

## *Supporting information*

### **A dual-response NIR fluorescent probe for separately and continuously recognizing H<sub>2</sub>S and Cys with different fluorescence signals and its applications**

Lisha Yue<sup>a</sup>, Yin Ai<sup>a</sup>, Gang Liu<sup>a</sup>, Haichang Ding<sup>a,\*</sup>, Shouzhi Pu<sup>a,b,\*</sup>

<sup>a</sup> Jiangxi Key Laboratory of Organic Chemistry, Jiangxi Science and Technology Normal University, Nanchang 330013, PR China

<sup>b</sup> Department of Ecology and Environment, Yuzhang Normal University, Nanchang 330103, P. R. China

\*Corresponding author: [dinghaichang@126.com](mailto:dinghaichang@126.com) (H. Ding), [pushouzhi@tsinghua.org.cn](mailto:pushouzhi@tsinghua.org.cn) (S. Pu)

#### **Contents:**

**Fig. S1.** <sup>1</sup>H NMR spectrum of **2C** in CD<sub>2</sub>Cl<sub>2</sub>.

**Fig. S2.** <sup>1</sup>H NMR spectrum of **Cy-S** in CD<sub>3</sub>CN.

**Fig. S3.** HRMS spectrum of **Cy-S** in CH<sub>3</sub>OH.

**Fig. S4.** <sup>1</sup>H NMR spectrum of **Cy-N** in DMSO-*d*<sub>6</sub>.

**Fig. S5.** HRMS spectrum of **Cy-N** in CH<sub>3</sub>OH.

**Fig. S6.** <sup>1</sup>H NMR spectrum of **Cy-NP** in DMSO-*d*<sub>6</sub>.

**Fig. S7.** <sup>13</sup>C NMR spectrum of **Cy-NP** in DMSO-*d*<sub>6</sub>.

**Fig. S8.** HRMS spectrum of **Cy-NP** in CH<sub>3</sub>OH.

**Fig. S9.** The linear range of **Cy-NP** to H<sub>2</sub>S and Cys.

**Fig. S10.** HRMS spectra of **Cy-NP**, **Cy-Cys**, **Cy-H<sub>2</sub>S** and **Cy-NP-NH<sub>2</sub>**.

**Fig. S11.** the sensing mechanism of **Cy-NP** to H<sub>2</sub>S.

**Fig. S12.** The structures used for DFT calculations.

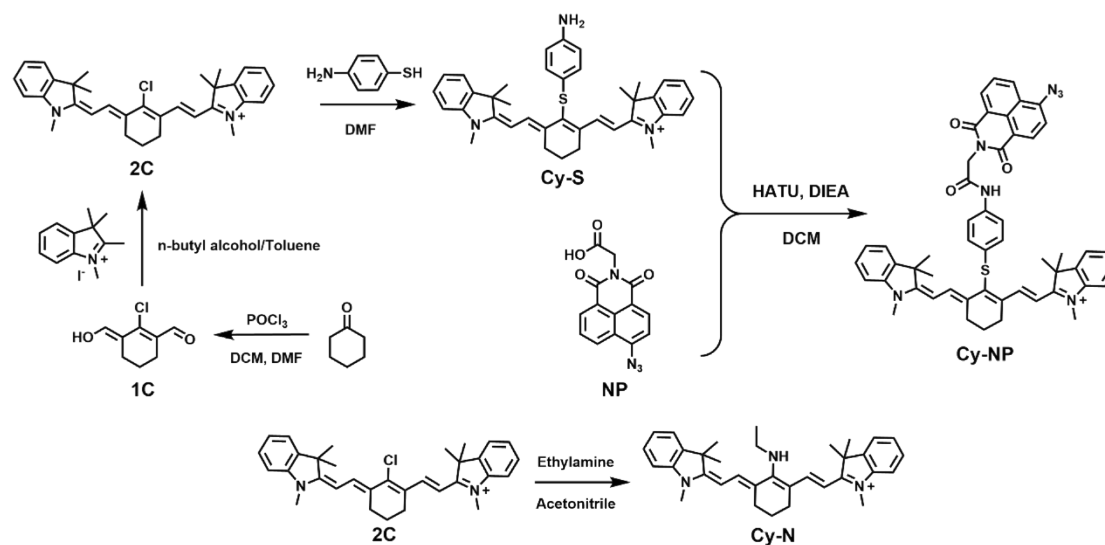
**Fig. S13.** The response of test strips immersed into different concentration of H<sub>2</sub>S solution.

**Fig. S14.** Optical images of **Cy-NP** test paper.

**Fig. S15.** Cytotoxicity Assay.

**Fig. S16.** The emission intensity changes of Cy-NP A) upon addition of Cys at 640 nm excitation. B) upon addition of Cys and H<sub>2</sub>S at 640 nm excitation. C) upon addition of H<sub>2</sub>S at 400 nm excitation. D) upon addition of Cys and H<sub>2</sub>S at 400 nm excitation. E) Change of fluorescence intensity at 640 nm excitation. F) Change of fluorescence intensity at 400 nm excitation.

**Table S1.** Comparison of Cy-NP with other fluorescent probes.



**Scheme S1.** Synthetic route of Cy-S, Cy-N, and Cy-NP.

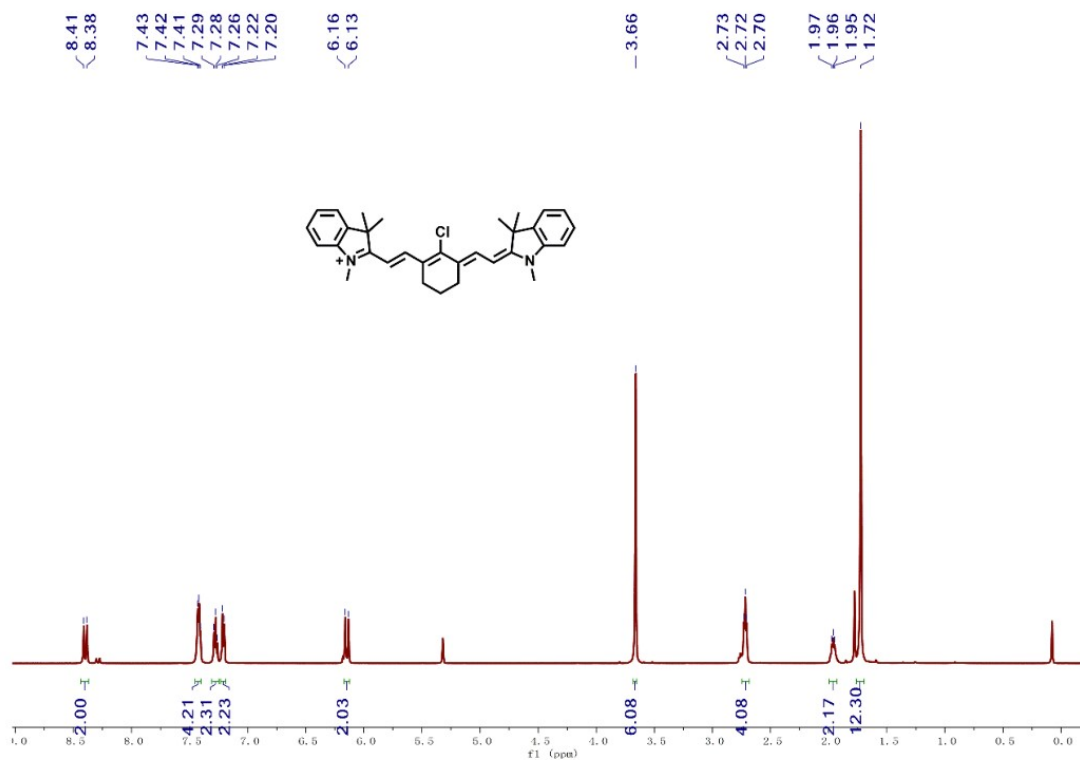


Fig. S1  $^1\text{H}$  NMR spectrum of 2C in  $\text{CD}_2\text{Cl}_2$ .

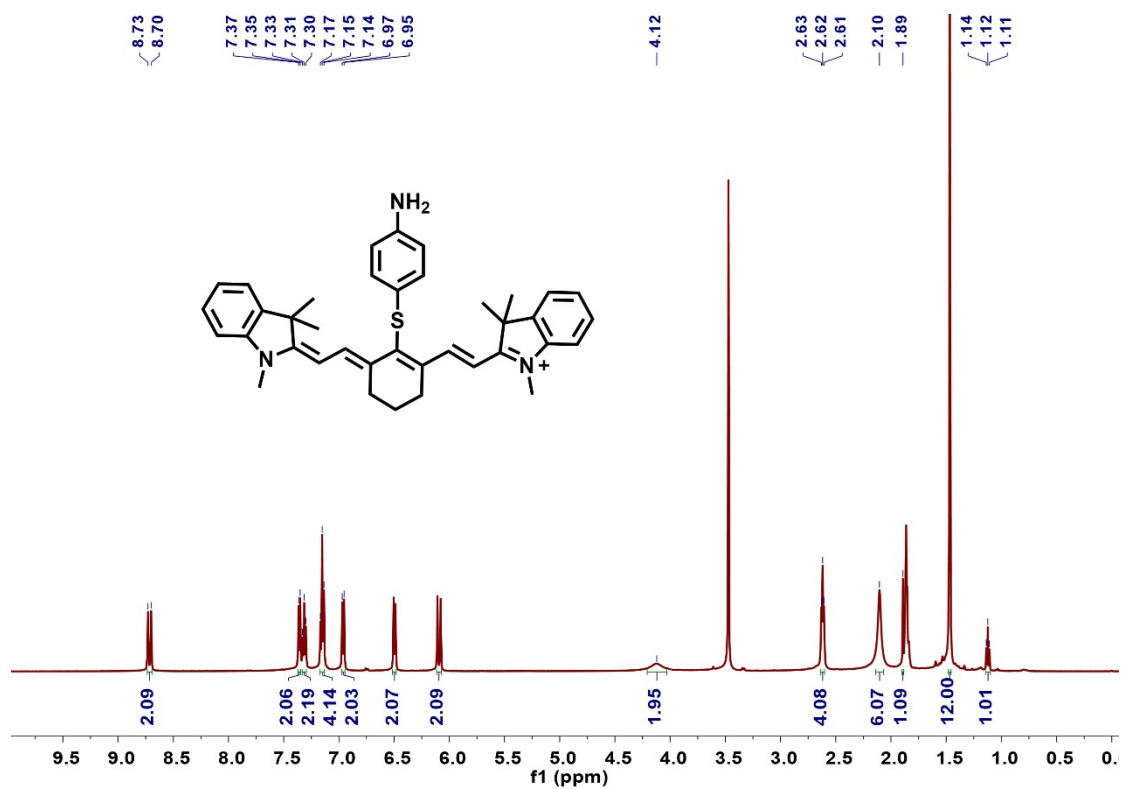


Fig. S2  $^1\text{H}$  NMR spectrum of Cy-S in  $\text{CD}_3\text{CN}$ .

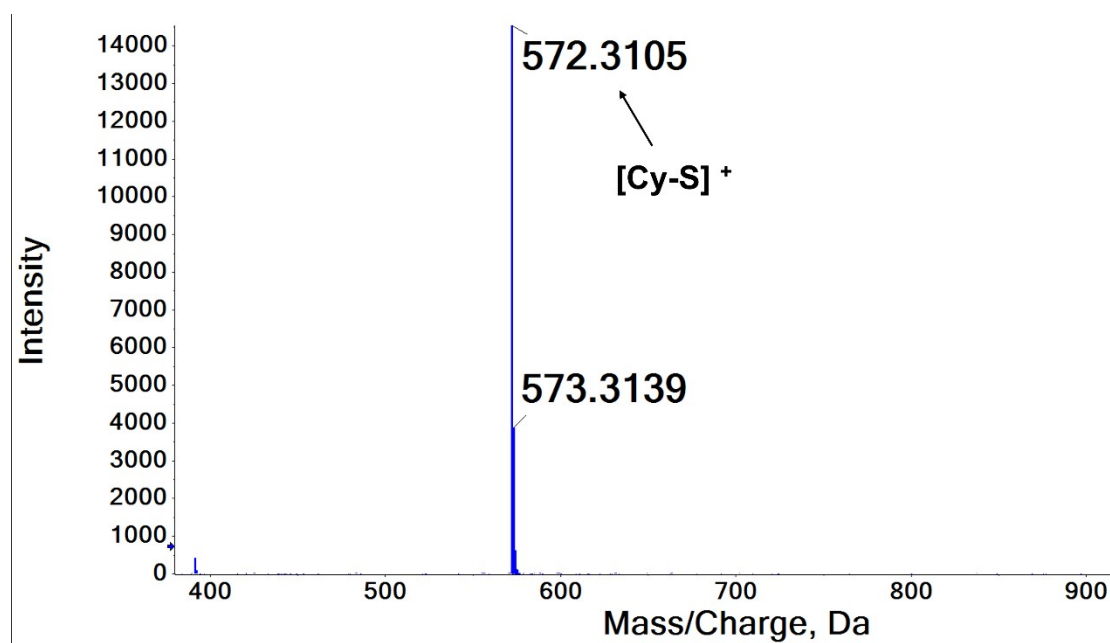


Fig. S3 HRMS spectrum of Cy-S in CH<sub>3</sub>OH.

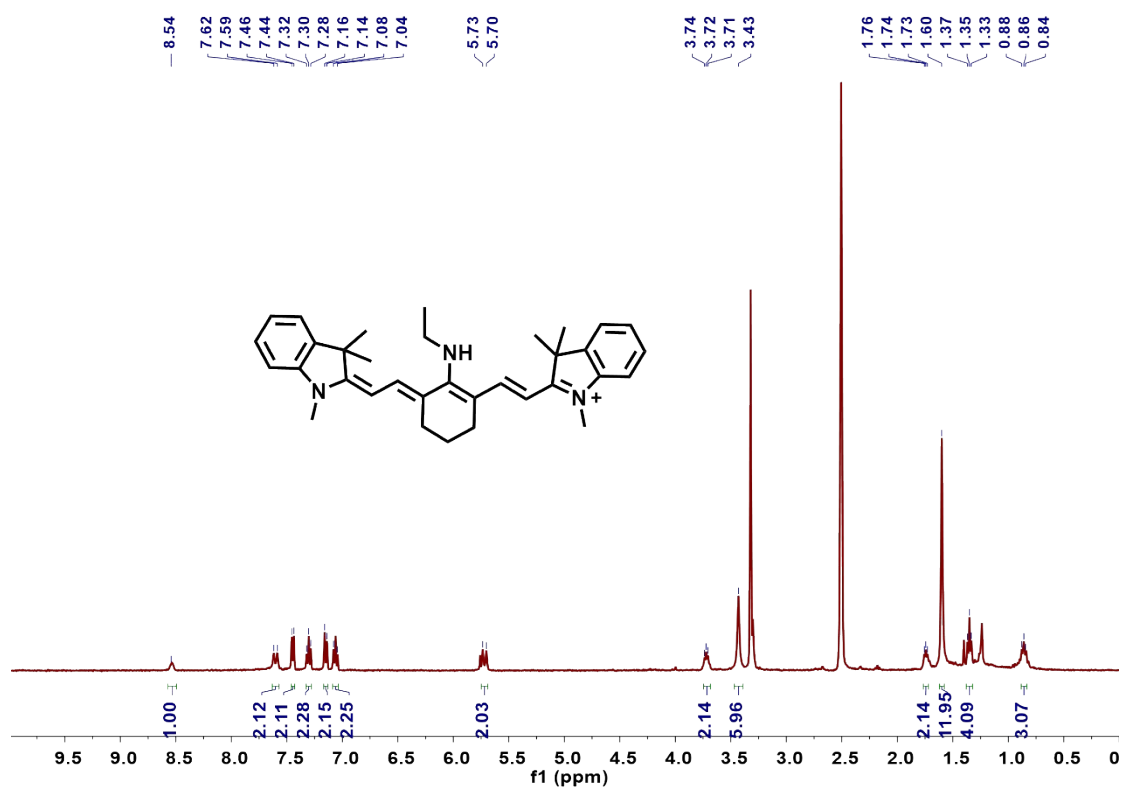


Fig. S4 <sup>1</sup>H NMR spectrum of Cy-N in DMSO-*d*<sub>6</sub>.

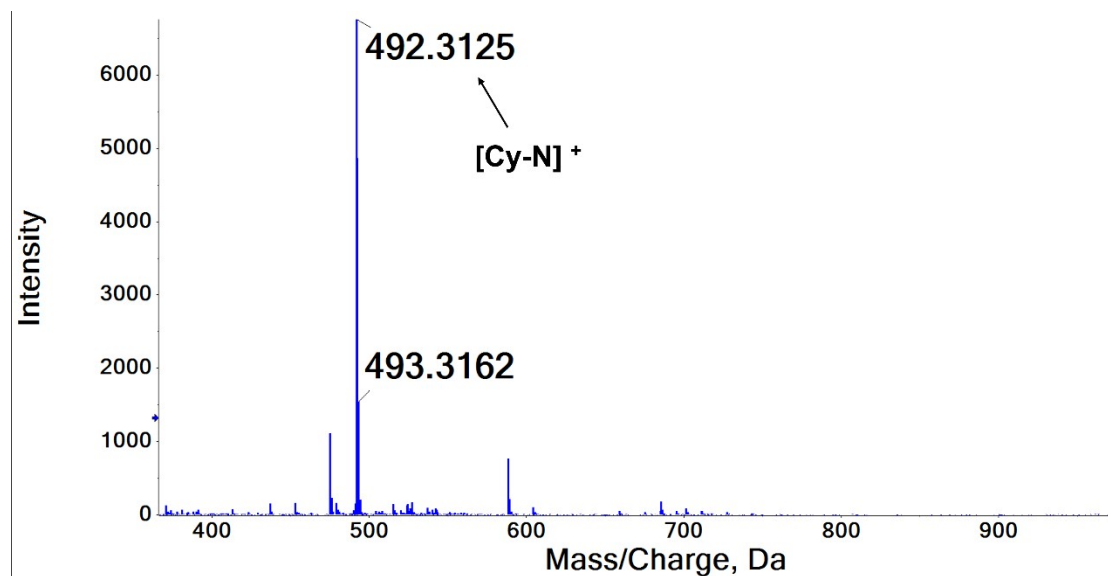


Fig. S5 HRMS spectrum of Cy-N in  $\text{CH}_3\text{OH}$ .

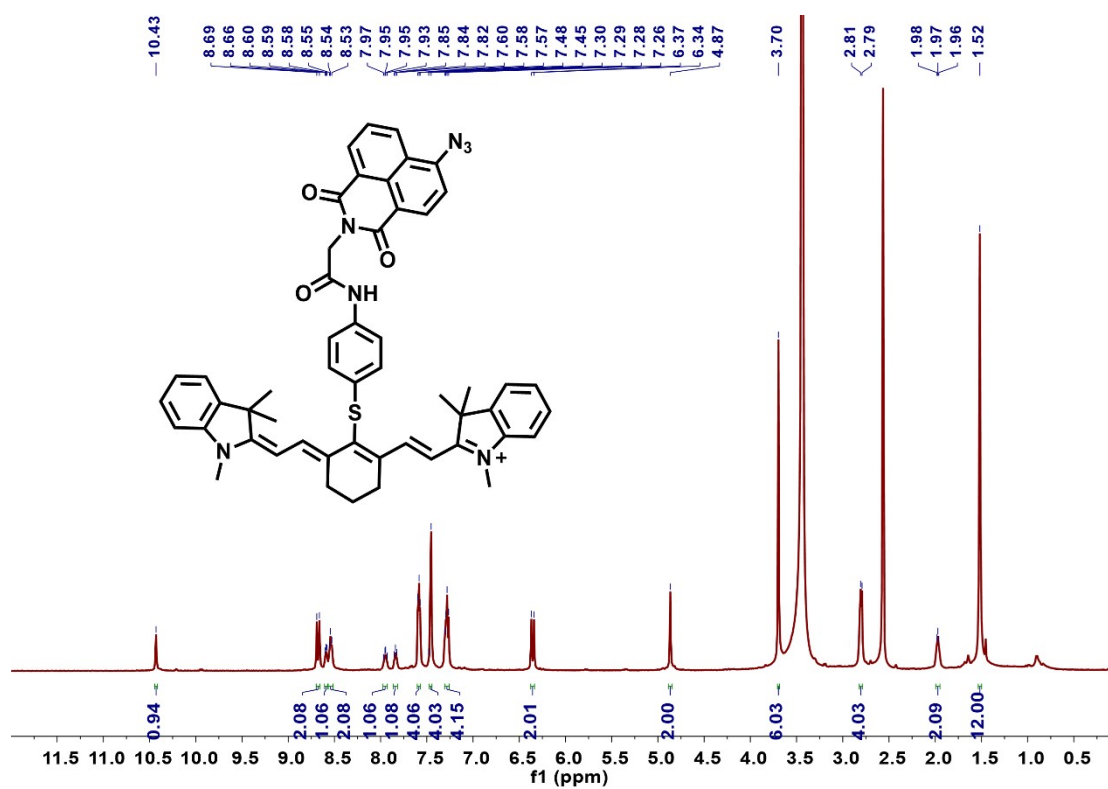


Fig. S6  $^1\text{H}$  NMR spectrum of Cy-NP in  $\text{DMSO-}d_6$ .

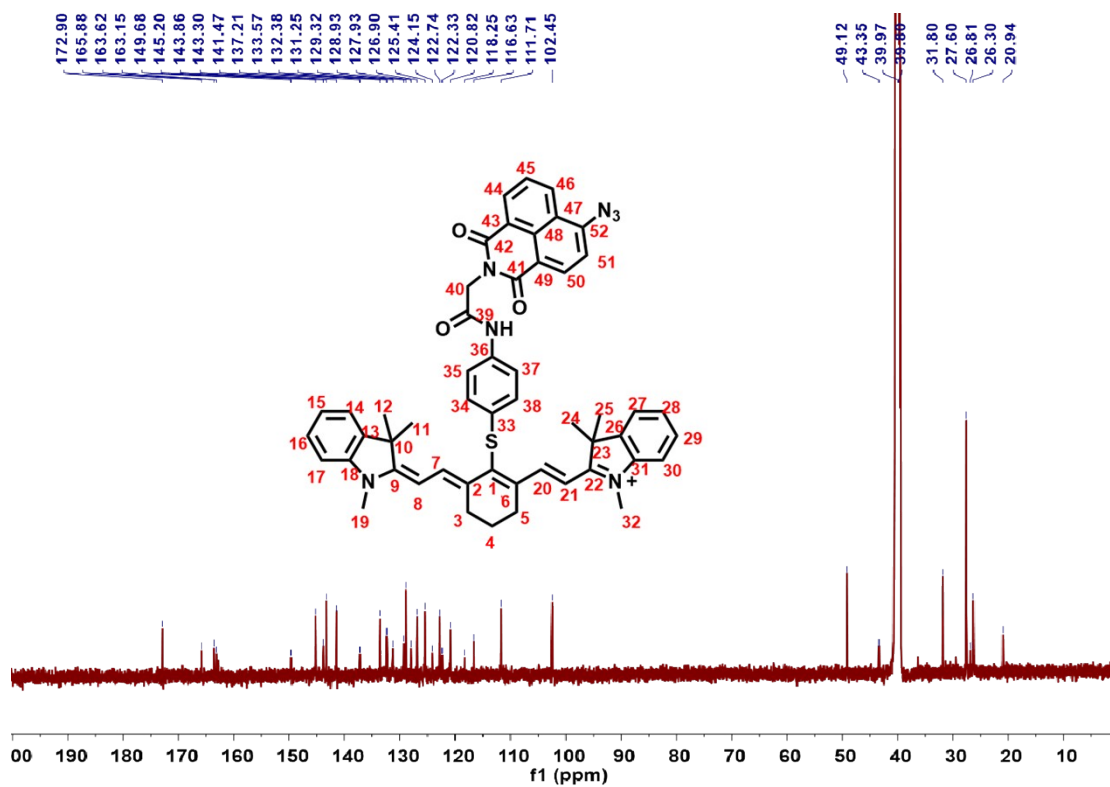


Fig. S7  $^{13}\text{C}$  NMR spectrum of Cy-NP in  $\text{DMSO-}d_6$ .

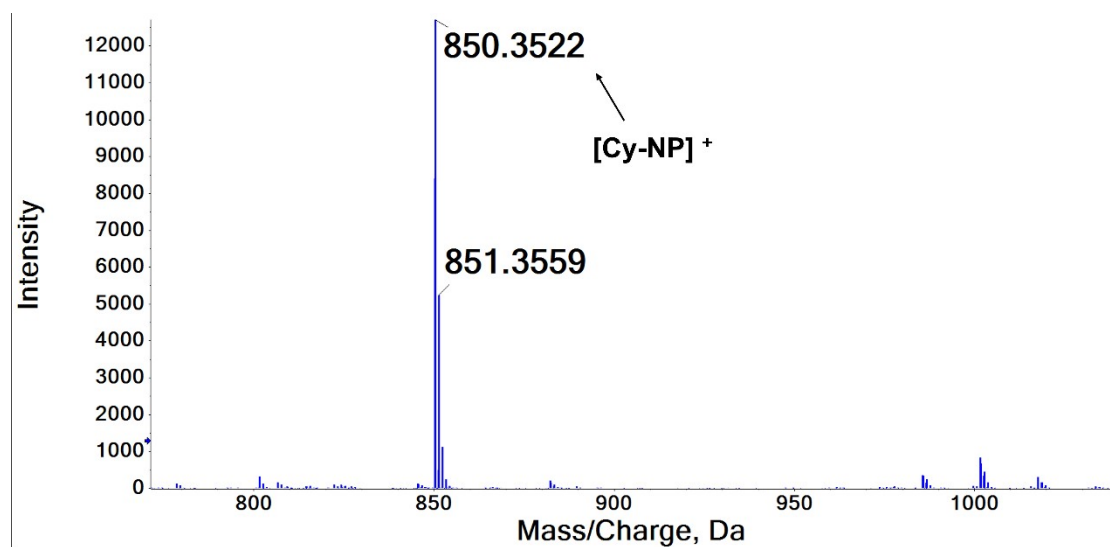


Fig. S8 HRMS spectrum of Cy-NP in  $\text{CH}_3\text{OH}$ .

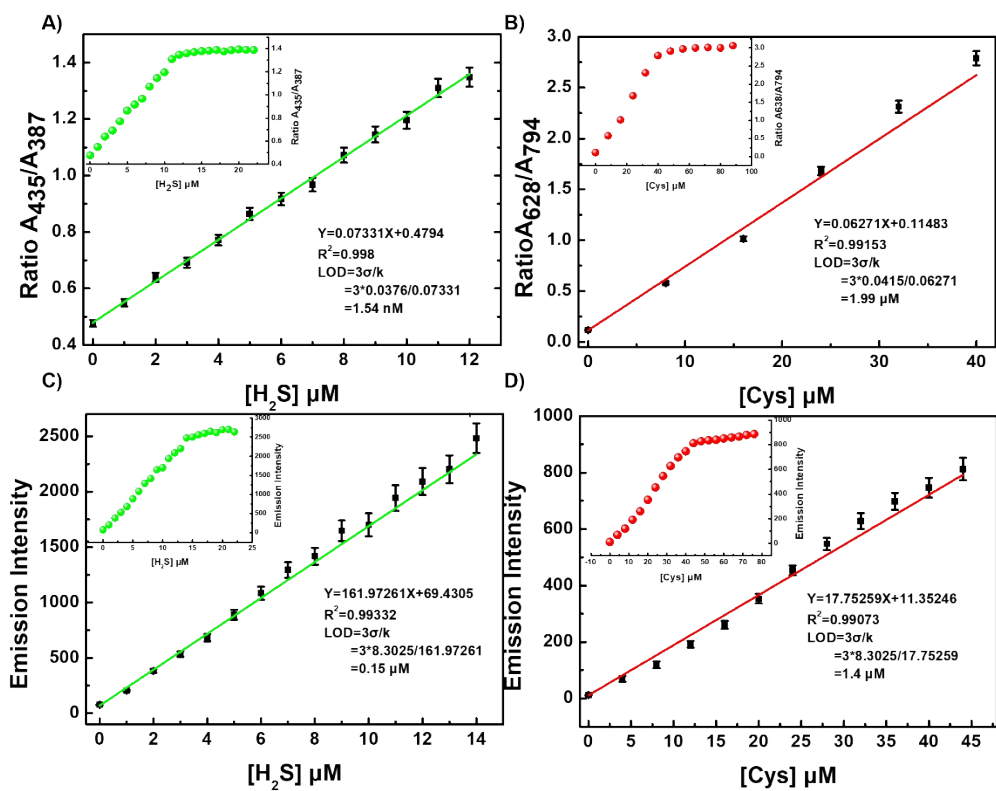


Figure S9. The linear range of Cy-NP to  $H_2S$  and Cys.

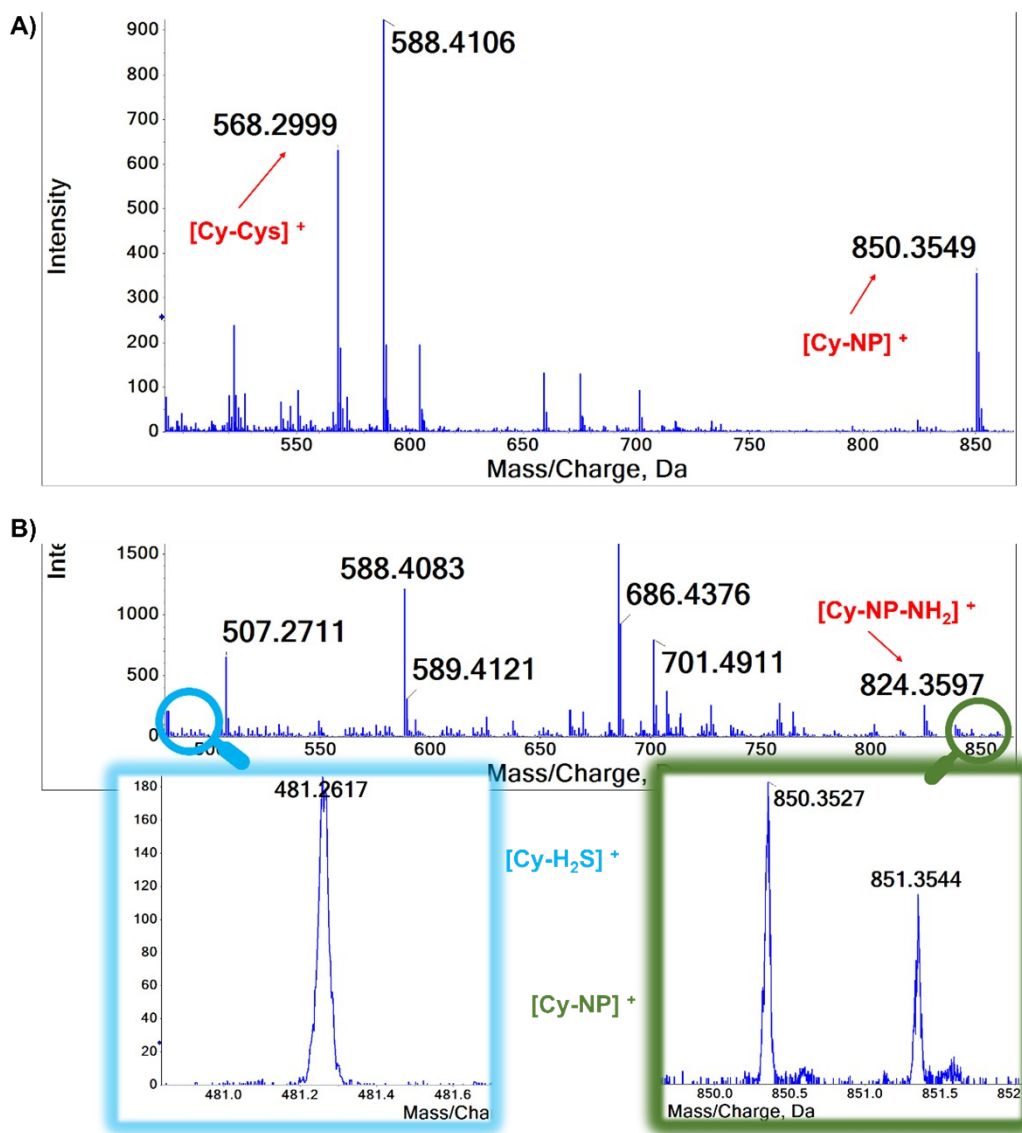


Fig. S10 HRMS spectra of Cy-NP, Cy-Cys, Cy-H<sub>2</sub>S and Cy-NP-NH<sub>2</sub> in CH<sub>3</sub>OH.

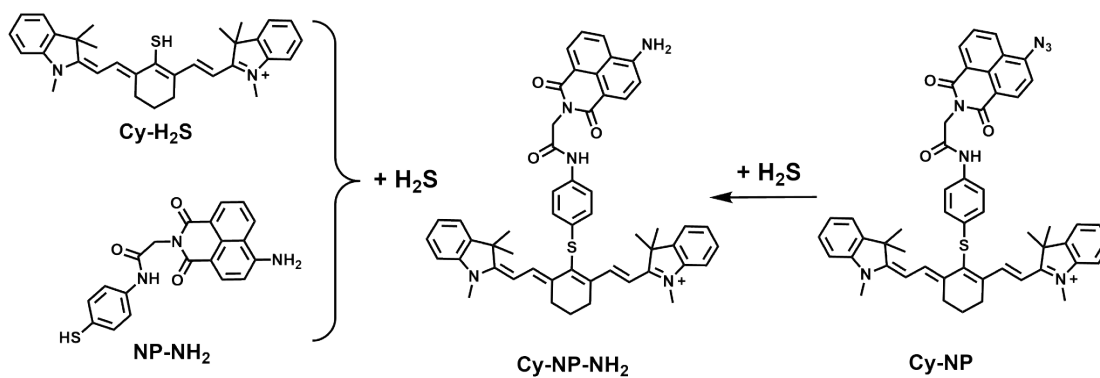
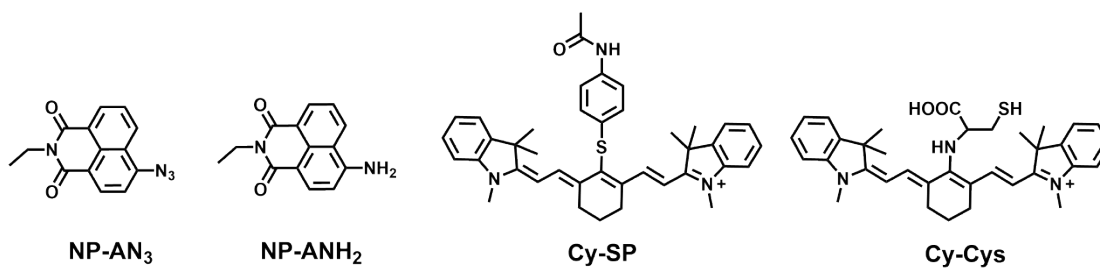
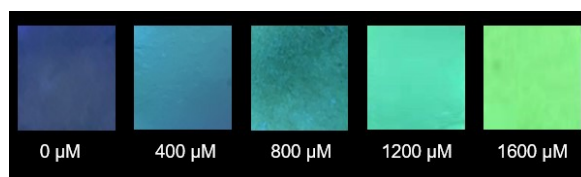


Fig. S11 the sensing mechanism of Cy-NP to H<sub>2</sub>S.

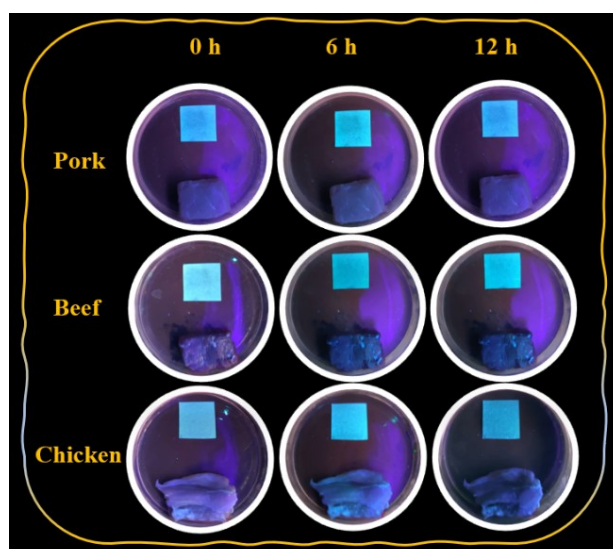




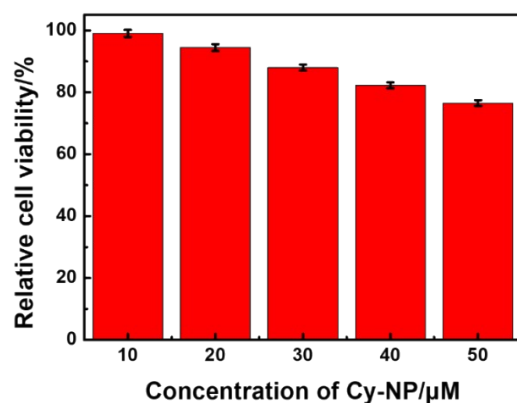
**Fig. S12** The structures used for DFT calculations.



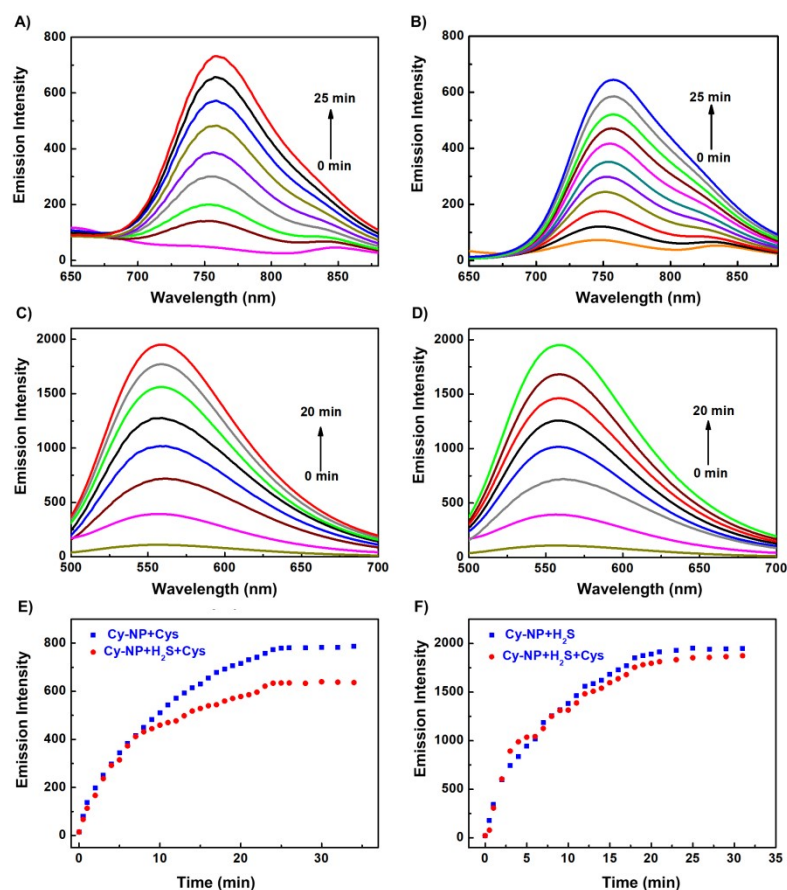
**Fig. S13** The response of test strips immersed into different concentration of H<sub>2</sub>S solution.



**Fig. S14** Optical images of Cy-NP test paper after being exposed to pork, beef, and chicken with different time intervals at 277 K in a refrigerator.



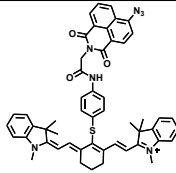
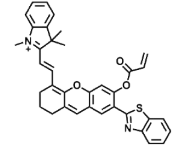
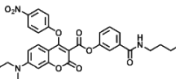
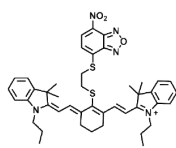
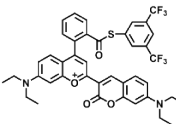
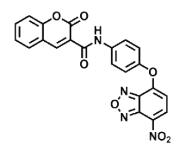
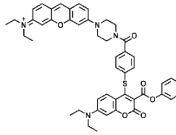
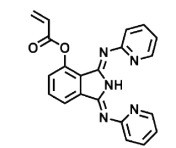
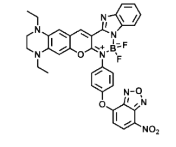
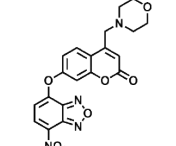
**Fig. S15** Percentage of viable MCF-7 cells after incubation with different concentrations of Cy-NP for 24 h.



**Fig. S16.** The emission intensity changes of Cy-NP A) upon addition of Cys at 640 nm excitation.

B) upon addition of Cys and H<sub>2</sub>S at 640 nm excitation. C) upon addition of H<sub>2</sub>S at 400 nm excitation. D) upon addition of Cys and H<sub>2</sub>S at 400 nm excitation. E) Change of fluorescence intensity at 640 nm excitation. F) Change of fluorescence intensity at 400 nm excitation.

**Table S1.** Comparison of Cy-NP with other fluorescent probes for Cys

Probe	Excitation mode	Selectivity	Emission (nm)	Detection	Reference
	Double	H <sub>2</sub> S Cys	560 760	0.15 μM 1.4 μM	This work
	Single	Cys/GSH	783	0.16 μM	1
	Single	Cys/Hcy	485	0.86 mM	2
	Double	Cys/Hcy GSH	550 810	94 nM 75 nM	3
	Single	Cys/Hcy	474/694	16 μM	4
	Double	Cys/Hcy GSH	520/550 520	0.43 μM 0.36 μM	5
	Double	Cys/Hcy GSH	472/584 542/584	95 nM 39 nM	6
	Single	Cys/Hcy	585	5.4 nM	7
	Double	Cys/Hcy GSH	565/630 630	95.6 nM 39.3 nM	8
	Single	Cys/Hcy GSH	490/580 490	1 μM 5 μM	9

**References**

- 1 X. Lu, M. Wu, S. Wang, J. Qin and P. Li, *Talanta*, 2021, **235**, 122771.
- 2 H. Zhang, L. Xu, W. Li, W. Chen and Q. Xiao, *RSC Adv.*, 2019, **9**, 7955-7960.
- 3 R. Li, H. Kassaye, Y. Pan, Y. Shen, W. Li and Y. Cheng, *Biomater. Sci.*, 2020, **8**, 5994-6003.
- 4 H. Lv, X. F. Yang, Y. Zhong, Y. Guo, Z. Li and H. Li, *Anal. Chem.*, 2014, **86**, 1800-1807.
- 5 Y. Z. Yang, Z. Y. Xu, L. Han, Y. Z. Fan, M. Qing and N. B. Li, *Dyes Pigm.*, 2021, **184**, 108722.
- 6 H. Zhang, B. Wang, Y. Ye, W. Chen and X. Song, *Org. Biomol. Chem.*, 2019, **17**, 9631-9635.
- 7 X. Liu, H. Tian, L. Yang, Y. Su, M. Guo and X. Song, *Tetrahedron Let.*, 2017, **58**, 3209-3213.
- 8 X. Ren, Y. Zhang, F. Zhang, H. Zhong, J. Wang and X. Liu, *Anal. Chim. Acta.*, 2020, **1097**, 245-253.
- 9 X. Song, Y. Tu, R. Wang and S. Pu, *Dyes Pigm.*, 2020, **177**, 180270 .