

A “Two-in-One” Pyrrolopyrrole Cyanine Fluorescent Probe for Discriminative Detection of Hydrazine and Hydrogen Sulfide in Real Samples

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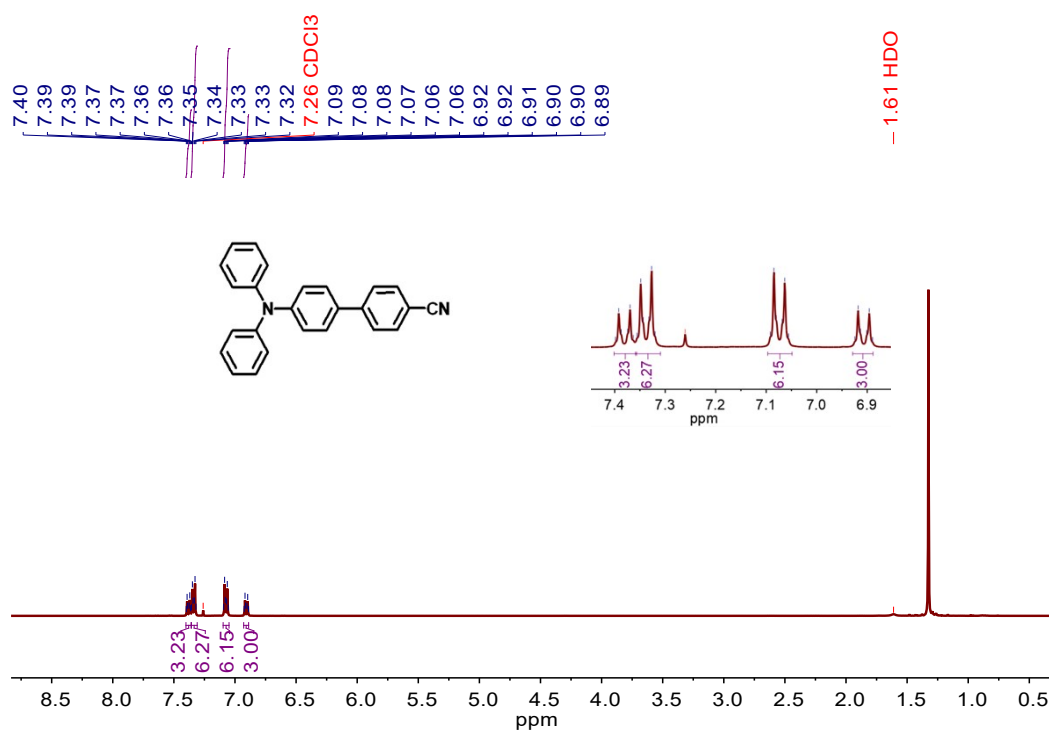


Figure S1. ^1H NMR spectrum of **1** in CDCl_3 .

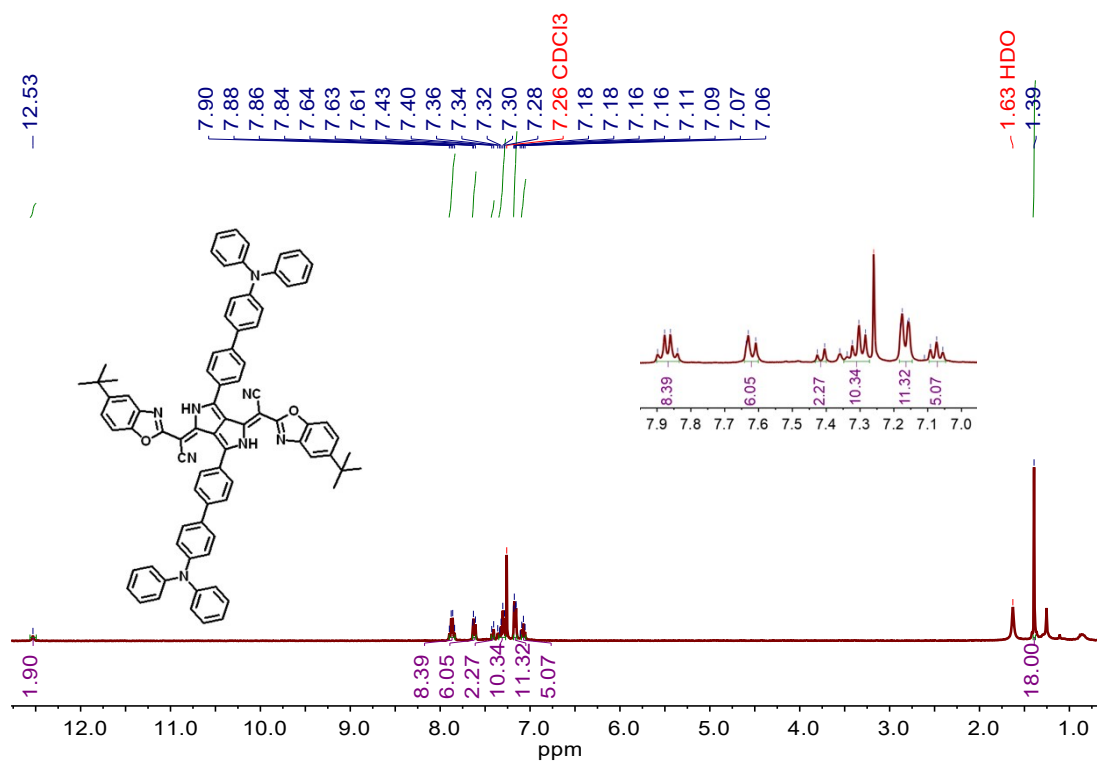


Figure S2. ^1H NMR spectrum of **PPCy-Ph-H** in CDCl_3 .

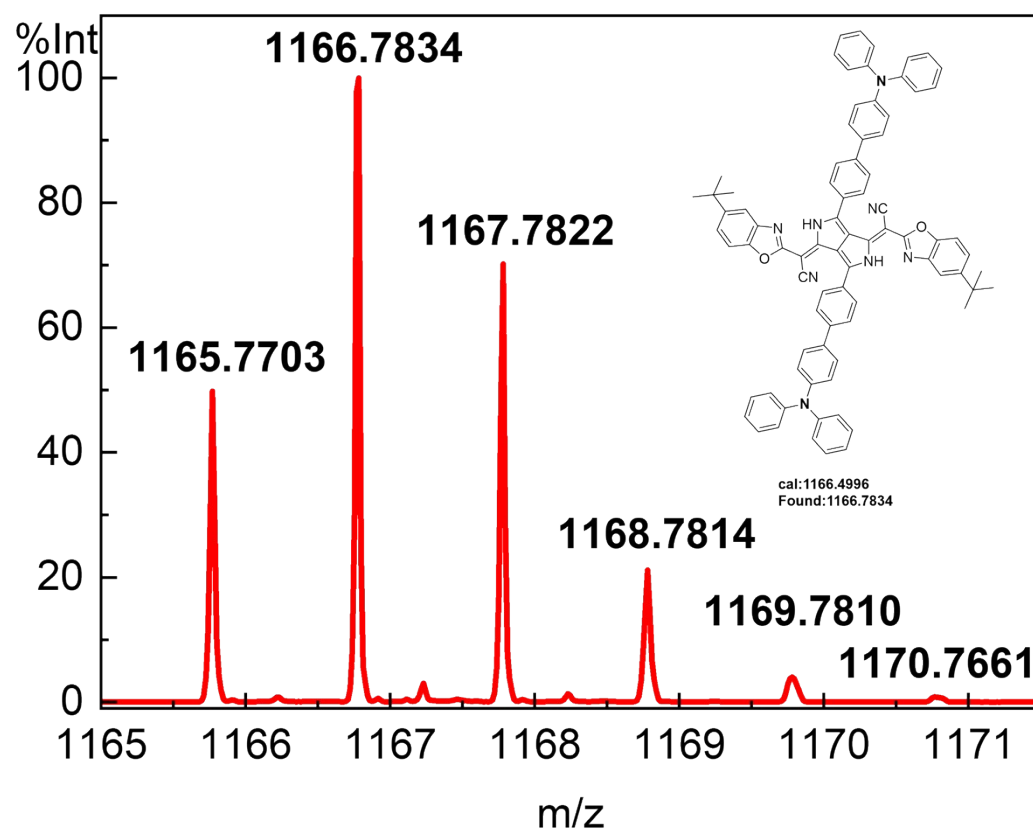


Figure S3. MALDI-TOF-MS of PPCy-Ph-H.

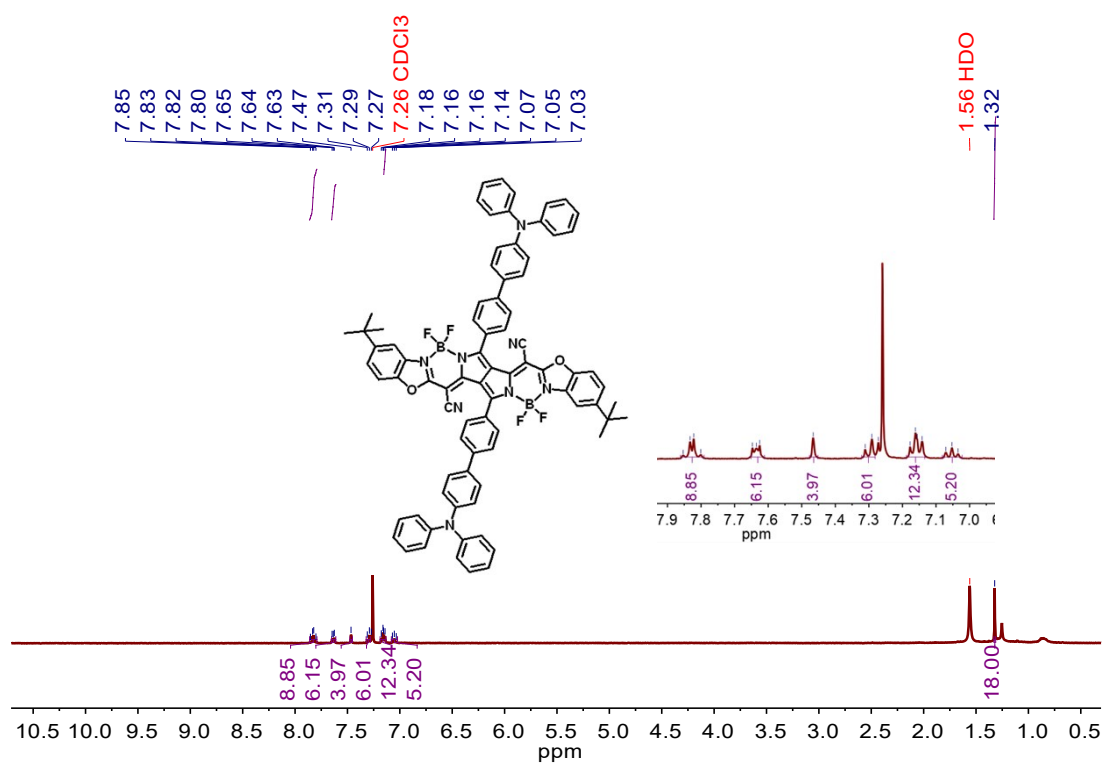


Figure S4. ¹H NMR spectrum of PPCy-Ph-BF₂ in CDCl₃.

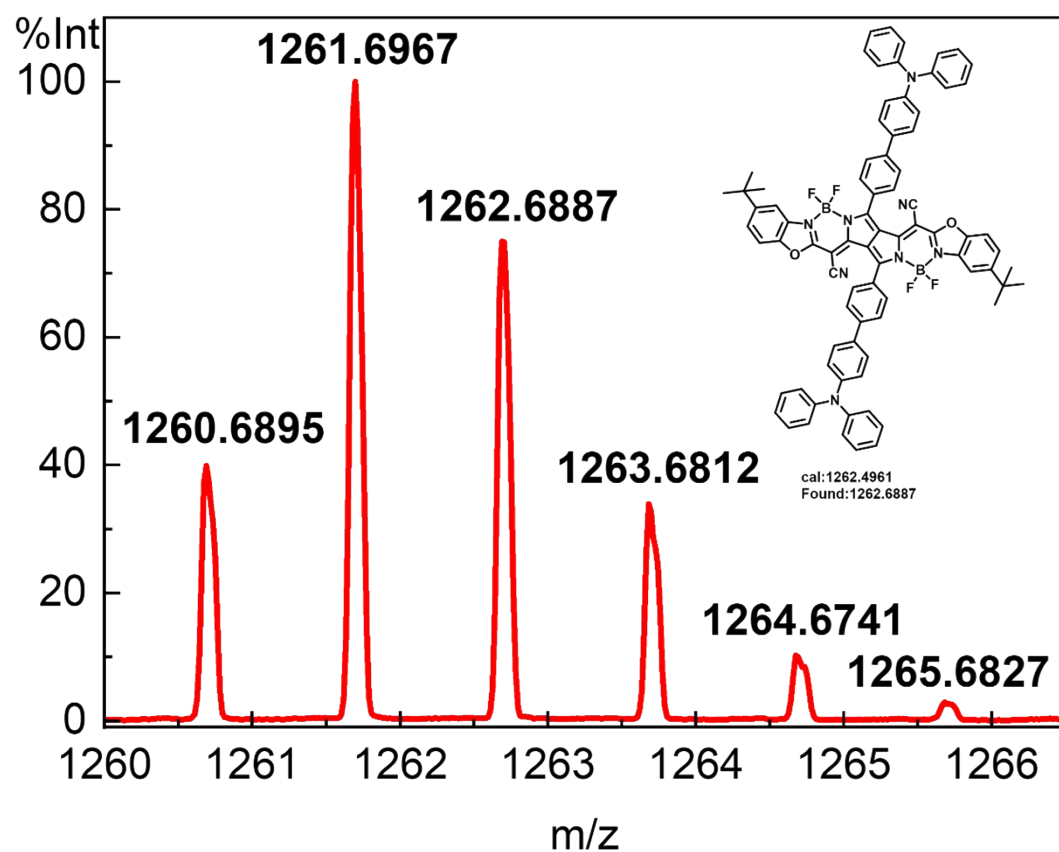


Figure S5. MALDI-TOF-MS of PPCy-Ph-BF2.

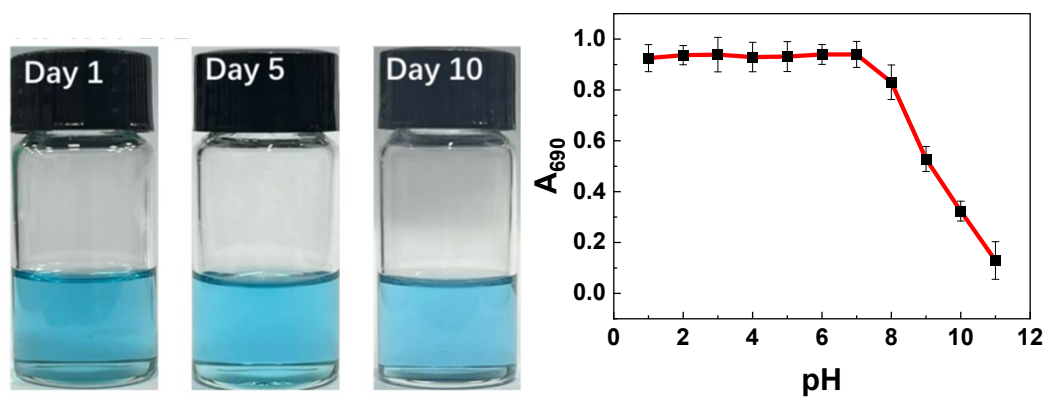


Figure S6. The photos of PPCy-Ph-BF2 in CH₂Cl₂ (a) after exposure of daylight in air for 10 days and (b) absorption maximum at 690 nm at different pH.

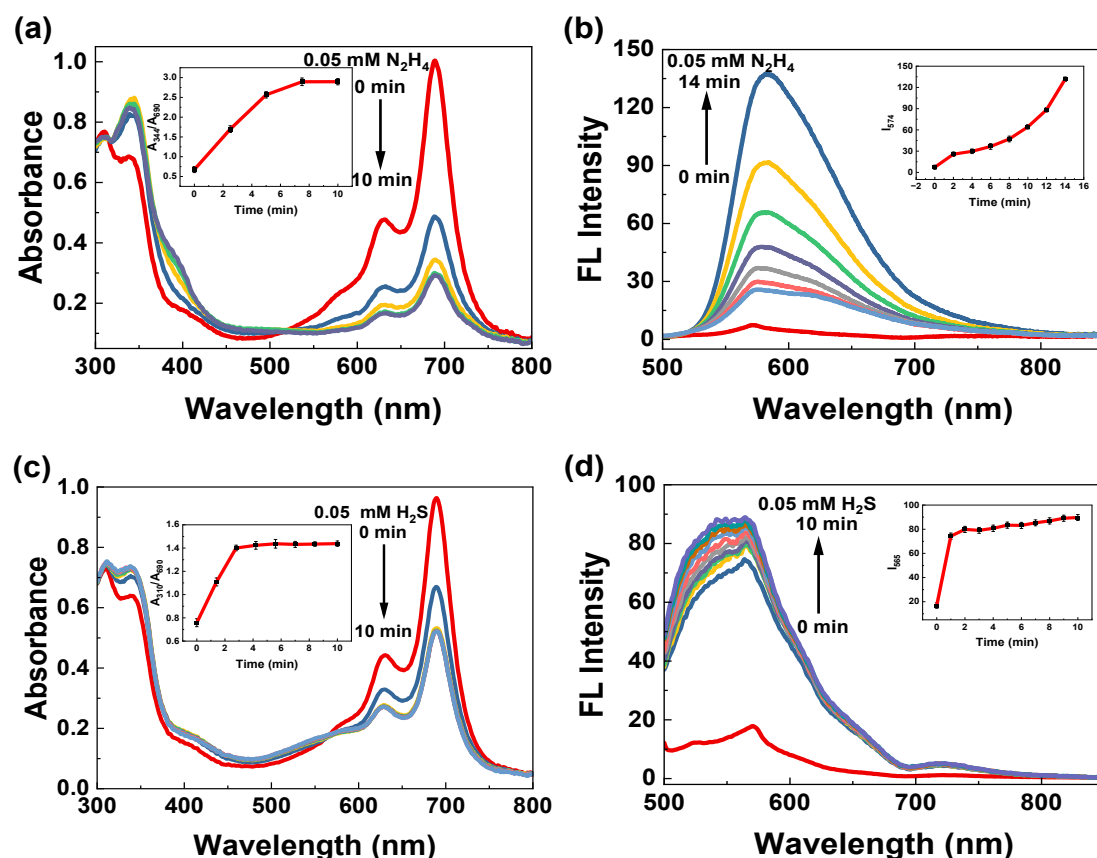


Figure S7. Time-dependent UV-vis absorption of PPCy-Ph-BF2 ($10\ \mu\text{M}$) towards (a) N_2H_4 and (c) H_2S ($0.05\ \text{mM}$). Time-dependent emission spectra of PPCy-Ph-BF2 towards (b) N_2H_4 and (d) H_2S .

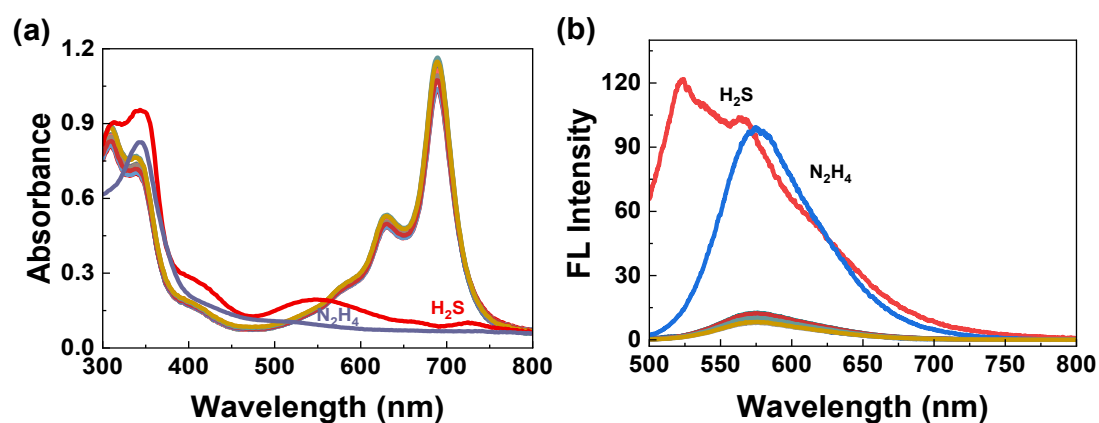


Figure S8. (a) UV-vis absorption and (b) emission spectra of PPCy-Ph-BF2 ($10\ \mu\text{M}$) in the presence of different analytes (Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Cr^{3+} , Mn^{2+} , Fe^{2+} , Fe^{3+} , Co^{2+} , Ni^{2+} , Cu^{2+} , Zn^{2+} , Cd^{2+} , Hg^{2+} , Pb^{2+} , NH_4^+ , F^- , Cl^- , Br^- , I^- , CO_3^{2-} , NO_3^- , NO_2^- , AcO^- , SO_4^{2-} , SO_3^{2-} , HSO_3^- , CN^-) at room temperature for 2 min.

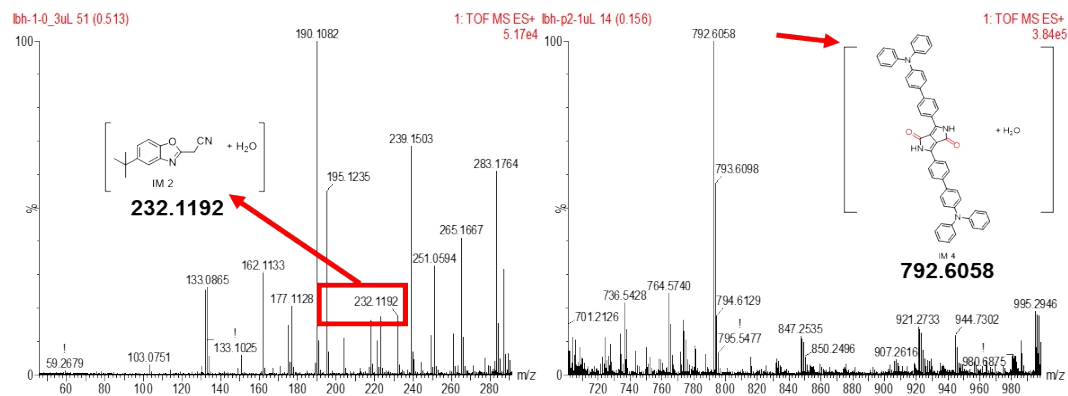


Figure S9. The HRMS spectra of PPCy-Ph-BF2 (10 μ M) in the presence of N_2H_4 .

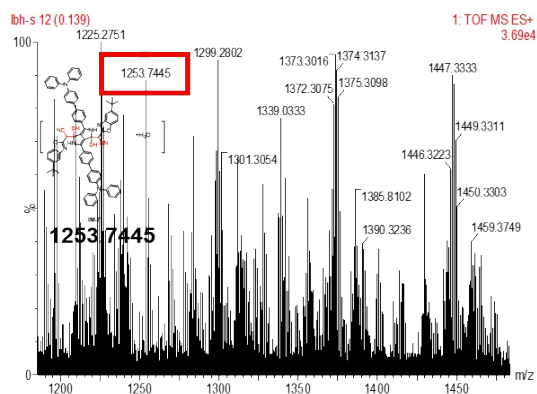


Figure S10. The HRMS spectrum of PPCy-Ph-BF2 (10 μ M) in the presence of H_2S .

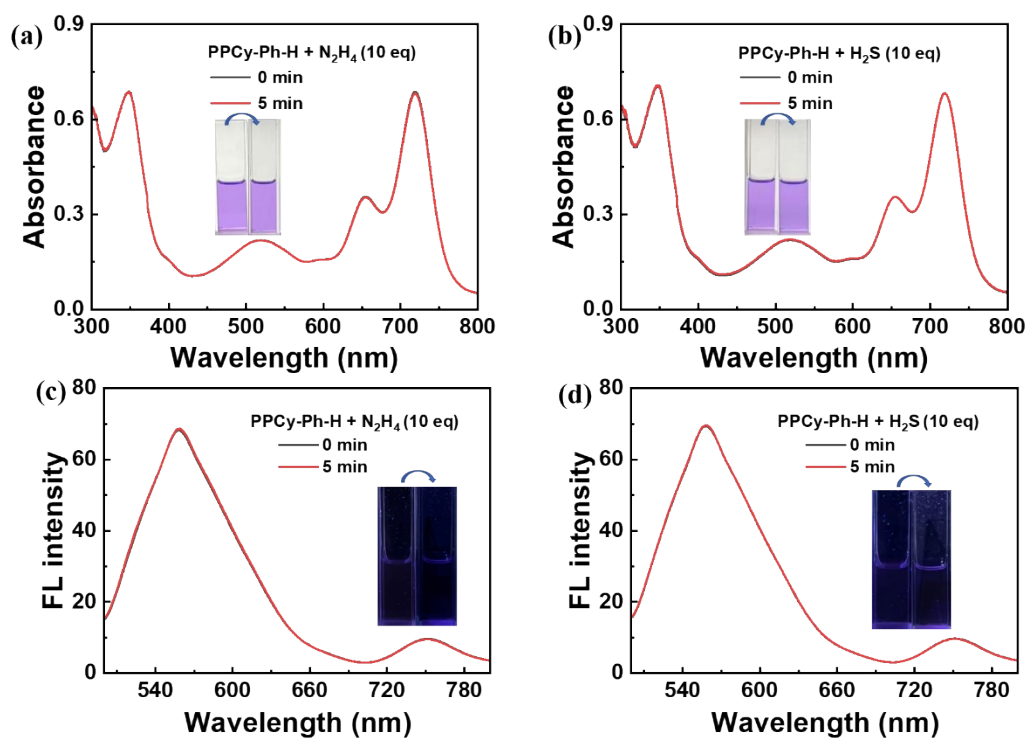


Figure S11 (a-d) The UV-vis and fluorescence spectra of model compound without BF_2 motif (**PPCy-Ph-H**) in presence of N_2H_4 or H_2S for 5 min.

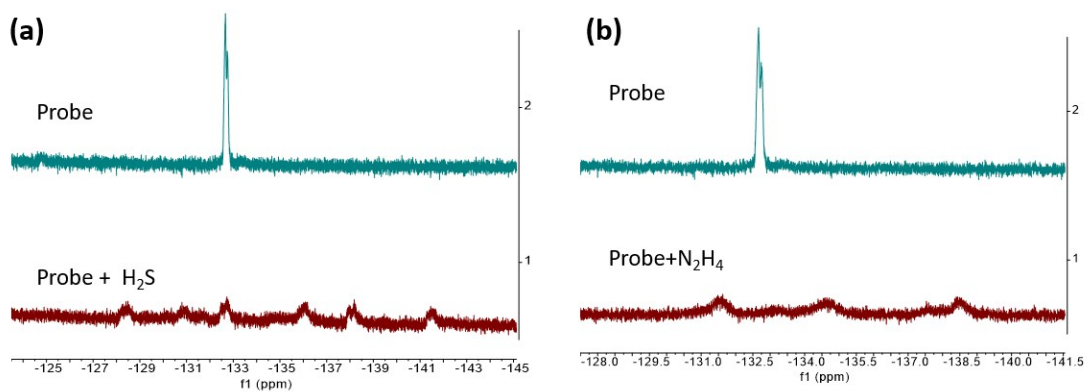


Figure S12 ^{19}F NMR spectra of **PPCy-Ph-BF₂** (10 mM) in the presence of (a) N_2H_4 and (b) H_2S in CDCl_3 at room temperature.

Table S1 The comparison of solution LODs and solid-state LQD values in this work with WHO/OSHA limits for N₂H₄ and typical H₂S levels

Analytes	OSHA	This work
N ₂ H ₄	0.048 ppm	(1) Detecting N ₂ H ₄ solution: 9.11 nM and 2.38 nM (UV-vis and Fluorescence method with PPCy-Ph-BF2 solution); 29.3 mM (with PPCy-Ph-BF2 -loading polyamide thin film and Color APP) (2) Detecting N ₂ H ₄ gas: 3.25 and 1.74 mM (with PPCy-Ph-BF2 -loading sponge and Color APP)
H ₂ S	10 ppm (8-hour average); 15 ppm (15 minutes)	(1) Detecting H ₂ S solution: 1.70 nM and 0.64 nM (UV-vis and Fluorescence method with PPCy-Ph-BF2 solution); 35.7 mM (with PPCy-Ph-BF2 -loading polyamide thin film and Color APP) (2) Detecting H ₂ S gas: 2.56 and 2.63 mM (with PPCy-Ph-BF2 -loading sponge and Color APP)

Table S2. Determination of N₂H₄ concentrations with **PPCy-Ph-BF2** and HPLC.

Sample	Spiked (μM)	Recovery (%) (by HPLC)	Recovery (%) (by probe)
Tap water	3.00	96.4	98.3
Lake water	3.00	97.8	99.6
Red wine	3.00	105.5	100.6
Beer	3.00	106.3	101.0