

Electronic supplementary information (ESI)

For

A Colorimetric and Fluorescent Merocyanine-Based Probe for Biological Thiols

Shu-Ping Wang, Wu-Jian Deng, Dan Sun, Min Yan, Hong Zheng* and Jin-Gou Xu
*Department of Chemistry and The Key Laboratory of Analytical Sciences of MOE, College of
Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China*
E-mail: hzheng@xmu.edu.cn

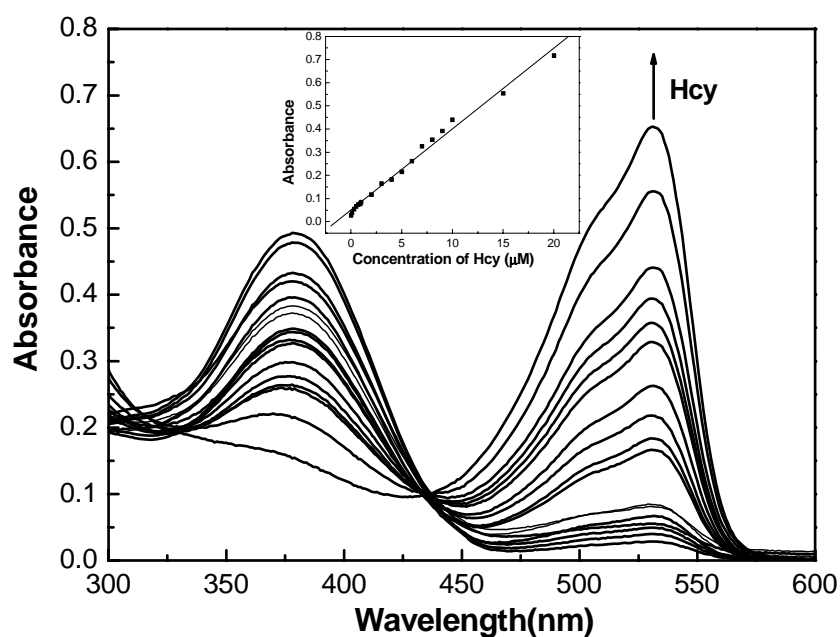


Figure S1. UV-vis spectra of **2** in the presence of Hcy in pH 7.40 phosphate buffer solution (MeOH/H₂O = 3:7, v/v). Each spectrum is recorded 15 min. after Hcy addition. Inset: plot of absorbance at 530 nm against concentration of Hcy. [2] = 2.0×10⁻⁵ M, [Hcy] = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10, 15 and 20.0 μM, respectively.

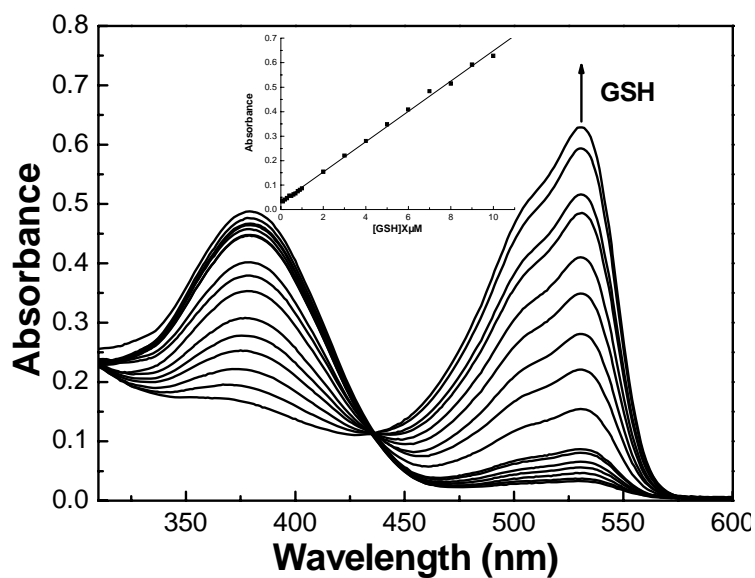


Figure S2. UV-vis spectra of **2** in the presence of GSH in pH 7.40 phosphate buffer solution (MeOH/H₂O = 3:7, v/v). Each spectrum is recorded 15 min. after GSH addition. Inset: plot of absorbance at 530 nm against concentration of GSH. [**2**] = 2.0×10^{-5} M, [GSH] = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, and 10.0 μ M.

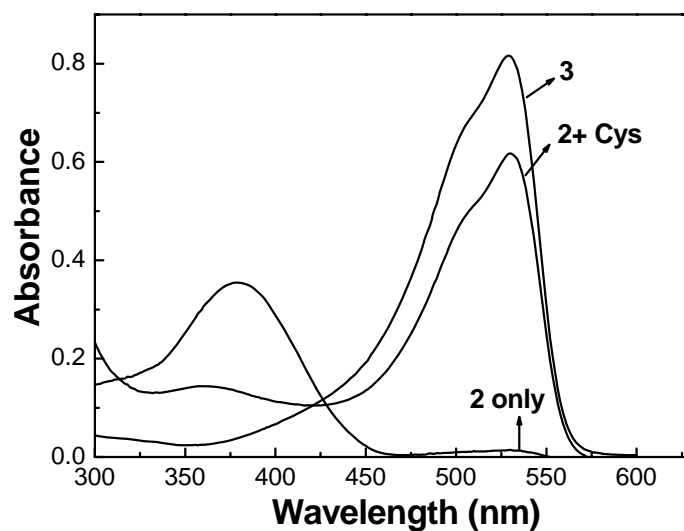


Figure S3. UV-vis spectra of **2** only, **2** with Cys, and **3** in pH 7.40 phosphate buffer solution (MeOH/H₂O = 3:7, v/v). [**2**] = 2.0×10^{-5} M, [**3**] = 1.0×10^{-5} M, [Cys] = 8.0×10^{-6} M.

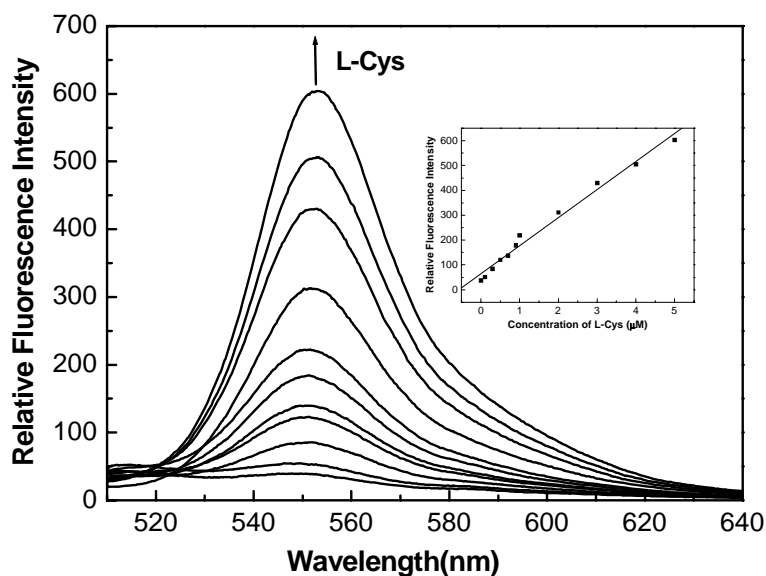


Figure S4. Fluorescence response of **2** in pH 7.40 of phosphate buffer (0.01 M) solution (MeOH/H₂O = 3:7, v/v) in the presence of Cys with an excitation at 490 nm. Inset: fluorescence intensity at 553 nm as a function of Cys concentration. [**2**] = 1.0×10^{-5} M, [Cys] = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0, 3.0, 4.0 and 5.0 μM, respectively.

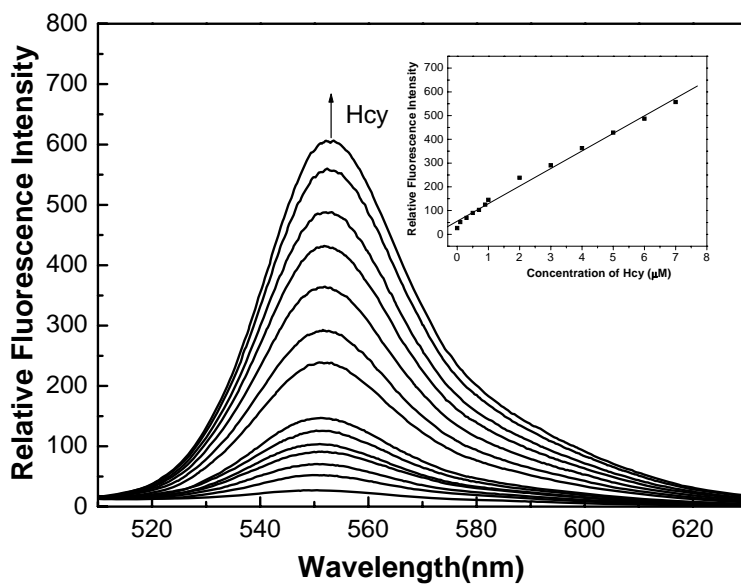


Figure S5. Fluorescence response of **2** in pH 7.40 of phosphate buffer (0.01 M) solution (MeOH/H₂O = 3:7, v/v) in the presence of Hcy with an excitation at 490 nm. Inset: fluorescence intensity at 553 nm as a function of Hcy concentration. [**2**] = 1.0×10^{-5} M, [Hcy] = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 and 7.0 μM, respectively.

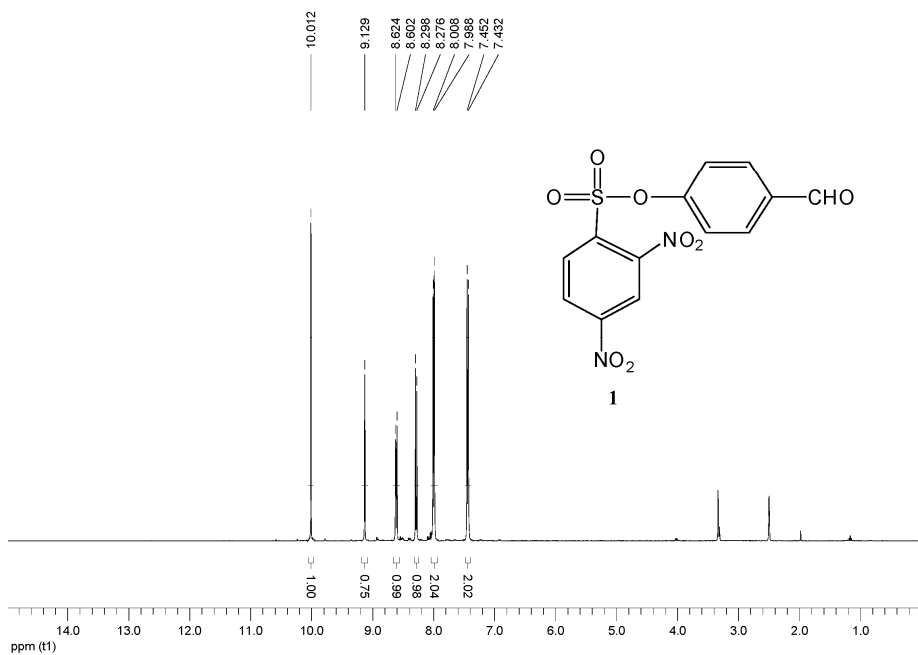


Figure S6. ¹H NMR spectra of compound **1** (DMSO-d₆).

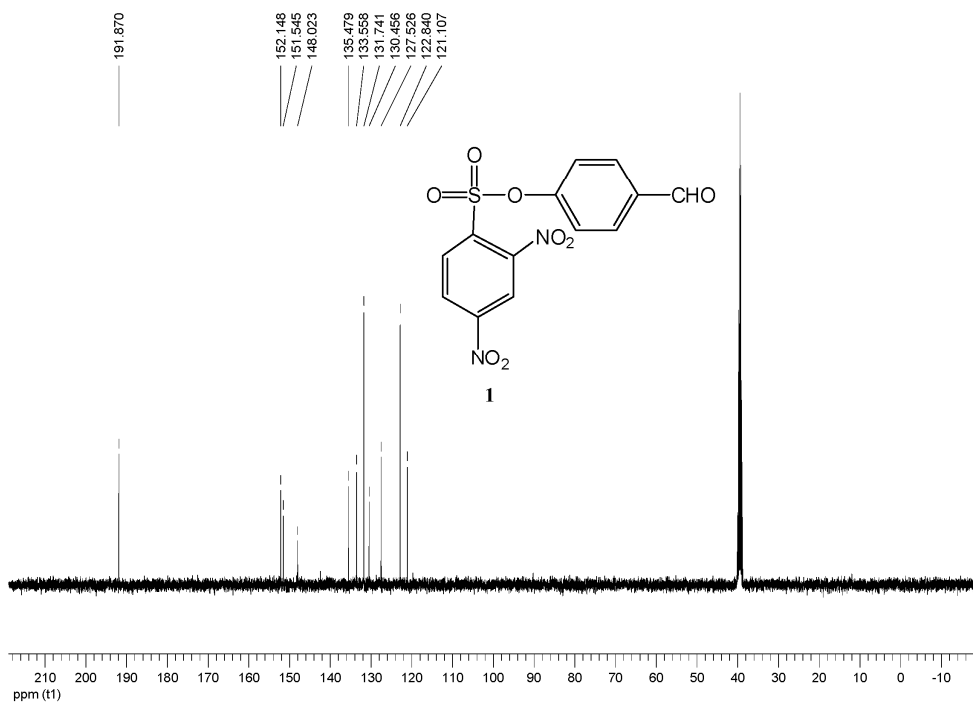


Figure S7. ¹³C NMR spectra of compound **1** (DMSO-d₆).

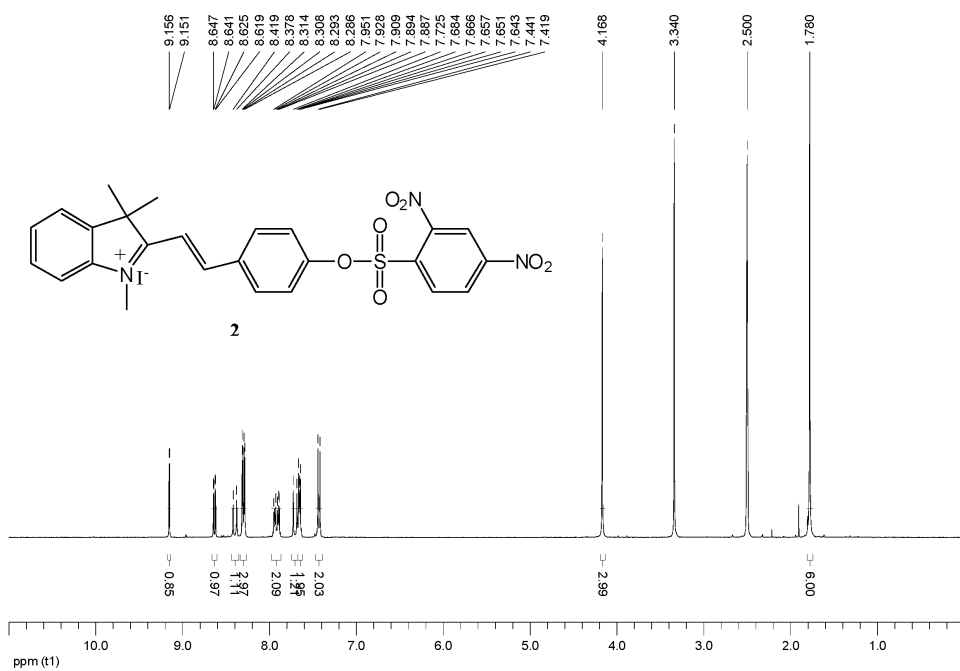


Figure S8. ¹H NMR spectra of compound **2** (DMSO-d₆). δ3.34(H₂O), δ2.50(DMSO residual peak)

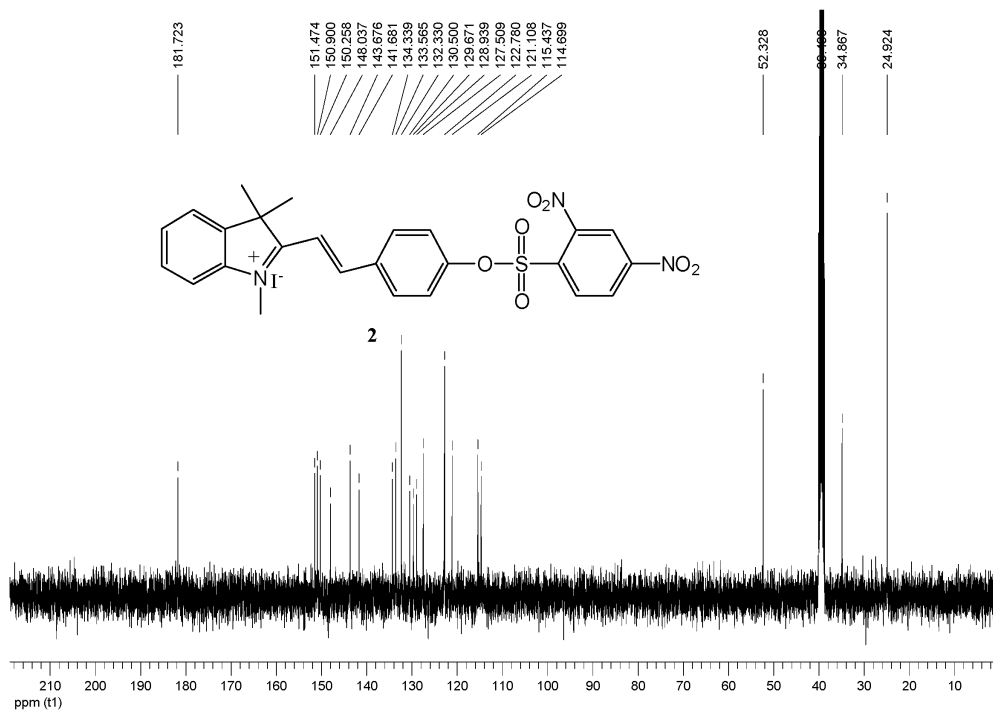


Figure S9. ¹³C NMR spectra of compound **2** (DMSO-d₆).

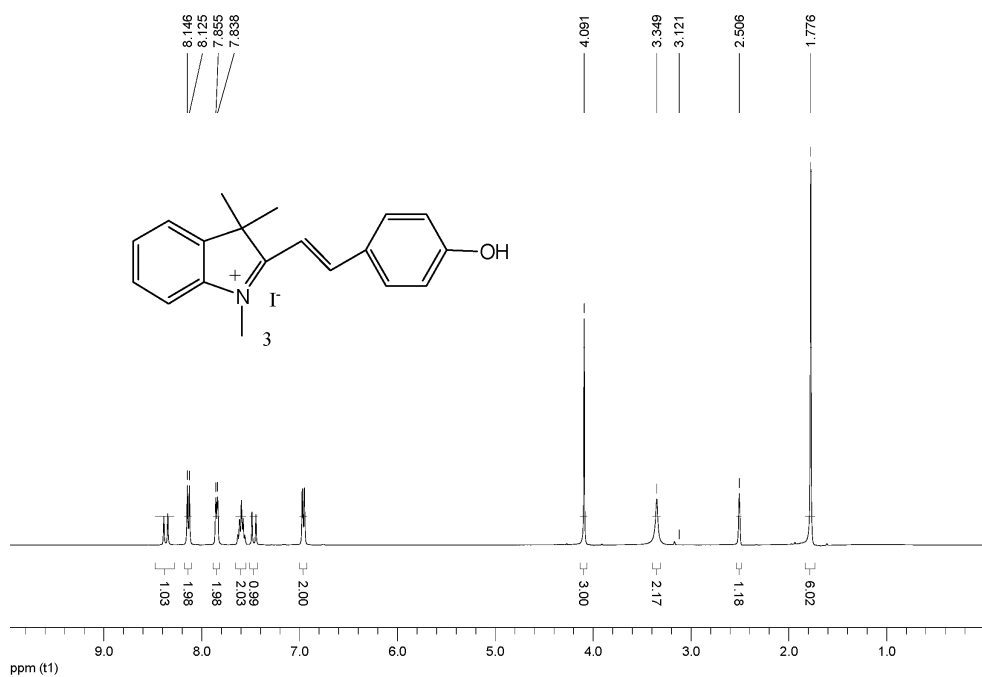


Figure S10. ¹H NMR spectra of compound 3 (DMSO-d₆).

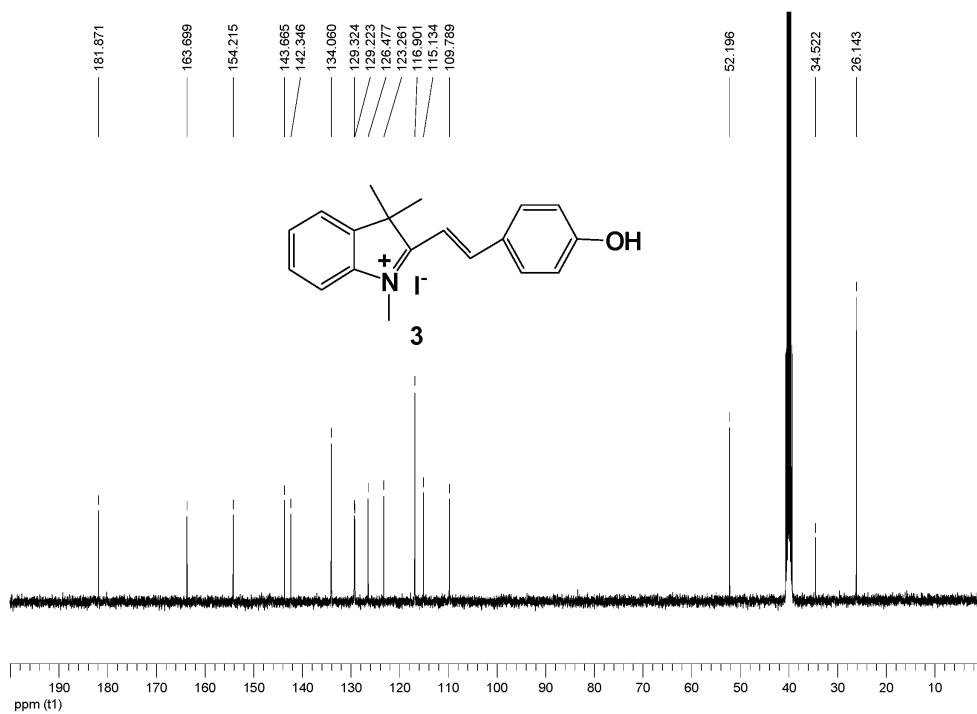


Figure S11. ¹³C NMR spectra of compound 3 (DMSO-d₆).