purification. $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded on a Bruker AV-400 spectrometer with chemical shifts reported in ppm at room temperature. Mass spectra were measured on a HP 1100 LC-MS spectrometer. UV-vis absorption spectra were recorded on a Varian Cary 100 spectrophotometer. Fluorescence spectra were measured with a Varian Cary Eclipse Fluorescence spectrophotometer. Spectral-grade solvents were used for measurements of UV-vis absorption and fluorescence. For absorption or fluorescence measurements, compounds were dissolved in $CH_3CN$ to obtain stock solutions (5.0 mM). The stock solutions were then diluted with aqueous solutions to the desired concentration.



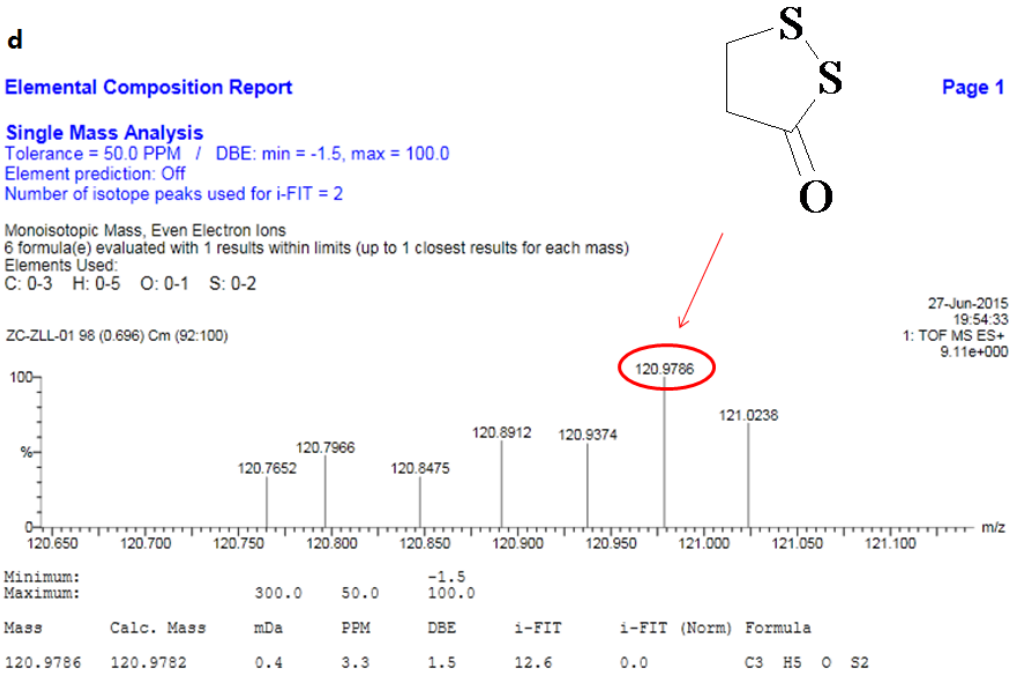




**Fig. S1.** Partial $^{1}$H NMR spectra of (a) **B601**, (b) the isolated product of **B601** + $H_2S$, (c) **BODIPY-OH**, (d) partial of HRMS spectra of **B601** + $H_2S$ for identification of the production a five membered cyclic lactone ring.

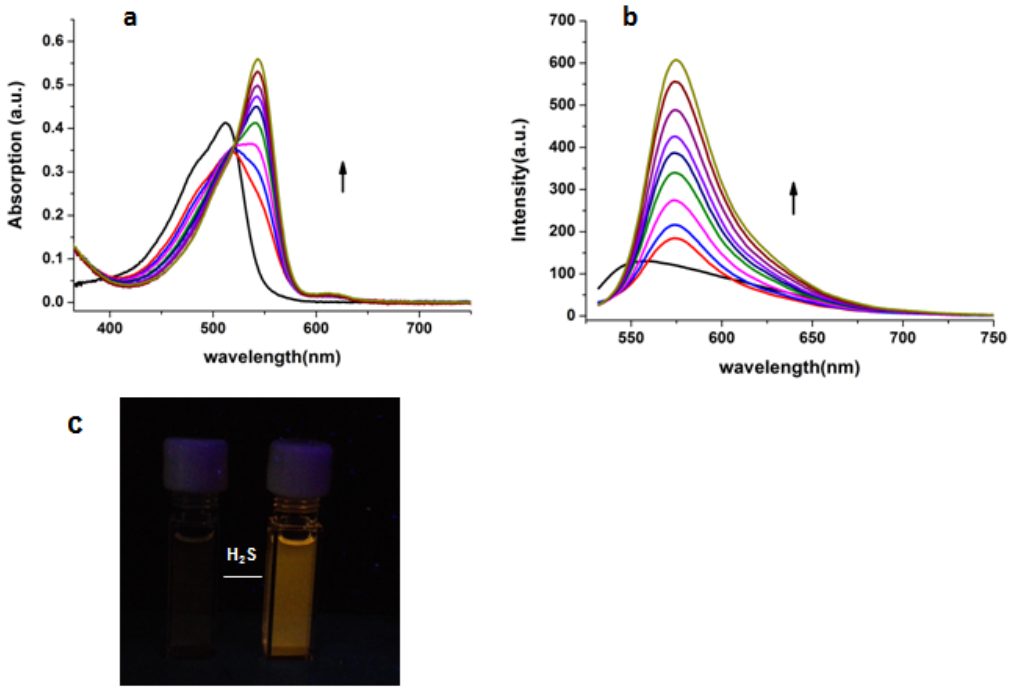



**Fig. S2.** (a) The absorption spectra **of B601** ($5\times10^{-6}$ M) in the presence of different concentrations of NaHS (0, 1, 2, 3, 4, 5, 6, 7, 8, 9,10 equiv.) in PBS buffer (pH=7.4, containing 30% of $CH_3CN$, v/v); (b) Time dependent fluorescence spectra changes of **B601** (10 μM) upon incubation with $H_2S$ (100 μM) in PBS buffer (pH=7.4, containing 30% of $CH_3CN$, v/v), (0, 1, 2, 3, 4, 5, 6, 7, 8, 9 min). (c) The fluorescence color changes of **B601** in the absence and presence of $H_2S$.

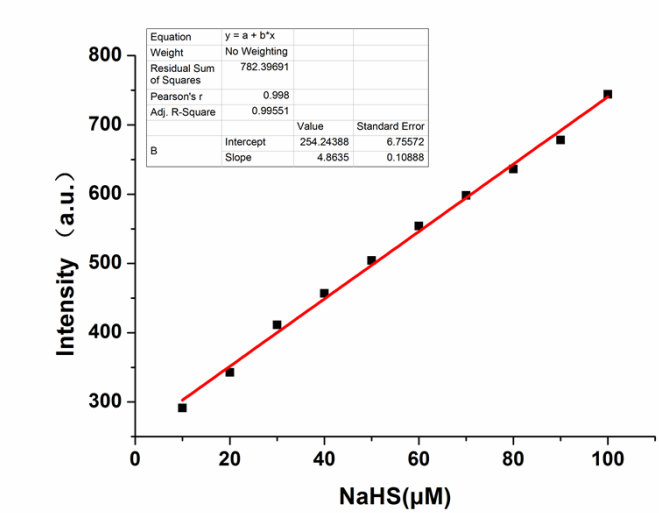
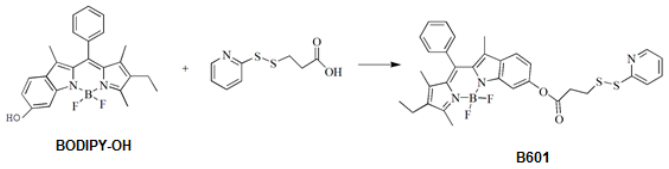


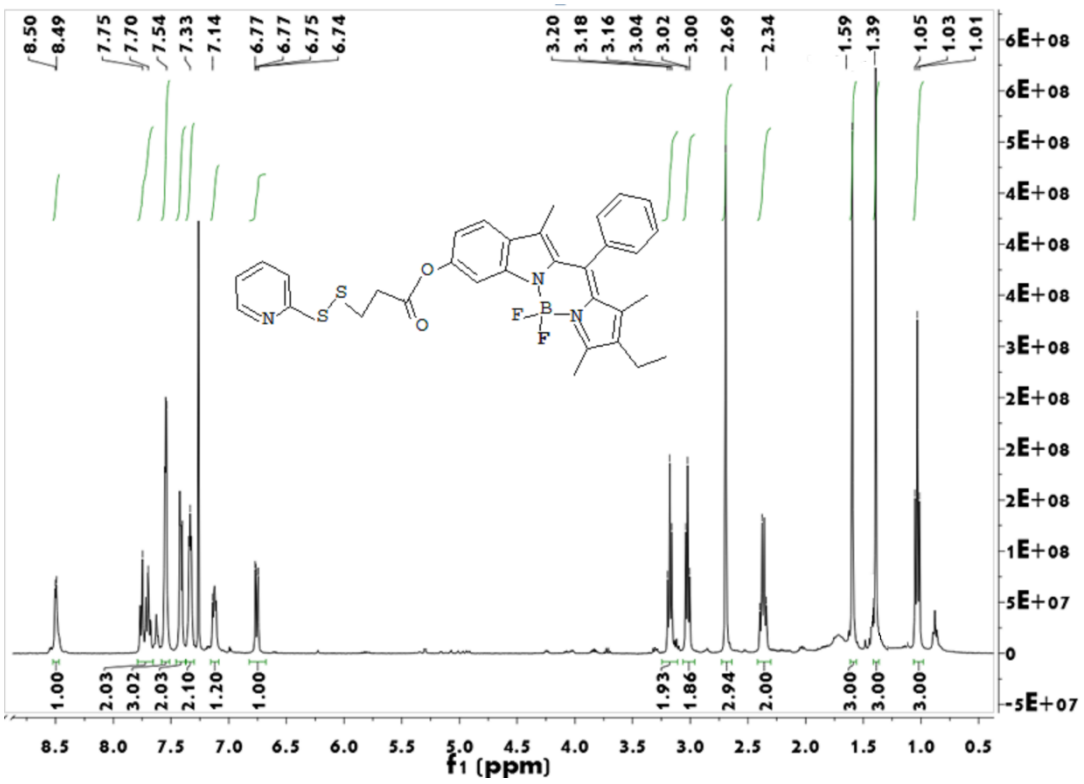

**Fig. S3.** Plots of fluorescence intensity as a function of $H_2S$ concentrations. The standard deviation was determined to be σ = 0.2481, the detection limit was then calculated by the formula (3σ/k) and given a result of $1.5\times10^{-7}$ M for $H_2S$.

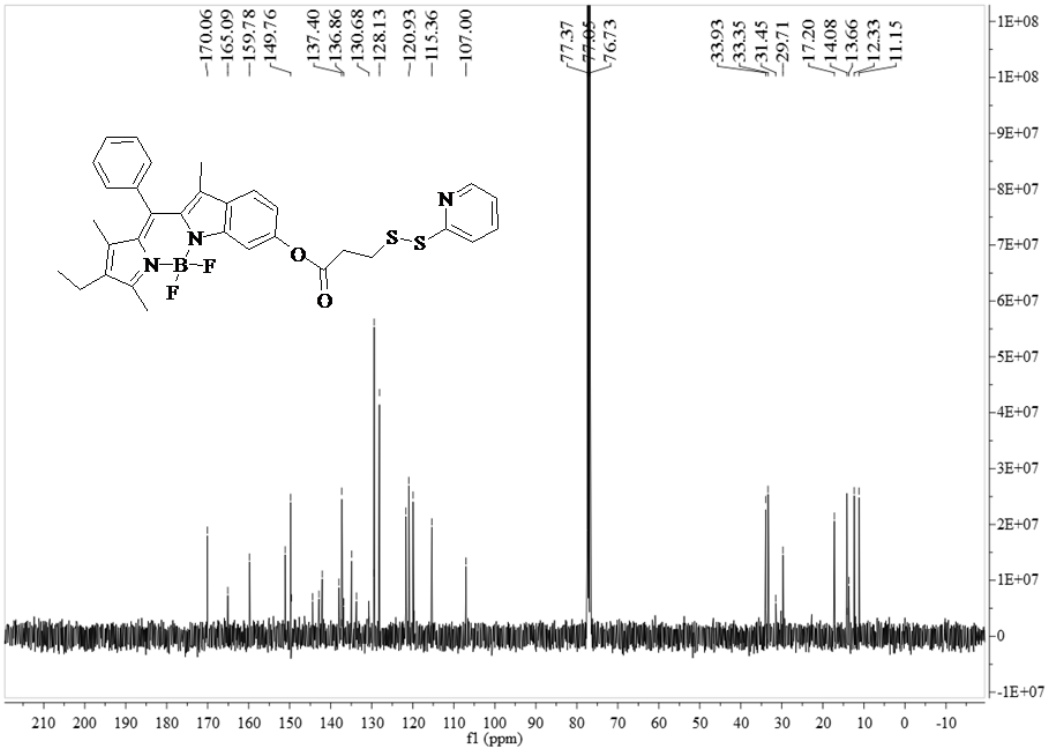
**Synthesis of B601**




**BODIPY-OH** (50 mg, 0.12 mmol) was dissolved in anhydrous dichloromethane (5 mL) in a round-bottom flask. 3-(2-Pyridyldithio) propionic acid (35 mg, 0.12 mmol) was added, followed by the addition of 4-(dimethylamino)-pyridinium-4-toluene sulfonate (DPTS) (37 mg, 0.12 mmol) and Diisopropylcarbodiimide (16 mg, 0.12 mmol). The reaction mixture was stirred for 2h, then diluted with dichloromethane, and washed with brine. The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and concentrated by rotary evaporation. The residue was further purified by column chromatography on silica gel to give the desired product **B601** as a dark red solid in 93% yield (68 mg). $^1$H NMR ($CDCl_3$,400 MHz, δ ppm): 8.50 (d, 2H) , 7.70 (m, 2H), 7.54 (m, 3H), 7.42 (m, 2H), 7.33 (m, 2H), 7.14 (t, 1H), 6.76 (dd, 1H), 3.18 (t, 2H), 3.02 (t, 2H), 2.69 (s, 3H), 2.38 (dd, 2H), 1.59 (s, 3H ) , 1.39 (s, 3H),1.03 (t, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz) δ(ppm) : 170.06, 165.09, 159.78, 151.12, 149.76, 149.60, 144.41, 142.85, 142.08, 137.28, 136.86, 133.75, 130.68, 129.50, 129.41, 128.13, 121.65, 120.93, 119.90, 115.36, 107.00, 77.37, 77.05, 76.73, 33.93, 33.35, 29.67, 17.20, 14.08, 13.66, 12.33, 11.15. HRMS: calcd for $[M+H]^+$ 602.1913, found 602.1907.

## $^{1}H$ and $^{13}C$ NMR of B601



**HRMS of B601**




| Compound Name (Library Hit) | Score | Formula | Intensity | Threshold | Expected m/z | Found at m/z | Error (ppm) | Expected RT (min) | Found RT (min) | RT Delta (min) | Isotope Diff (%) | Library Score(%) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 601.184057904 | 47% | C32H30BF2N3O2S2 | 73568 | 100 | 602.1913 | 602.1907 | -1.0 | 0.00 | 2.06 | 2.06 | 34.8% | N/A |