Electronic Supplementary Information

A turn-on homodimer fluorescent probe based on homo-FRET for sensing of biothiols in lysosome: a trial of new turn-on strategy

Ying-Jie Tang, Wen-Le Fang, Kui Ren, Xiao-Feng Guo*, Hong Wang*

College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, China

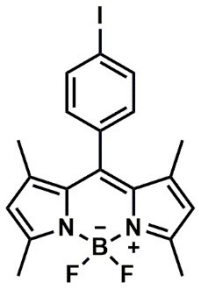
Corresponding authors:

ggxxff123@163.com (Xiao-Feng Guo)

hongwang@whu.edu.cn (Hong Wang)

Content Table

Synthesis of compound a



4-iodobenzaldehyde (0.6 g, 2.4 mmol) and 2, 4-dimethylpyrrole (0.5 mL, 4.9 mmol) were dissolved in dichloromethane (300 mL). The reaction mixture was stirred 10 min and TFA (3 drops) was added. The resulted dark red solution was stirred at 20 °C overnight in the dark. TLC monitoring showed a complete consumption of 4-iodobenzaldehyde (silica; EtOAc/cyclohexane 2:8). A suspension of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (0.6 g, 2.4 mmol) in dichloromethane (20 mL) was added and strirring was continued for 5 h. Triethylamine (10.2 mL, 73 mmol) and boron trifluoride diethyl etherate complex (12 mL, 97 mmol) were then successively added to the reaction mixture leading to a dark green solution. Stirring was continued 2 h and the reaction mixture was successively washed with water (500 mL) and an aqueous solution of sodium hydroxide (2N, 500 mL). The organic layer was dried over Na_2SO_4, filtered and the volatiles were evapored under reduced pressure. The dark green crude material was purified by chromatography over silica gel (dichloromethane/cyclohexane 1:1.5) to provide an orange powder (460 mg, yield 43 %). 1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.0 Hz, 2H), 5.99 (s, 2H), 2.55 (s, 6H), 1.42 (s, 6H).

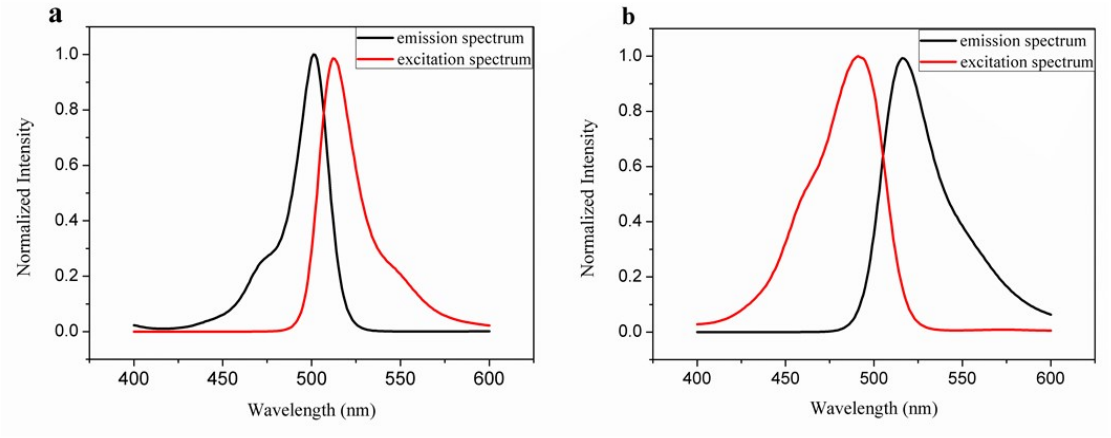


Fig. S1. (a) The excitation and emission spectra of TMPB, $\lambda_{ex}/\lambda_{em}$=500/512 nm (b) The excitation and emission spectra of fluorescein, $\lambda_{ex}/\lambda_{em}$=493/517 nm.

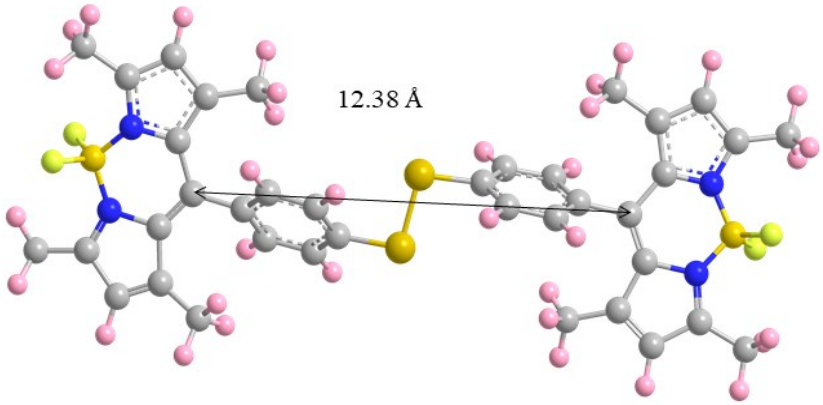


Fig. S2. A geometry optimized molecular model of probe was created using the Chem3D software package (Chem Office, USA) running under Microsoft Windows 10. Energy minimization was performed using molecular mechanics (MM2 force field).

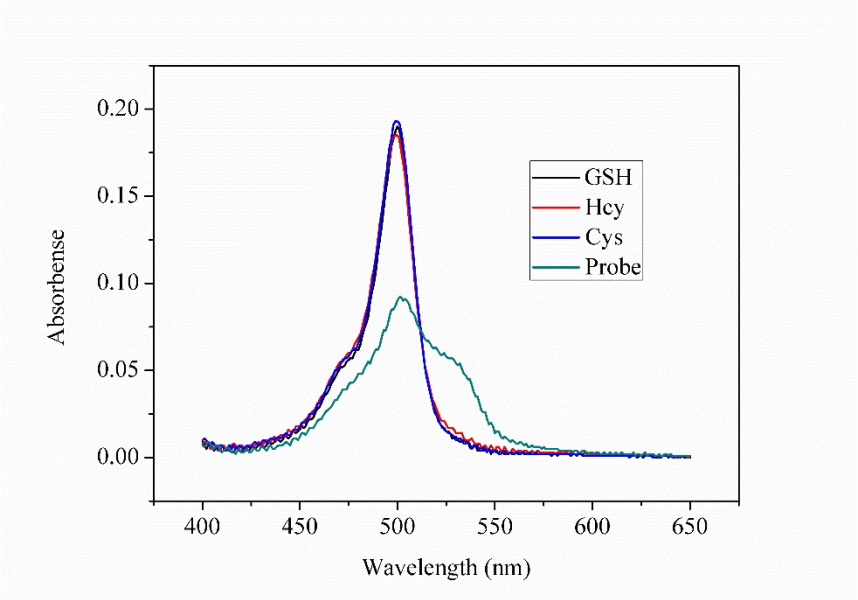


Fig. S3. The UV-vis spectra of D-TMSPB, D-TMSPB + GSH, D-TMSPB + Hcy, D-TMSPB + Cys in PB buffer (0.05 M, pH 5, containing 50% DMSO, v/v) for 30min.

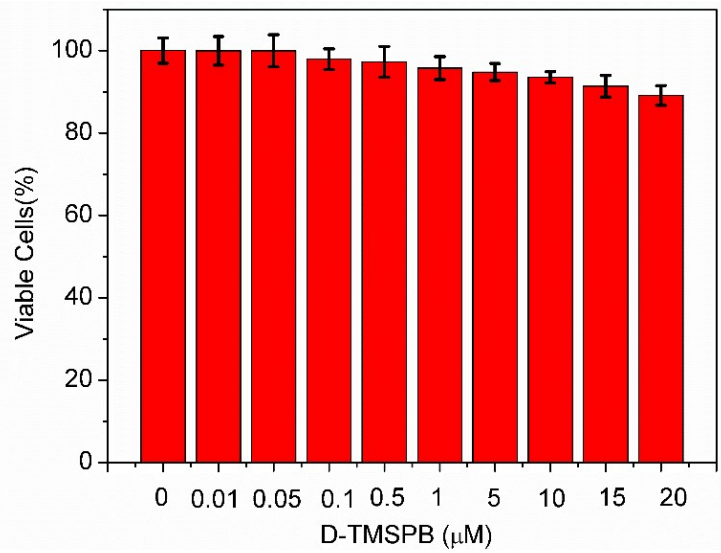


Fig. S4. Cytotoxicity assays of D-TMSPB at different concentrations for MCF-7 cells.

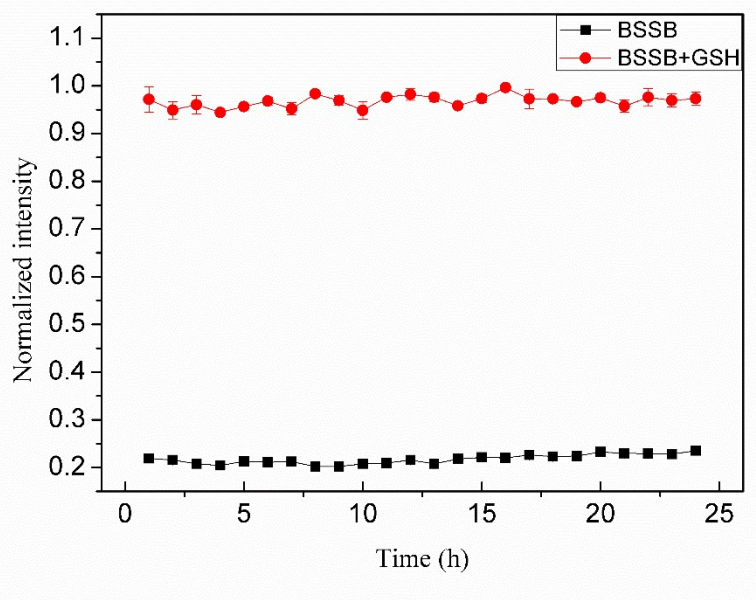


Fig. S5. Photostability of 5 μM D-TMSPB and the derivative with GSH in PB buffer (0.05 M, pH 5, containing 50% DMSO, v/v). Slit widths: 3 and 3 nm for excitation and emission spectra.

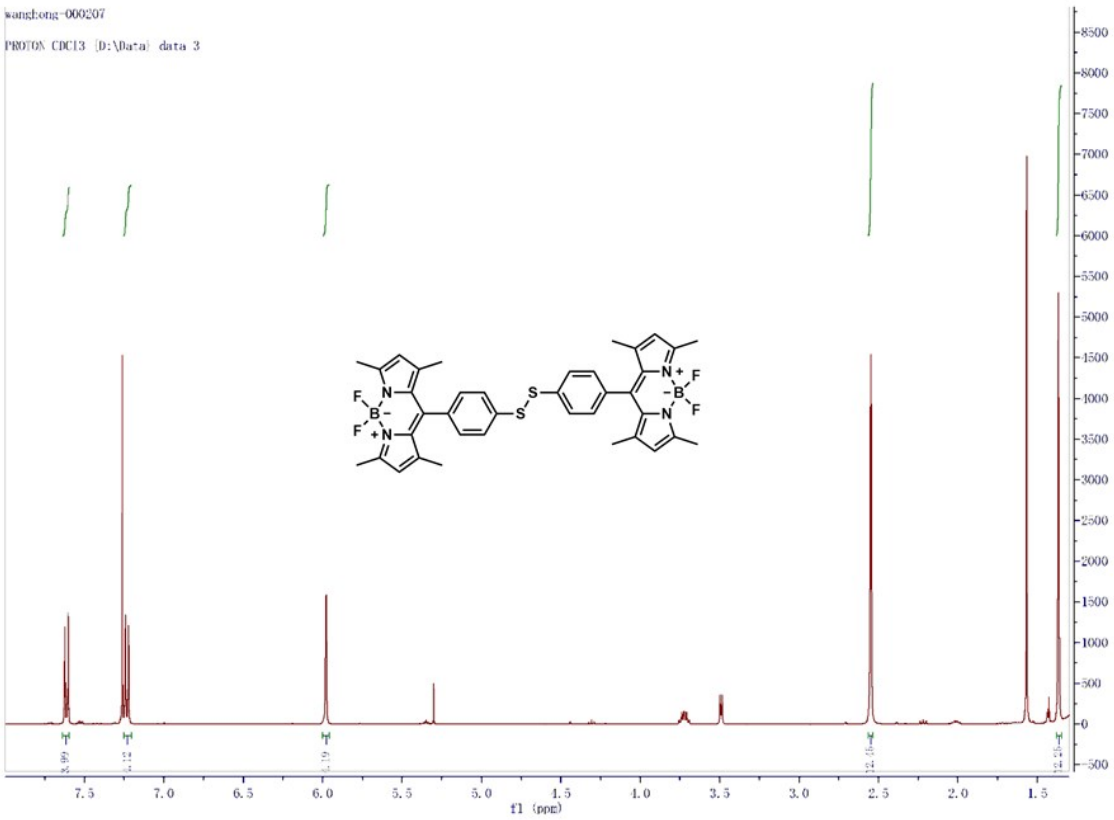


Fig. S6. ^{1}H NMR spectrum of BSSB in $CDCl_3$ solvent.

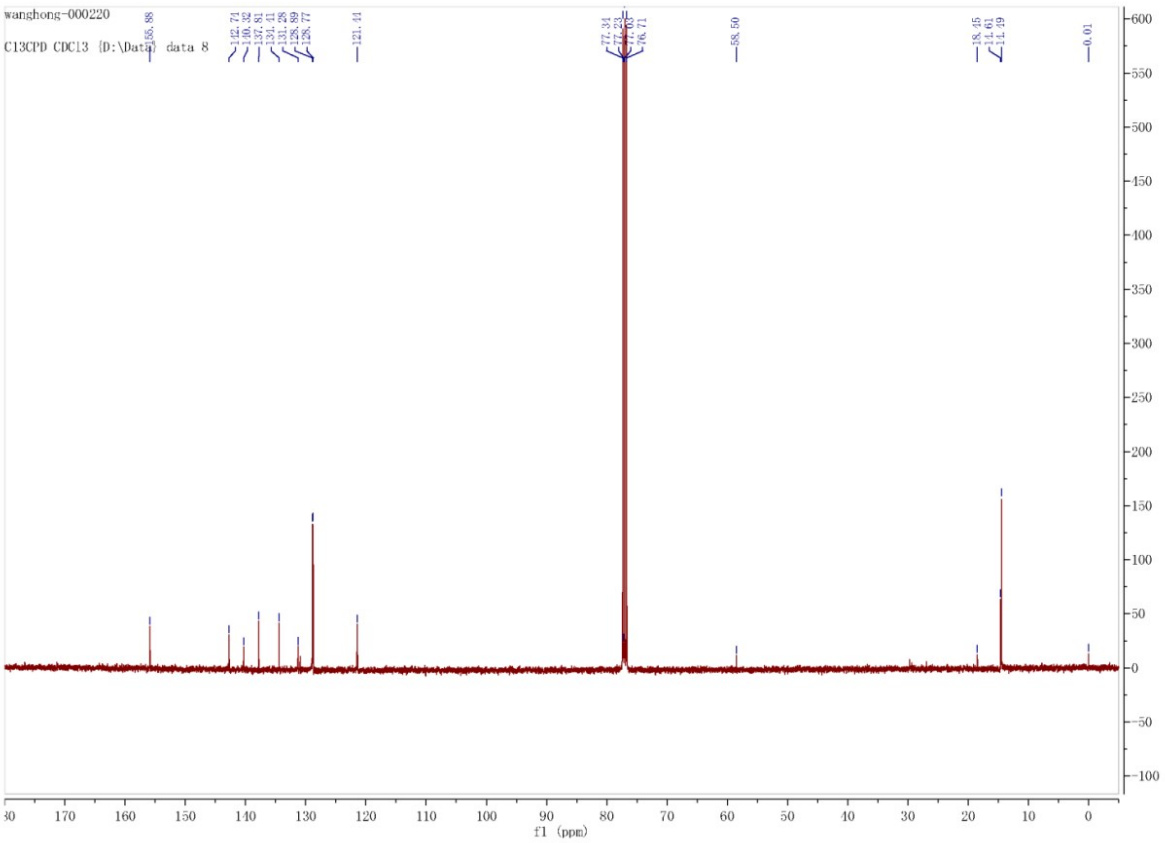


Fig. S7. ^{13}C NMR spectrum of BSSB in $CDCl_3$ solvent.