

Supporting information

A near-infrared fluorescent probe for the discrimination of cysteine in aqueous solution and imaging of cysteine in hepatocellular carcinoma cells with facile cell-compatible ability

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Figure S1. ¹HNMR spectra of M₃ in DMSO-d₆

Figure S2. ¹HNMR spectra of M₄ in DMSO-d₆

Figure S3. ¹HNMR spectra of probe AySA in DMSO-d₆

Figure S4. ¹³CNMR spectra of probe AySA in DMSO-d₆

Figure S5. HRMS spectrum of probe AySA

Figure S6. The color of probe added amino acids under sunlight in pure water solution (PBS solution)

Figure S7. The blue bar is the histogram of Fig. 1 (a), the red bar is the fluorescence intensity of probe (10 μM) upon the addition of other amino acids (10 μM) in the presence of Cys (10 μM) in pure water solution (PBS buffer solution, pH = 7.4).

Figure S8. Fluorescence intensity of the free probe (10 μM) and in the presence of Cys (10 μM) under different pH values in pure water solution (PBS buffer solution, pH = 7.4).

Table 1 The detailed photophysical properties of AySA in the absence and presence of Cys.

Experimental Section

Fluorescence intensity normalization method

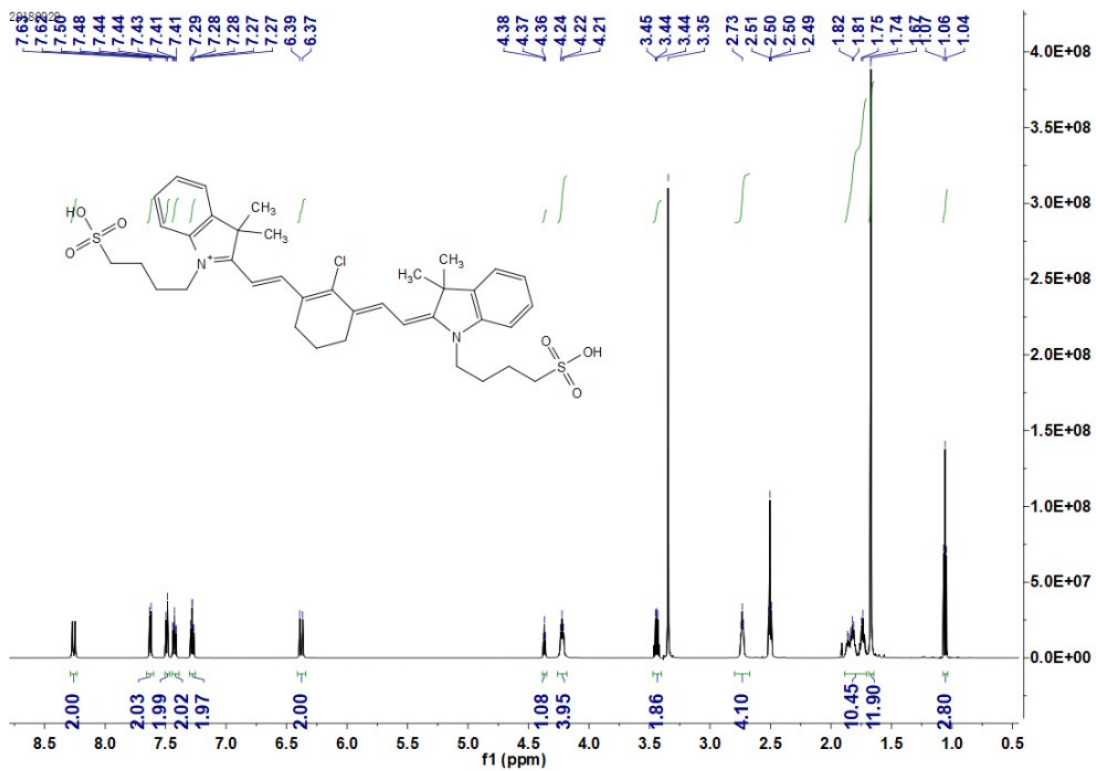


Fig. S1. ¹H NMR spectra of M₃ in DMSO-d₆

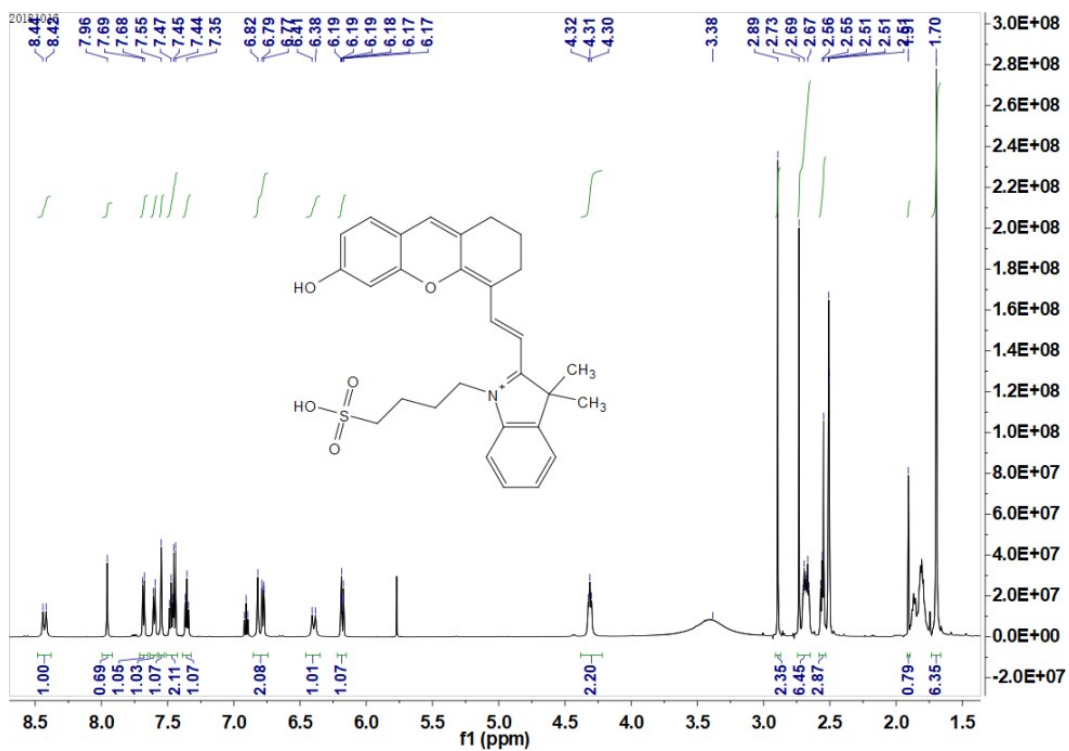


Fig.S2 ¹H NMR spectra of M₄ in DMSO-d₆

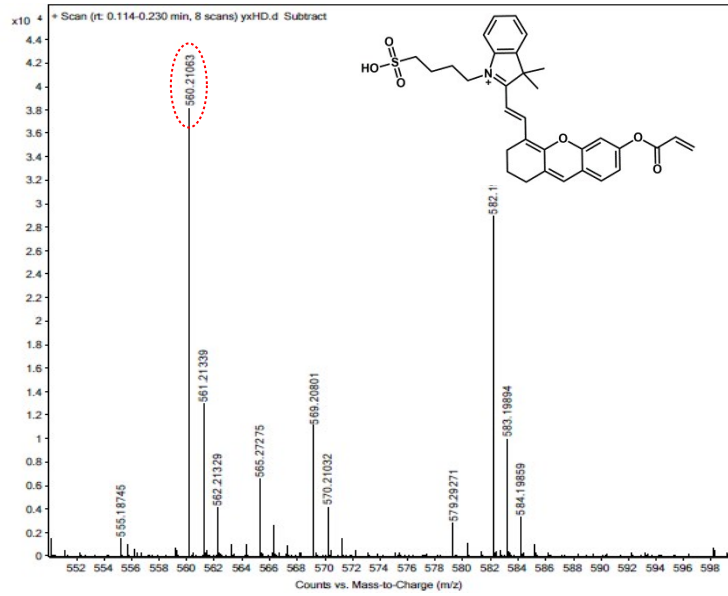


Fig.S5 ^1H RMR spectra of probe AySA in CH_3OH

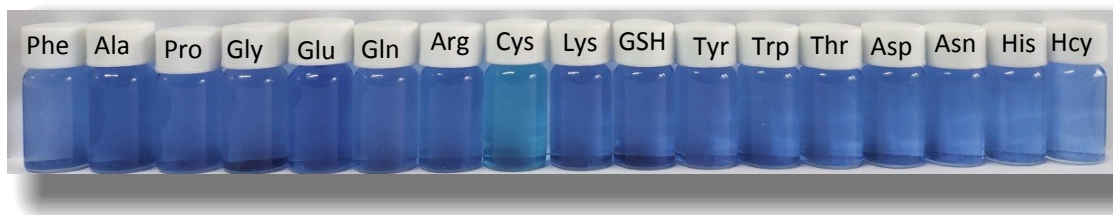


Fig.S6 The color of probe added amino acids under sunlight in pure water solution (PBS solution)

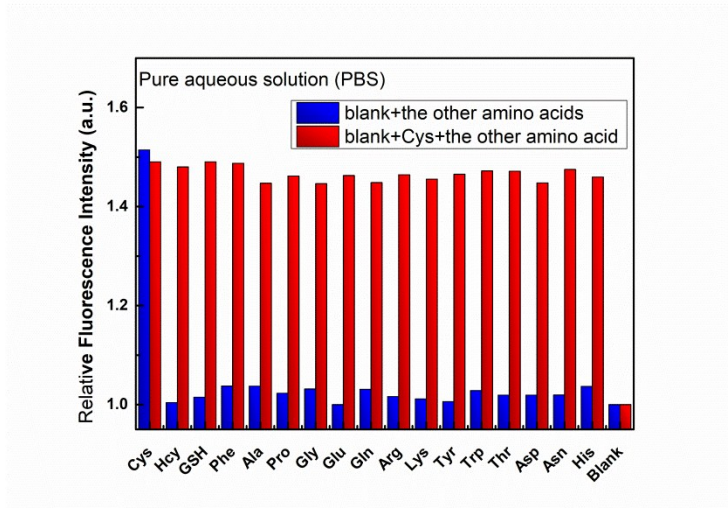


Fig.S7 The green bar is the histogram of Fig. 1 (b), the red bar is the fluorescence intensity of probe ($10\ \mu\text{M}$) upon the addition of other amino acids ($10\ \mu\text{M}$) in the presence of cys ($10\ \mu\text{M}$) in PBS buffer solution ($\text{pH} = 7.4$).

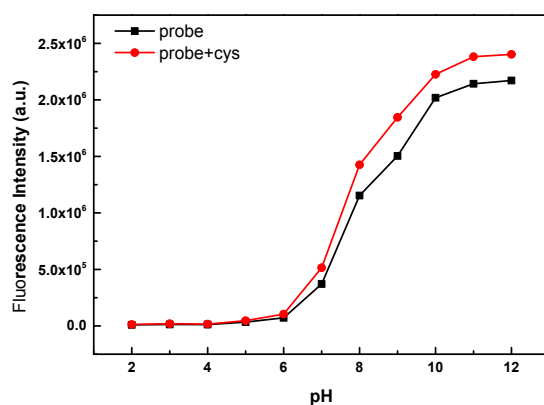


Fig.S8 Fluorescence intensity of the free probe (10 μM) and in the presence of Cys (10 μM) under different pH values in pure PBS buffer solution (pH = 7.4).

Table 1 Comparison of probe molecular quantum yield toward Cys

	λ_{abs} (nm)	ϵ_{max} ($10^4 \text{ M}^{-1} \text{ cm}^{-1}$)	λ_{em} (nm)	quantum yield(%)	the color under sunlight
Probe	592	0.92	701	6.5	purple
	615	0.73			
	669	0.47			
Probe+Cys	603	0.86	701	7.6	Green- blue
	652	1.14			
	678	1.05			

λ_{abs} : UV absorption maximum; ϵ_{max} : maximum molar extinction coefficient; λ_{em} : maximum emission wavelength $\Phi_{\text{F}(x)}$ was calculated according to the equation: $\Phi_{\text{F}(x)} = \Phi_{\text{F}(s)} (A_s F_x / A_x F_s) (n_x / n_s)^2$.

Fluorescence intensity normalization method

In this paper, the fluorescence intensity measured in selectivity and interference experiment was normalized. Using the fluorescence intensity of the blank probe as a standard, all readings at 701 nm were subjected to the fluorescence intensity values of the blank probes to obtain normalized values. The error is expressed by the standard deviation of the three tests.