

Supplementary Data

A Highly Sensitive Near-infrared Fluorescent Probe for Detection of Hydrogen Sulfide and Its Application in Living Cells and Mice

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Fluorescence quantum yield measurement

The quantum yield of the compound was calculated according to the equation:

$$\Phi_u = \Phi_s \frac{I_u}{I_s} \times \frac{A_s}{A_u} \times \left(\frac{n_u}{n_s}\right)^2$$

Φ denotes the quantum yield; I denotes the area under the fluorescence curve; A denotes the absorbance at the excitation wavelength; n denotes the refractive index of the solvent. Quinine sulfate ($\Phi = 0.542$ in 0.05 M sulfuric acid solution) was used as the reference standard.

The limit of detection measurement

The detection limit of **Cy-PBA** towards H₂S was determined through fluorescence titration, which was measured ten times. The standard deviation of the blank solution was also measured for 15 times. After the linear slope of fluorescence intensity vs. concentrations of H₂S was obtained, the detection of limit (LOD) was calculated by following equation:

$$LOD = 3\sigma/\kappa$$

Where σ denotes the standard deviation of blank measurement, κ denotes the slope of the fluorescence intensity vs. H₂S concentrations.

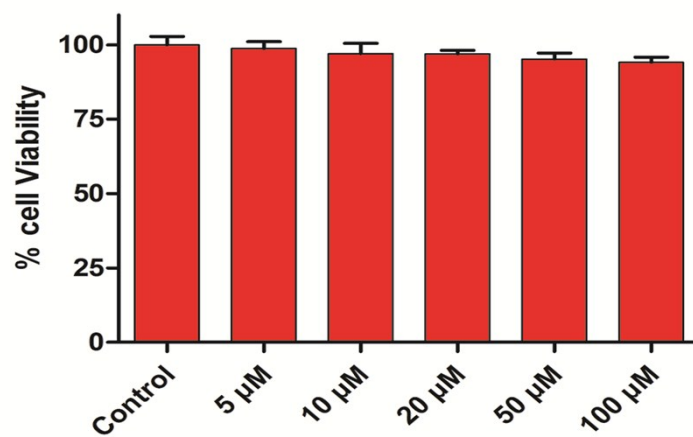


Figure S1. Cytotoxicity studies of **Cy-PBA** (5 μ M; 10 μ M; 20 μ M; 50 μ M; 100 μ M) for A549 cells.

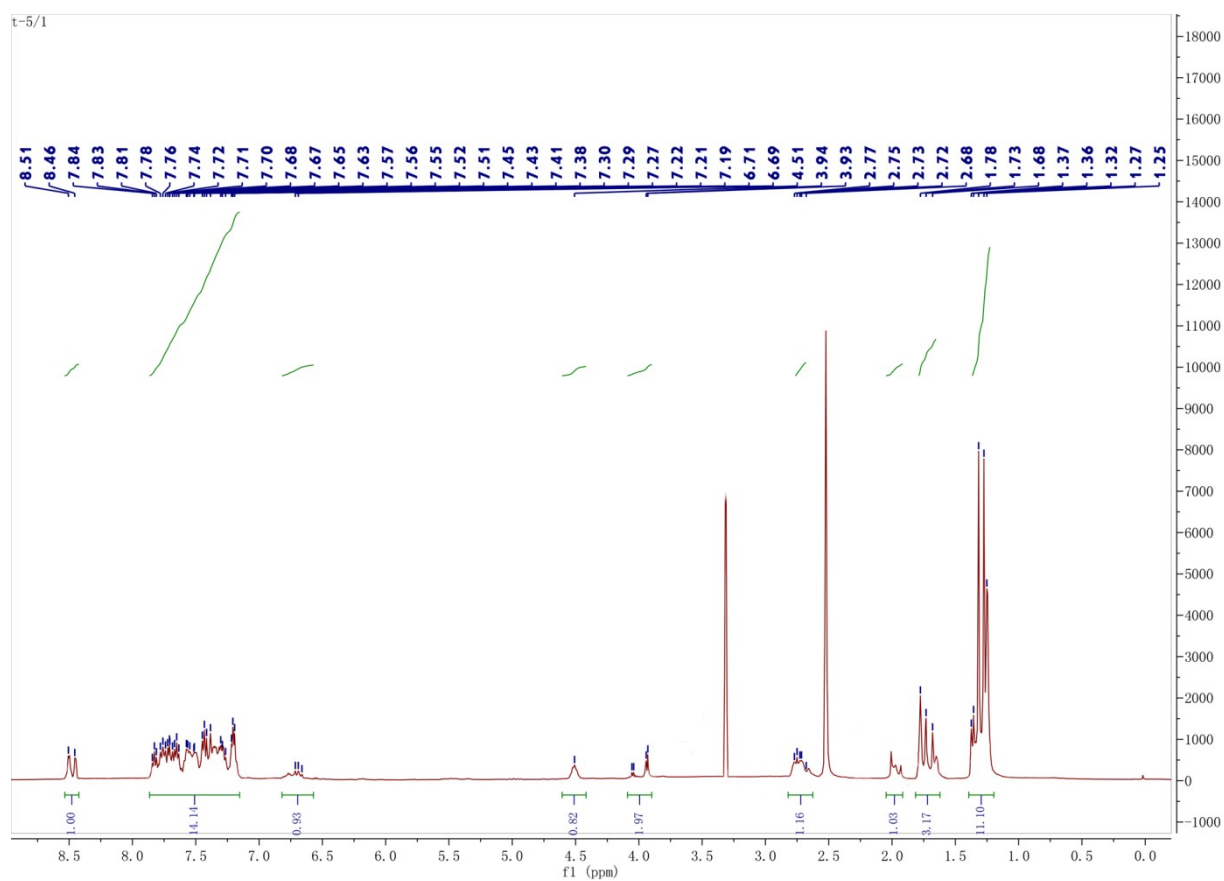


Figure S2. ^1H NMR spectrum of the probe **Cy-PBA**.

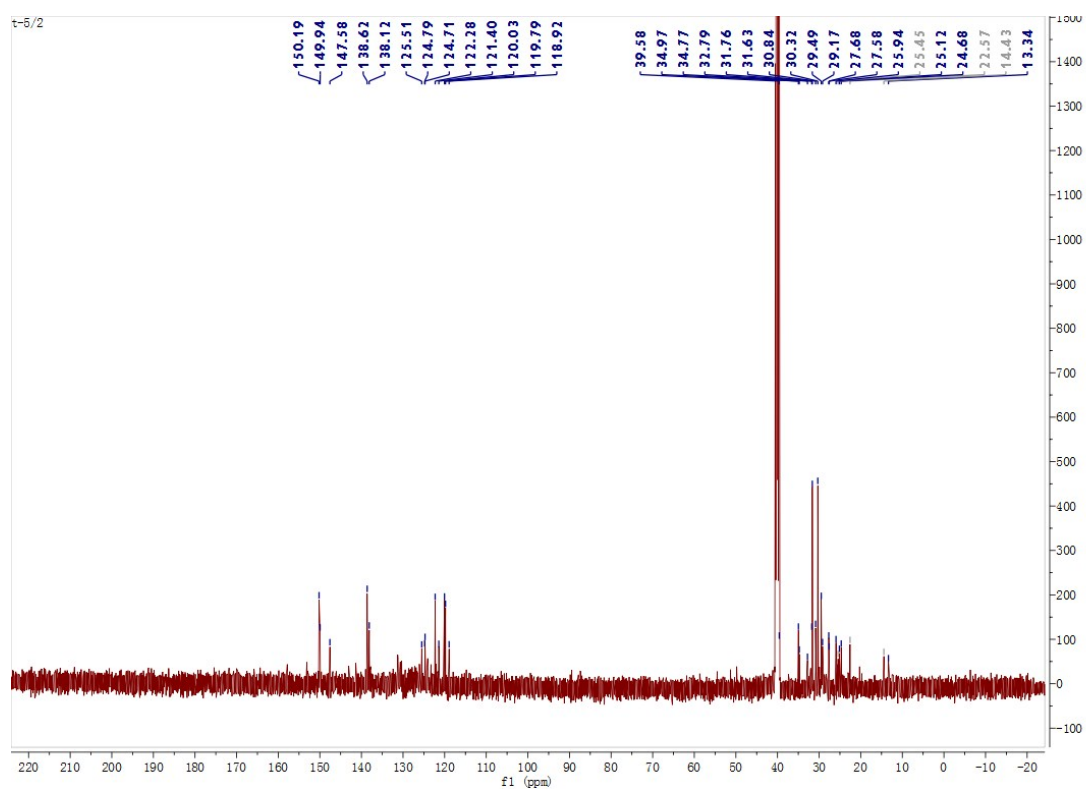


Figure S3. ^{13}C NMR spectrum of the probe Cy-PBA.

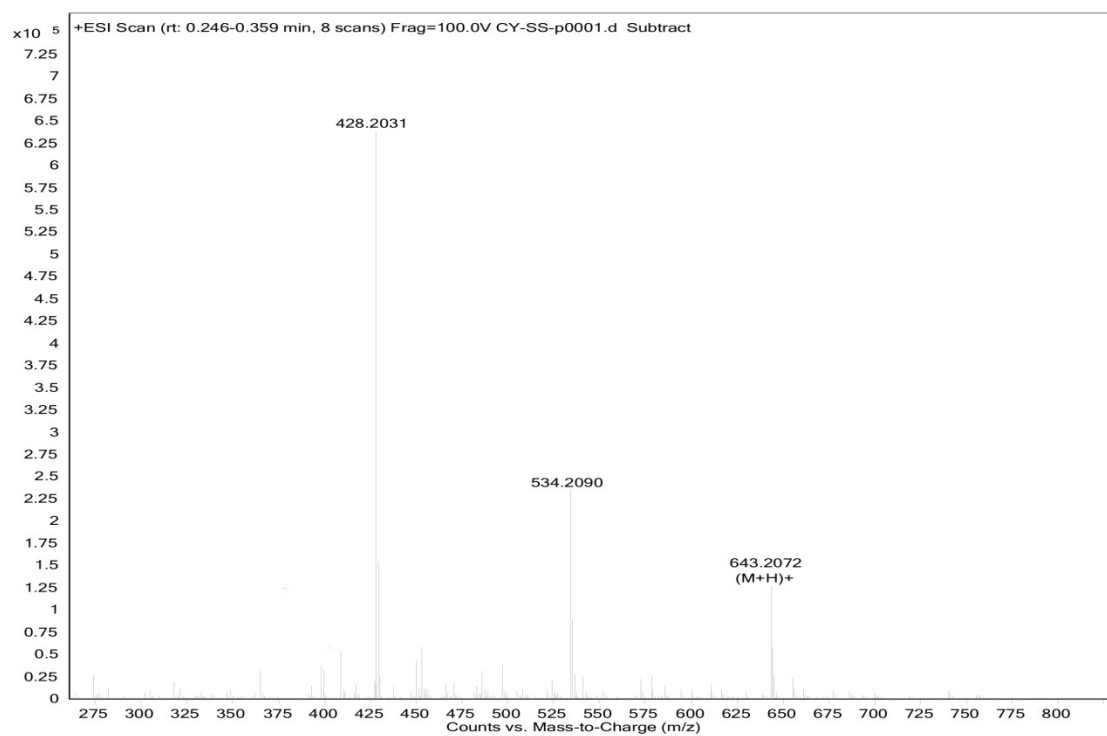


Figure S4. HRMS spectrum of the probe Cy-PBA.

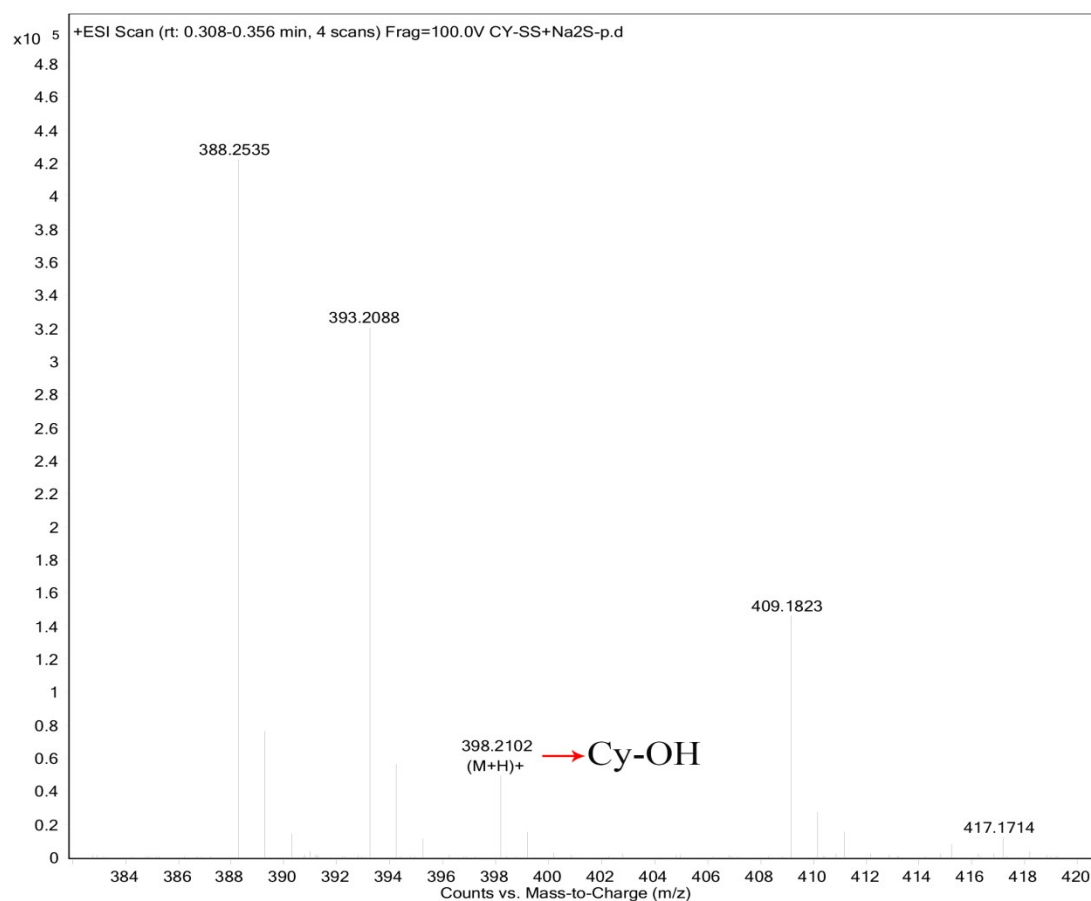


Figure S5. HRMS spectrum of the reaction product of the probe **Cy-PBA** with Na₂S.