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Supplementary Information

BODIPY-based fluorescent probe for the simultaneous detection of glutathione and cysteine/homocysteine at different excitation wavelengths

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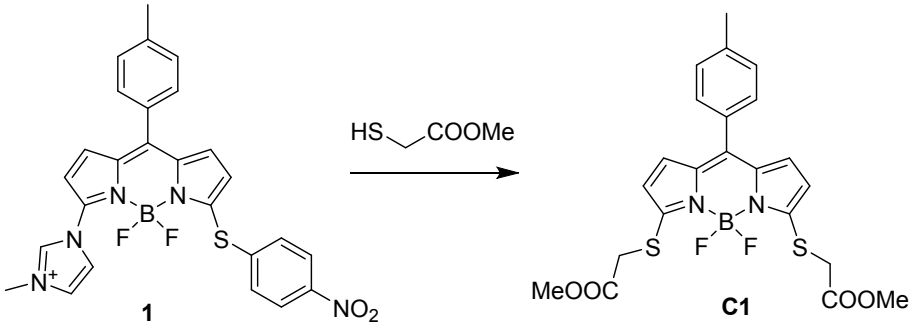
Synthesis of Compound C1



Compound **1** (36 mg, 0.07 mmol) was dissolved in 20 mL acetonitrile and one drop of triethylamine and mercaptopropionic acid (25 μL, 0.28 mmol) was added. The mixture was stirred at r.t for 10 min and then evaporated. The residue was purified by column chromatography on silica gel (dichloromethane / petroleum ether = 1/1 as eluent) to give **C1** (28 mg, 83%) as a purple solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, 2H, J = 8.0 Hz), 7.30 (d, 2H, J = 8.0 Hz), 6.80 (d, 1H, J = 4.0 Hz), 6.51 (d, 1H, J = 4.4 Hz), 3.81 (s, 4H), 3.77 (s, 6H), 2.45 (s, 3H).

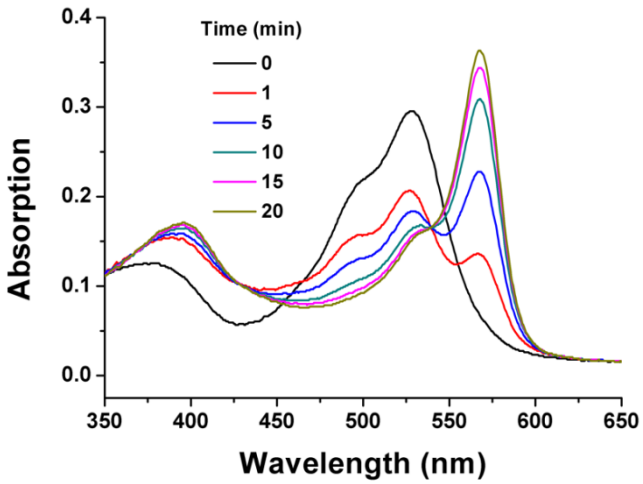


Fig. S1 Time-dependent absorption spectra of **1** (10 μM) in addition of GSH (1 mM) in acetonitrile/ HEPES buffer (1:99, v/v, 20 mM, pH 7.4).

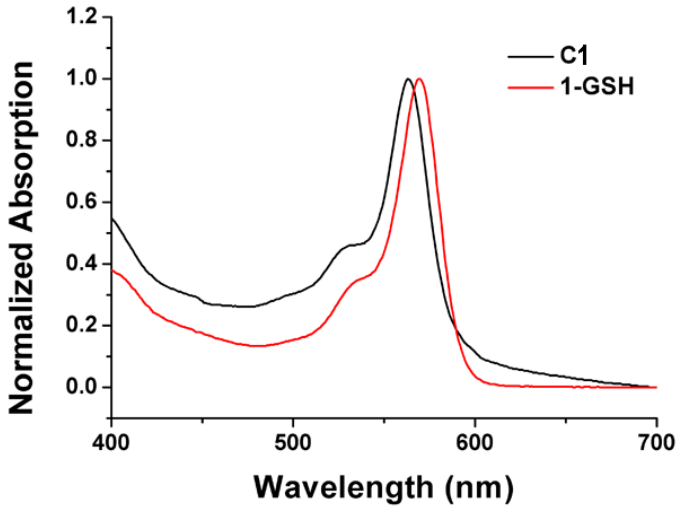


Fig. S2 Normalized absorption spectra of **C1** and **1**-GSH.

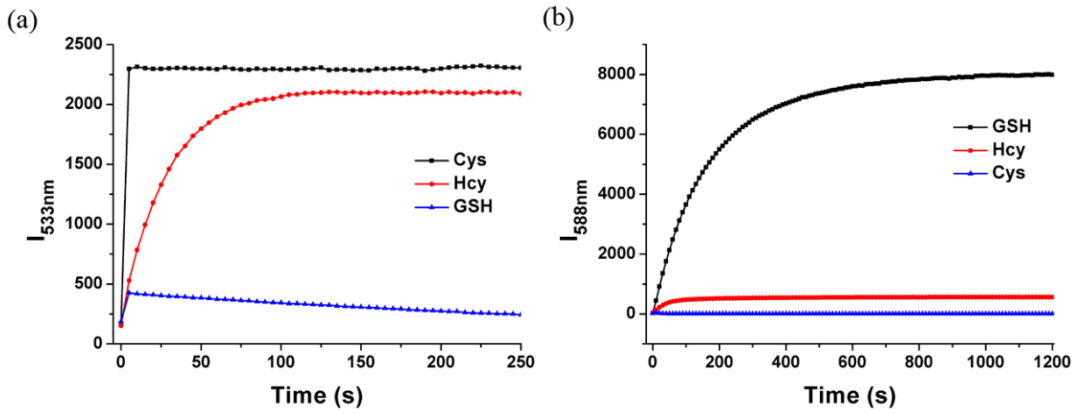


Fig. S3 Time-dependent emission intensity changes in addition of Cys, Hcy and GSH at (a) 533 nm (λ_{ex} = 443 nm), (b) 588 nm (λ_{ex} = 568 nm) in acetonitrile/ HEPES buffer (1:99, v/v, 20 mM, pH 7.4).

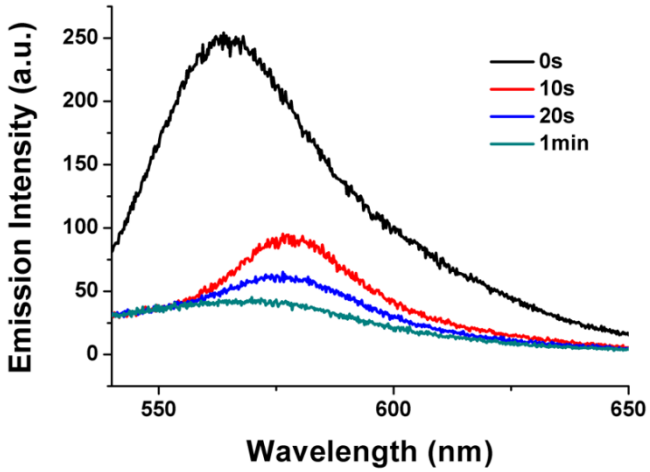


Fig. S4 Time-dependent fluorescence spectra of **1** (10 μM) with addition of (a) GSH (1 mM) and (b) Hcy (1 mM) in acetonitrile/ HEPES buffer (1:99, v/v, 20 mM, pH 7.4). λ_{ex} = 528 nm.

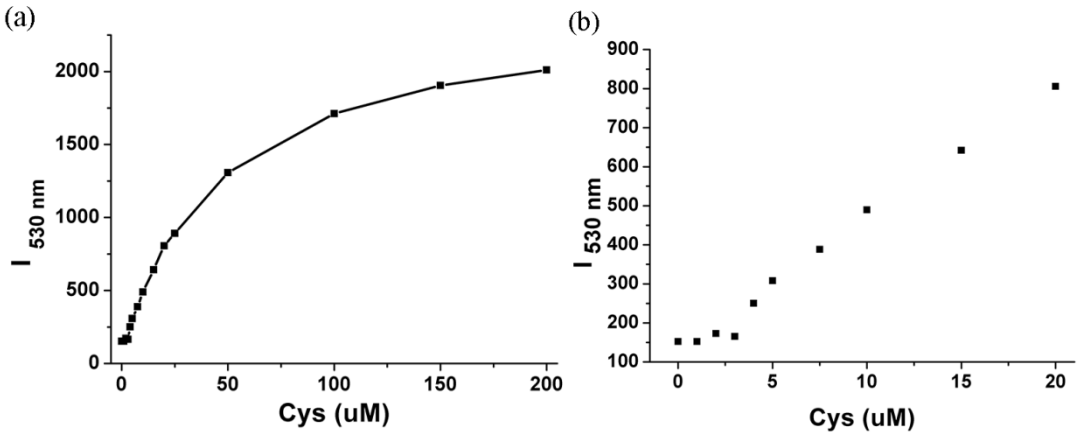


Fig. S5 Plot of the fluorescence intensity as a function of Cys concentrations. Each data was acquired 1 min after Cys addition in acetonitrile/ HEPES buffer (1:99, v/v, 20 mM, pH 7.4). λ_{ex} = 443 nm.

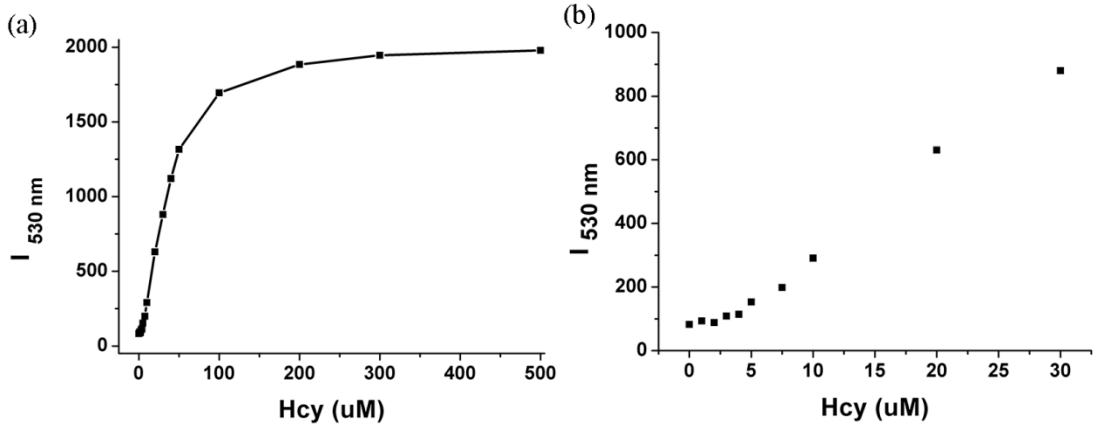


Fig. S6 Plot of the fluorescence intensity as a function of Hcy concentrations. Each data was acquired 5 min after Cys addition in acetonitrile/ HEPES buffer (1:99, v/v, 20 mM, pH 7.4). λ_{ex} = 443 nm.

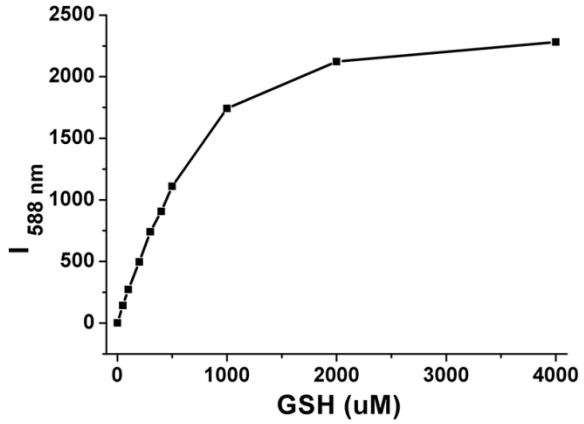
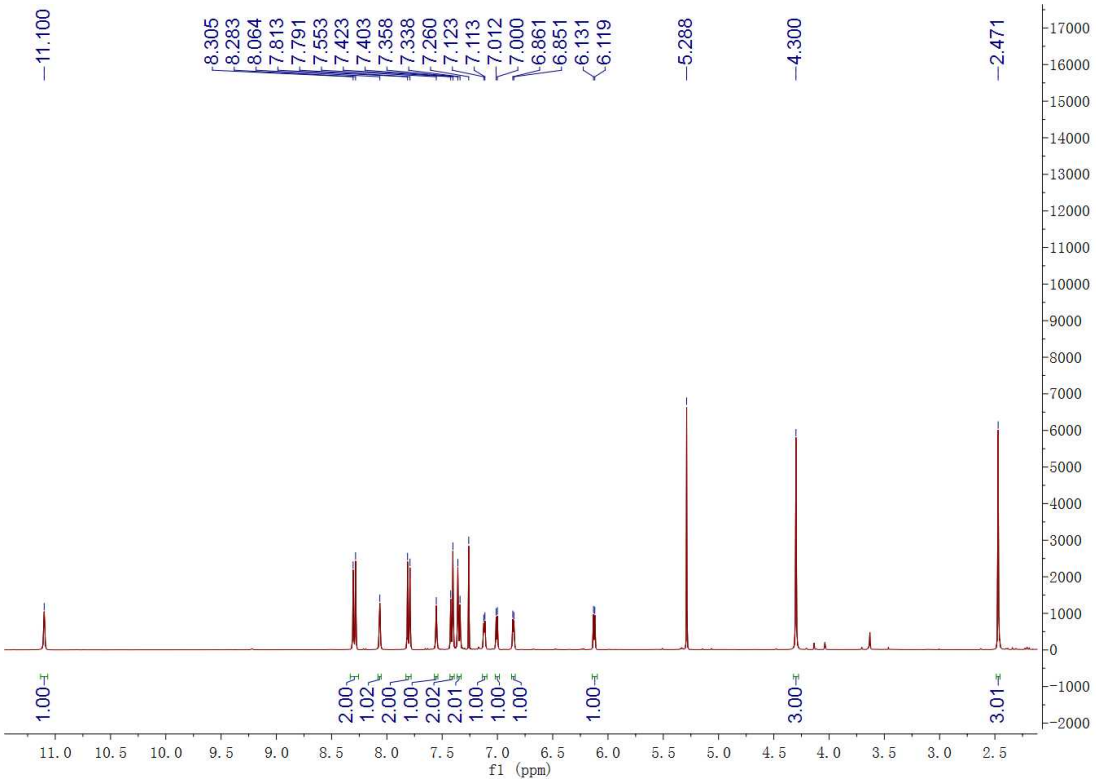
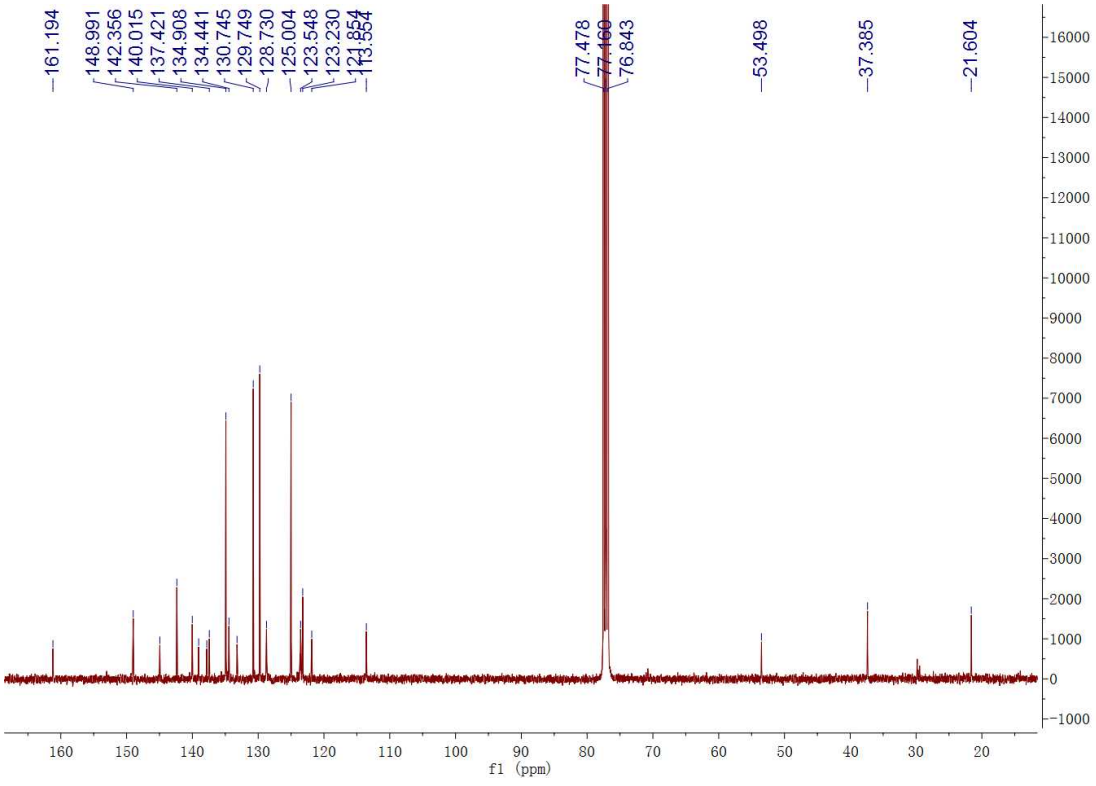


Fig. S7 Plot of the fluorescence intensity as a function of GSH concentrations. Each data was acquired 5 min after Cys addition in acetonitrile/ HEPES buffer (1:99, v/v, 20 mM, pH 7.4). λ_{ex} = 568 nm.

^{1}H NMR, ^{13}C NMR and HRMS of 1





Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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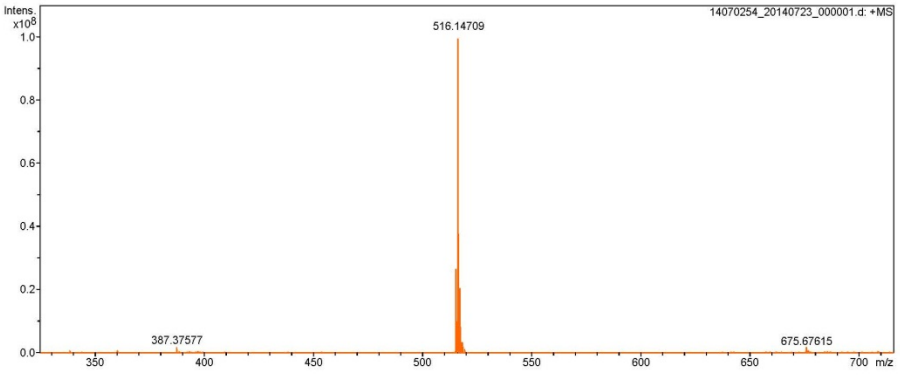
Comment	ESI Positive	Operator	Peking University



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
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