Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

A human serum albumin-binding-based fluorescent probe for monitoring hydrogen sulfide and bioimaging

Table of Contents

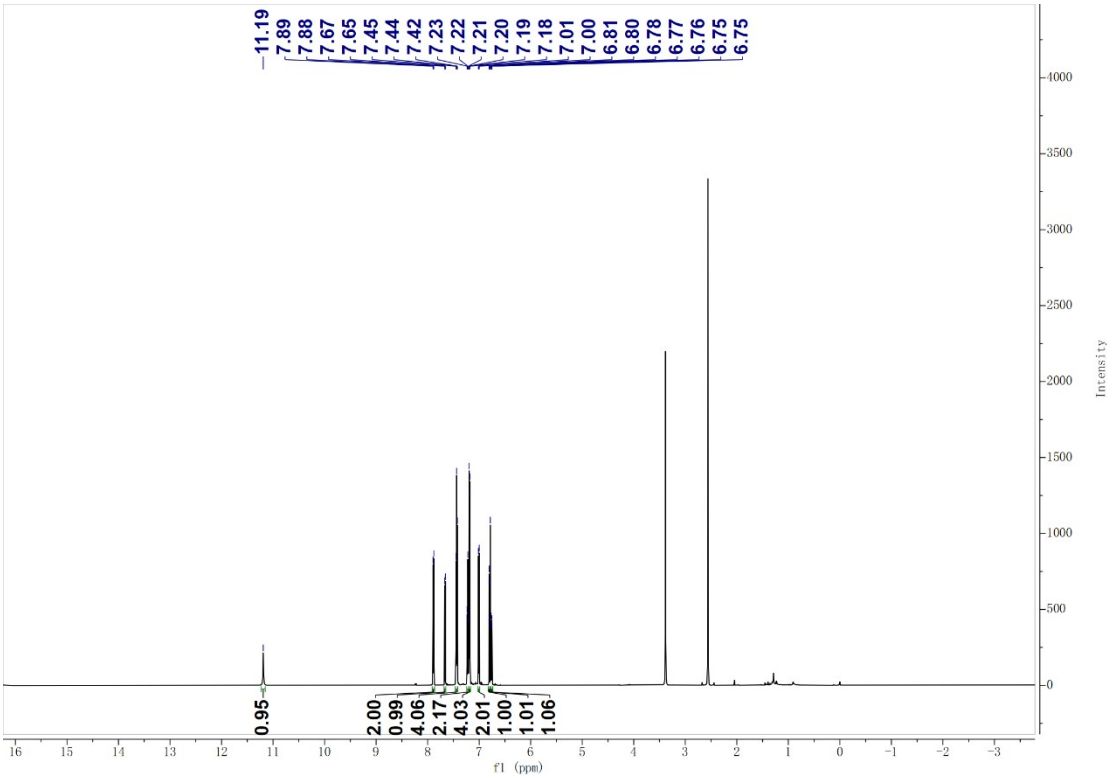


Figure S1. ^{1}H NMR spectrum of the compound **TPABF** (600 MHz, in DMSO-d_6).

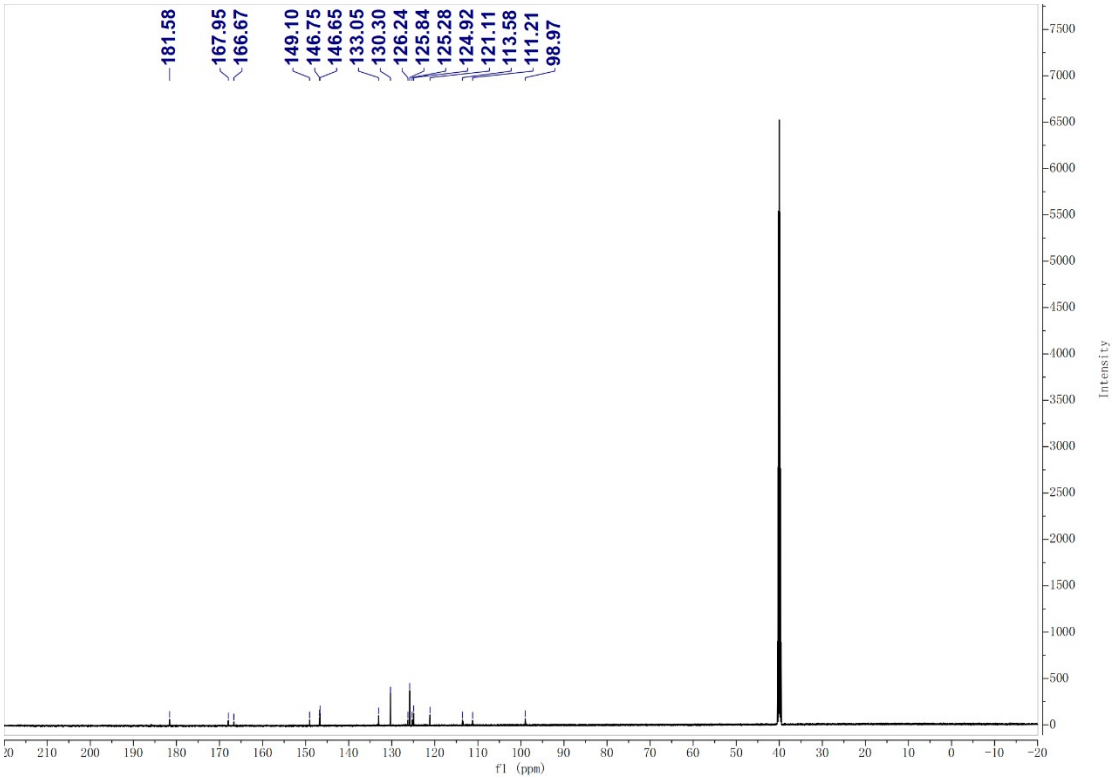


Figure S2. ^{13}C NMR spectrum of the compound **TPABF** (151 MHz, in DMSO-d_6).

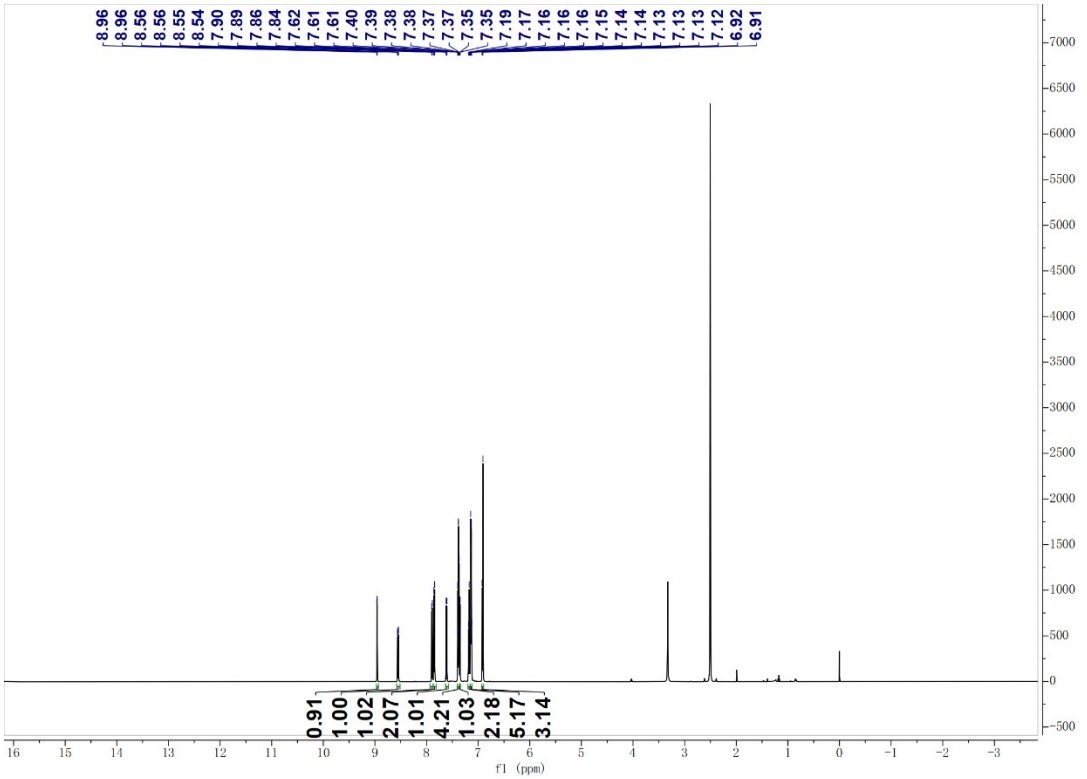


Figure S3. ^{1}H NMR spectrum of the probe **TPABF-HS** (600 MHz, in DMSO-d_6).

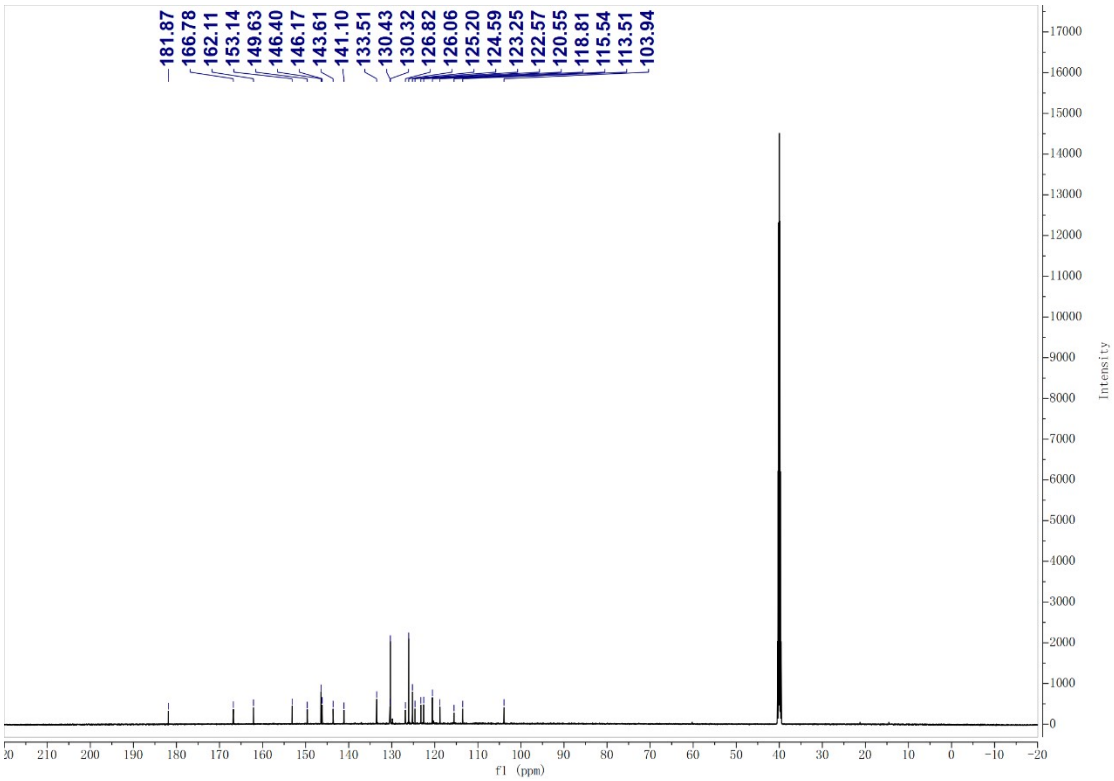


Figure S4. ^{13}C NMR spectrum of the probe **TPABF-HS** (151 MHz, in DMSO-d_6).

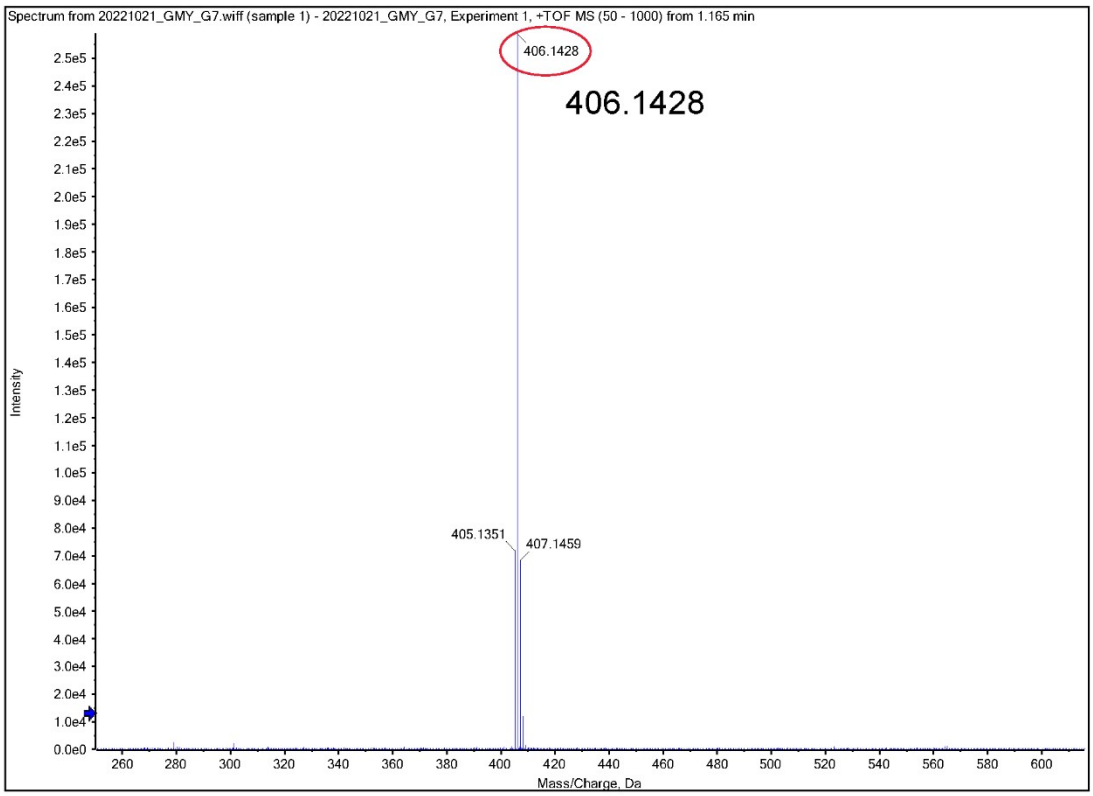


Figure S5. HRMS spectrum of the probe **TPABF** in acetonitrile.

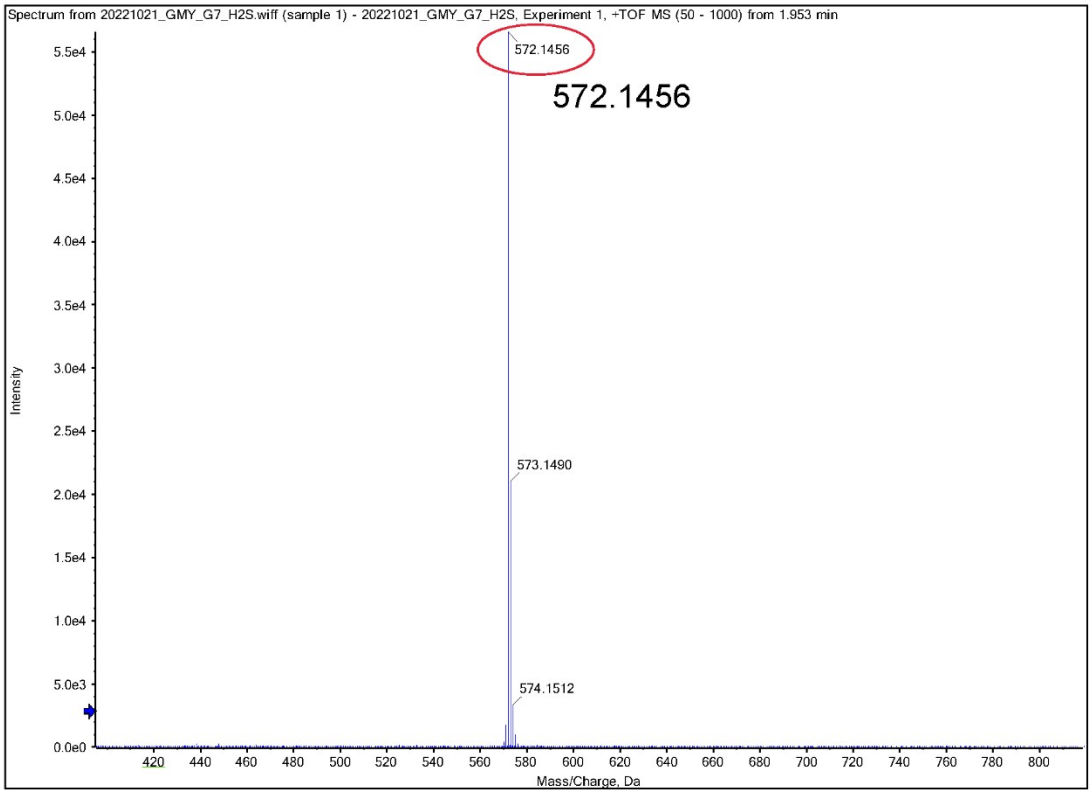


Figure S6. HRMS spectrum of the detecting product **TPABF-HS** in acetonitrile.

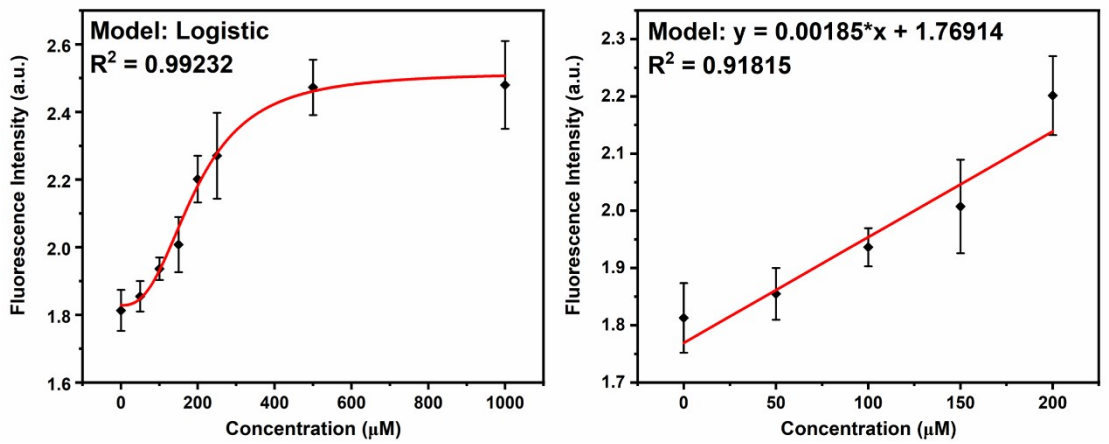


Figure S7. The fluorescence spectra of the detecting system containing **TPABF-HS** (10 μM) and H_2S of various concentrations (0-1000 μM) without HSA. Conditions: pH 7.4, 37 °C, 100 min, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

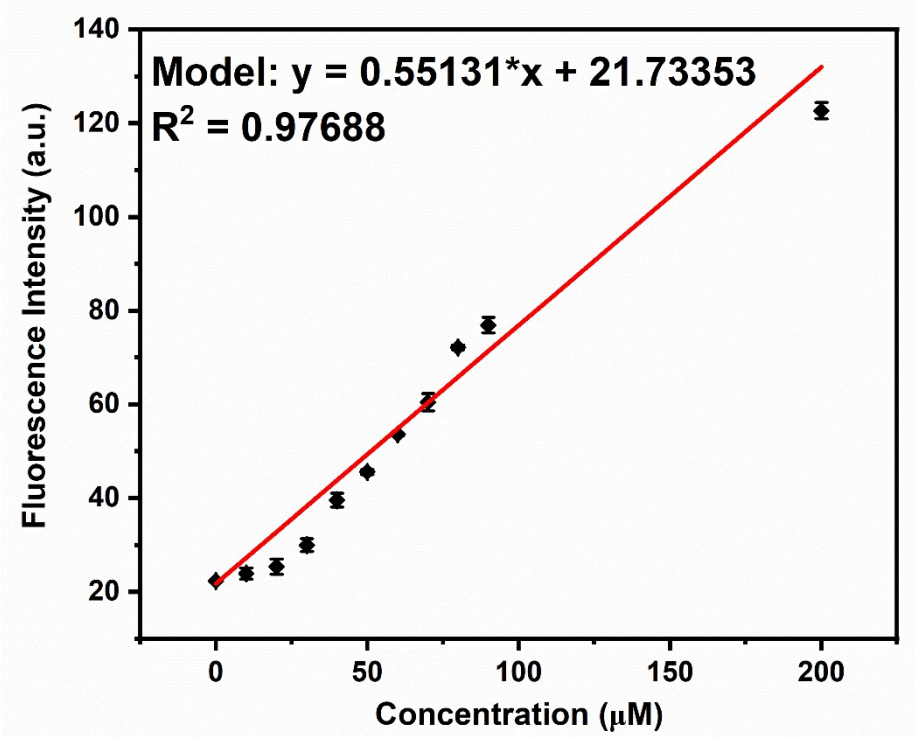


Figure S8. The fluorescence spectra of the detecting system containing TPABF-HS (10 μM) and HSA (0.6 mg/mL) with various concentrations (0-200 μM) of H2S. Conditions: pH 7.4, 37 °C, 100 min, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

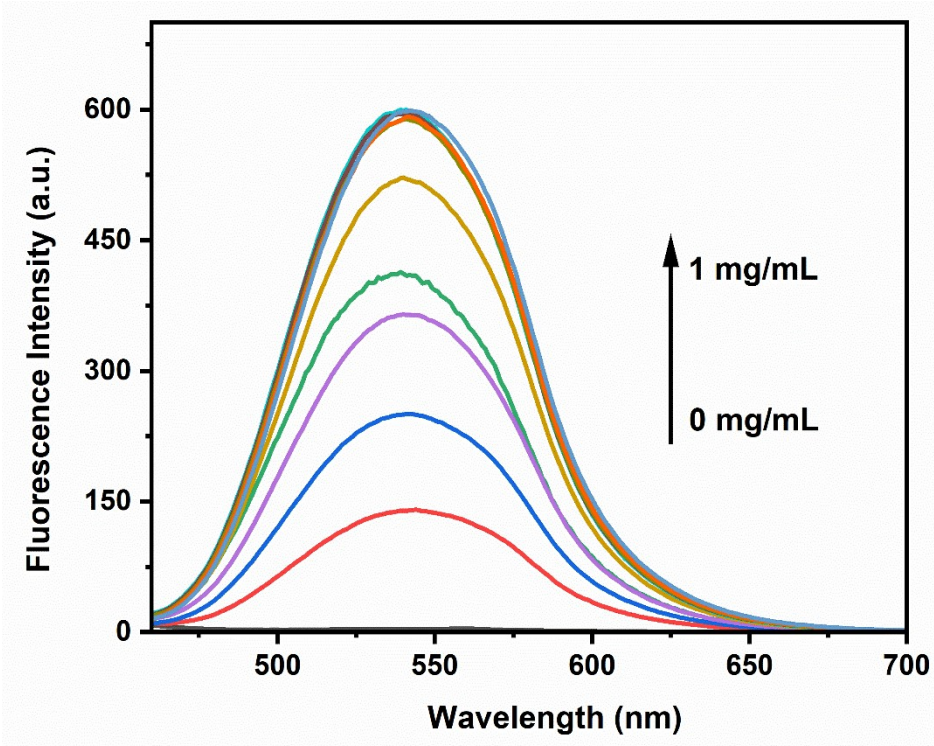


Figure S9. The fluorescence spectra of the detecting system containing **TPABF-HS** (10 μM) and H_2S (1 mM) with various concentrations (0-1 mg/mL) of HSA. Conditions: pH 7.4, 37 °C, 100 min, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

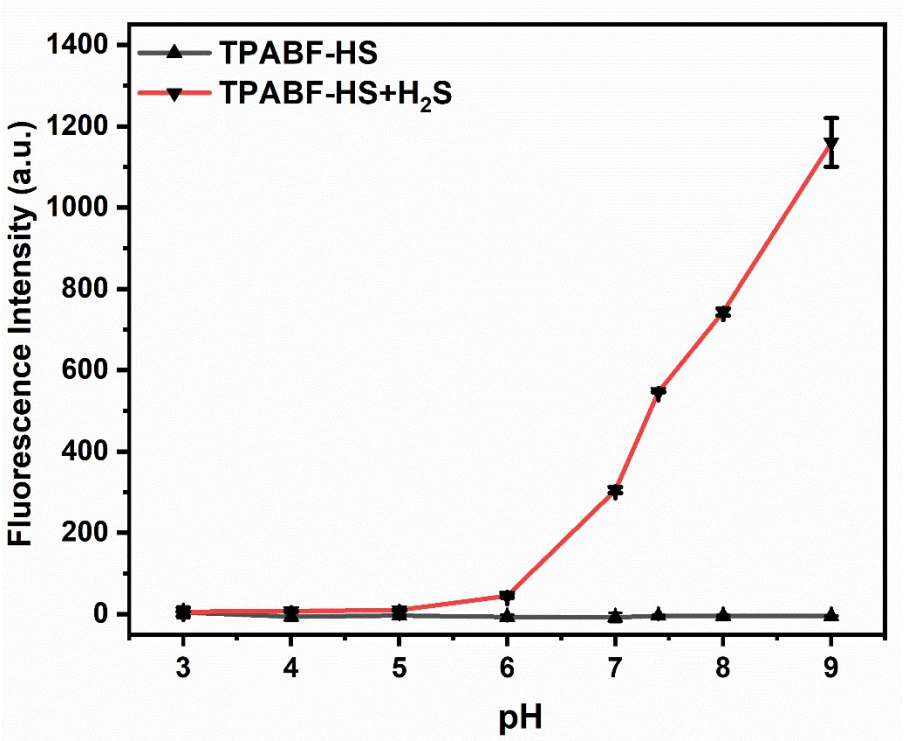


Figure S10. The fluorescence intensity of **TPABF-HS** (10 μM) and **TPABF-HS** (10 μM) with H_2S (1 mM) were detected in buffer liquid systems with different pH (3.0-9.0). Conditions: 37 °C, 100 min, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

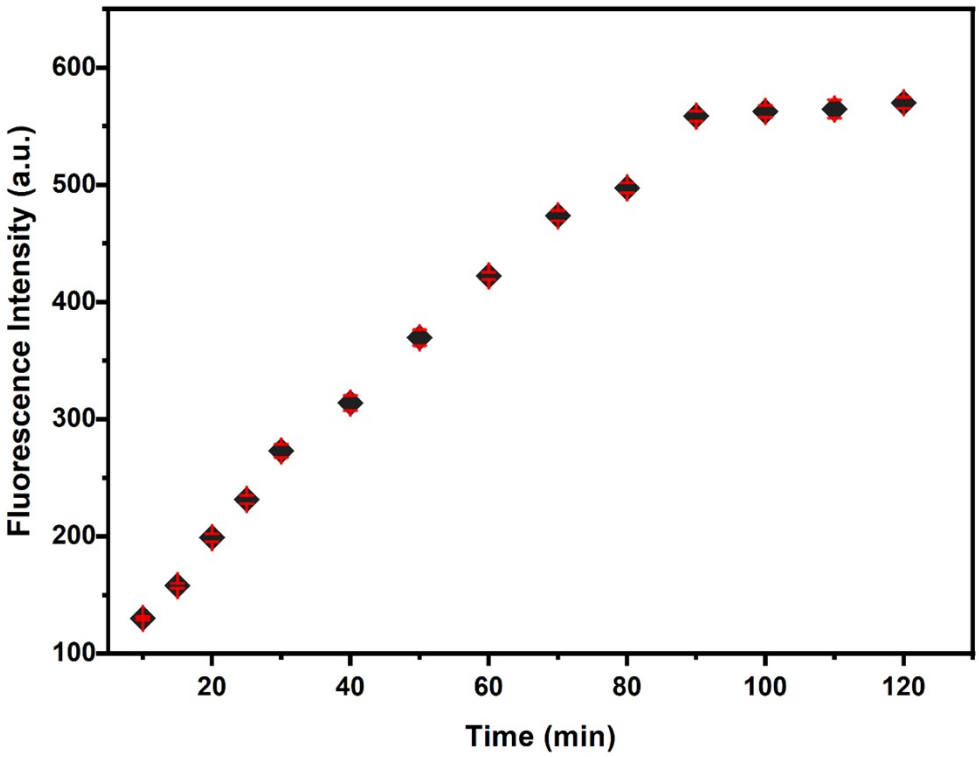


Figure S11. The fluorescence intensity of **TPABF-HS** (10 μM) with H_2S (1 mM) were detected under different reaction time (10-120 min). Conditions: pH 7.4, 37 °C, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

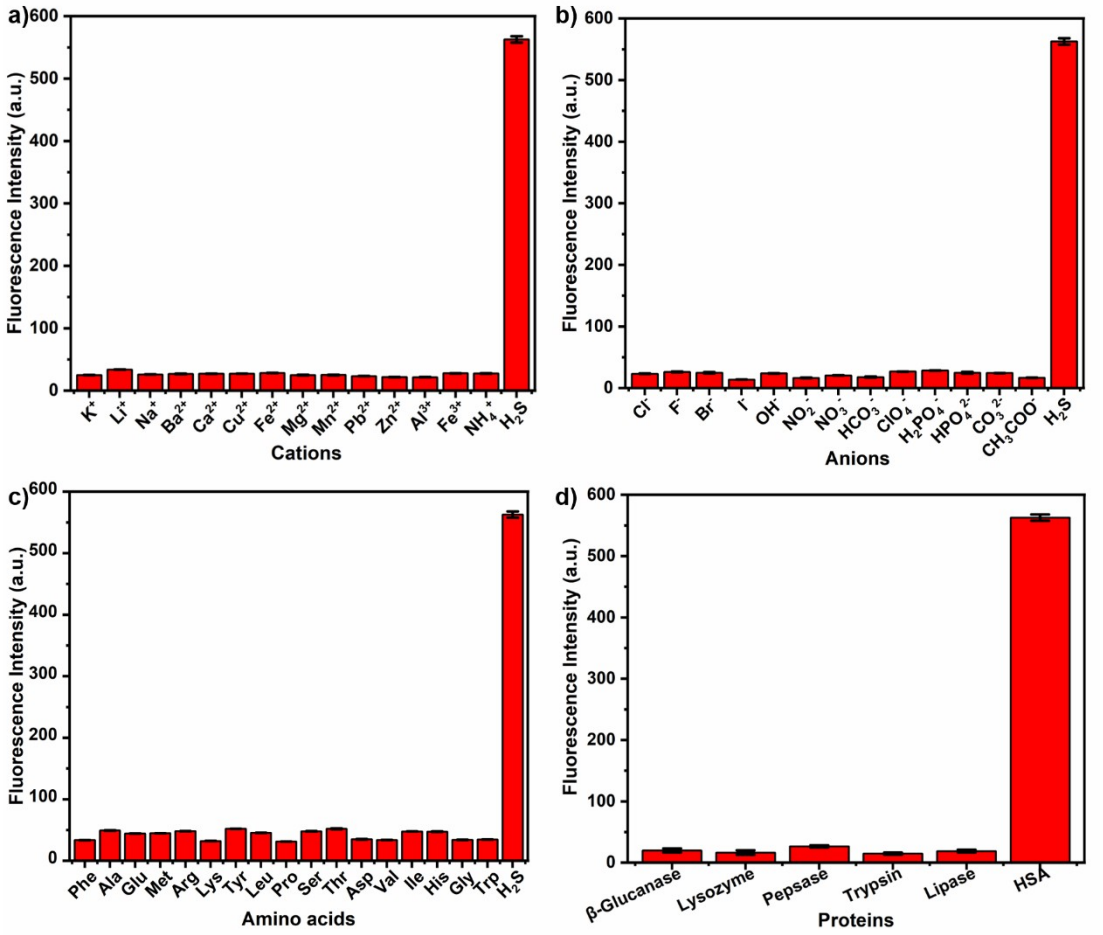


Figure S12. The fluorescence intensity at 540 nm of **TPABF-HS** (10 μM) with HSA (0.6 mg/mL) after the incubation of various cations, anions, amino acids and proteins (1 mM); (a) cations: K^+, Li^+, Na^+, Ba^{2+}, Ca^{2+}, Cu^{2+}, Fe^{2+}, Mg^{2+}, Mn^{2+}, Pb^{2+}, Zn^{2+}, Al^{3+}, Fe^{3+}, NH_4^+; (b) anions: Cl^-, F^-, Br^-, I^-, OH^-, NO_2^-, NO_3^-, HCO_3^-, ClO_4^-, $H_2PO_4^-$, HPO_4^{2-}, CO_3^{2-}, CH_3COO^-; (c) amino acids: Phe, Ala, Glu, Met, Arg, Lys, Tyr, Leu, Pro, Ser, Thr, Asp, Val, Ile, His, Gly, Trp; (d) proteins: *β*-glucanase, lysozyme, pepsase, trypsin, lipase; Conditions: pH 7.4, 37 °C, 100 min, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

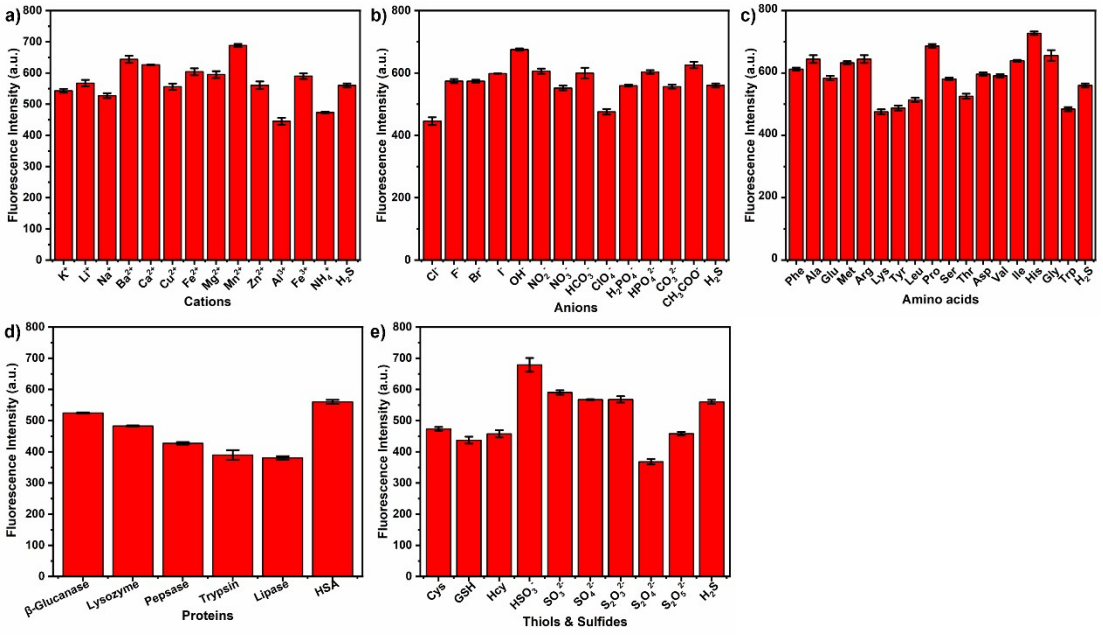


Figure S13. The fluorescence intensity at 540 nm of **TPABF-HS** (10 μM) with HSA (0.6 mg/mL) and H_2S (1mM) after the incubation of various cations, anions, amino acids, proteins, thiols and sulfides (1 mM); (a) cations: K^+, Li^+, Na^+, Ba^{2+}, Ca^{2+}, Cu^{2+}, Fe^{2+}, Mg^{2+}, Mn^{2+}, Zn^{2+}, Al^{3+}, Fe^{3+}, NH_4^+; (b) anions: Cl^-, F^-, Br^-, I^-, OH^-, NO_2^-, NO_3^-, HCO_3^-, ClO_4^-, $H_2PO_4^-$, HPO_4^{2-}, CO_3^{2-}, CH_3COO^-; (c) amino acids: Phe, Ala, Glu, Met, Arg, Lys, Tyr, Leu, Pro, Ser, Thr, Asp,

Val, Ile, His, Gly, Trp; (d) proteins: *β*-glucanase, lysozyme, pepsase, trypsin, lipase; (e) thiols and sulfides: Cys, GSH, Hcy, SO_3^{2-}, SO_4^{2-}, $S_2O_3^{2-}$, $S_2O_4^{2-}$, $S_2O_5^{2-}$; Conditions: pH 7.4, 37 °C, 100 min, 5 nm * 5 nm, 650 V, λ_{ex} = 445 nm.

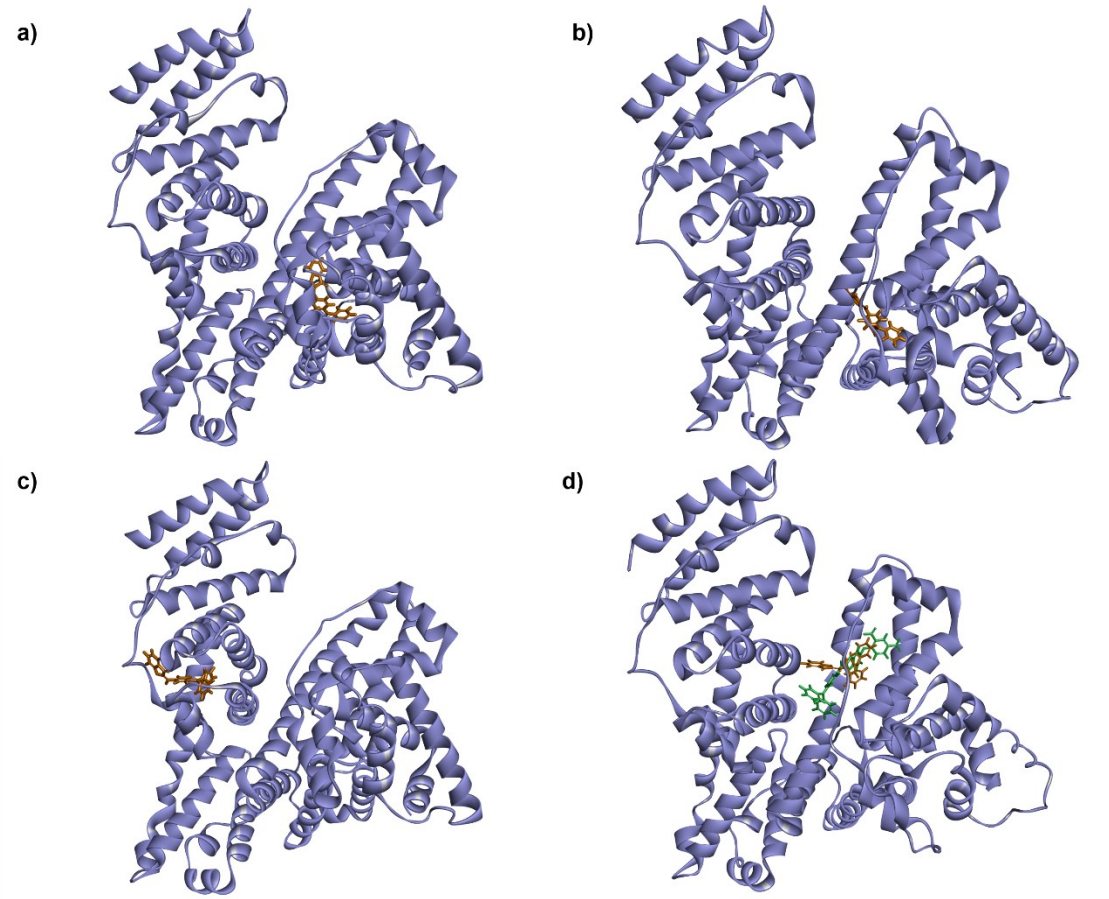


Figure S14. Molecular docking diagram of **TPABF** and **TPABF-HS** and HSA proteins. (a)The binding patterns of TPABF into the phenylbutazone - binding site; (b)The binding patterns of **TPABF** into the salicylic acid-binding site; (c)The binding patterns of **TPABF** into the ibuprofen-binding site; (d)The binding patterns of **TPABF** and **TPABF-HS** into the naproxen-binding site.

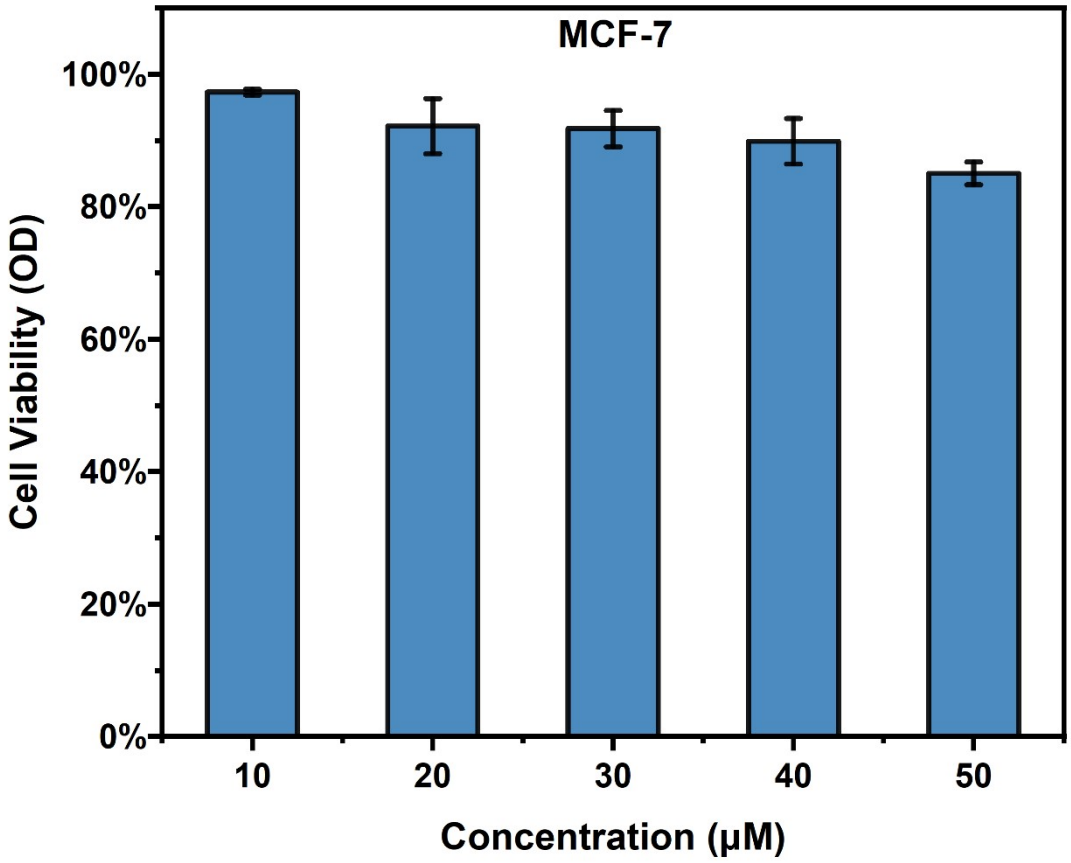
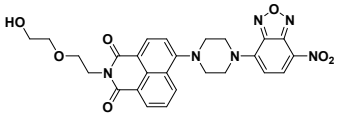
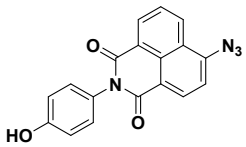
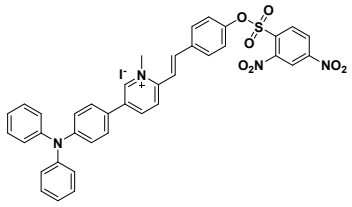
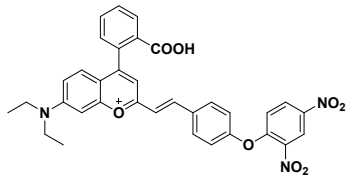
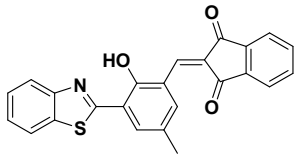
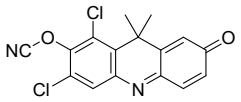
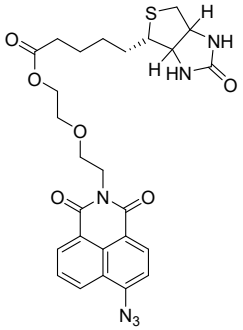
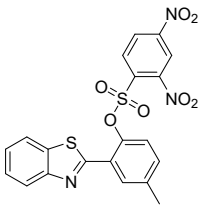
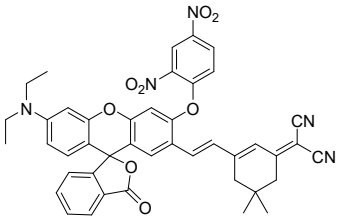
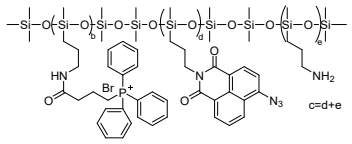
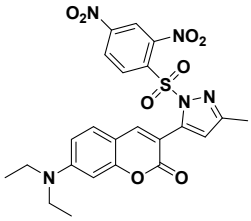
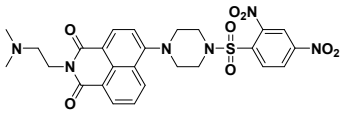
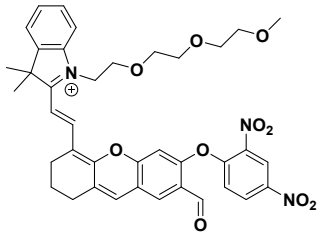
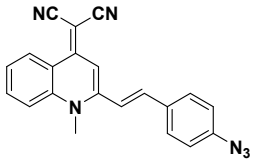
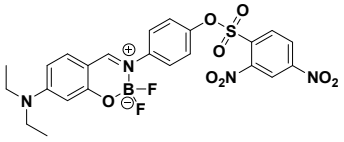
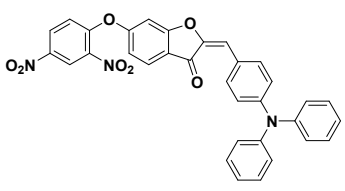


Figure S15. Cell viability of MCF-7 cells treated with different concentrations (10-50 μM) of **TPABF-HS** for 36 h at 37 ℃.

Table S1. The comparison between the probe in this work and those previously reported.

Probe	$\lambda_{ex}/\lambda_{em}$ (nm)	Linear interval (μM)	LOD (μM)	Application	Refere -nce
	420/430	10	0.41	HeLa cells	[25]
	465/527	17	1.18	HeLa cells	[26]

	530/623	130	0.04	Foodstuff, Water samples, HeLa cells	[27]
	686/736	100	/	HeLa cells	[28]
	390/542 390/630	1000	212.3	HepG2 cells	[29]
	600/658	70	0.004	Food samples, HeLa cells	[30]
	430/545	10	1.15	A549 cells	[31]
	-/487	100	0.372	Water samples, Test strips, Fluorescent films	[32]
	580/760	9	0.04	HeLa cells	[33]

	488/550	70	0.1	HeLa cells, Zebrafish	[34]
	440/500	500	0.019	Water samples, MCF-7 cells	[35]
	400/530	20	0.152	CaKi-1 cells	[36]
	685/718	20	0.75	Raw meal, Wheat seeds	[37]
	475/610	80	0.01	HeLa cells	[38]
	420/500	40	/	HeLa cells	[39]
	445/540	1000	0.42	MCF-7 cells, *C. elegans*	**This work**