Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

A naphthalimide-indole fused chromophore-based fluorescent probe for detection of biothiol with a red emission and a large Stokes shift

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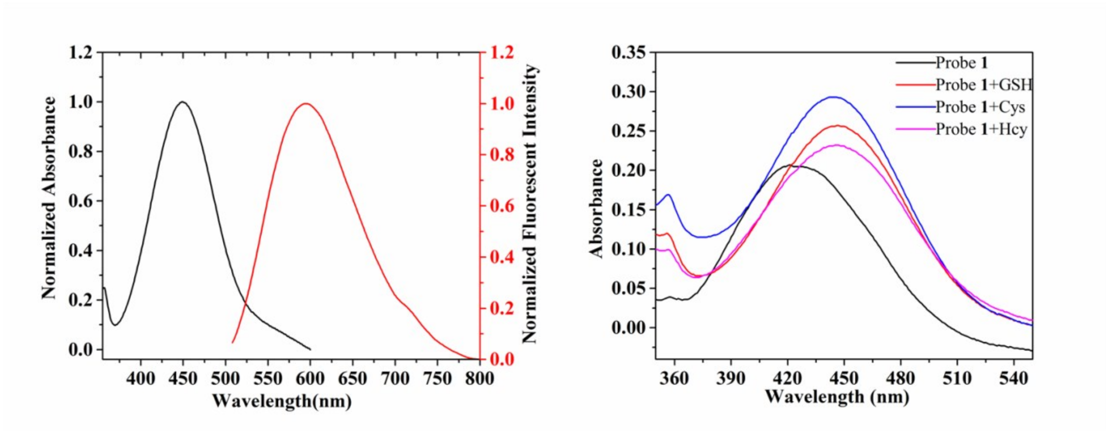


Fig. S1. Left: The normalized absorption and emission spectra of Compound **4** in PBS buffer (10.0 mM, 1.0 mM CTAB, pH = 7.4). Right: The absorption and emission spectra of probe **1** in the absence and presence of Cys, Hcy and GSH in PBS buffer (10.0 mM, 1.0 mM CTAB, pH = 7.4).

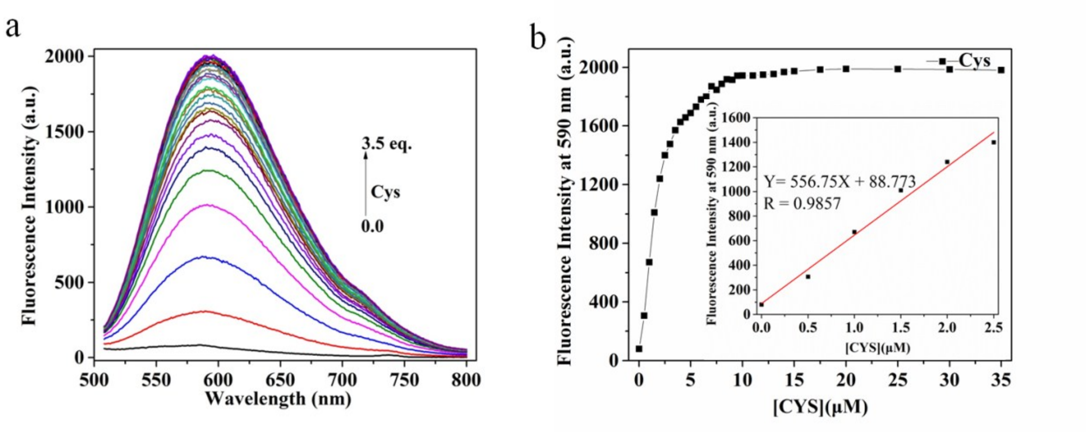


Fig. S2. (a) Fluorescence spectra of Probe **1** (10.0 μM) after reacting with Cys (0.0-3.5 equiv.) in PBS buffer (10.0 mM, 1.0 mM CTAB, pH = 7.4) for 4 min at 25 °C (λ_{ex} = 488 nm). (b) Fluorescence intensity at 590 nm of Probe **1** (10.0 μM) against Cys concentration. Inset: the linear correlation between fluorescence intensity at 590 nm and the concentration of Cys (0-2.5 μM).

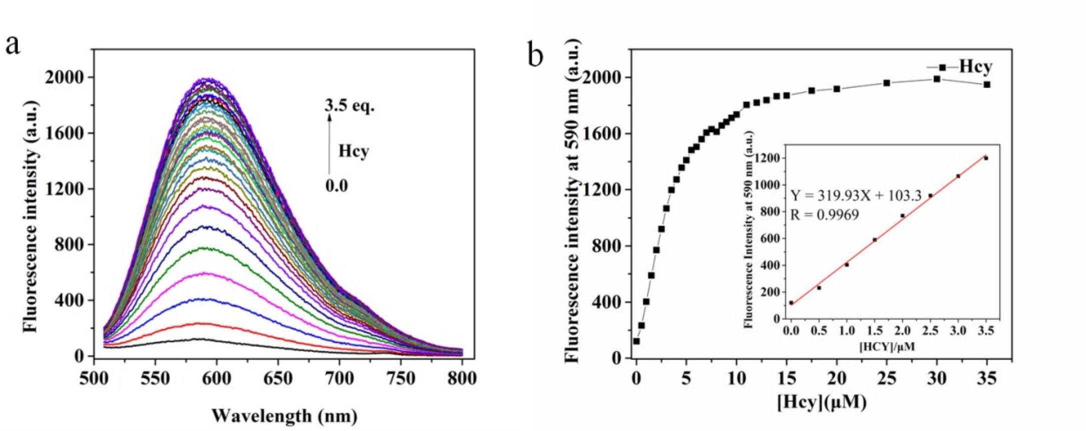


Fig. S3. (a) Fluorescence spectra of Probe **1** (10.0 μM) and after reacting with Hcy (0.0-3.5 equiv.) in PBS buffer (10.0 mM, 1.0 mM CTAB, pH = 7.4) for 4 min at 25 °C (λ_{ex} = 488 nm). (b) Fluorescence intensity at 590 nm of Probe **1** (10.0 μM) against Hcy concentration. Inset: the linear correlation between fluorescence intensity at 590 nm and the concentration of Hcy (0-3.5 μM).

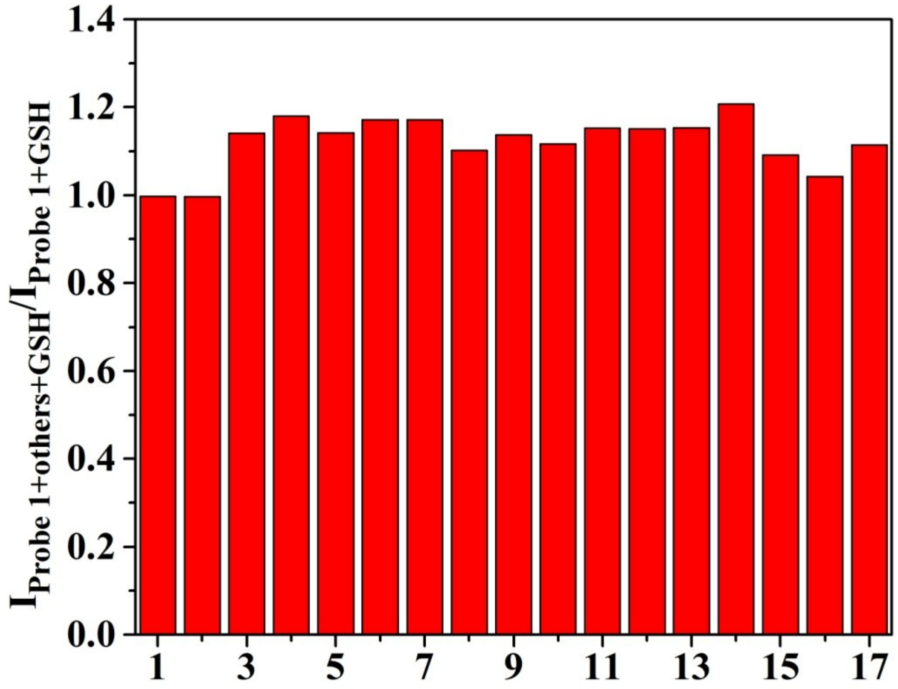


Fig. S4. Fluorescence spectra of Probe **1** (10.0 μM) towards GSH (3.5 equiv.) with other relevant species (3.5 equiv.) in PBS buffer (10.0 mM, 1.0 mM CTAB, pH = 7.4). The spectra were recorded after reacting 4 min at 25 °C. λ_{em} = 590 nm, λ_{ex} = 488 nm. (1. Arg, 2. Ile, 3. Ser, 4. His, 5. Ala, 6. Phe, 7. Glu, 8. Trp, 9. Thr, 10. Val, 11. Lys, 12. Asp, 13. Tyr, 14. Leu, 15. Gly, 16. Pro, 17. Met)

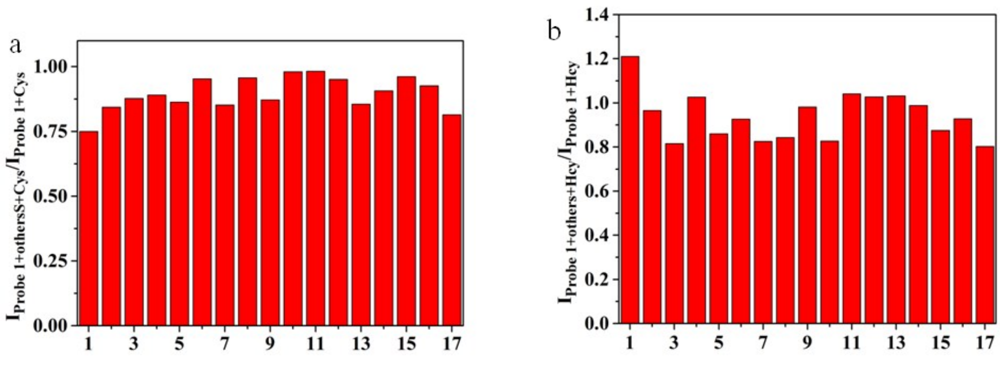


Fig. S5. Fluorescence spectra of Probe **1** (10.0 μM) towards (a) Cys and (b) Hcy (3.5 equiv). with some relevant species (3.5 equiv.) in PBS buffer (10.0 mM, 1.0 mM CTAB, pH = 7.4). The spectra were recorded after reacting 4 min at 25 °C. λ_{em} = 590 nm, λ_{ex} = 488 nm. (1. Arg, 2. Ile, 3. Ser, 4. His, 5. Ala, 6. Phe, 7. Glu, 8. Trp, 9. Thr, 10. Val, 11. Lys, 12. Asp, 13. Tyr, 14. Leu, 15. Gly, 16. Pro, 17. Met)

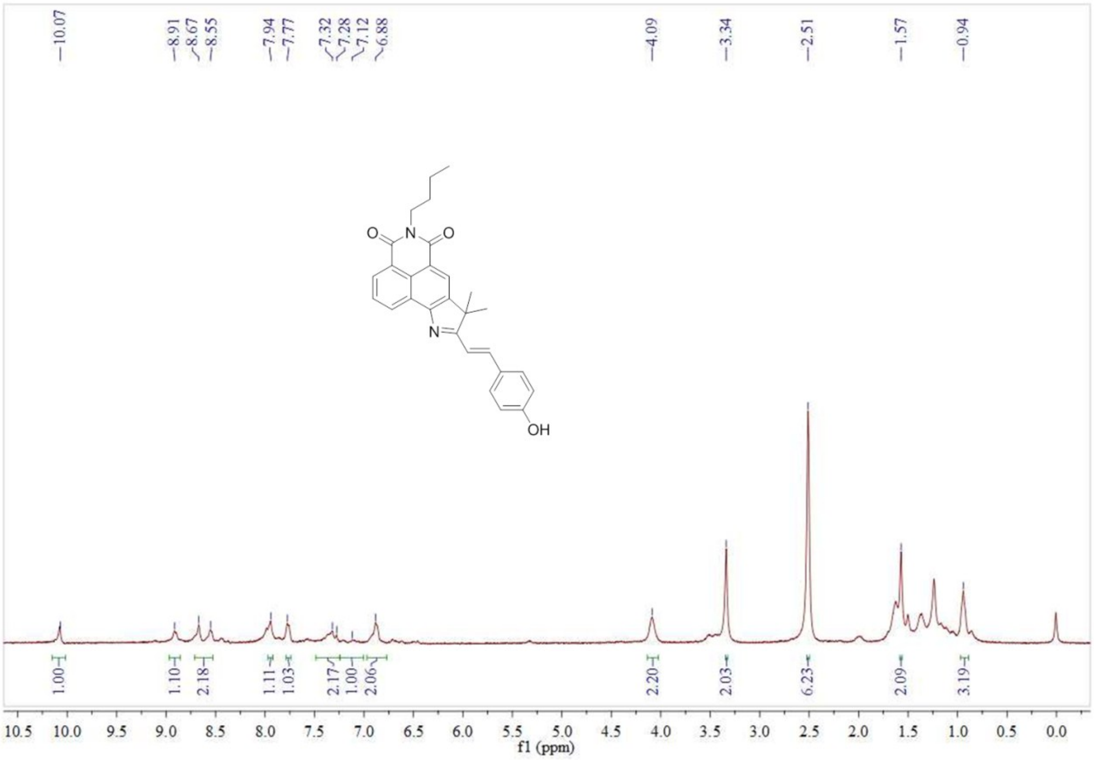


Fig. S6. The [1]H NMR spectrum of reaction product between Probe **1** and Cys in DMSO-d_6.

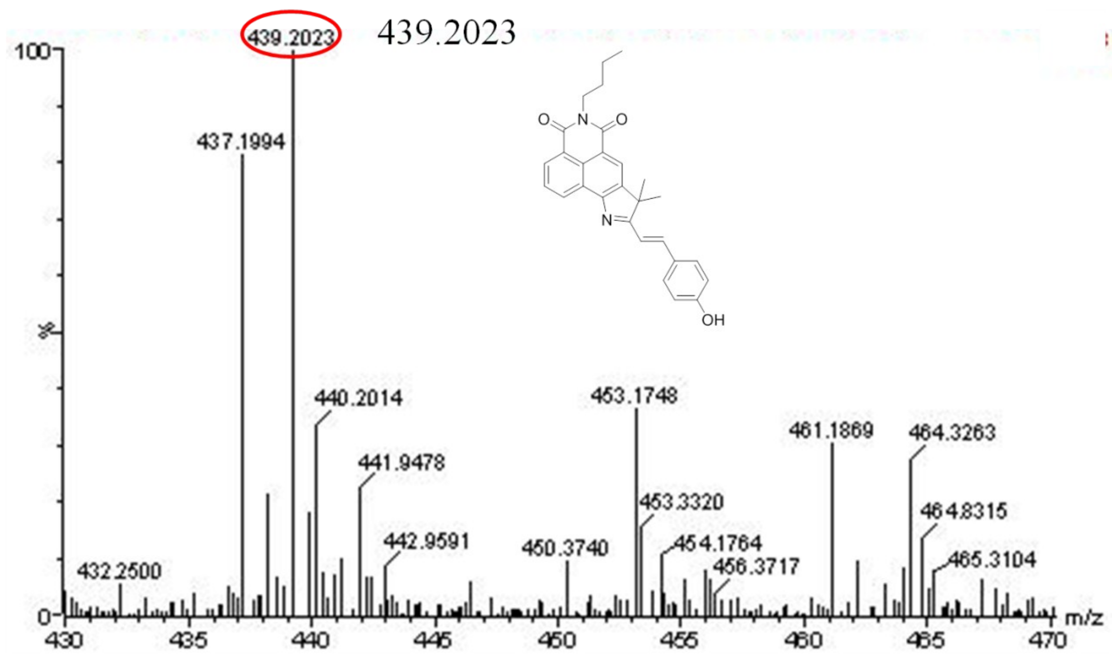


Fig. S7. The HRMS spectrum of reaction product between Probe **1** and Cys.

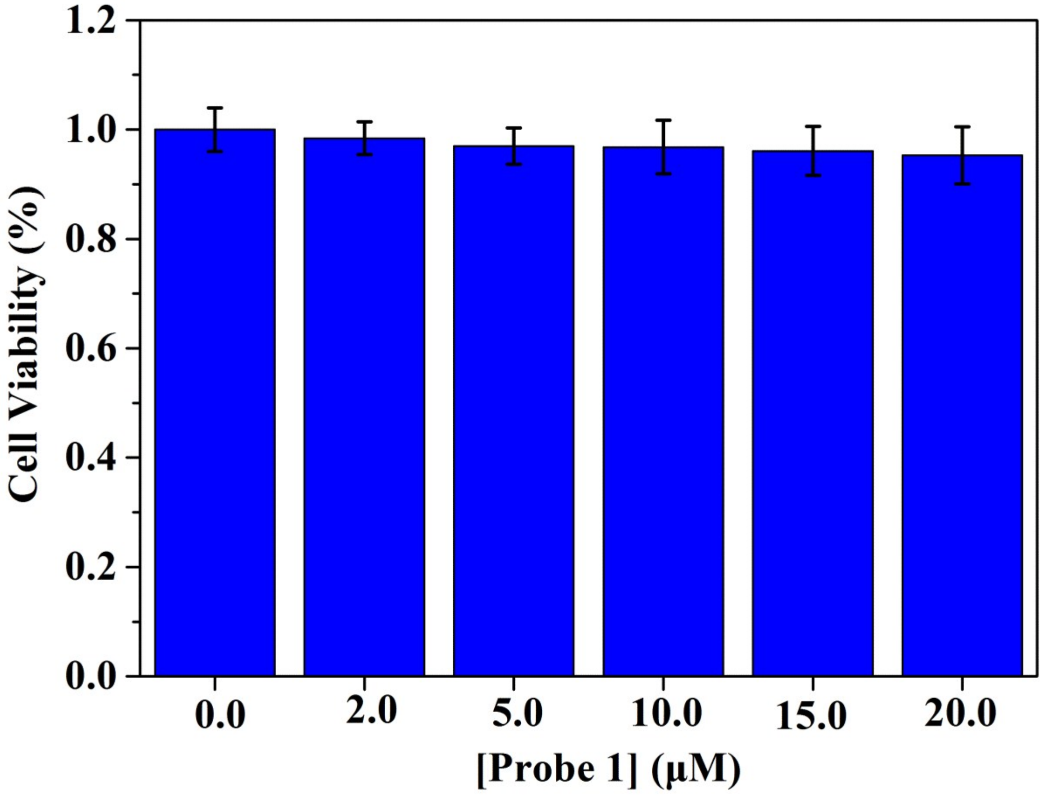


Fig. S8. The cytotoxicity of Probe **1** at different concentrations (0 μM, 2 μM, 5 μM, 10 μM, 15 μM and 20 μM) in MCF - 7 cells for 24 hours.

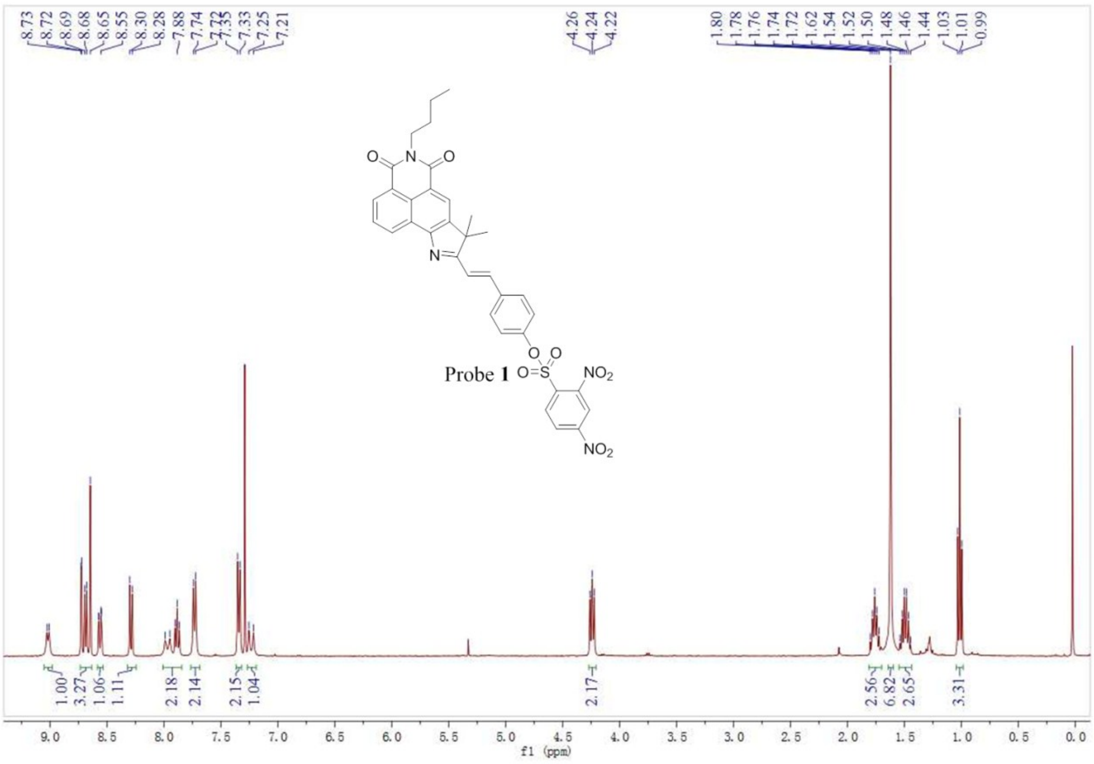


Fig. S9. The ^1H NMR spectrum of Probe **1** in $CDCl_3$.

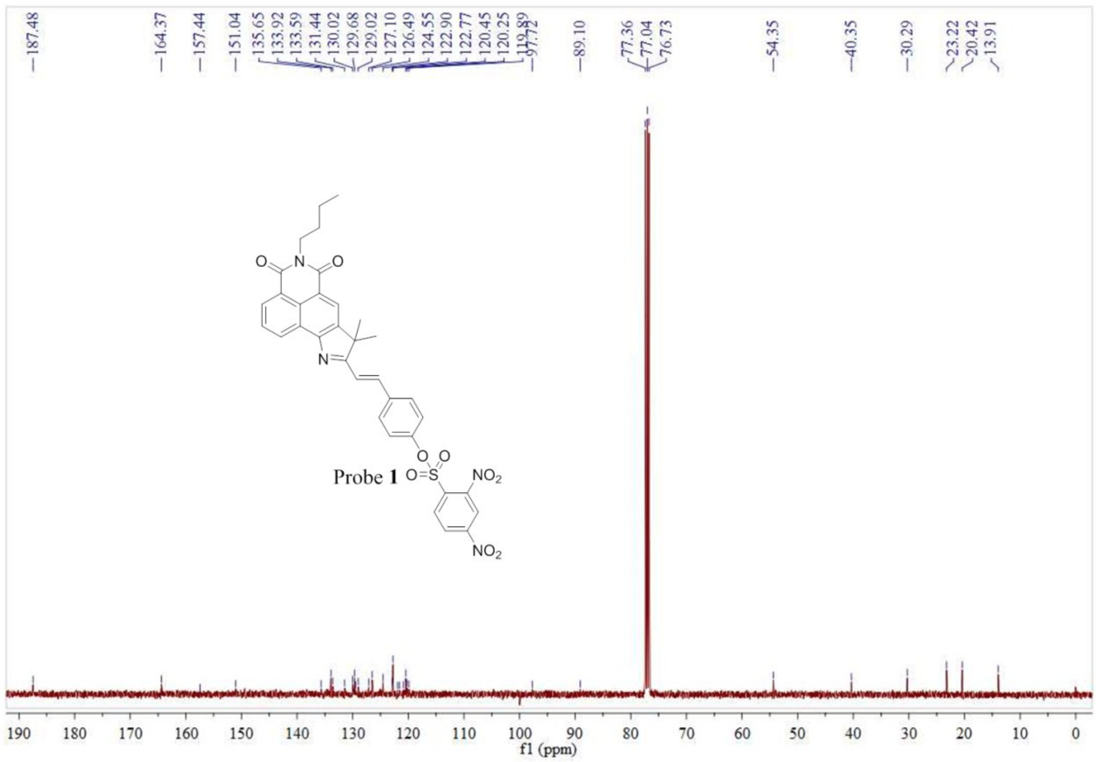


Fig. S10. The ^{13}C NMR spectrum of Probe **1** in $CDCl_3$.

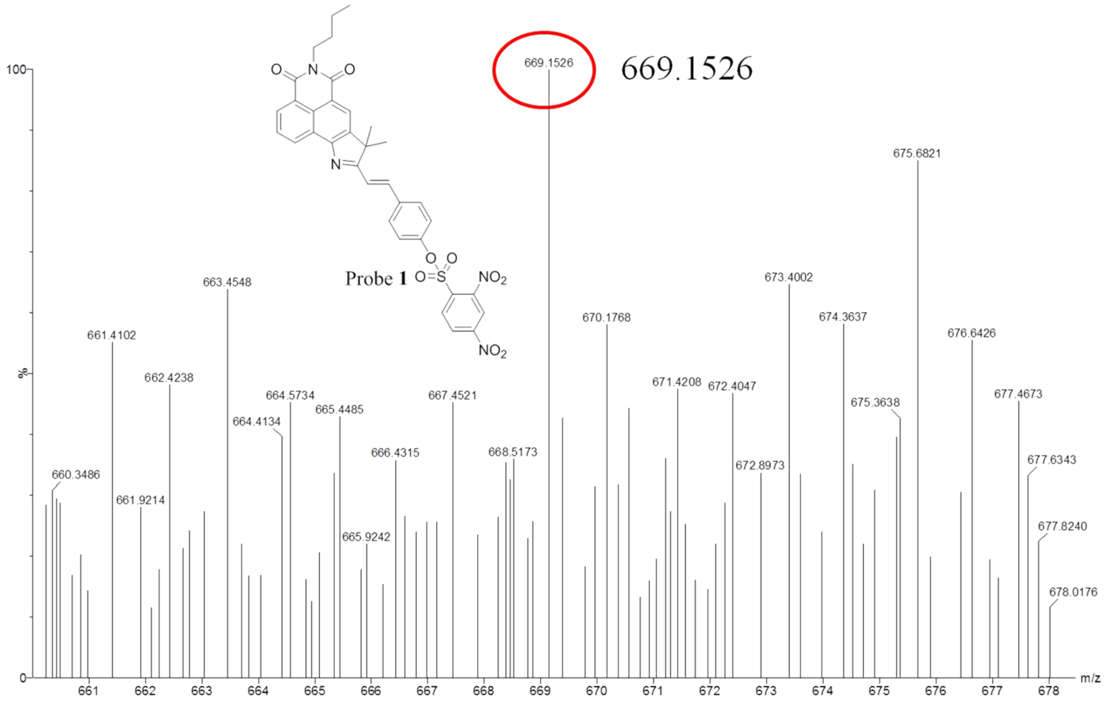


Fig. S11. The HRMS of Probe **1**.

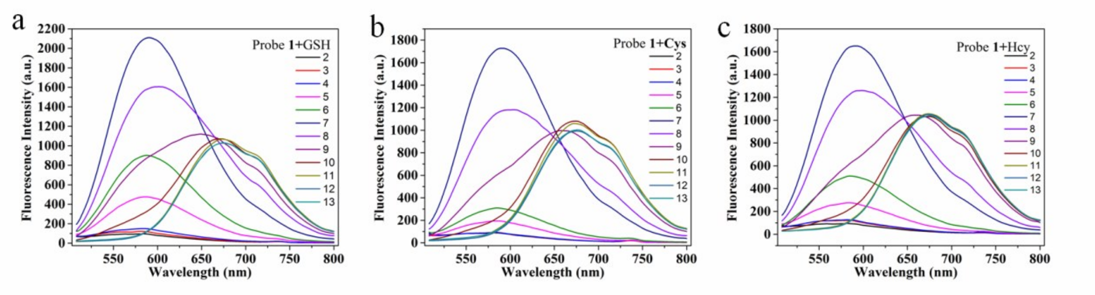
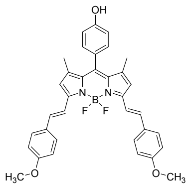
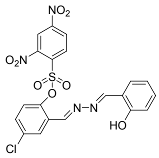
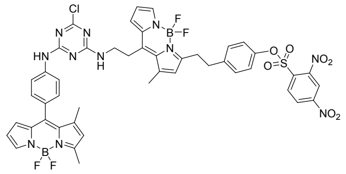
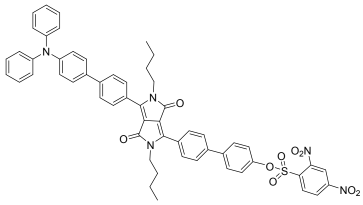
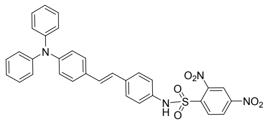
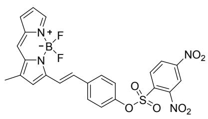
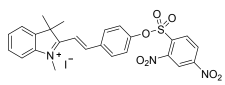
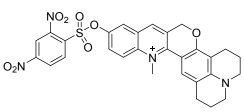
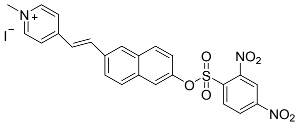
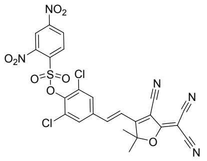
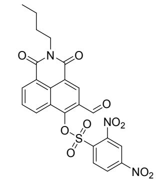
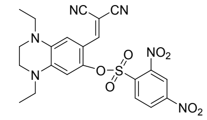
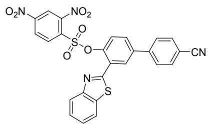
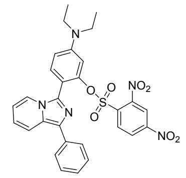
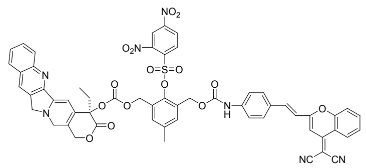
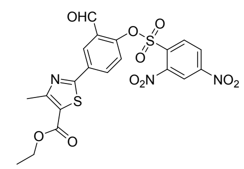
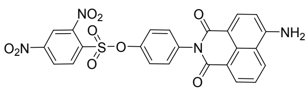
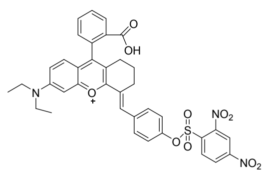
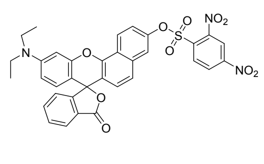
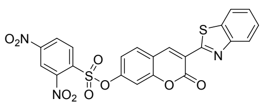
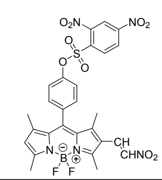
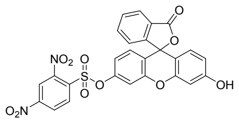


Fig. S12. The emission spectra of probe **1** in response to biothiols at different pH values.

Table. S1 Fluorescent probes for biothiols.

Probe	$\lambda_{ex}/\lambda_{em}$	Stokes shift	Response time	Literature
	646 nm/656 nm	10 nm	90 min	Dyes and Pigments, 2018, 152, 85-92
	365 nm/558 nm	193 nm	40 min	Dyes Pigments, 2014, 108 24-31
	490 nm/580 nm	90 nm	60 min	Biomaterials, 2014, 35 6078-6085
	510 nm/615 nm	105 nm	30 min	Sensor. Actuat. B-Chem., 2015, 211, 275-282.
	365 nm/440 nm	75 nm	/	Sensor. Actuat. B-Chem., 2016, 233, 307-313.
	527 nm/570 nm	43 nm	60 min	Org. Biomol. Chem., 2010, 8, 3627-3630.
	490 nm/553 nm	63 nm	/	Org. Biomol. Chem., 2009, 7 4017-4020
	498 nm/613 nm	115 nm	120 min	Chinese Chem. Lett., 2019, 30, 563-565.
	392 nm/583 nm	191 nm	2 min	Analyst, 2019, 144, 439-447.
	560 nm/625 nm	65 nm	15 min	Chem. Commun. 2018, 54, 4786-4789

	450nm/525nm	75 nm	20 min	Talanta, 2018, 179, 326-330.
	485nm/619nm	134 nm	100 min	Tetrahedron, 2016, 72, 6909-6913
	320nm/482nm	162 nm	20 min	Tetrahedron, 2017, 73, 589-593.
	309nm/510nm	201 nm	10 min	Tetrahedron Lett., 2017, 58, 2654-2657
	365 nm/437 nm 500 nm/674 nm	72 nm 174 nm	5 h	Biomaterials,2017, 139, 139-150
	346 nm/500 nm	155 nm	30 min	Dyes Pigments, 2018, 156, 338-347.
	420 nm/550 nm	130 nm	25 min	Anal. Chem., 2017, 89 8097-8103.
	580 nm/660 nm	80 nm	10 min	J. Mater. Chem. B, 2017, 5, 3836-3841.
	586 nm/635 nm	49 nm	30 min	Res. Chem. Intermediat., 2017, 43, 7387-7398.
	453 nm/493 nm	40 nm	30 min	Dyes Pigments, 2018, 149 475-480
	504 nm/517 nm	13 nm	10 min	Dyes Pigments, 2018, 152, 29-35.

	337 nm/347 nm	10 nm	27 min	Food Chem., 2018, 262, 67-71