Supplementary Data

For

A novel near-infrared and naked-eyes turn on fluorescent probe for detection of biothiols with a large stokes shift and its application in living cells

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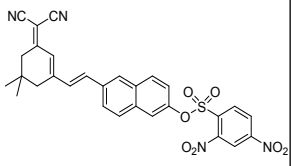
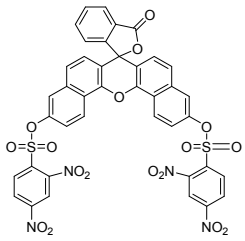
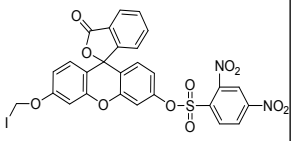
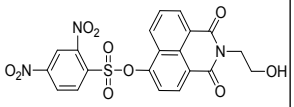
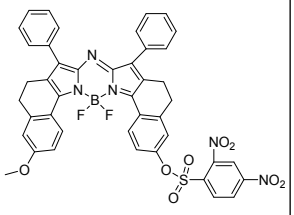
Content

15. Figsure S14. Absorbance spectra and fluorescent spectra analysis.

16. Figsure S15. The color of probe **DDND** with different concentration of Cys under UV light.

17. Figsure S16. Cell viabiality to Hela cells of probe **DDND**.

	Probe	**Solvent (pH=7.4)**	**Dose of Cys (eq.)**	**Time (min)**	**Stokes shift （nm ）**	**Naked eyes**	**Detection Limit (μM)**	**Reference**
1	 (Ex=492nm,Em=623nm)	DMSO-PBS (1/1,v/v)	3	5	131	Yes	Cys 0.23 Hcy 0.34 GSH 0.41	**This work**
2	 (Ex=620nm,Em=688 nm)	DMSO-PBS (1/1,v/v)	2	20	68	No	Cys 2.93 Hcy 1.29 GSH 0.59	[1]
3	 (Ex=454nm,Em=521 nm)	DMSO-PBS (3/7,v/v)	5	2	67	Yes	Cys 0.16 Hcy no data GSH no data	[2]
4	 (Ex=450nm,Em=560nm)	DMSO-PBS (containing 1% DMSO)	3	6	110	No	Cys 0.78 Hcy 0.54 GSH 1.01	[3]
5	 (Ex=670nm,Em=755 nm)	CH_3CN-H_2O (3:7,v/v)	20	120	75	No	Cys 0.50 Hcy no data GSH no data	[4]

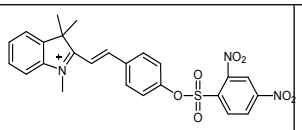
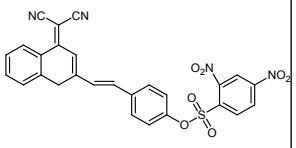
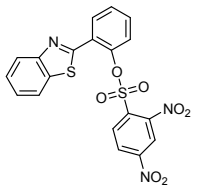
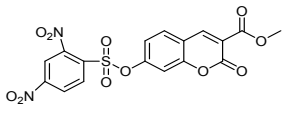
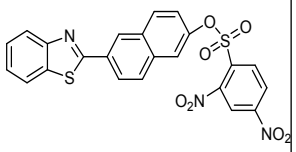
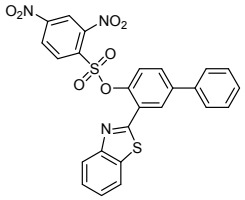
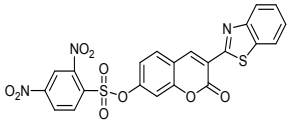
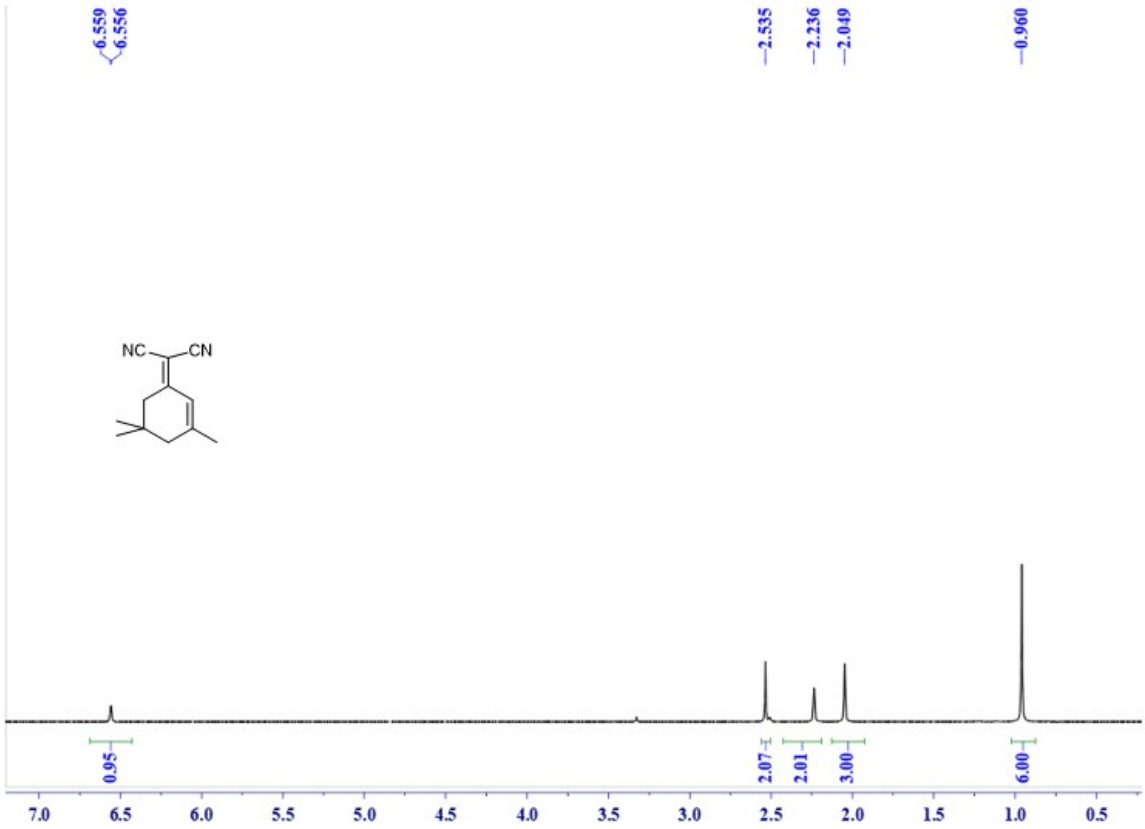
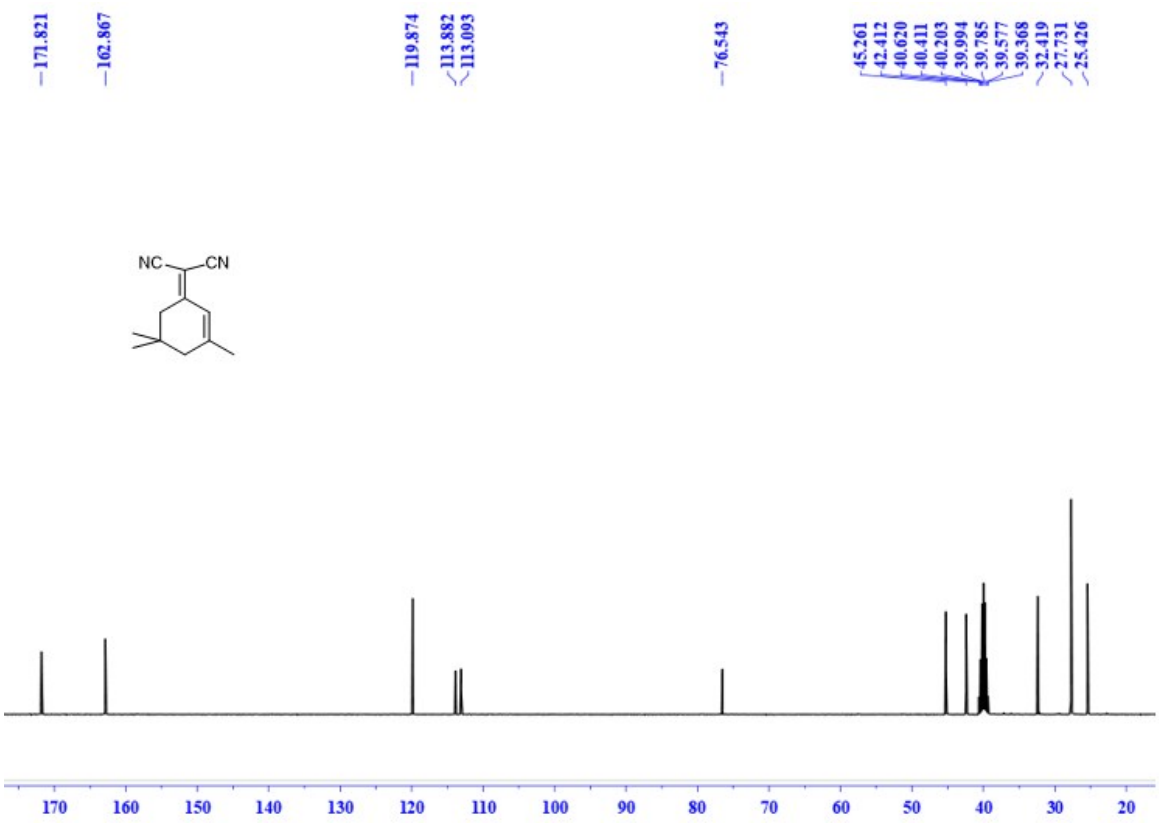
6	 (Ex=425nm,Em=530 nm)	EtOH-H_2O (3:7,v/v)	4	15	105	Yes	Cys no data Hcy no data GSH 0.24	[5]
7	 (Ex=560nm,Em=690 nm)	DMSO-water (1/1,v/v)	5	3	130	No	Cys no data Hcy no data GSH 0.18	[6]
8	 (Ex=340 nm,Em=445 nm)	DMSO-PBS (1/1,v/v)	4	5	105	No	No data	[7]
9	 (Ex=370nm,Em=473 nm)	EtOH-PBS (3/7, v/v)	10	20	103	No	No data	[8]
10	 (Ex=430nm,Em=503 nm)	EtOH-PBS (1:1, v/v)	20	5	73	No	No data	[9]
11	 (Ex=320nm,Em=482 nm)	DMSO-HEPES (2:8, v/v)	8	15	162	No	Cys 0.2 Hcy 0.17 GSH 0.12	[10]
12	 (Ex=390nm,Em=510 nm)	DMSO-PBS (1/1,v/v)	20	50	120	No	No data	[11]

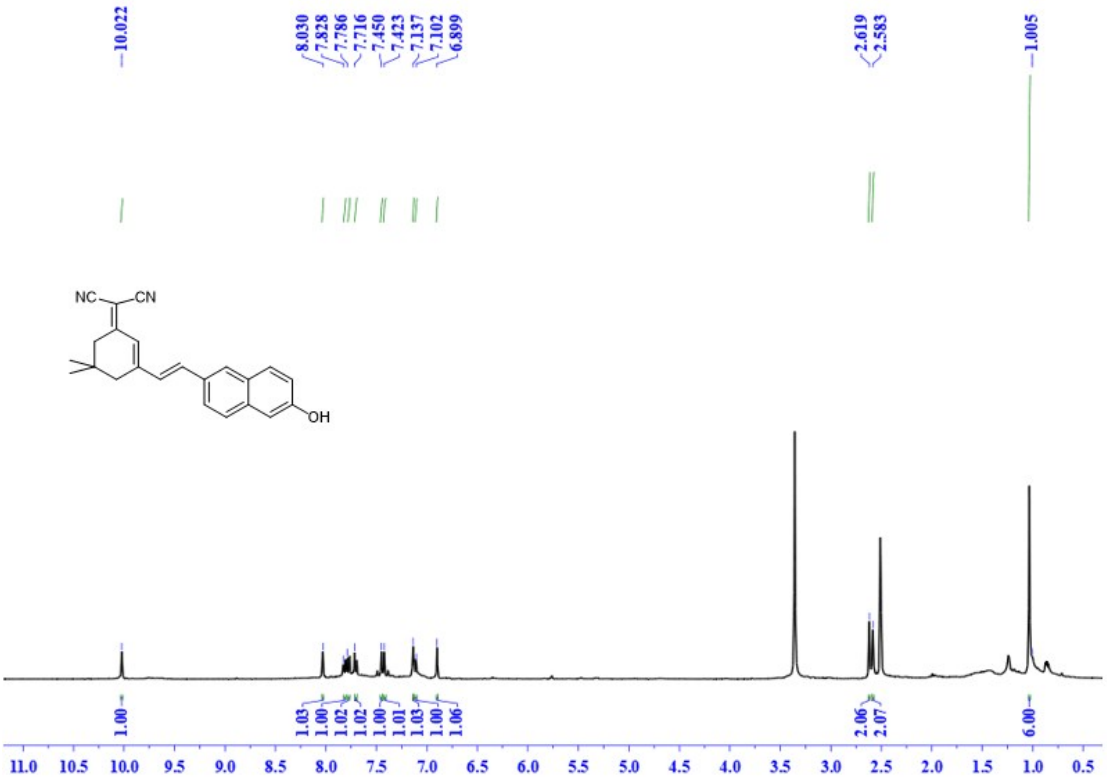
Table S1. Some similar functionalized probes for the detection of biothiols



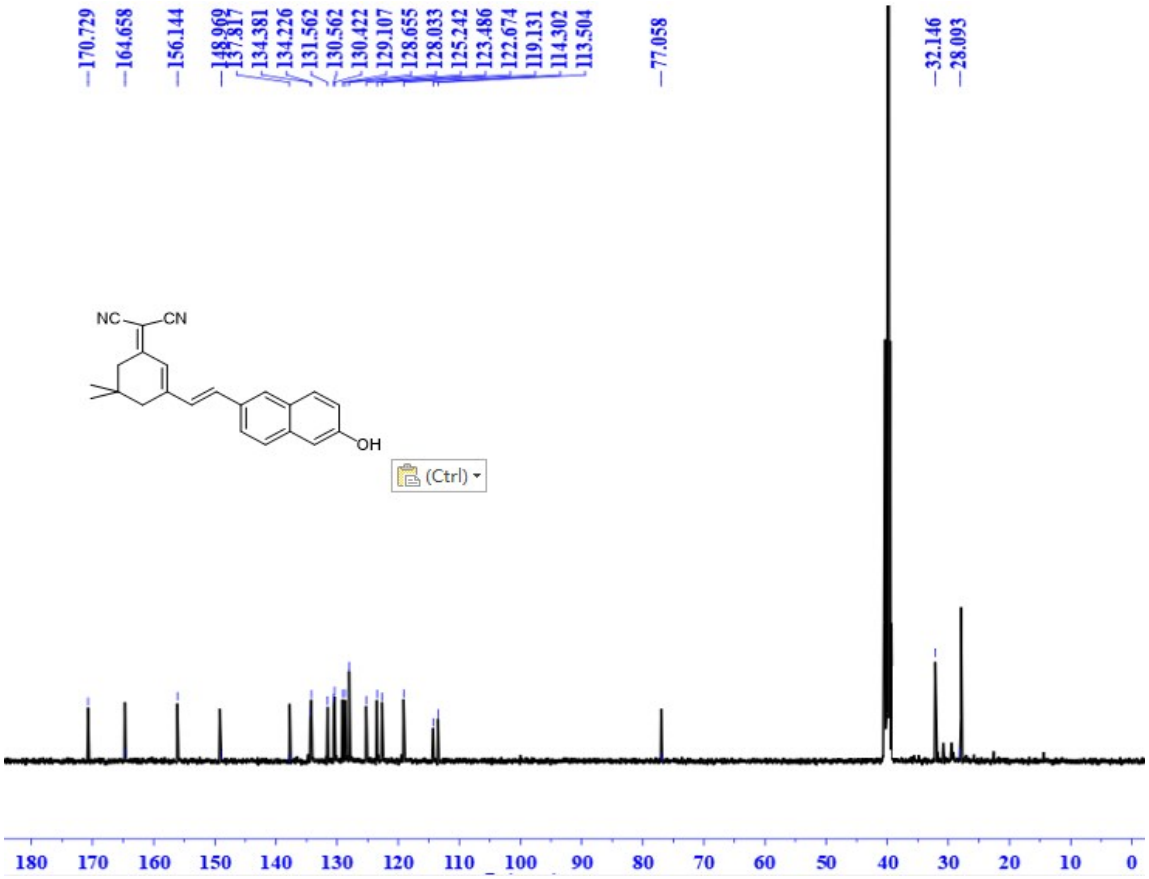
Figsure S1. ^{1}H NMR (400 MHz) spectrum of compound **1** in DMSO-d_6



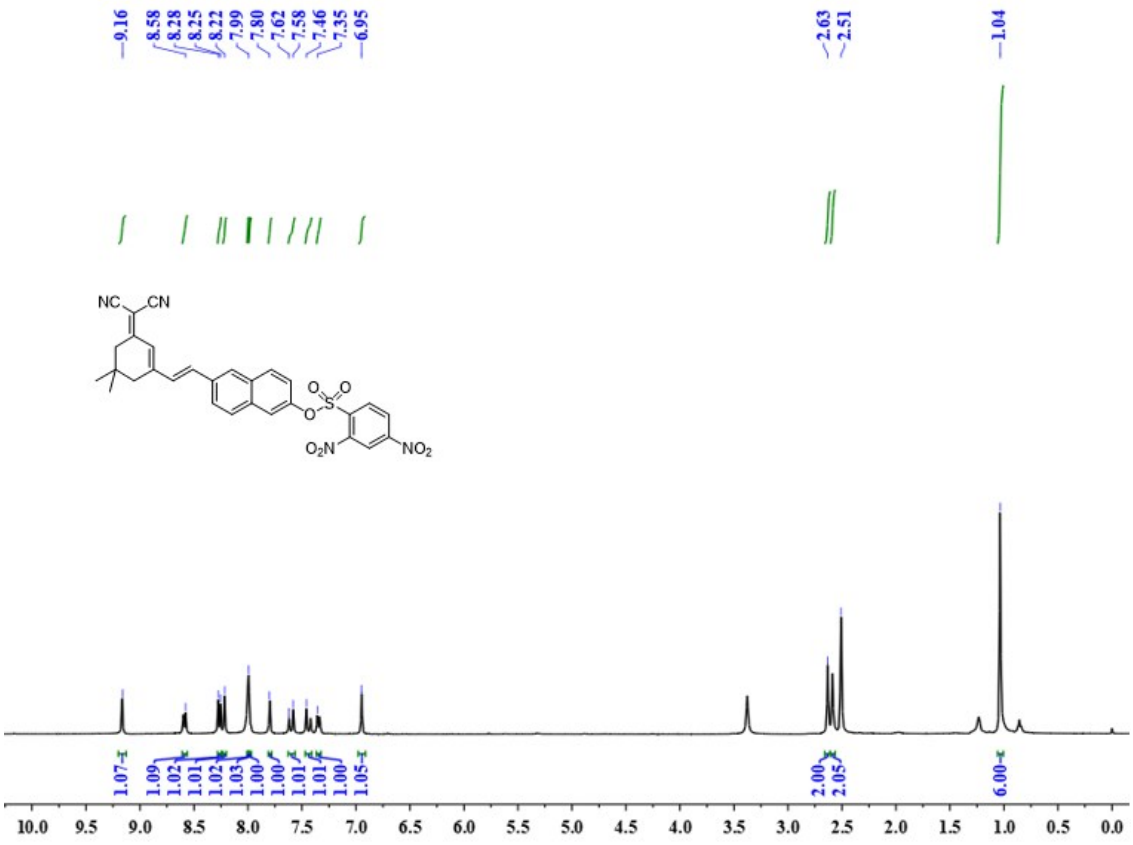
Figsure S2. ^{13}C NMR (100 MHz) spectrum of compound **1** in DMSO-d_6.



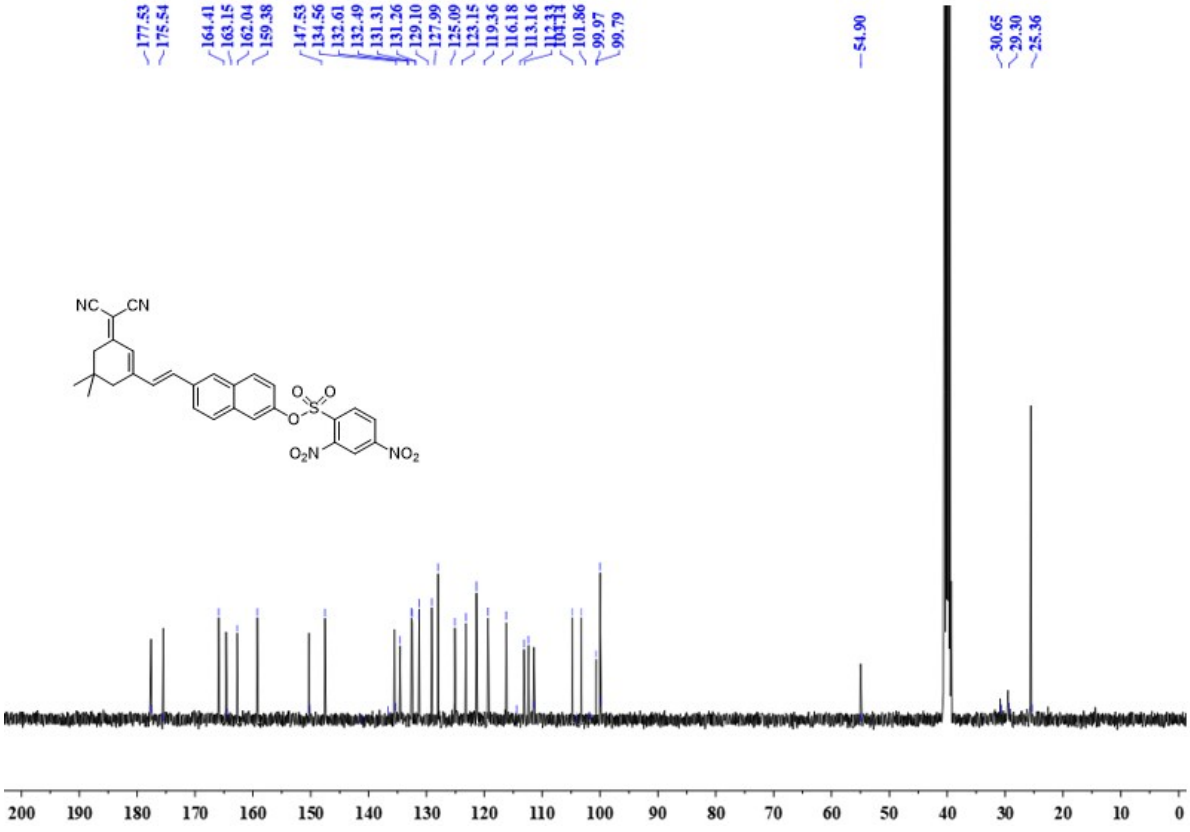
Figsure S3. ^{1}H NMR (400 MHz) spectrum of **HDM** in DMSO-d_6.



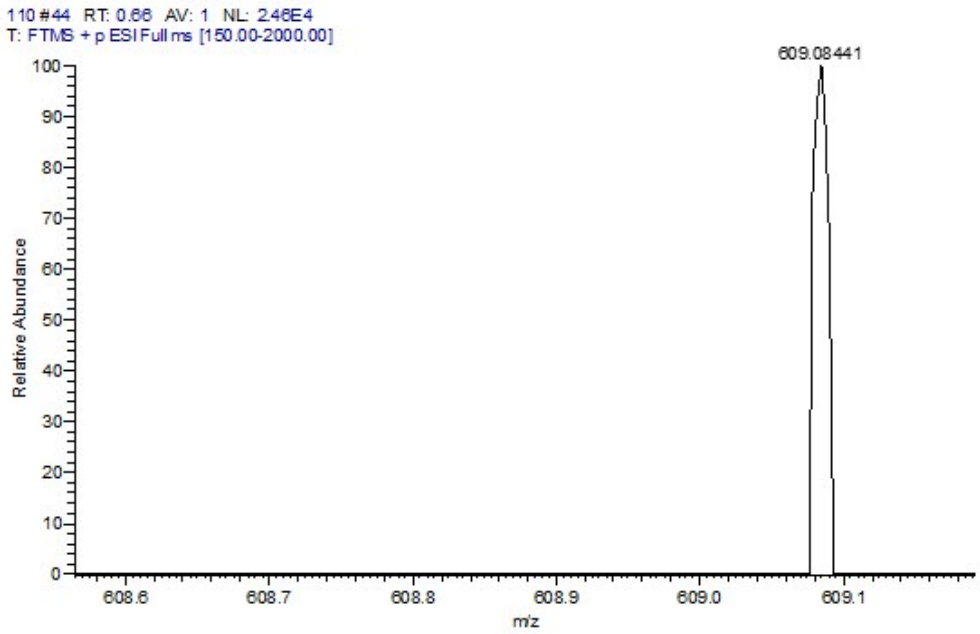
Figsure S4. ^{13}C NMR (100 MHz) spectrum of **HDM** in DMSO-d_6.



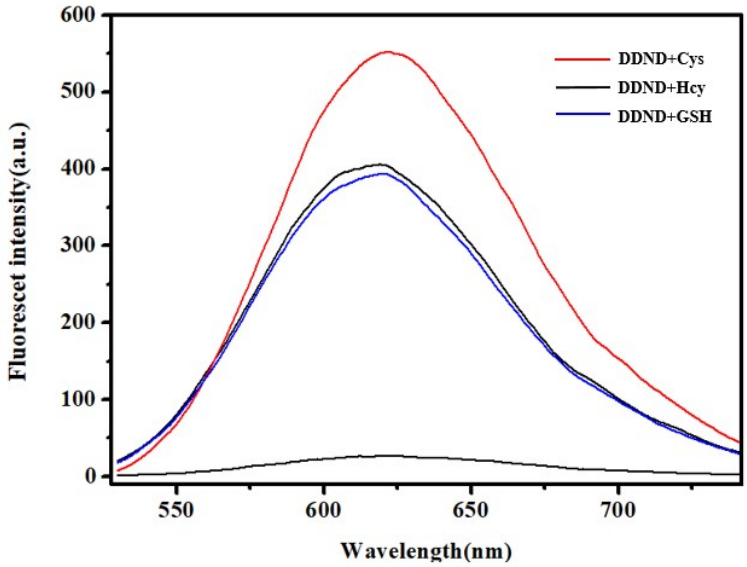
Figsure S5. [1]H NMR (400 MHz) spectrum of probe **DDND** in DMSO-d_6.



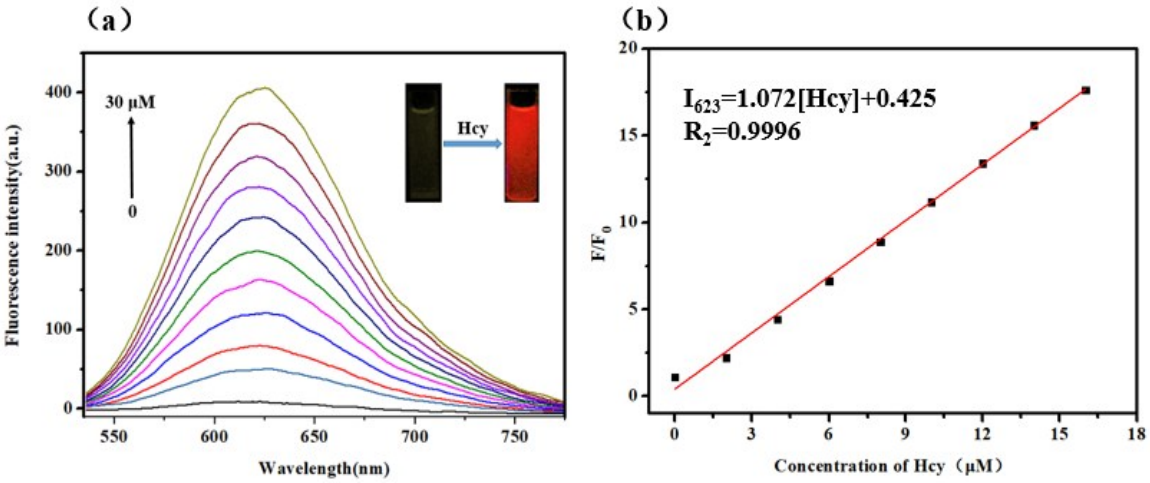
Figsure S6. [13]C NMR (100 MHz) spectrum of probe **DDND** in DMSO-d_6.



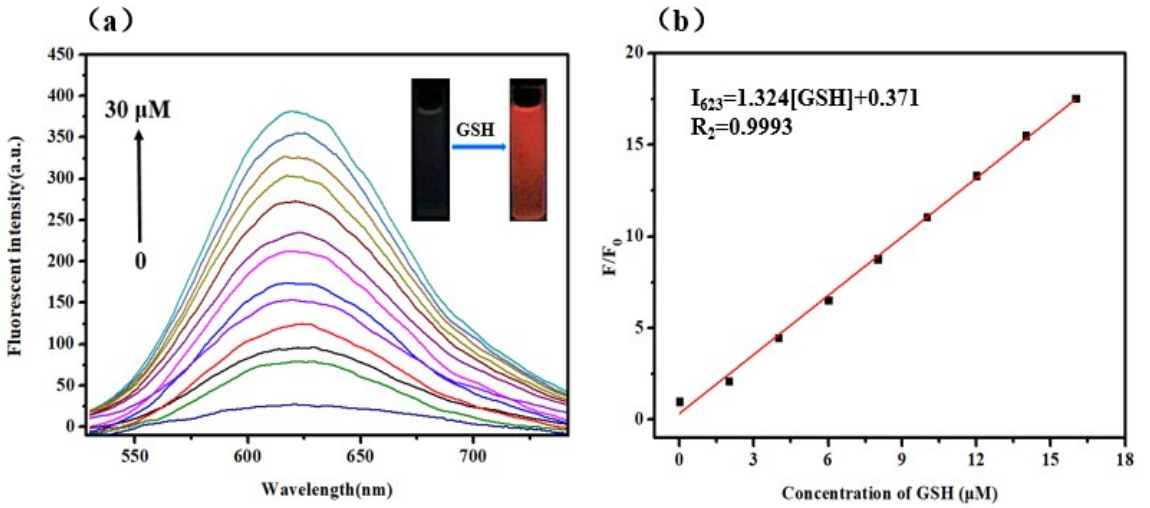
Figsure S7. HRMS (ESI^+) spectrum of probe **DDND**



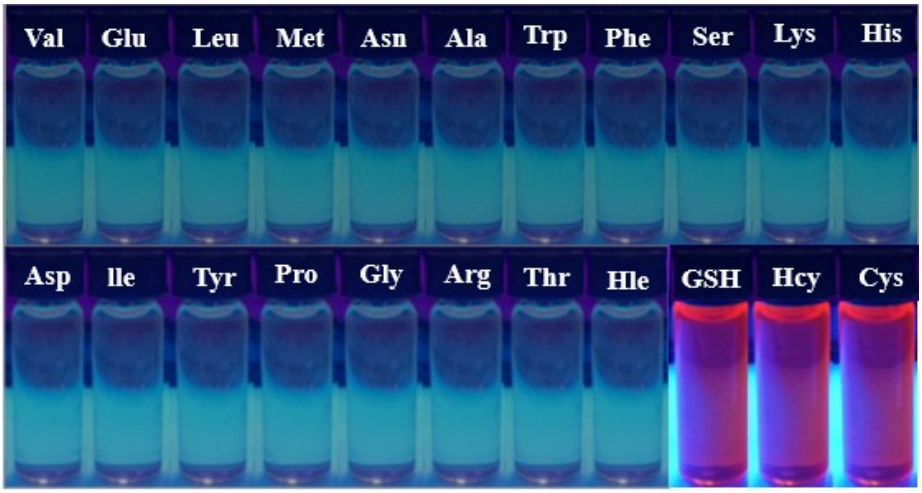
Figsure 8. Fluorescence spectra of **DDND** by itself (10 μM, gray line), and **DDNA** (10 μM) in the prescence of Cys (1 mM, red line), Hcy (1 mM, black line) and GSH (1 mM, blue line). Ex=492 nm.



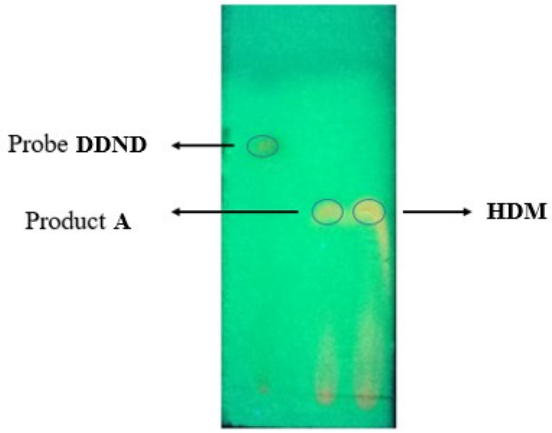
Figsure S9. (a) Fluorescence titration of **DDND** (10 μM) upon addition of Hcy (0-30 μM). Ex =492 nm, slit: 5.0 nm/5.0 nm; (b) Stand curve of F/F_0 at 623 nm versus Hcy concentration (from 0 to 16 μM). F_0 and F are the fluorescence intensity in the absence and presence of Hcy, respectively. Ex =492 nm, slit: 5.0 nm/5.0 nm.



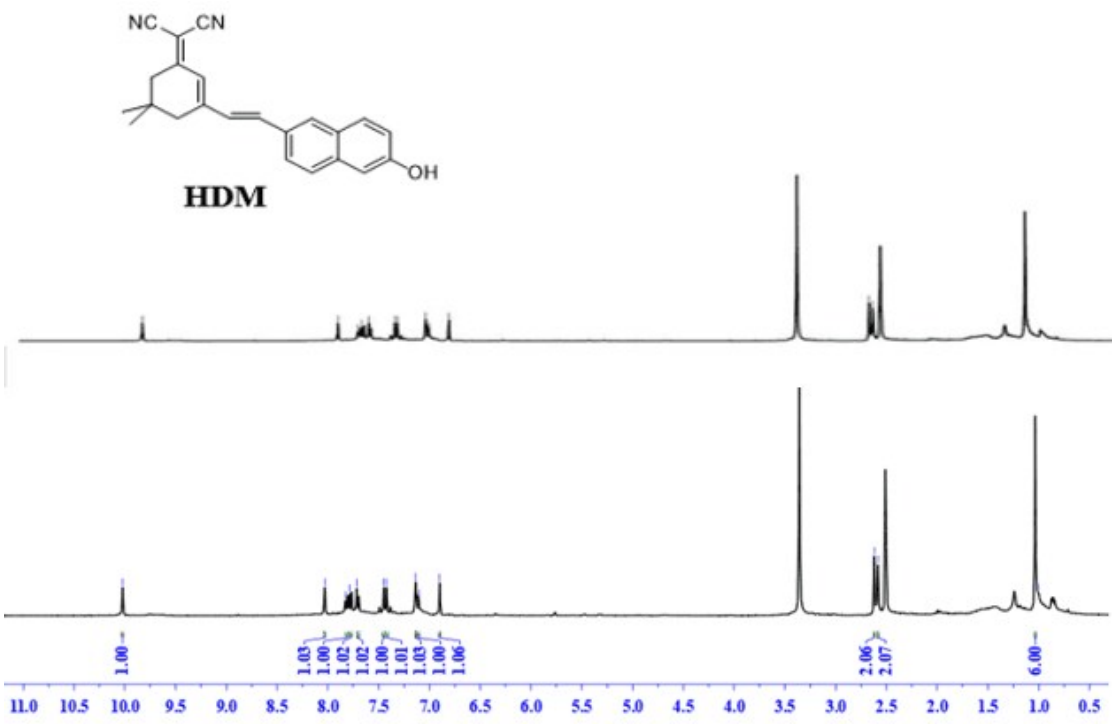
Figsure S10. (a) Fluorescence titration of **DDND** (10 μM) upon addition of GSH (0-30 μM). Ex =492 nm, slit: 5.0 nm/5.0 nm; (b) Stand curve of F/F_0 at 623 nm versus GSH concentration (from 0 to 16 μM). F_0 and F are the fluorescence intensity in the absence and presence of Hcy, respectively. Ex =492 nm, slit: 5.0 nm/5.0 nm.



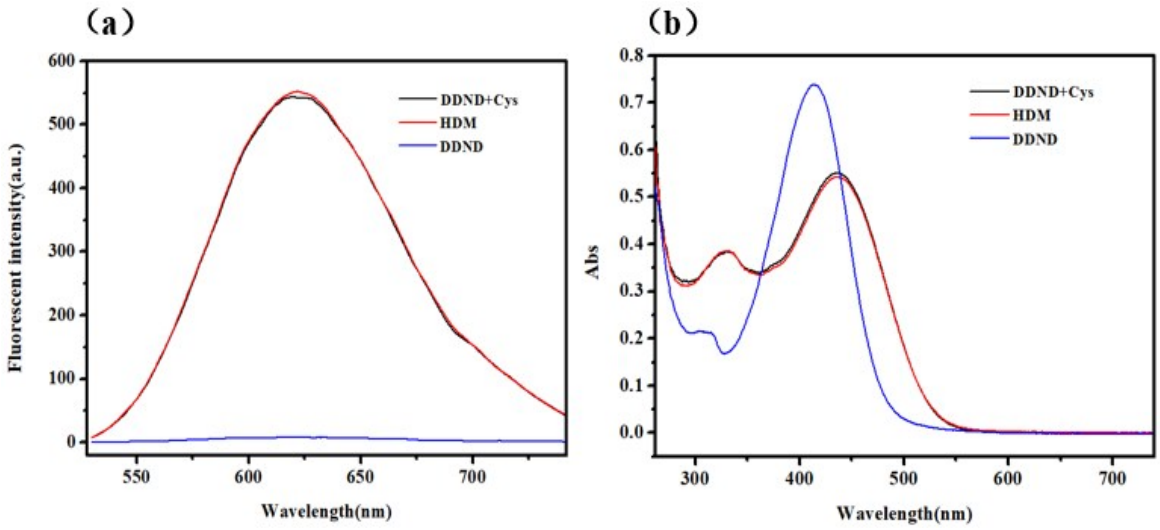
Figsure S11. Emission color changes of probe **DDND** with various analytes.



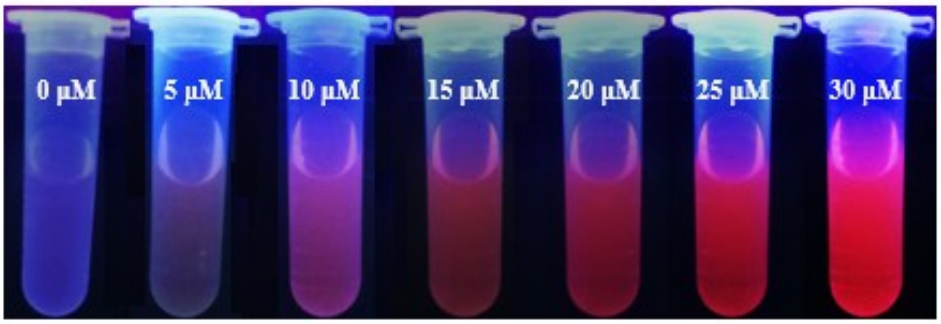
Figsure S12. TLC analysis of the reaction product A with the reference compound **HDM** and probe **DDND**. The TLC plate was observed under a light of 256 nm. The eluent for TLC: petroleum ether:ethyl acetate = 1:4 (v/v). This data showed that compound A was compound **HDM**



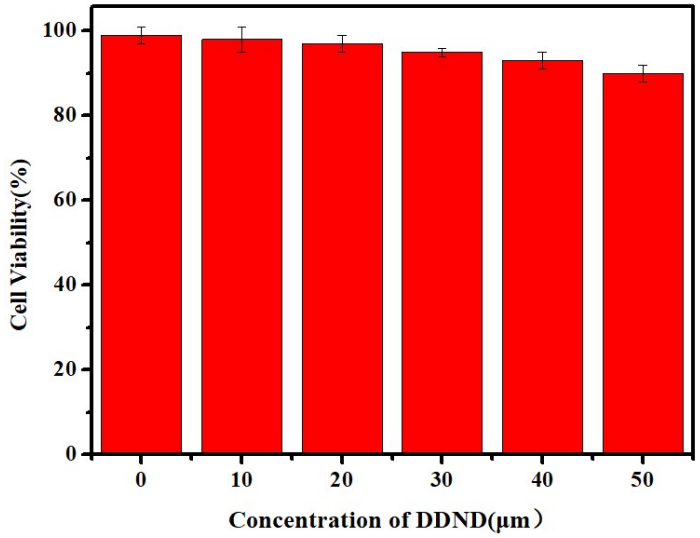
Figsure S13. ^{1}H NMR spectrum analysis of product **A** with the reference compound **HDM**.



Figsure S14. A comparison of (a) fluorescent spectra and (b) absorbance spectra of probe **DDND** (10 μM), compound **HDM** (10 μM), and the mixture of probe **DDND** (10 μM) + Cys (50 μM) after 15 min in PBS buffer (50% DMSO) solution.



Figsure S15. Probe **DDND** with different concentration of Cys under UV irradiation (365 nm).



Figsure S16. Viable HeLa cells after treatment with indicated concentrations of probe after 24 hours. The cell viability was observed via MTT assay.

References

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