Supporting Information for

A novel near-infrared fluorescent probe with "donor-π-acceptor" type structure and its application in the selective detection of cysteine in living cells

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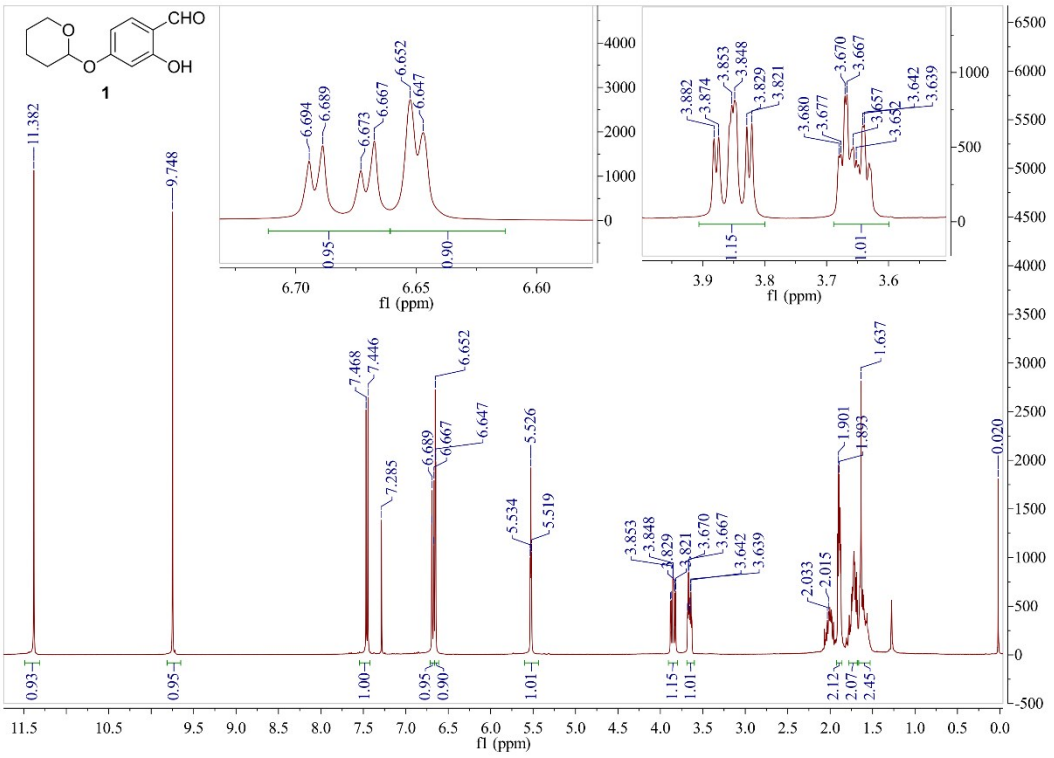

Fig. S1. ^{1}H NMR of compound **1** in $CDCl_3$

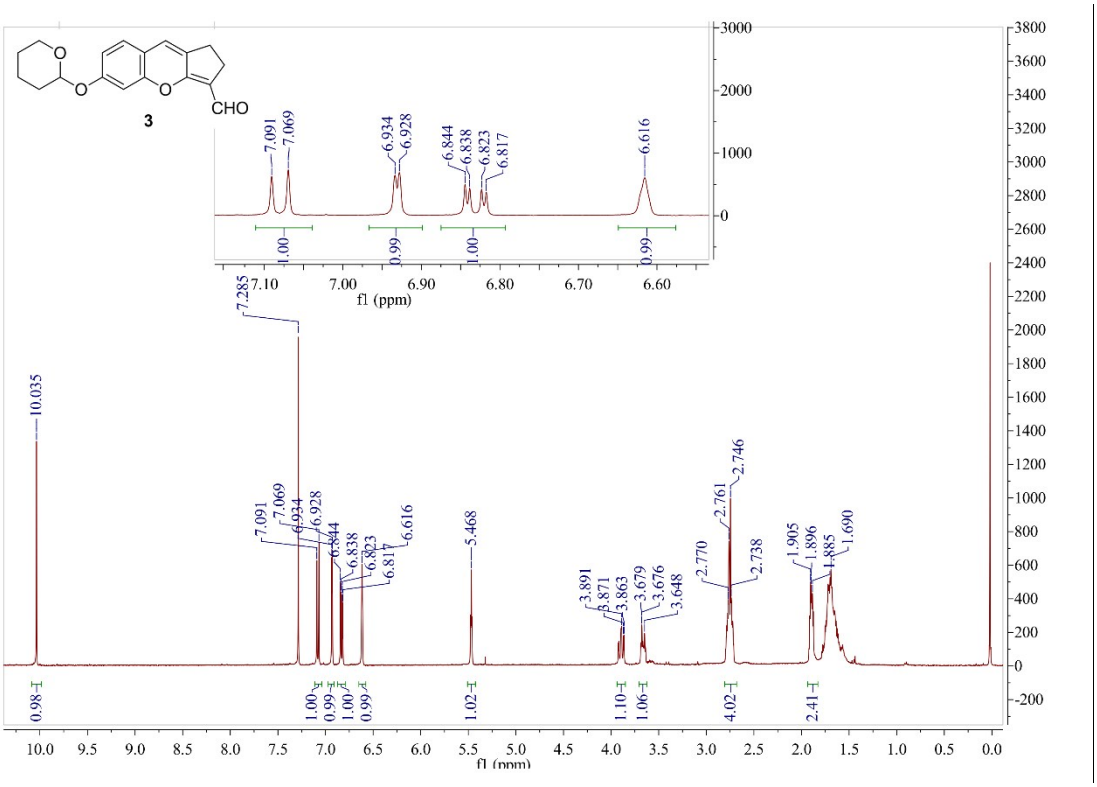

Fig. S2. ^{1}H NMR of compound **3** in $CDCl_3$**.**

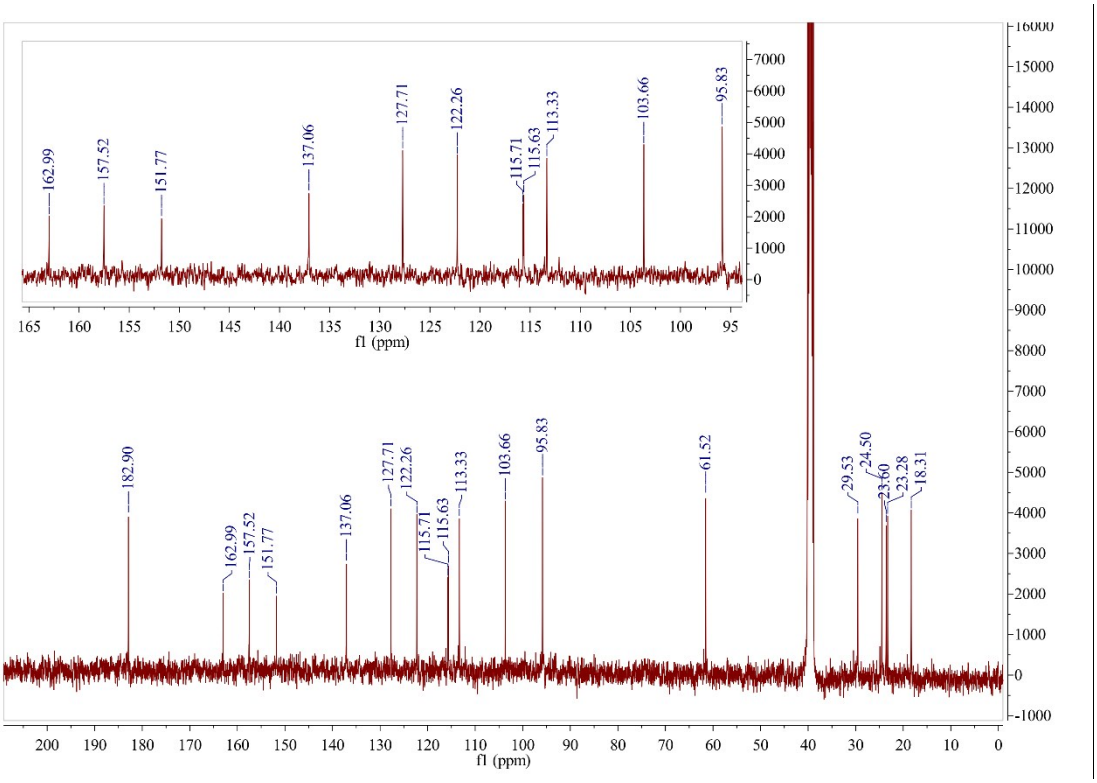

Fig. S3. ^{13}C NMR of compound **3** in d_6-DMSO**.**

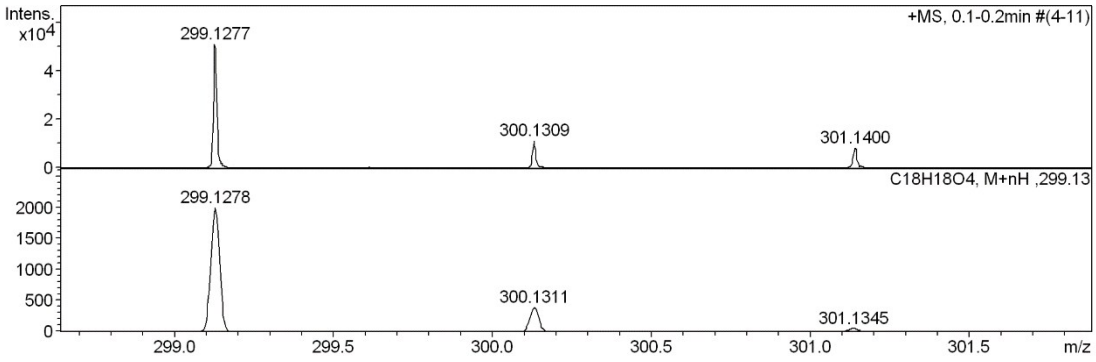

Fig. S4. HRMS(ESI) spectrum of compound **3.**

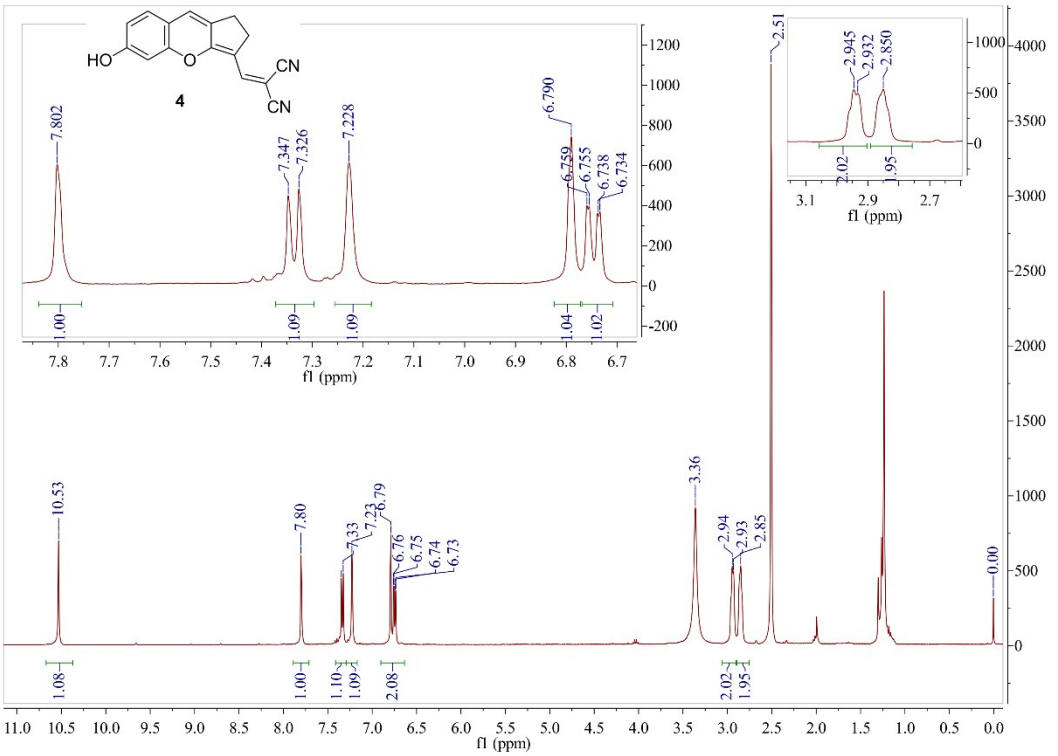

Fig. S5. ^{1}H NMR of compound **4** in d_6-DMSO**.**

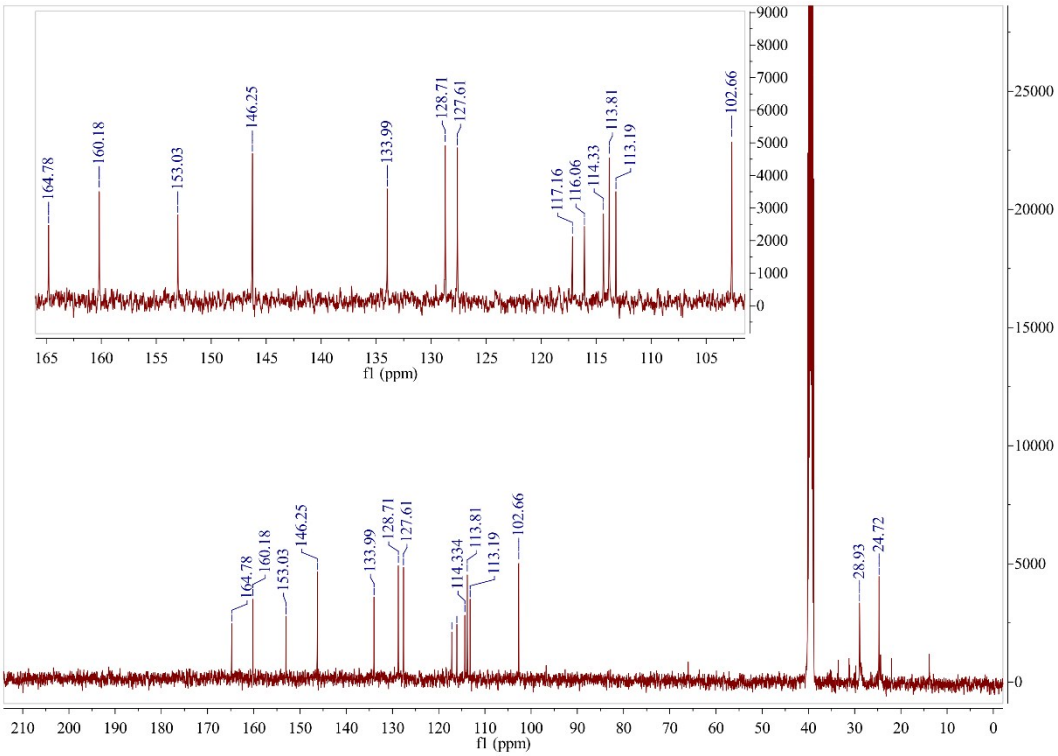

Fig. S6. ^{13}C NMR of compound **4** in d_6-DMSO**.**

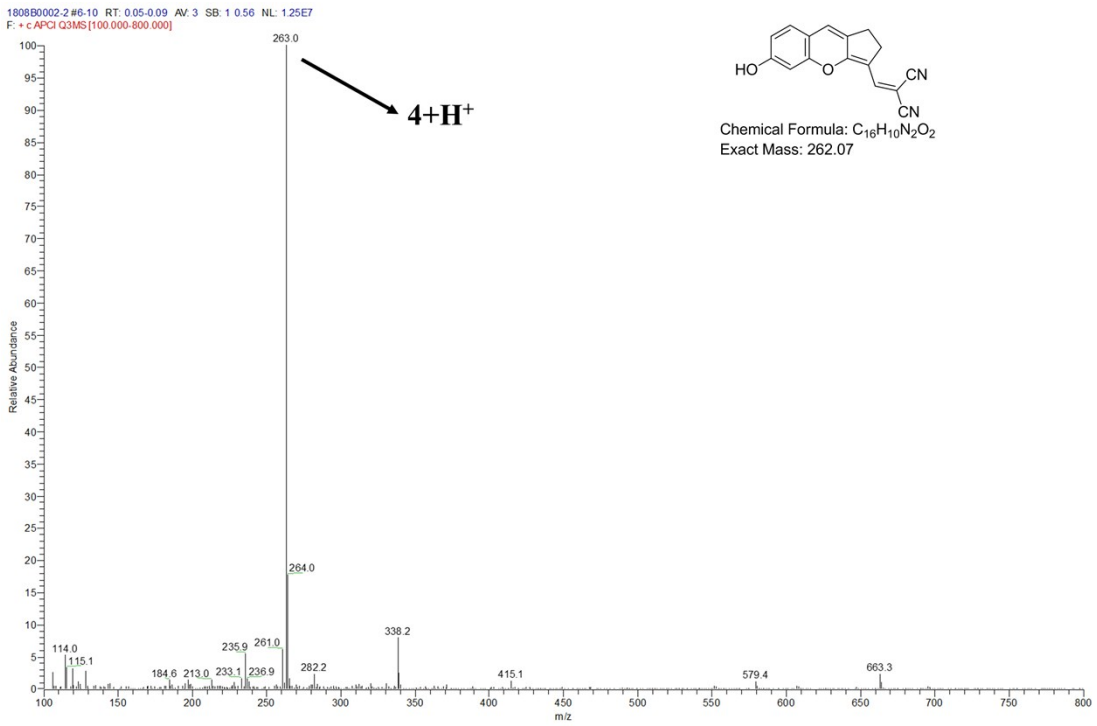

Fig. S7. MS spectrum (APCI) of compound **4.**

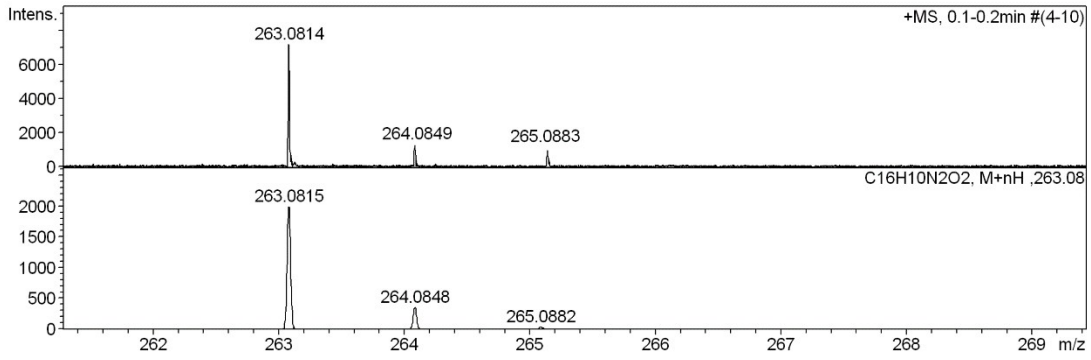

Fig. S8. HRMS(ESI) spectrum of compound **4.**

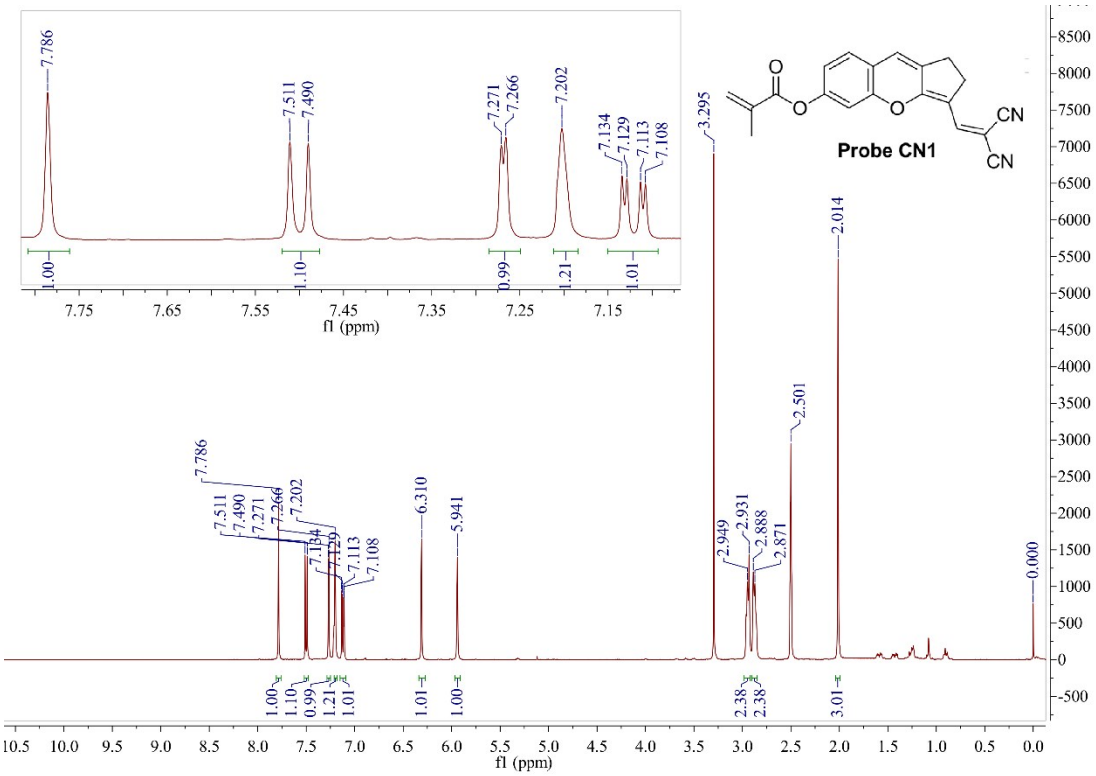

Fig. S9. ^{1}H NMR of Probe **CMC** in d_6-DMSO**.**

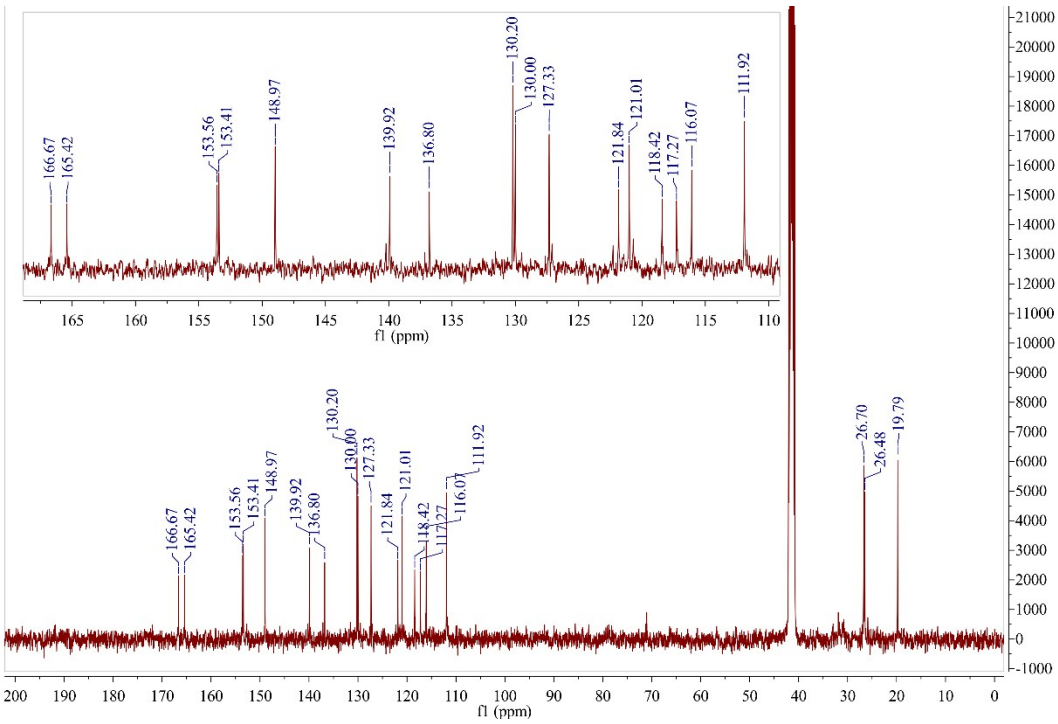

Fig. S10. ^{13}C NMR of Probe **CMC** in d_6-DMSO**.**

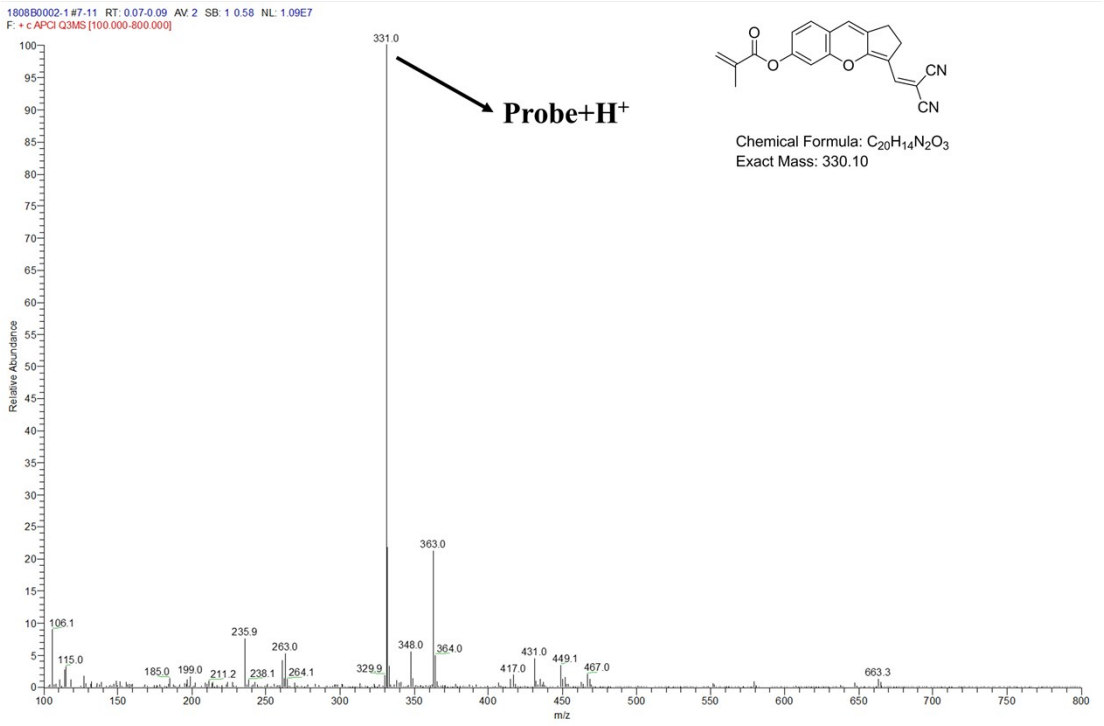

Fig. S11. MS spectrum (APCI) of Probe **CMC.**

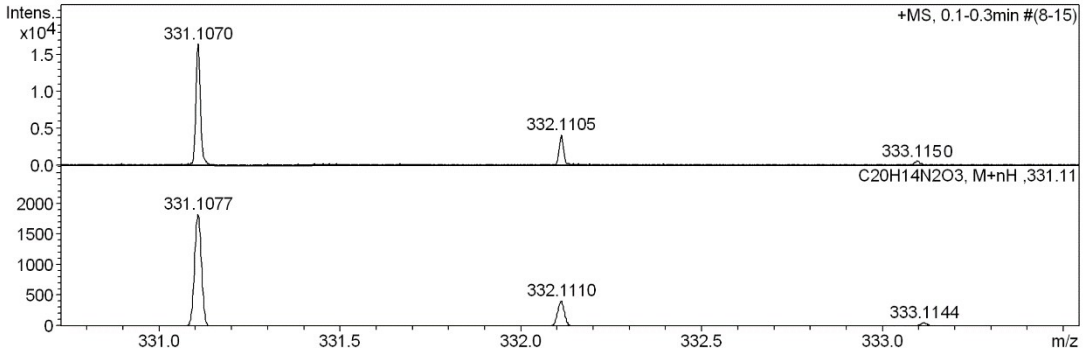

Fig. S12. HRMS spectrum (ESI) of Probe **CMC.**

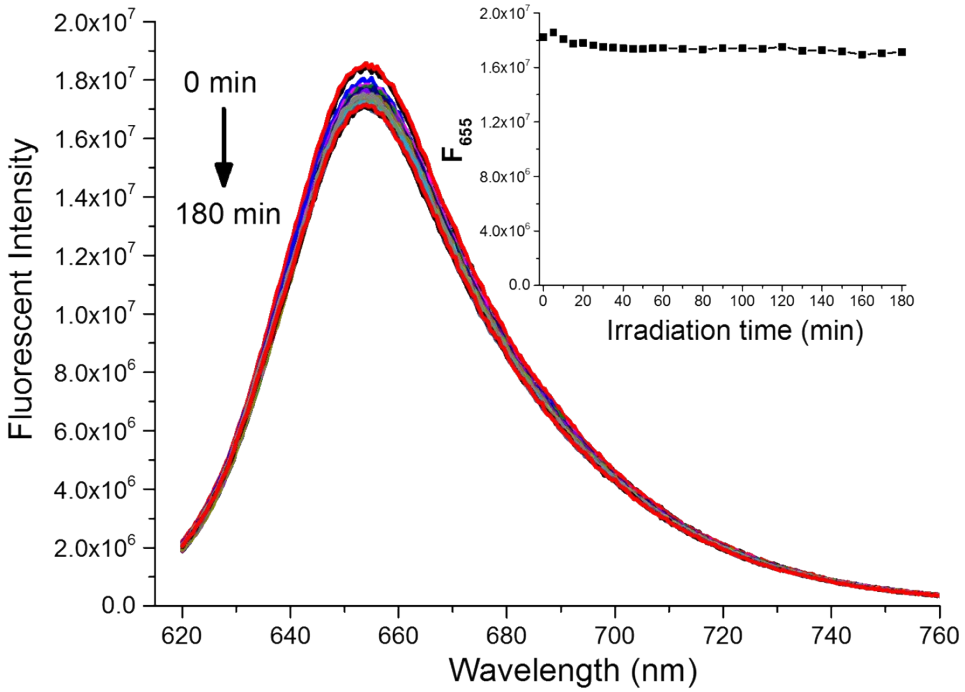

Fig. S13. Changes of fluorescence intensity of Probe **CMC** in the mixture of DMF/PBS buffer (pH 7.4, *v*/*v* = 1:1) under the irradiation of 150 W Xe lamp (λ_{ex} = 614 nm, slit width as 0.5 nm and 2.5 nm).

Table S1. UV/vis and Photoluminescence (PL) Data of Compound **4**

	Ethanol	Dioxane	Acetonitrile	DMSO	DMF	PBS/DMF (*v*/*v* = 1:1)
[a]UV/vis λ_{max} (nm)	511	498	504	518	670	614
ε (L mol^{-1} cm^{-1})	30500	27000	30100	21700	32300	37000
[b]λ_{em} (nm)	647.5	603	673	684.5	683.5	655
[c]Δλ(nm)	30.5	125	21	13.5	12.5	41
[d]Φ_F	20.00%	0.28%	18.14%	26.30%	30.50%	19.20%

[a]The slit was set as 5 nm, and the concentration of compound **4** was 10 μmol/L. [b]The λ_{exc} was set at the maximum wavelength of UV-vis absorption, and the concentration of compound **4** was 10 μmol/L. [c]Stokes shift. [d]The absolute fluorescence quantum yield (Φ) values were determined by using an integral sphere.

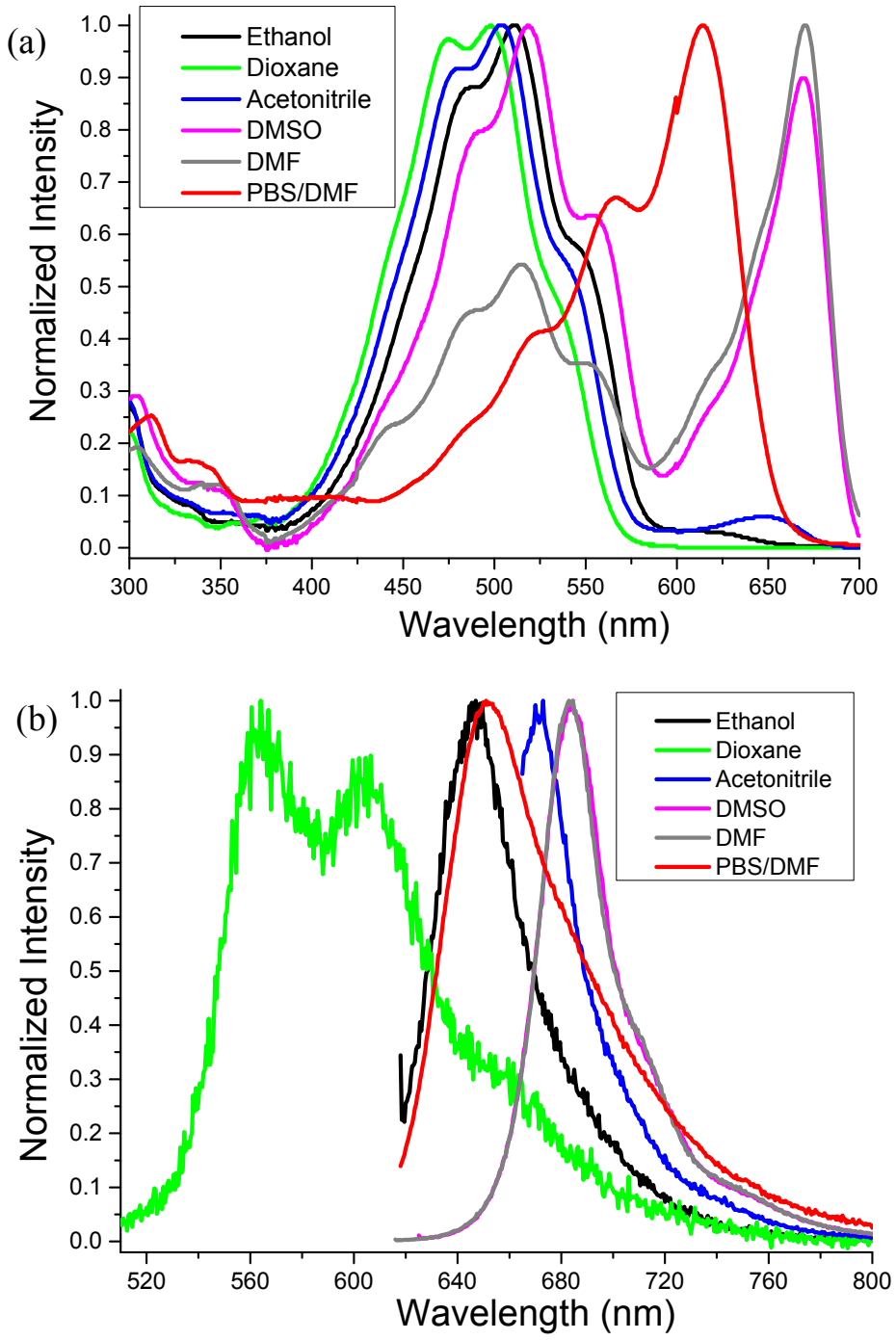

Fig. S14. Normalized UV/vis (a) and emission spectra (b) of compound **4** (10 μmol/L) in different solvents.

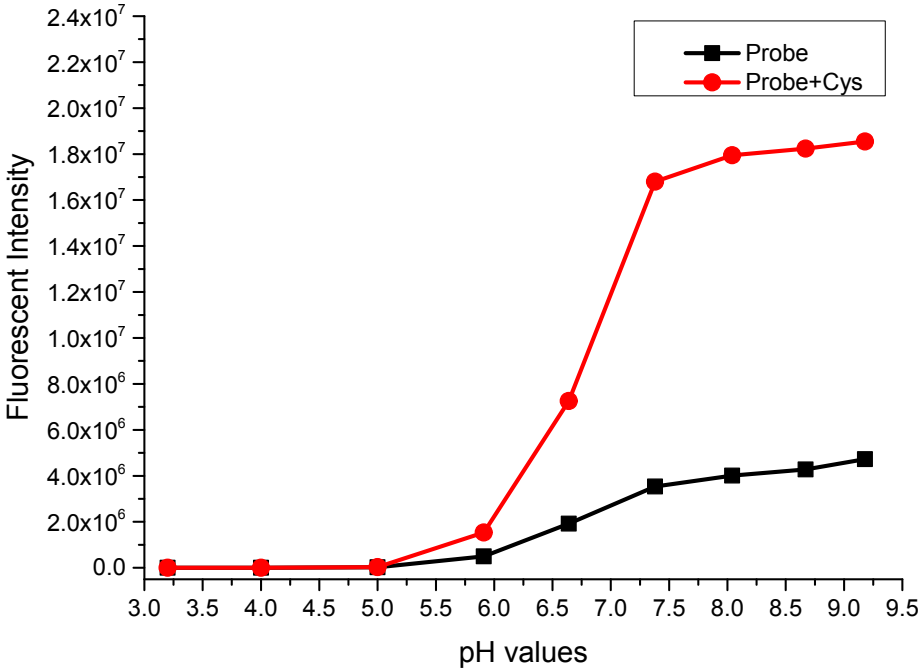

Fig. S15. The effect of pH on the fluorescent intensity of probe **CMC** (10 μmol/L) at 655 nm after 30 min of addition of 10 equiv. of Cys. All these data were measured in the mixture of DMF/PBS buffer (pH 7.4, *v*/*v* = 1:1) at 25 °C under the excitation at 614 nm. Slit width: (0.5, 2.5).

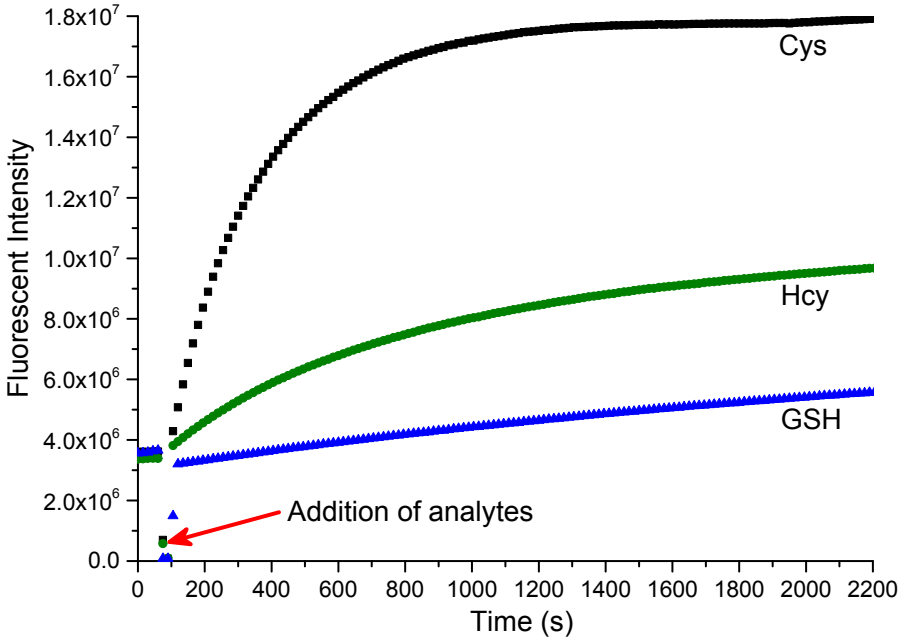

Fig. S16. Fluorescent kinetics study of probe **CMC** (10 μmol/L) upon addition of Cys, Hcy and GSH (100 μmol/L) in the mixture of DMF/PBS buffer (pH 7.4, *v*/*v* = 1:1) at 25 °C. The reactions were monitored at 655 nm under the excitation at 614 nm. Slit width: (0.5, 2.5).

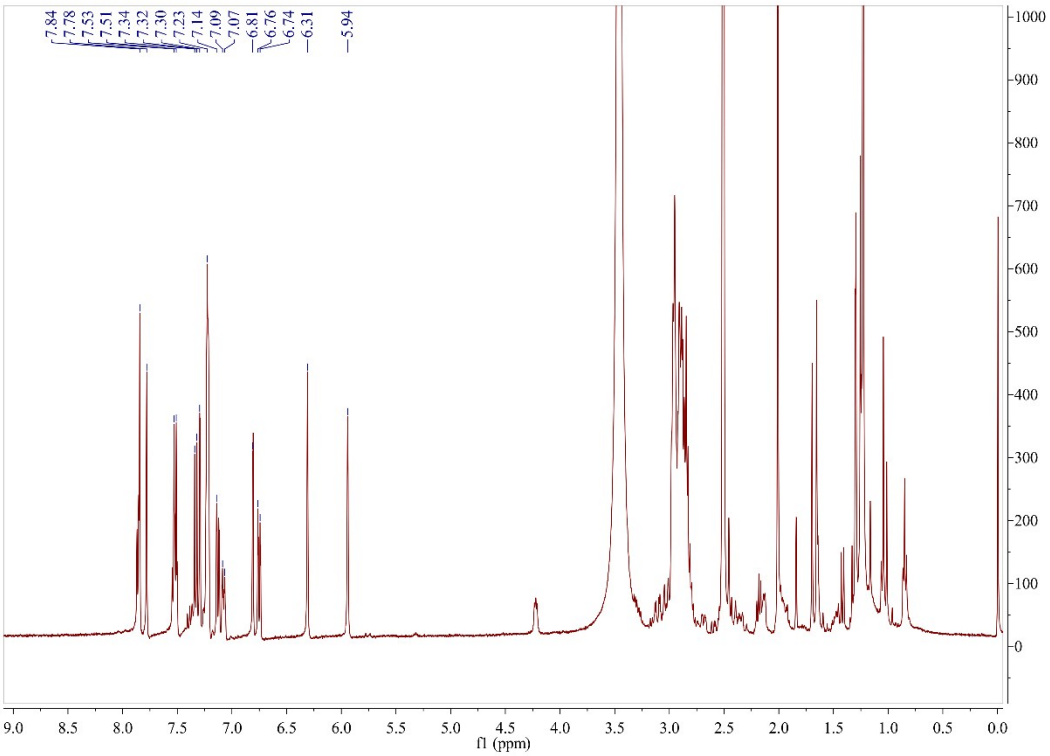

Fig. S17. ^{1}H NMR of the reaction mixture of Probe **CMC** in d_6-DMSO with Cys (3 eq) in D_2O**.**

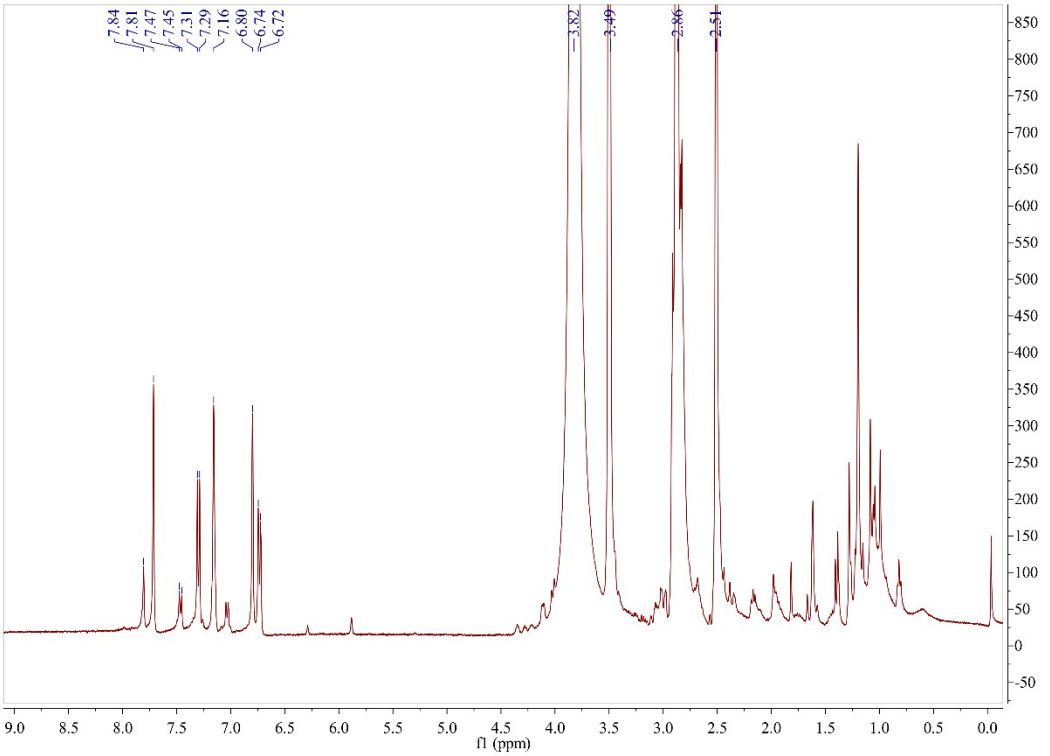

Fig. S18. ^{1}H NMR of the reaction mixture of Probe **CMC** in d_6-DMSO with Cys (10 eq) in D_2O**.**

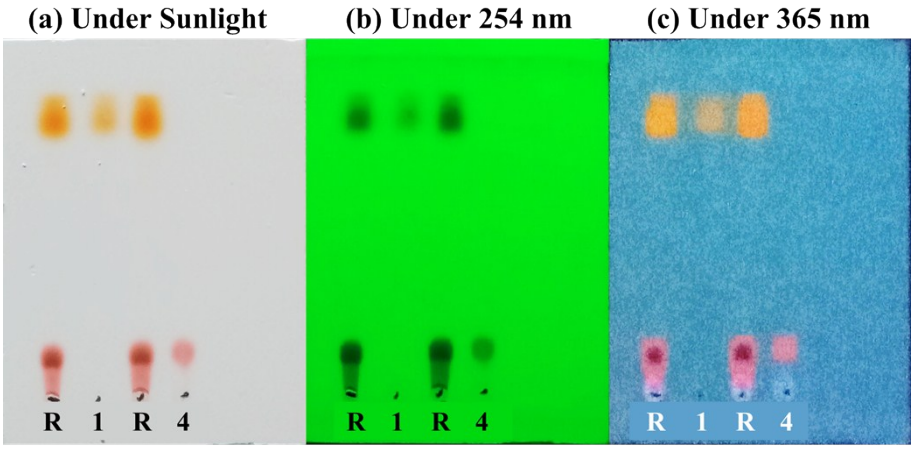

Fig. S19. The photos of the TLC plate under different light by comparing probe **CMC** (label **1**), compound **4** (label **4**) and ethyl acetate layer extracted from the reaction mixture of probe **CMC** with Cys in DMF/H_2O (label **R**). (A) under Sunlight, (B) under light of 254 nm, (C) under light of 365 nm. The eluent for TLC: CH_2Cl_2 /ethyl acetate (*v*/*v* = 20:1).

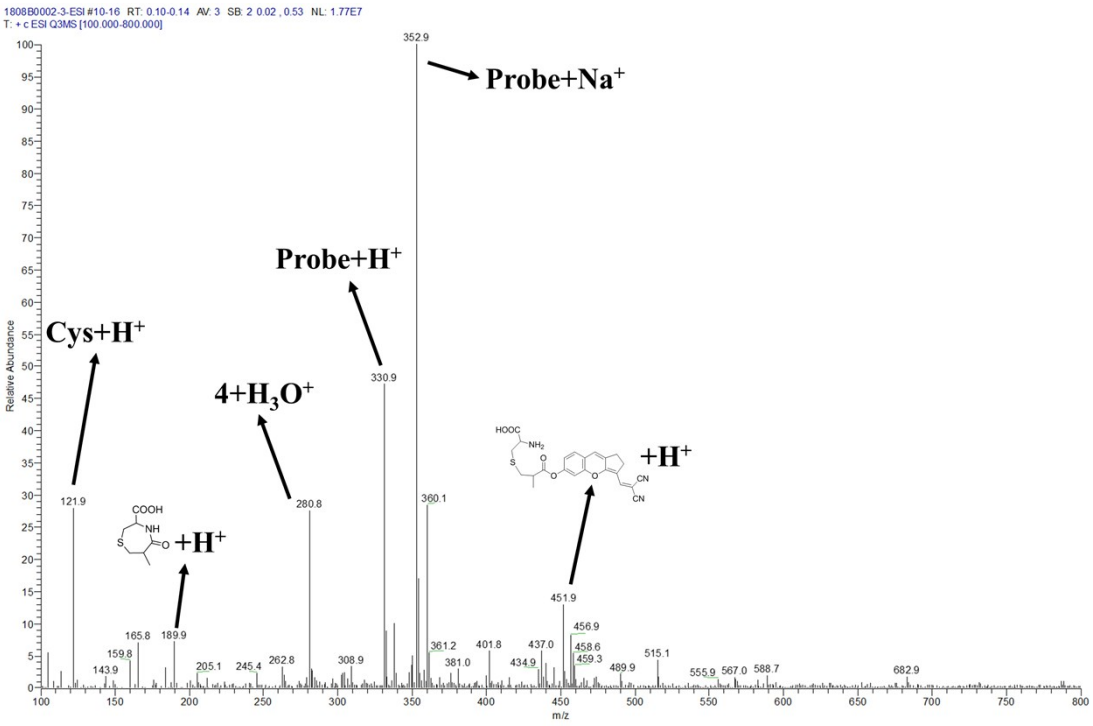

Fig. S20. MS(ESI) spectrum of the reaction mixture after 5 min of the adding 6 eq Cys into the probe **CMC** solution in CH_3CN/H_2O (*v*/*v* = 1:1).

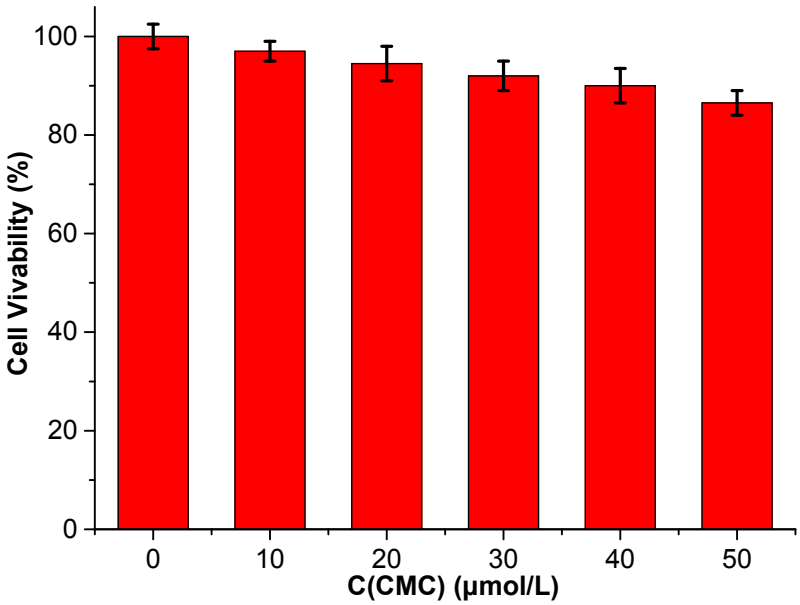

Fig. S21. Viable HeLa cells after indication with different concentrations of probe **CMC** at 37 °C after 24 hours, and the cell viability was estimated via MTT assay.