

Supplementary Information

A green-emitting fluorescent probe based on benzothiazole derivative for imaging thiols in living cells

Xiaohua Ma ^{1,2}, Yuanqiang Hao ^{2,*}, Guoguang Wu ^{1,*}, and Lin Liu ^{3,*}

¹ School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou 221000, China; mayingjie518@sohu.com (X.M.); b12040004@cumt.edu.cn (G.W)

² Henan Key Laboratory of Biomolecular Recognition and Sensing, College of Chemistry and Chemical Engineering, Shangqiu Normal University, Shangqiu 476000, China; haoyuanqiang@aliyun.com (Y.H.)

³ Key Laboratory of New Optoelectronic Functional Materials (Henan Province), College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang 455000, China; liulin@aynu.edu.cn (L.L.)

* Correspondence: haoyuanqiang@aliyun.com (Y.H.); b12040004@cumt.edu.cn; liulin@aynu.edu.cn (L.L.), Tel.: +86-0370-3112844 (Y.H.)

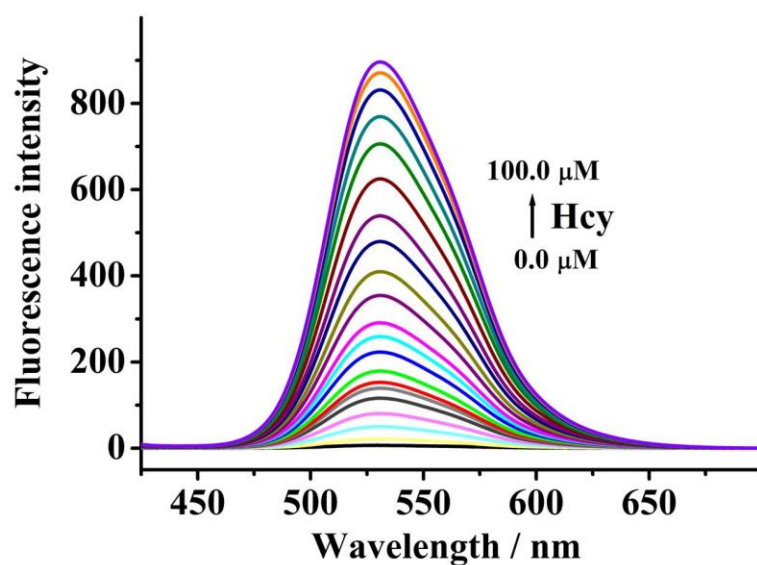


Figure S1 Fluorescence spectra changes of probe **1** ($5.0\ \mu\text{M}$) upon the addition of Hcy ($0.0\text{--}100.0\ \mu\text{M}$) in PBS buffer ($\lambda_{\text{exc}} = 413\ \text{nm}$, and $t = 15\ \text{min}$).

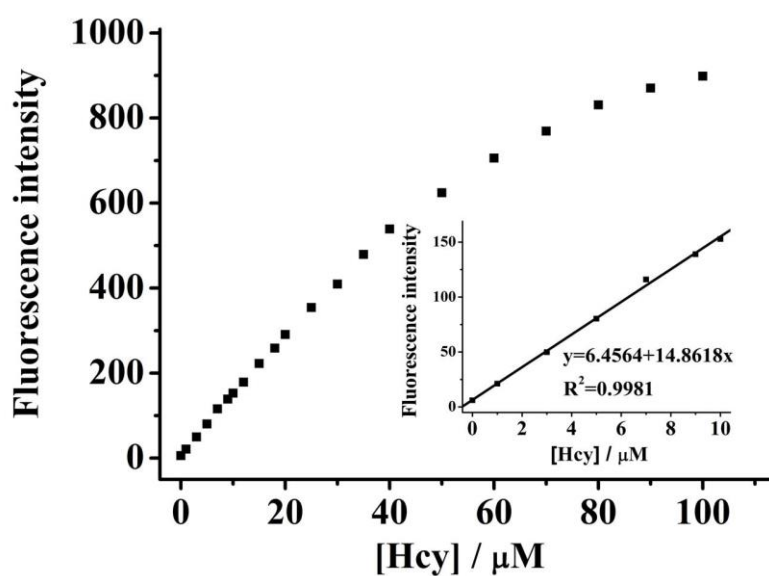


Figure S2 Fluorescence intensity of probe **1** ($5.0\ \mu\text{M}$) at $530\ \text{nm}$ as a function of Hcy concentration ($0.0\text{--}100.0\ \mu\text{M}$) in PBS buffer ($\lambda_{\text{exc}} = 413\ \text{nm}$, and $t = 15\ \text{min}$). Inset: the linear relationship between fluorescence intensity and Hcy at low concentrations.

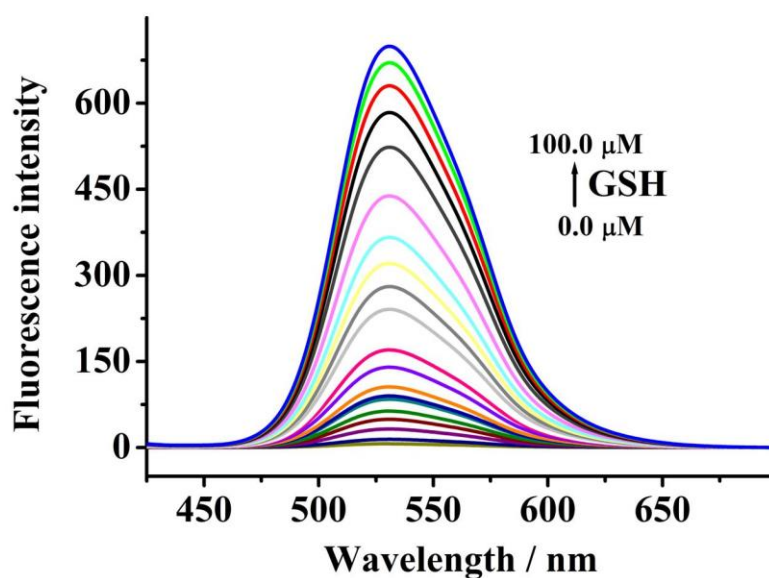


Figure S3 Fluorescence spectra changes of probe **1** ($5.0 \mu\text{M}$) upon the addition of GSH (0.0 – $100.0 \mu\text{M}$) in PBS buffer ($\lambda_{\text{exc}} = 413 \text{ nm}$, and $t = 15 \text{ min}$).

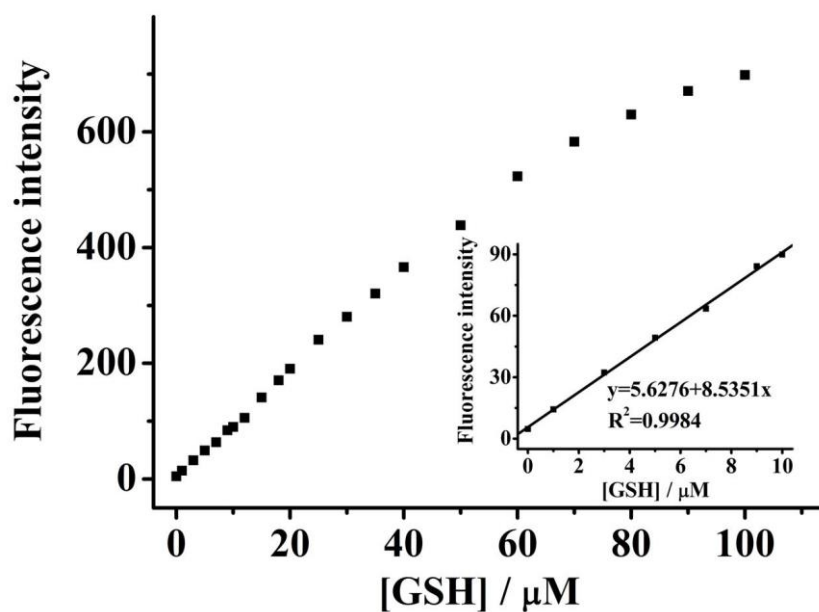


Figure S4 Fluorescence intensity of probe **1** ($5.0 \mu\text{M}$) at 530 nm as a function of GSH concentration (0.0 – $100.0 \mu\text{M}$) in PBS buffer ($\lambda_{\text{exc}} = 413 \text{ nm}$, and $t = 15 \text{ min}$). Inset: the linear relationship between fluorescence intensity and GSH at low concentrations.

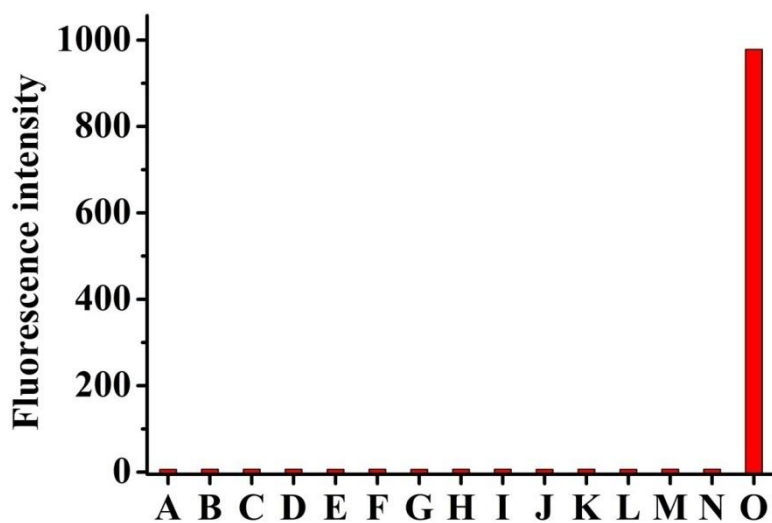


Figure S5 The fluorescence intensity at 530 nm of probe **1** (5.0 μM) upon the addition of the various common amino acid (A-O: 100.0 μM for K^+ , Na^+ , Mg^{2+} , Ca^{2+} , Zn^{2+} , Fe^{3+} , SO_4^{2-} , SCN^- , AcO^- , CO_3^{2-} , NO_3^- , PO_4^{3-} , NO_2^- , H_2O_2 , Cys) ($\lambda_{\text{exc}} = 413 \text{ nm}$, and $t = 15 \text{ min}$).

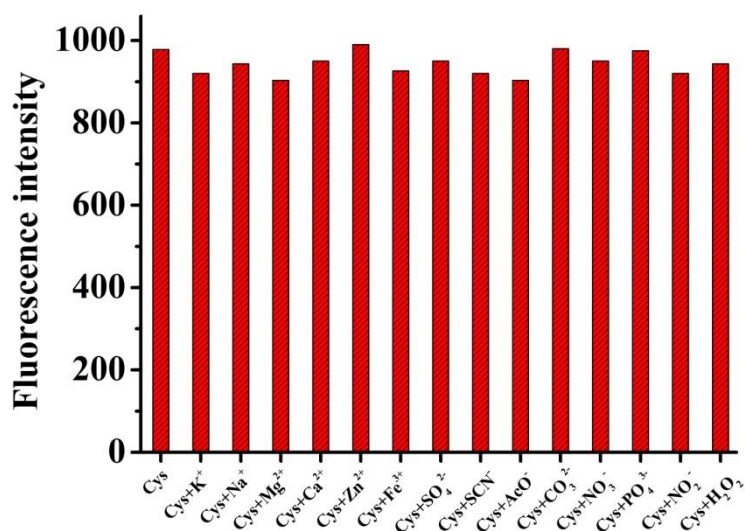


Figure S6 The fluorescence intensity at 530 nm of probe **1** (5.0 μM) to Cys (100.0 μM) with the competition analytes in PBS buffer ($\lambda_{\text{exc}} = 413 \text{ nm}$, and $t = 15 \text{ min}$).

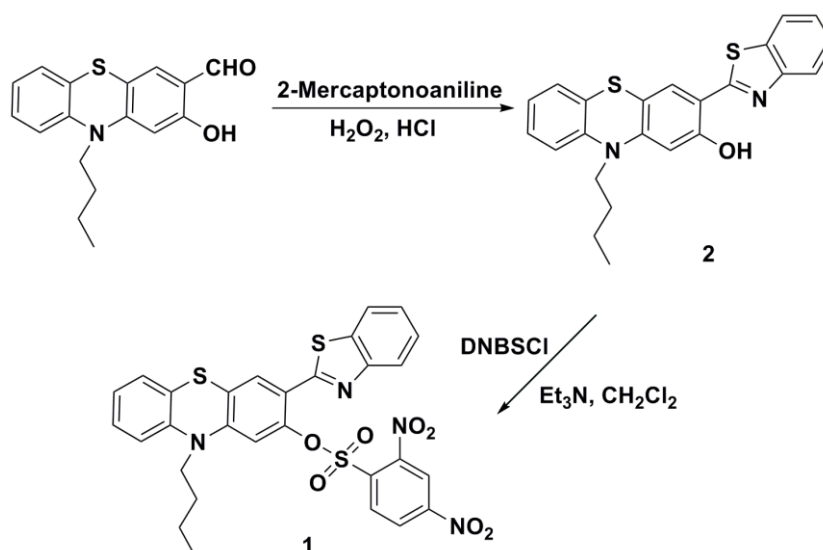


Figure S7 Synthetic route to probe **1**.

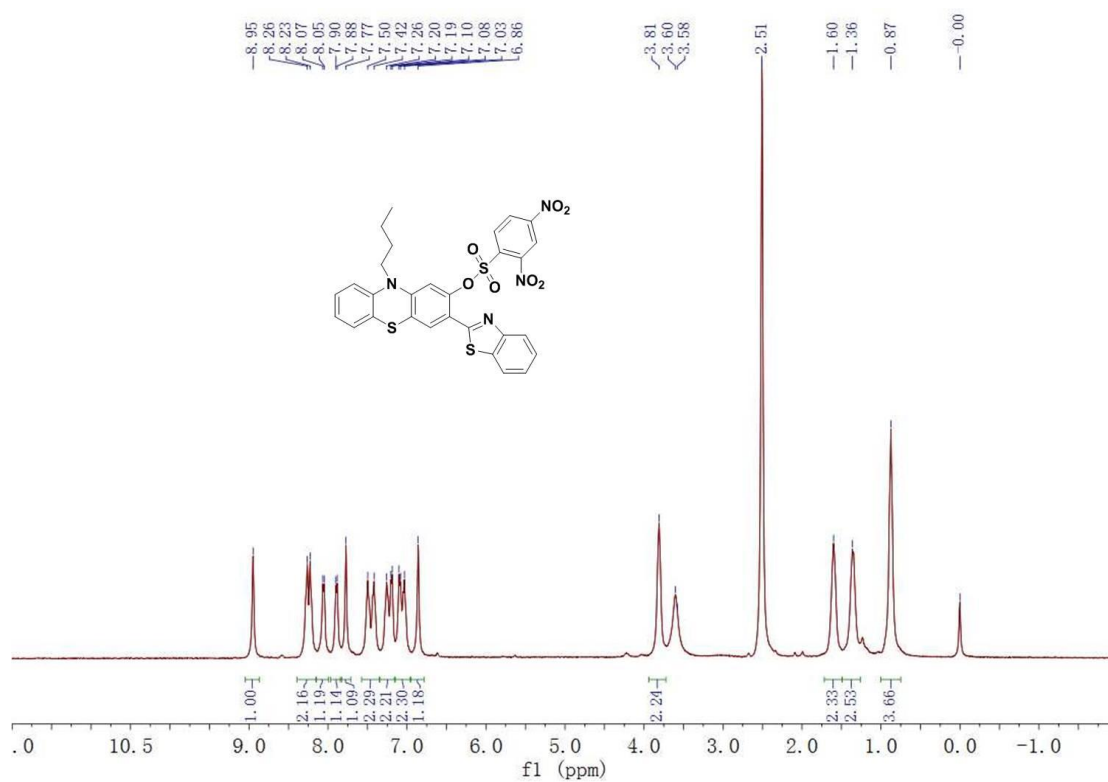


Figure S8 ¹H NMR spectrum of probe **1** in DMSO-*d*₆.

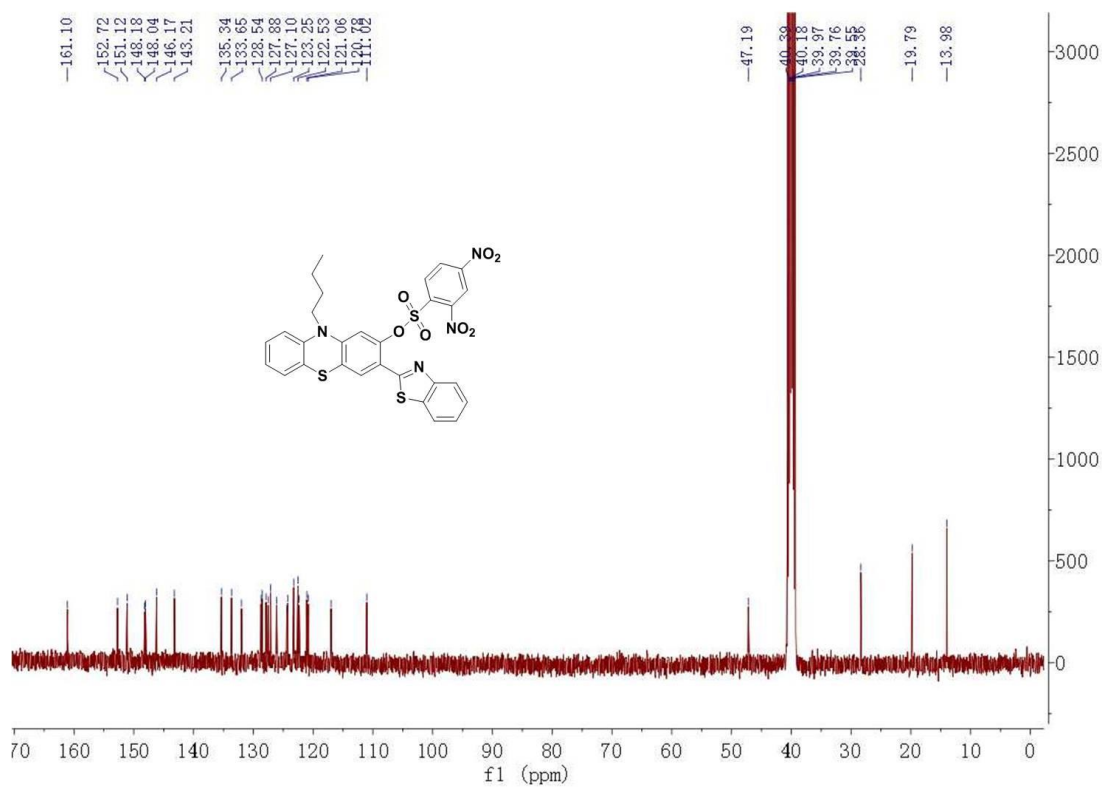


Figure S9 ¹³C NMR spectrum of probe **1** in DMSO-*d*₆.

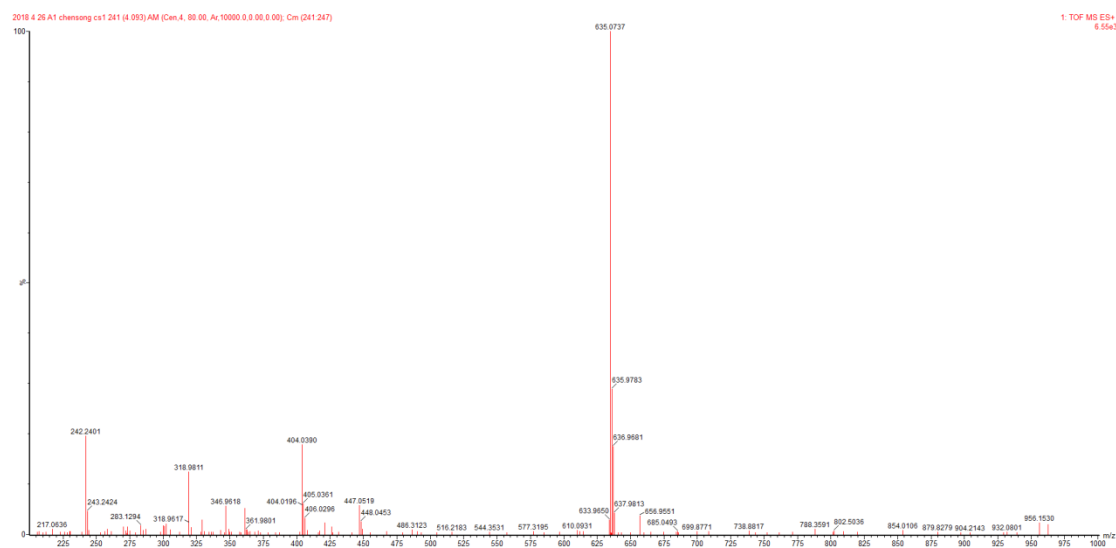


Figure S10 Mass spectrum of probe **1**.

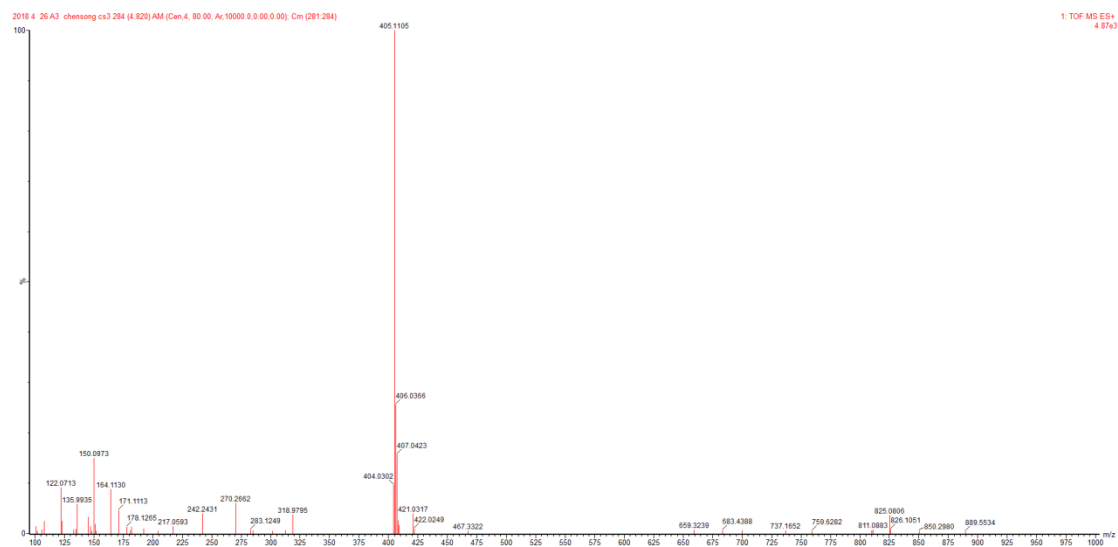


Figure S11 Mass spectrum of probe 1+Cys.

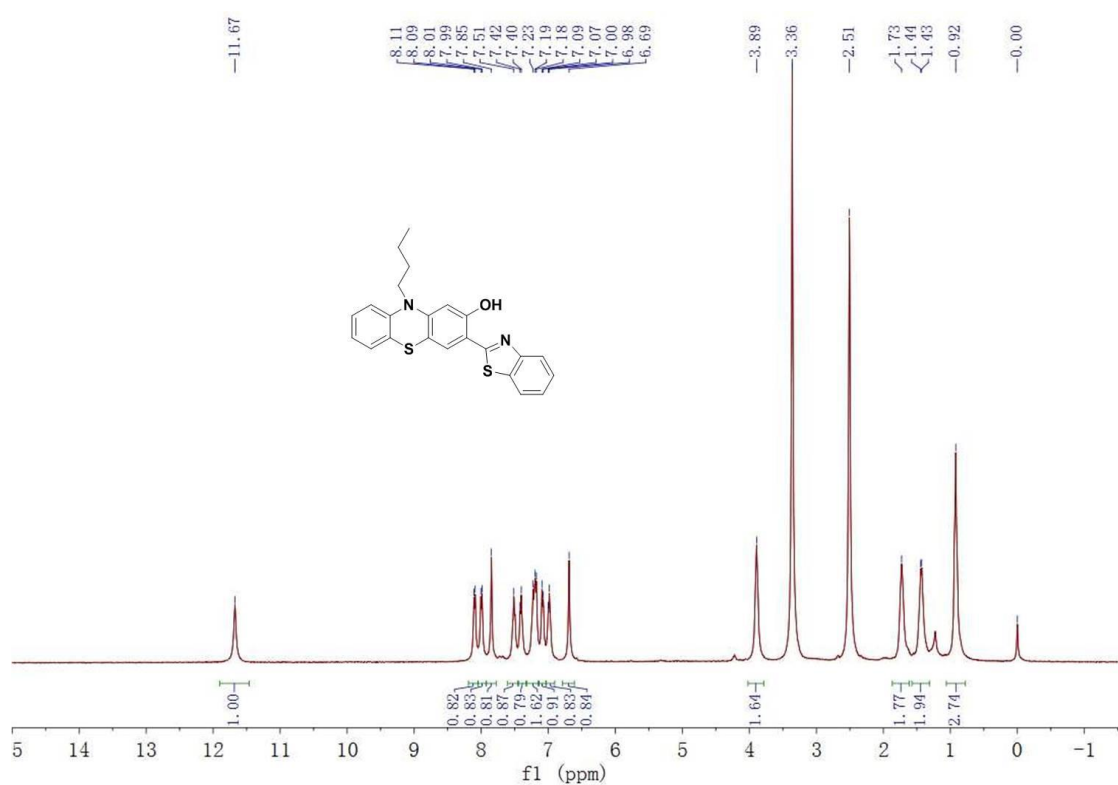


Figure S12 ¹H NMR spectrum of dye 2 in DMSO-*d*₆.

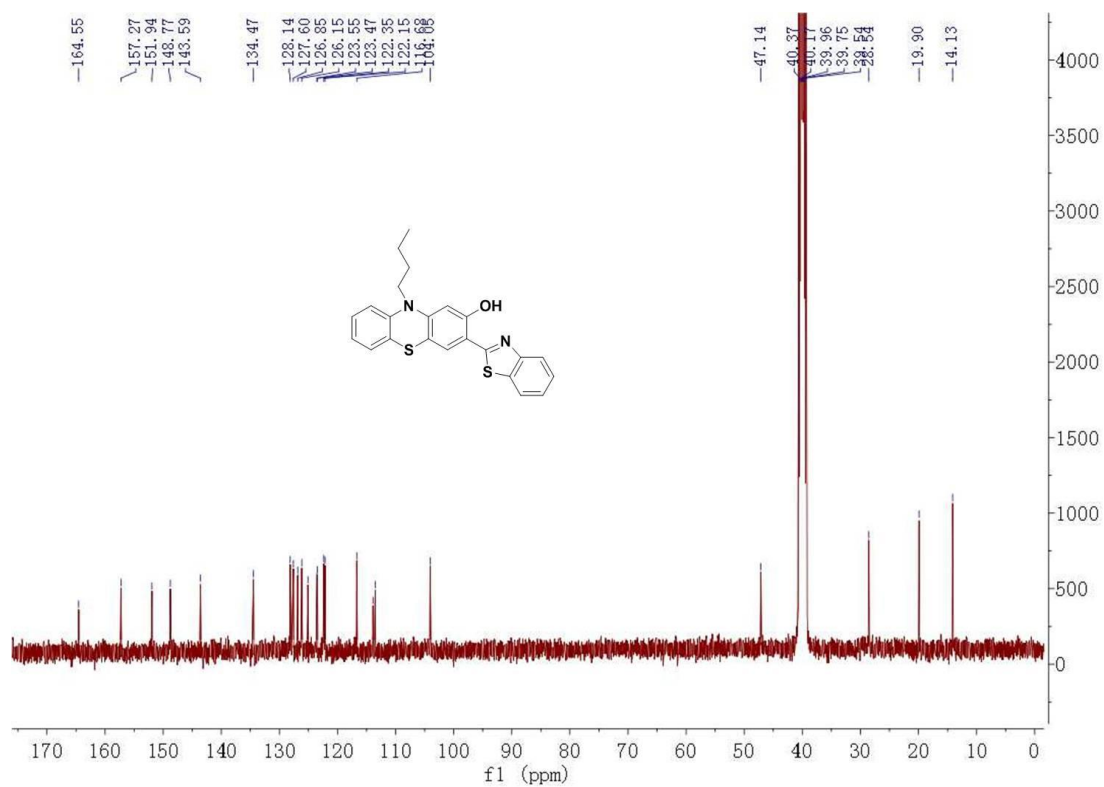


Figure S13 ¹³C NMR spectrum of dye 2 in DMSO-*d*₆.

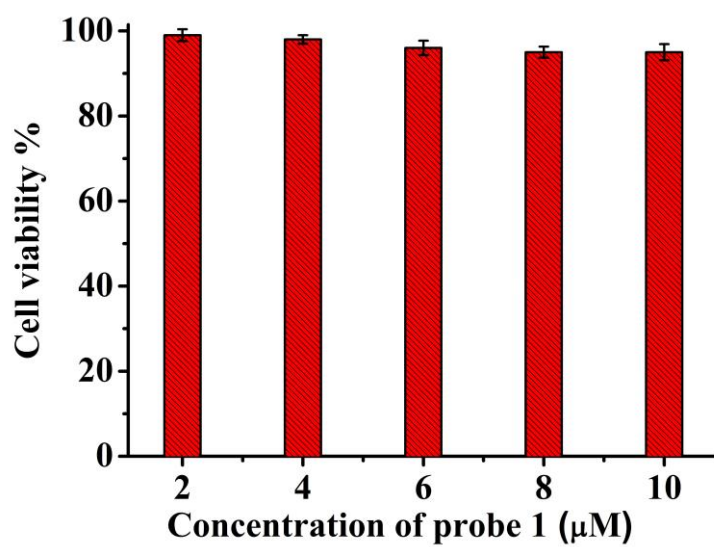


Figure S14 Percentage of viable A549 cells after treatment with different concentrations of probe 1 for 24 hours.

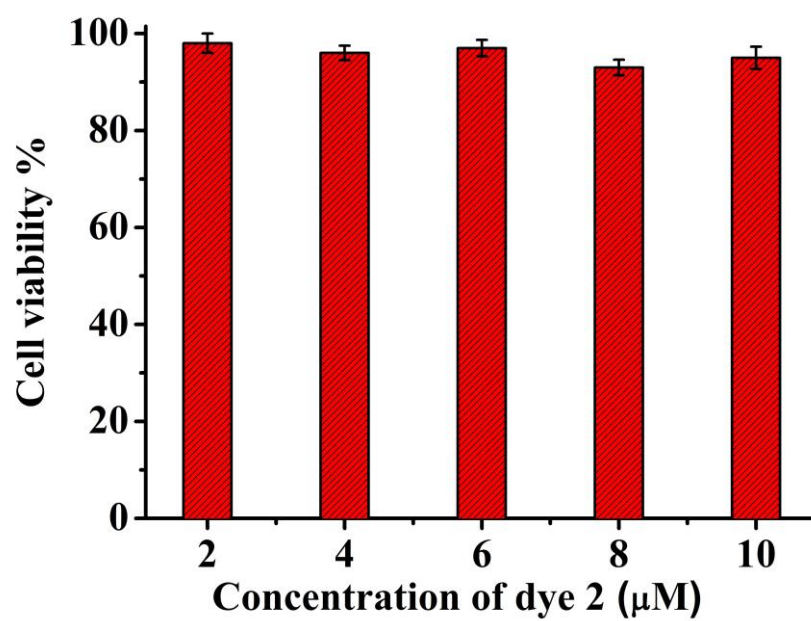
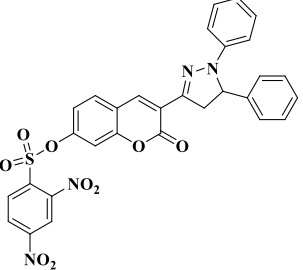
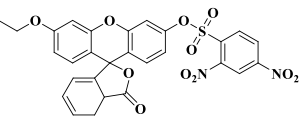
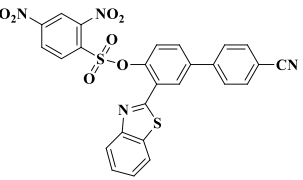
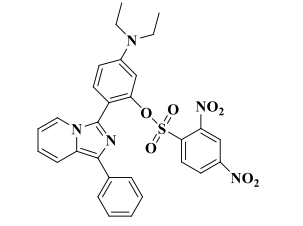
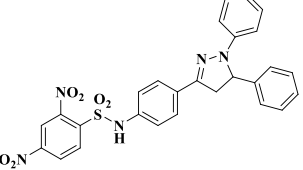
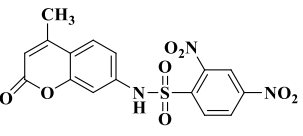
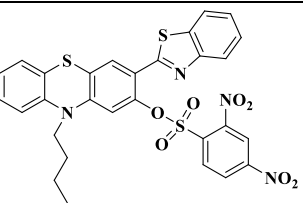


Figure S15 Percentage of viable A549 cells after treatment with different concentrations of dye 2 for 24 hours.

Table S1. Comparison of fluorescent probes for biothiols.

Probes	$\lambda_{\text{ex}}/\lambda_{\text{em}}$ (nm)	Stokes shift (nm)	Limit of detection	Response time	Reference
	450/540	90	$1.5 \times 10^{-8} \text{ M}$	10 min	Sensors actuat B-Chem, 2016, 223, 274-279.
	454/521	67	$0.16 \mu\text{M}$	10 min	Tetrahedron Letters, 2016, 57, 2478-2483
	280/482	202	$2.0 \times 10^{-8} \text{ M}$	20 min	Tetrahedron, 2017, 73, 589-593
	309/510	201	$0.17 \mu\text{M}$	10 min	Tetrahedron Letters, 2017, 58, 2654-2657.
	370/464	94	$4.11 \times 10^{-7} \text{ M}$	12 h	Analyst, 2013, 138, 7169-7174.
	353/450	97	30 nM	2 h	Chem Commun, 2013, 49,4640-4642.
	413/530	117	$0.12 \mu\text{M}$	15 min	This work

