Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.
This journal is © The Royal Society of Chemistry 2017

Supporting information for

A Novel Near-infrared Fluorescent Probe with Large Stokes Shift for Biothiols and the Application for *in vitro* and *in vivo* Fluorescence Imaging

Keyin Liu, Huiming Shang, Xiuqi Kong, Weiying Lin*

Institute of Fluorescent Probes for Biological Imaging, School of Materials Science and Engineering, School of Chemistry and Chemical Engineering, University of Jinan, Jinan, Shandong 250022, PR China.

E-mail: weiyinglin2013@163.com

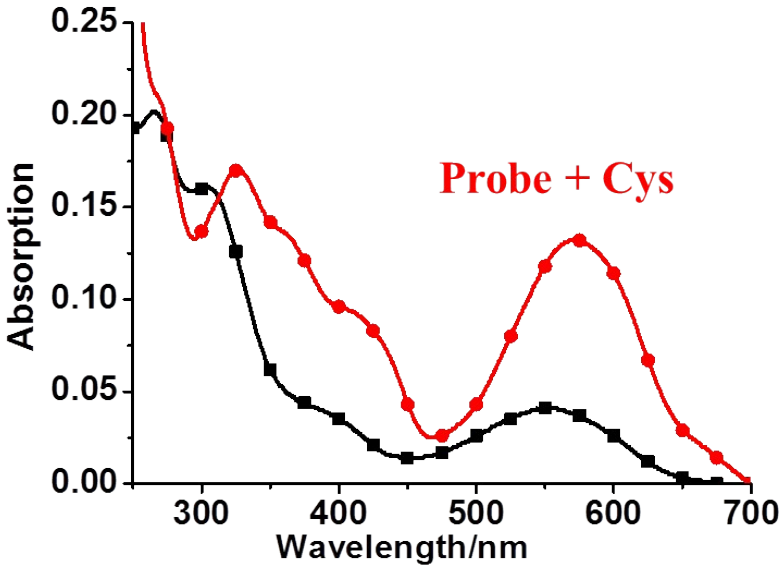


Fig. S1 The absorption spectra of **CS-thiols** with Cys, 10 μM of **CS-thiols** in PBS (Black line), 10 μM of **CS-thiols** in the presence of 100 eq. of Cys (Red line).

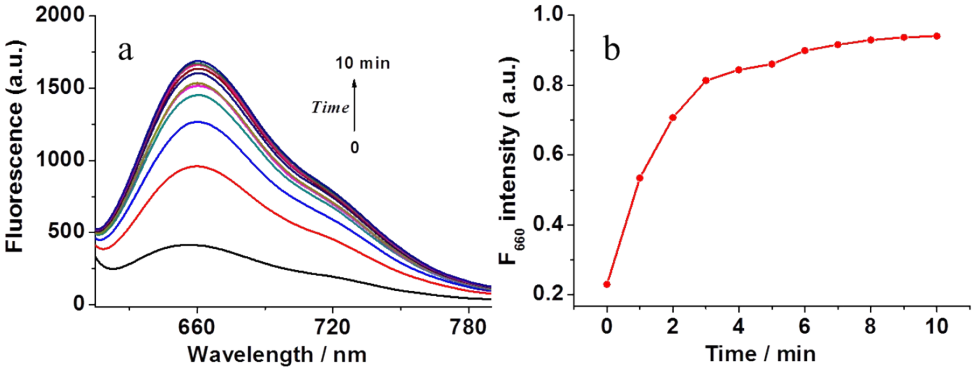


Fig. S2 (a) The fluorescence change of 10 μM **CS-thiols** and (b) the fluorescence intensity change at 660 nm with time in the presence of 100 eq. of Cys, λ_{ex} = 580 nm, 25 ^{o}C.

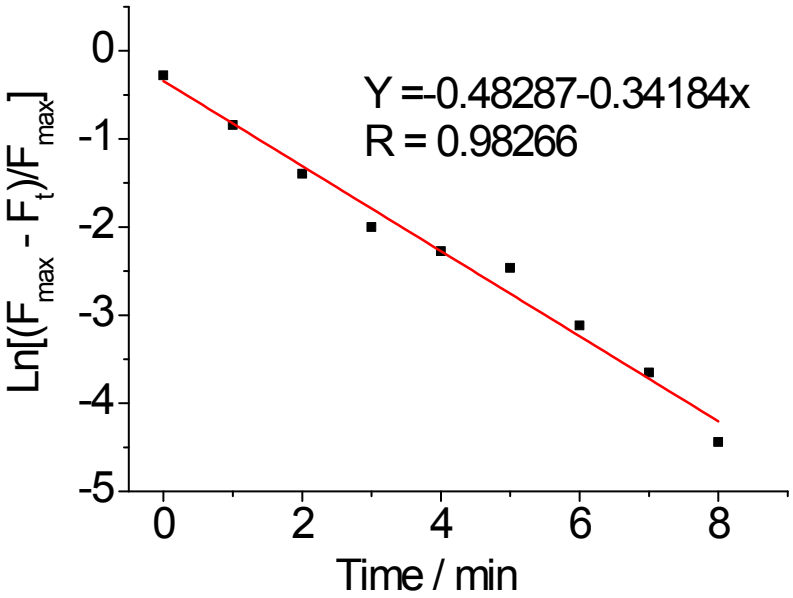


Fig. S3 *Pseudo* first-order kinetic plot of **CS-thiols** reacted with Cys in pH 7.2, 10 mM PBS buffer/DMSO (8:2 v/v). Slop = 0.3418 min^{-1}. 10 μM **CS-thiols** in the presence of 100 eq. of Cys, the fluorescence intensity change at 660 nm with time, λ_{ex} = 580 nm, 25 ^{o}C.

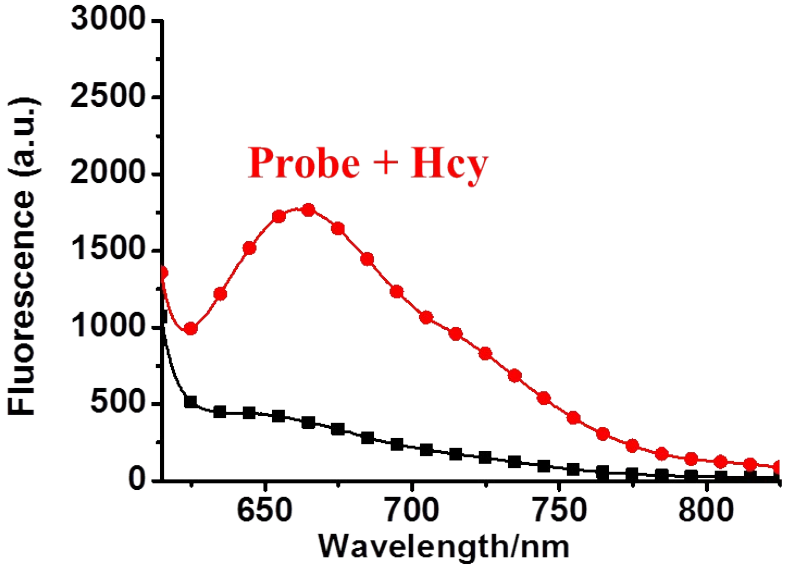


Fig. S4 The emission spectra of **CS-thiols** with Hcy, 10 μM of **CS-thiols** in PBS (Black line), 10 μM of **CS-thiols** in the presence of 100 eq. of Hcy (Red line), λ_{ex} = 580 nm.

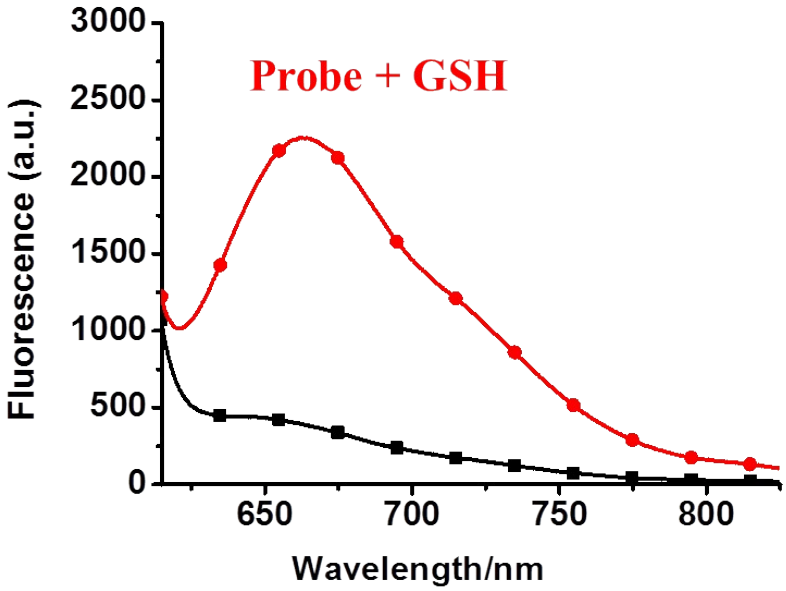
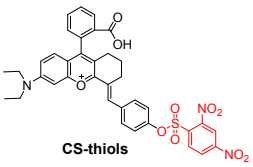
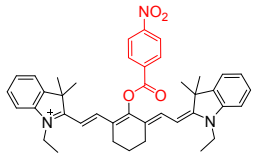
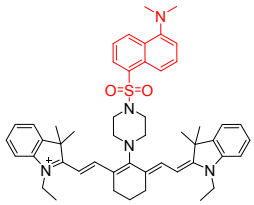
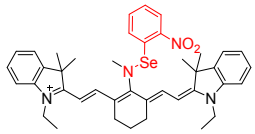
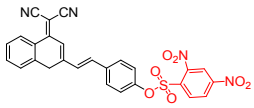
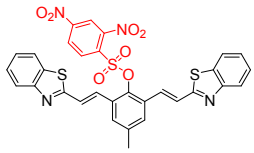
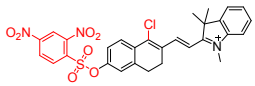
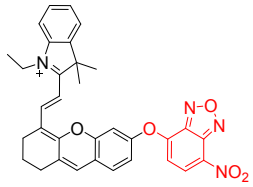
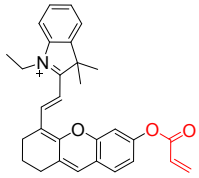
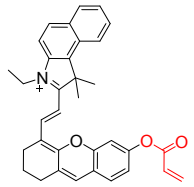
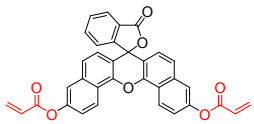
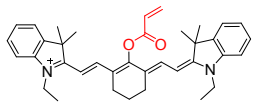
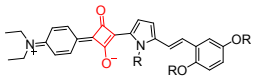
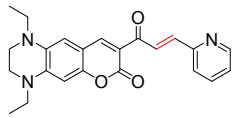
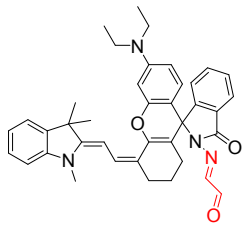
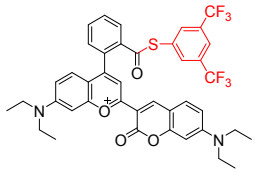


Fig. S5 The emission spectra of **CS-thiols** with GSH, 10 μM of **CS-thiols** in PBS (Black line), 10 μM of **CS-thiols** in the presence of 100 eq. of GSH (Red line), λ_{ex} = 580 nm.

Table S1. Comparison of **CS-thiols** with other representative near infrared fluorescent

probes for thiols detection reported in the literature.

Ref.	Probes	λ_{em} / nm	Design mechanism	Response time/ min	Selectivity	Imaging application	Stokes Shift/nm
This work		660/ 720	Deprotection	10	Thiols	HeLa cells, animals	110
Biosens. Bioelectron., 2015, **74**, 156-164.		640/ 785	Deprotection	10	Cys	HepG2 animals	20
J. Am. Chem. Soc., 2014, **136**, 5351-5358.		736	Deprotection	20	GSH	HeLa, animals	Not given
Chem. Eur. J., 2012, **18**, 11343-11349.		750	Deprotection	3	Not given	RAW 264.7, tissue	Not given
Chem. Commun., 2014, **50**, 1751-1753.		690	Deprotection	Not given	Thiols	HeLa cells	130
J. Mater. Chem. B, 2016, **4**, 6662-6669.		679	Deprotection	30	Thiols	Fibroblast L929 cells	Not given
Chem. Sci., 2016, **7**, 1896-1903.		642/ 700	Substitution and deprotection	60	Thiols	HeLa cells, animals	Not given
Biosens. Bioelectron., 2016, **81**, 341-348.		550/ 716	Deprotection	5	GSH and Cys/Hcy	HeLa cells	23
Anal. Chem., 2015, **87**, 4856-4863.		697	Addition and deprotection	5	Cys	HeLa cells	23

Acs Appl. Mater. Interface, 2015, **7**, 27968-27975.		735	Addition and deprotection	10	Cys	HeLa cells; animals	25
Biosens. Bioelectron., 2015, **68**, 316-321.		690	Addition and deprotection	10	Cys	HeLa cells	78
Chem. Sci., 2012, **3**, 2760-2765.		560/ 740	Addition and deprotection	30	Cys	MCF-7 cells	20
Chem. Sci., 2016, **7**, 4110-4116.		520/ 700	Addition	10	Thiols	Huh-7 cell, animals	20
Tetrahedron Lett., 2015, **56**, 7176-7179.		660	Addition	37.5	Cys	HeLa cells	Not given
Anal. Chem., 2016, **88**, 9746-9752.		735	Addition and deprotection	3	GSH	HeLa cells, tissue	37
Anal. Chem., 2014, **86**, 1800-1807.		474/ 694	Deprotection	10	Cys / Hcy	HeLa cells	Not given

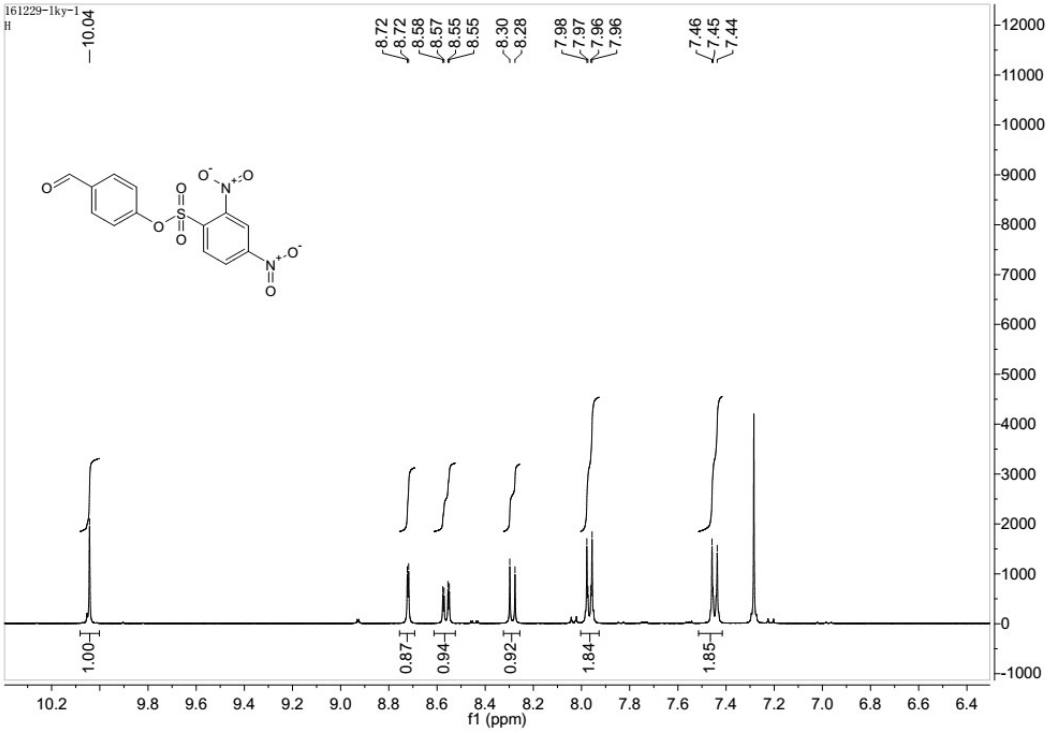


Fig. S6 ^{1}H NMR (400 MHz, CCl_3D) spectrum of compound **9**.

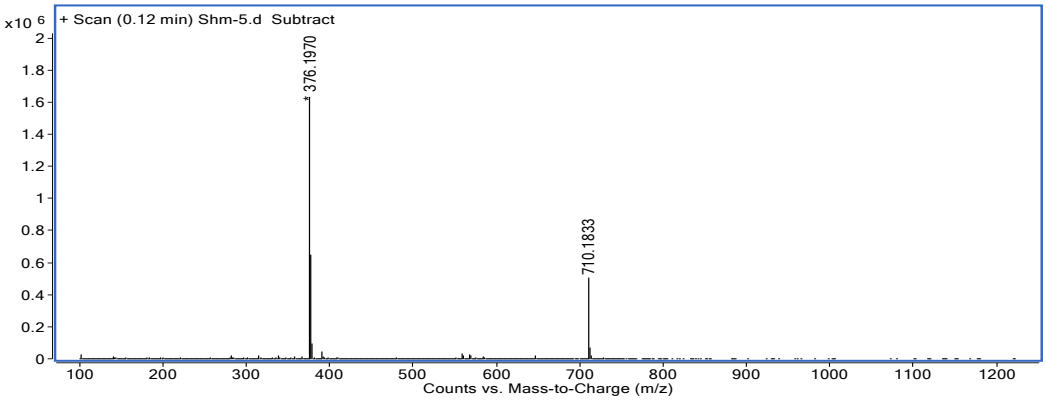


Fig. S7 HRMS spectrum of **CS-thiols**.

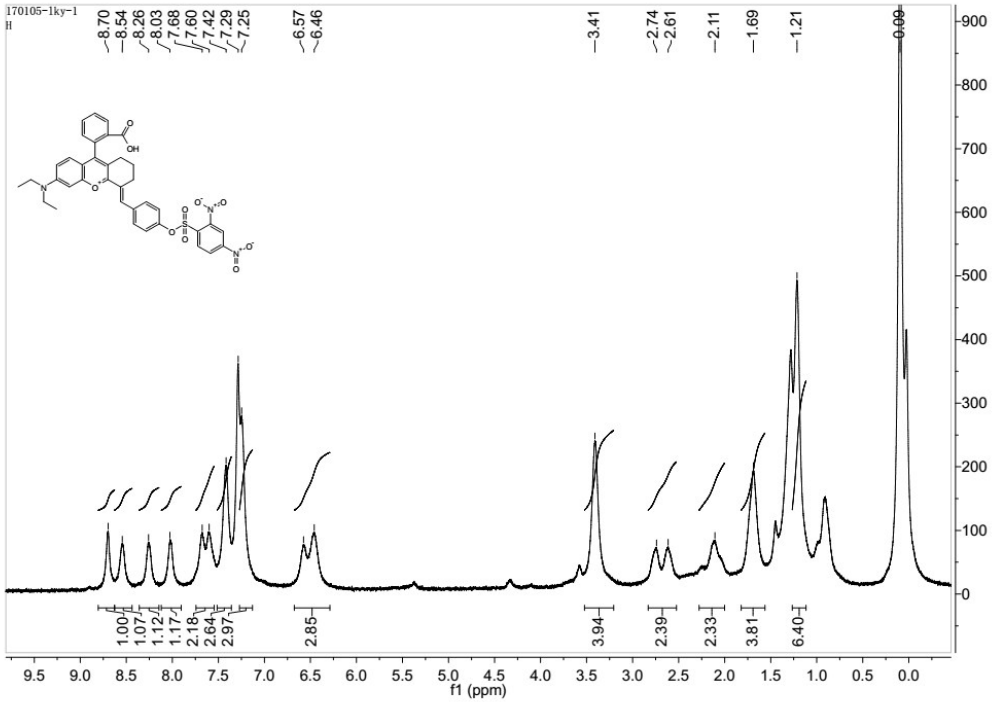


Fig. S8 ^{1}H NMR (400 MHz, CCl_3D) spectrum of **CS-thiols**.

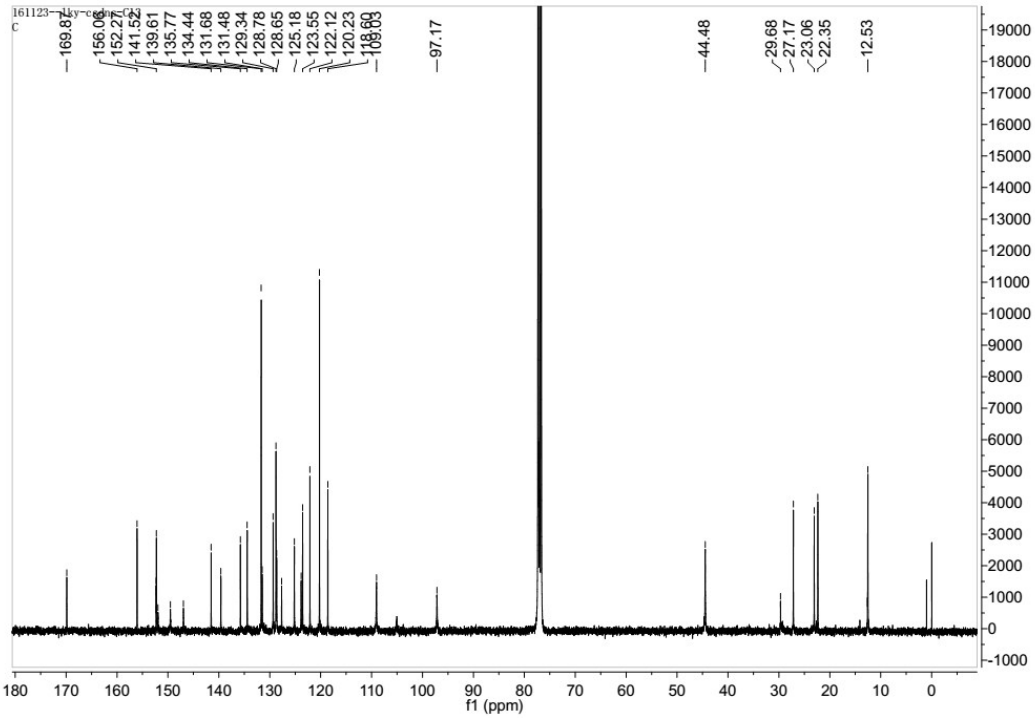


Fig. S9 ^{13}C NMR (100 MHz, CCl_3D) spectrum of **CS-thiols**.