Supporting Information

Near-infrared turn-on fluorescent probe for discriminative detection of Cys and application in vivo imaging

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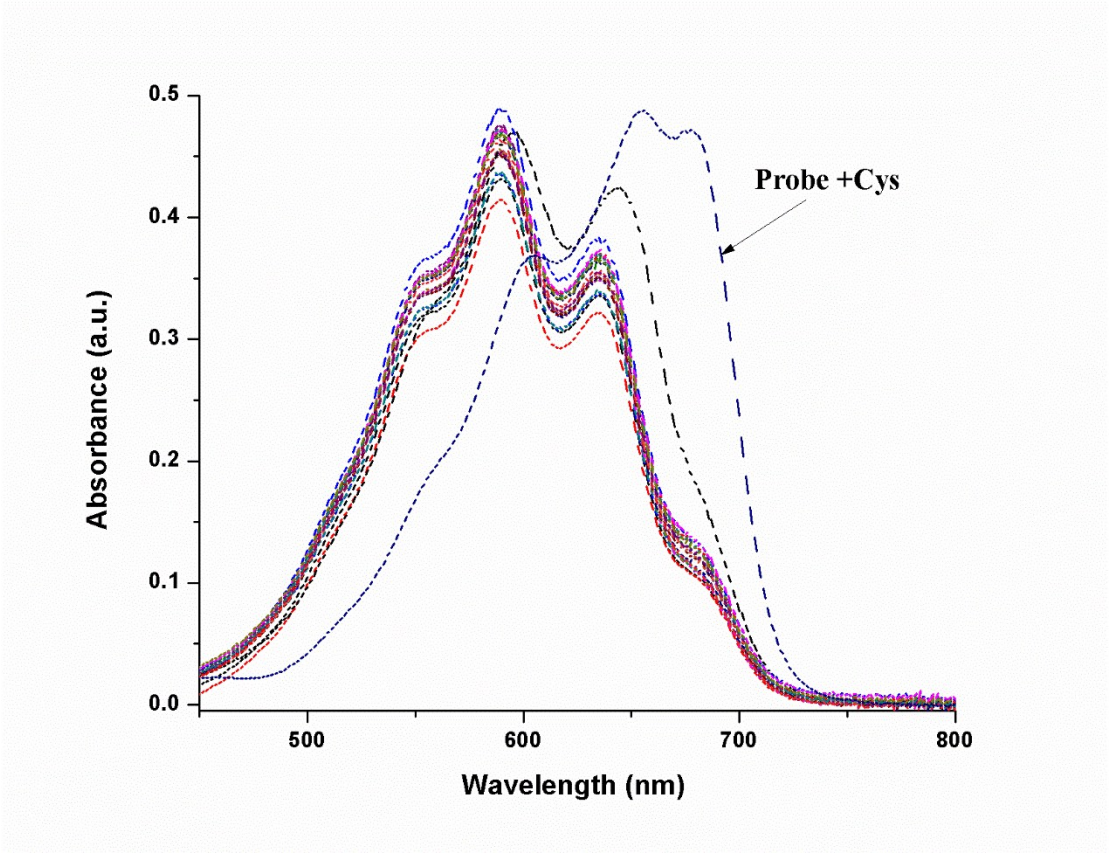

Fig. S1 Absorption of NIRHA in the presence of 4.8 eq Cys, 480 eq GSH and 48 eq other interfering substance.

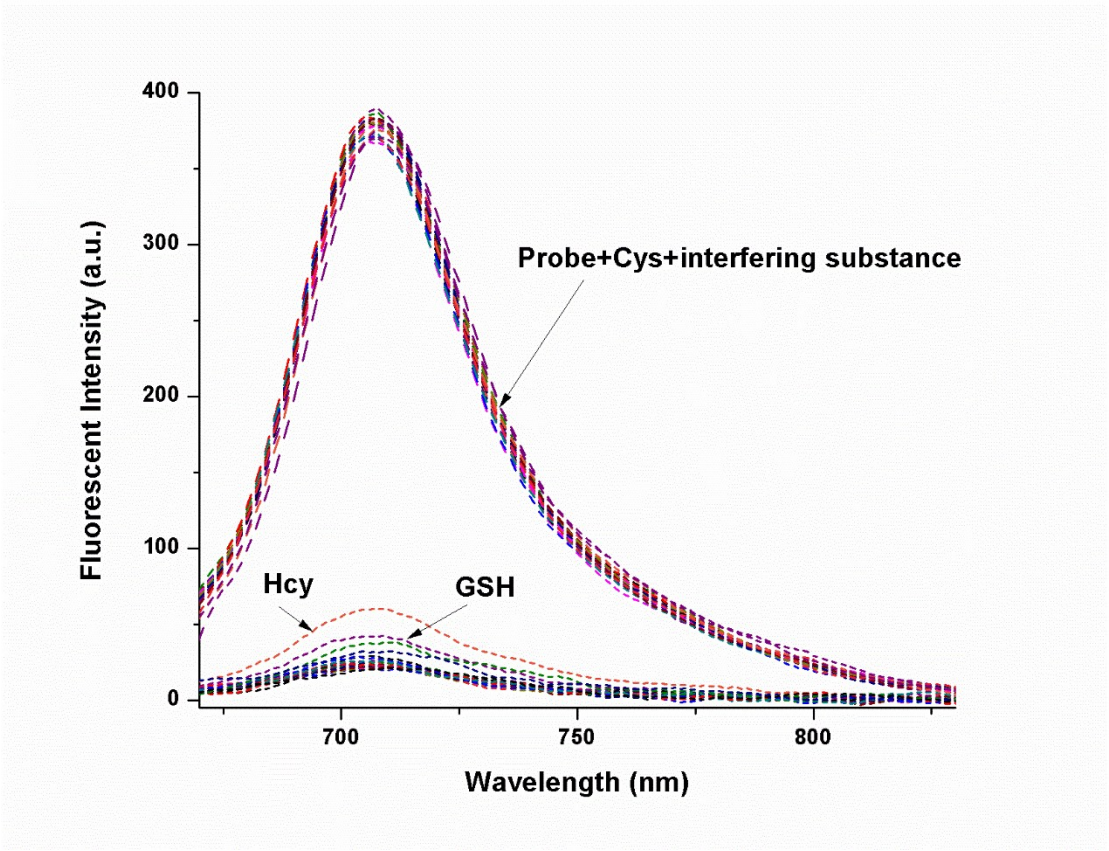

Fig. S2 Fluorescence of NIRHA in the presence of various interfering substance: 480 eq GSH and 48 eq other

competitive substance. Fluorescence of NIRHA in the presence of 4.8 eq Cys, 480 eq GSH and 48 eq other competitive analytes.

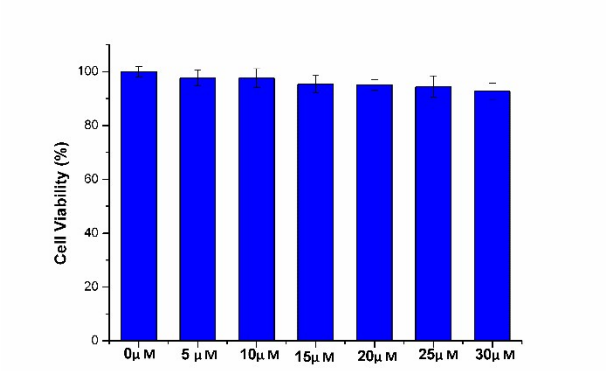

Fig. S3 Cell viability of NIRHA via the standard MTT assay of HeLa cells.

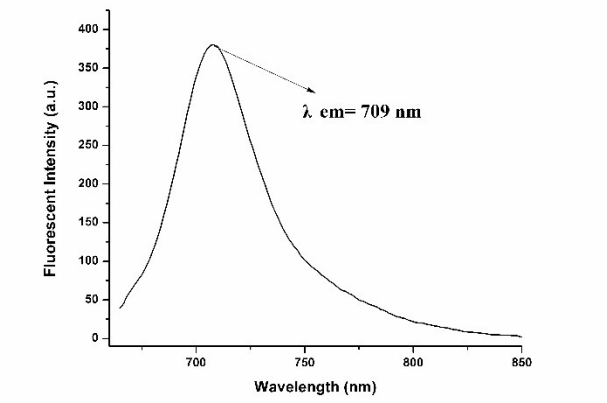

Fig. S4 fluorescence signal of compound *2*.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	C:\Users\ÇàÄê\Desktop\°ëë×°±Ëá\±íÕ÷ÊÖ¶Î\·´Ó¦Ö®ºóµÄ·Ö×ÓÁ¿ÖÊÆ×-»úÀíÑÐ¾¿	Acquisition Date	2019/5/28 15:16:49
Method	lc-ms-hr-low.m	Operator	zlwei
Sample Name	zlb2	Instrument / Ser#	micrOTOF-Q II 10351
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
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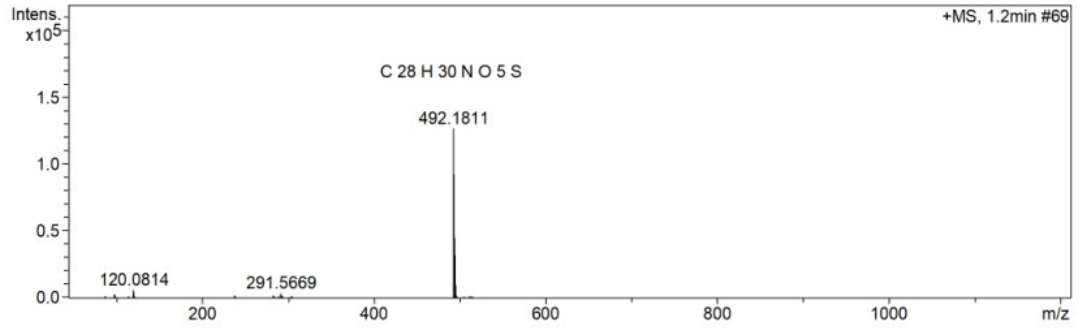
Scan End	1200 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
492.1811	1	C 28 H 30 N O 5 S	492.1839	5.6	5.1	14.5	ok	even	21.15	0.0322	0.0029	0.0106	0.0036	0.8427

Fig. S5 HR-MS spectrum of released compound *2*.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	C:\Users\ÇàÄê\Desktop\°ëë×°±Ëá\±íÕ÷ÊÖ¶Î\·´Ó¦Ö®ºóµÄ·Ö×ÓÁ¿ÖÊÆ×-»úÀíÑÐ¾¿	Acquisition Date	2019/5/28 15:16:49
Method	lc-ms-hr-low.m	Operator	zlwei
Sample Name	zlb2	Instrument / Ser#	micrOTOF-Q II 10351
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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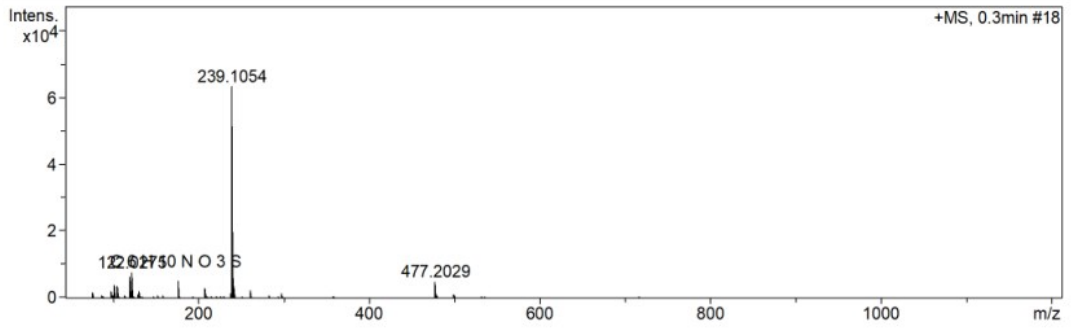
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
176.0375	1	C 6 H 10 N O 3 S	176.0376	0.3	2.6	2.5	ok	even	31.28	0.0514	0.0014	0.0349	0.0049	0.8427

Fig. S6 HR-MS spectrum of released seven-membered ring compound.

Mass Spectrum SmartFormula Report

Analysis Info

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Method	lc-ms-hr-low.m	Operator	zlwei
Sample Name	ZLB	Instrument / Ser#	micrOTOF-Q II 10351
Comment			

Acquisition Parameter

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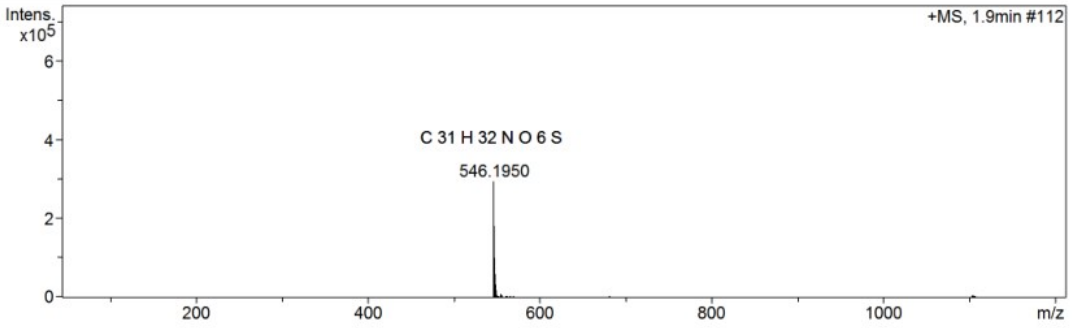
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
546.1950	1	C 31 H 32 N O 6 S	546.1945	-1.0	-0.3	16.5	ok	even	5.88	0.0090	0.0014	0.0030	0.0032	0.8427

Fig. S7 HR-MS spectrum of probe NIRHA.

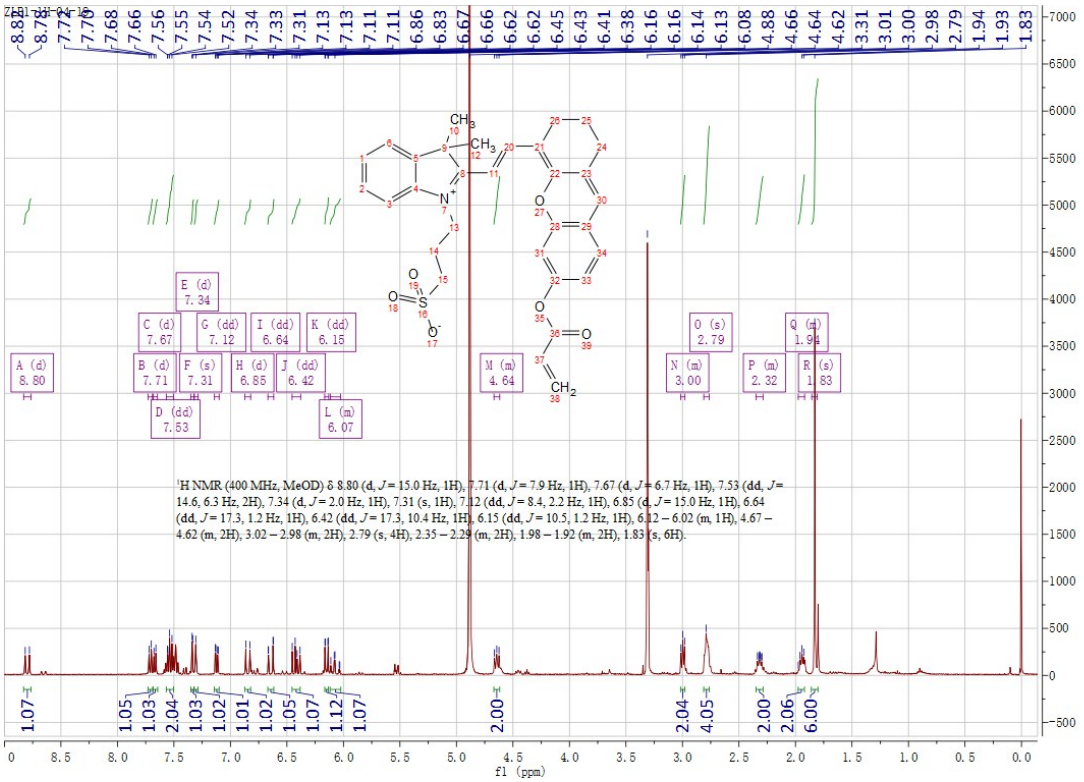


Fig. S8 ^{1}H NMR of probe NIRHA.

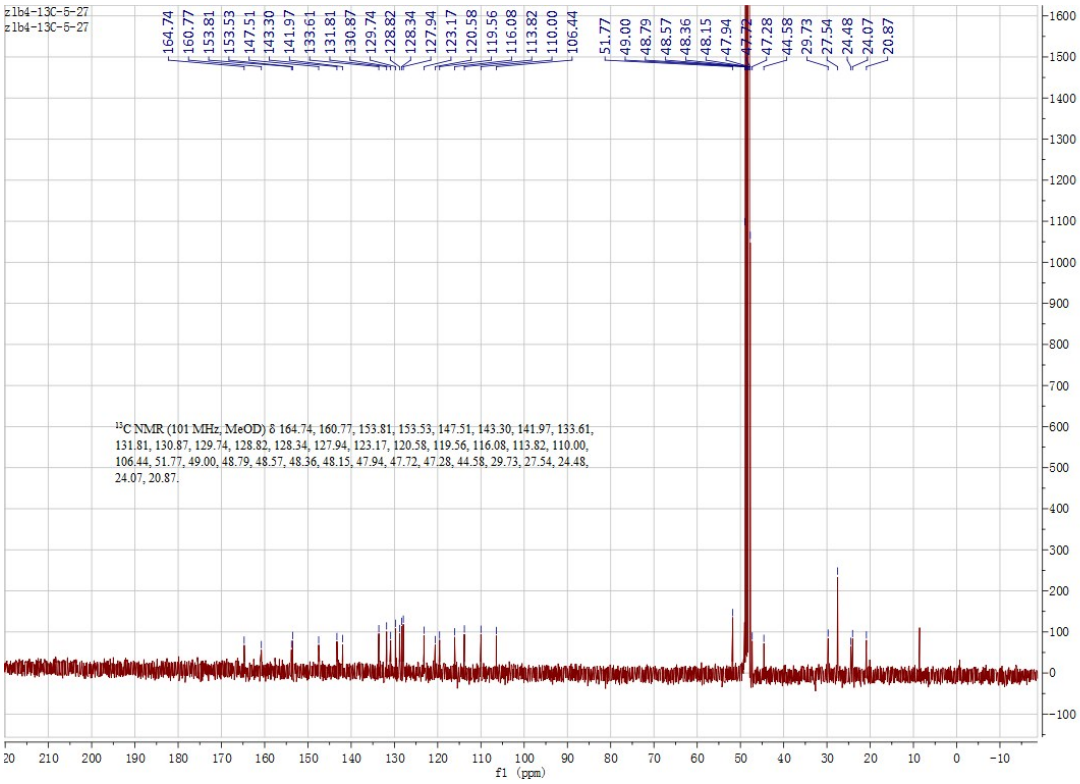


Fig. S9 [1]C NMR of probe NIRHA.

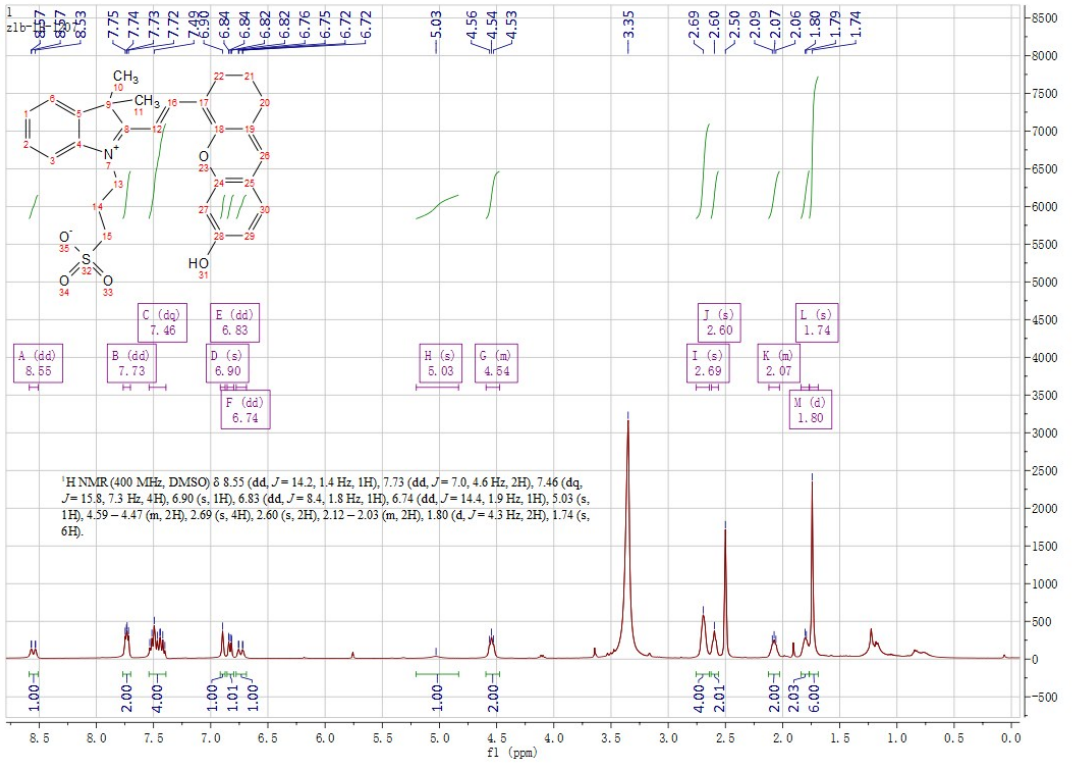


Fig. S10 [1]H NMR of compound *2*.

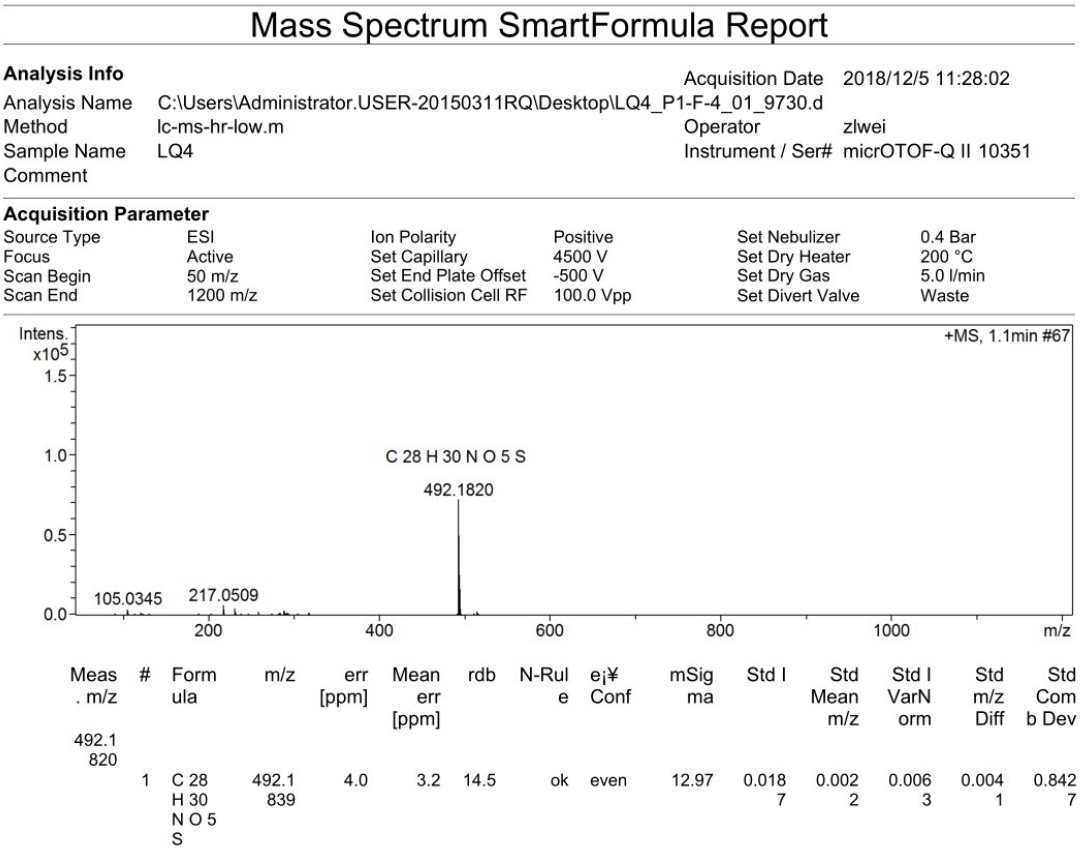


Fig. S11 HR-MS spectrum of compound *2*

Table S1. Comparison of the representative Cys probes with the present work[1-7].

Previous literatures	Solvent system	LOD	time	λex/λem
Angewandte Chemie International Edition, 2011, **50**, 10690-10693	PBS	0.13 μM	10 min	470/585 nm
Chemical Communications, 2012, **48**, 8341-8343	EtOH/PBS = 2:8	0.11 uM	9 min	304/ 487 nm
Sensors and Actuators B: Chemical, 2019, **290**, 47-52	C_2H_5OH/PBS = 1:99	0.12 μM	30 min	570/615 nm
Analytical Chemistry, 2015, **87**, 4856-4863	DMSO/H_2O = 1:19	0.16 μM	5 min	670 /697 nm
RSC Advances, 2017, **7**, 18867-18873	CAN/ HEPES = 2:8	0.158 μM	90 min	470/565 nm
Sensors and Actuators B: Chemical, 2018, **267**, 76-82	PBS/DMSO = 4/1	0.122 μM	5 min	445/500 nm
Sensors and Actuators B: Chemical, 2019, **298**, 126844	H_2O/CH3CN = 3/1	2.31 μM	10 min	370/464 nm
This work	PBS/DMF =99:1	0.0776 μM	15 min	650/710 nm

References:

1. X. Yang, Y. Guo and R. M. Strongin, *Angewandte Chemie International Edition*, 2011, **50**, 10690-10693.
2. H. Wang, G. Zhou, H. Gai and X. Chen, *Chemical Communications*, 2012, **48**, 8341-8343.
3. S. Jiao, X. He, L. Xu, P. Ma, C. Liu, Y. Huang, Y. Sun, X. Wang and D. Song, *Sensors and Actuators B: Chemical*, 2019, **290**, 47-52.
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5. J. Guo, Z. Kuai, Z. Zhang, Q. Yang, Y. Shan and Y. Li, *RSC Advances*, 2017, **7**, 18867-18873.
6. X. Xie, C. Yin, Y. Yue and F. Huo, *Sensors and Actuators B: Chemical*, 2018, **267**, 76-82.
7. J. Chao, M. Li, Y. Liu, Y. Zhang, F. Huo and C. Yin, *Sensors and Actuators B: Chemical*, 2019, **298**, 126844.