

## Supporting Information

### **Cancer Cell-Specific Benzoxadiazole-based Fluorescent Probe for Hydrogen Sulfide Detection in Mitochondria**

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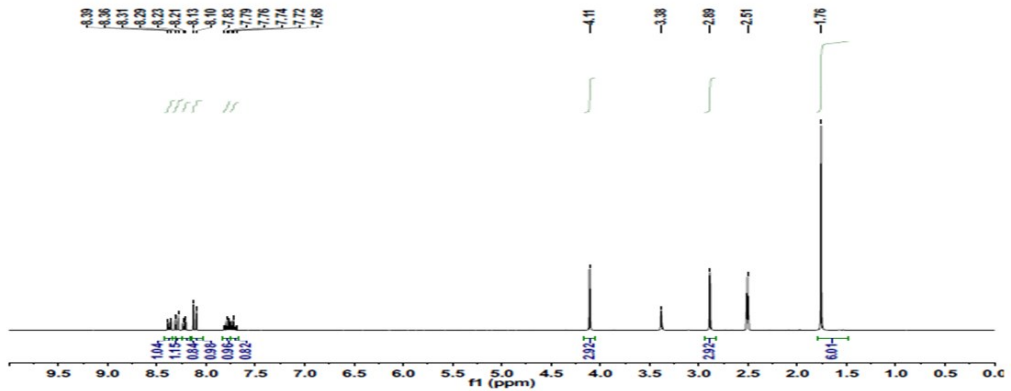


Figure S1.  $^1\text{H-NMR}$  of compound **1a** in  $\text{DMSO-}d_6$ .

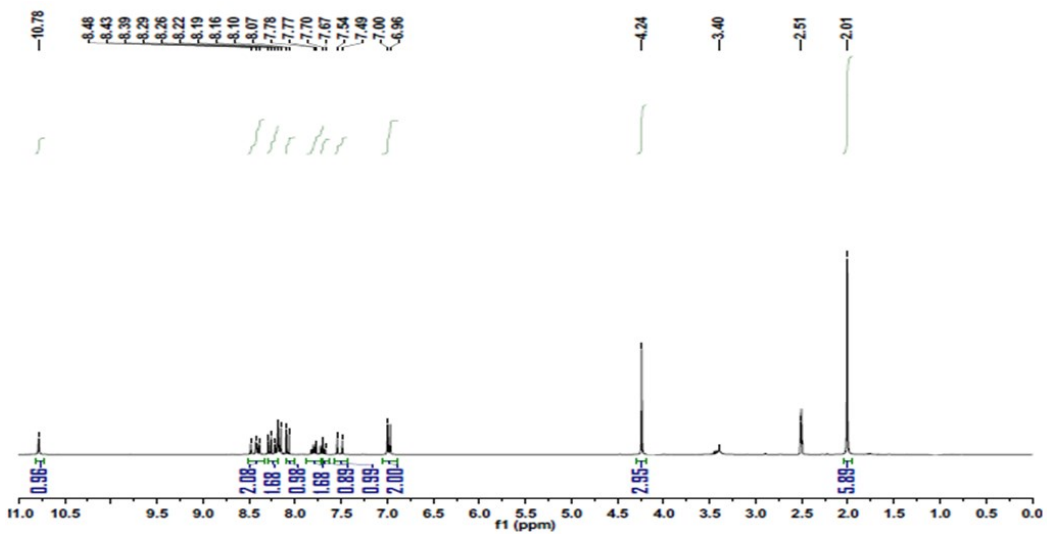
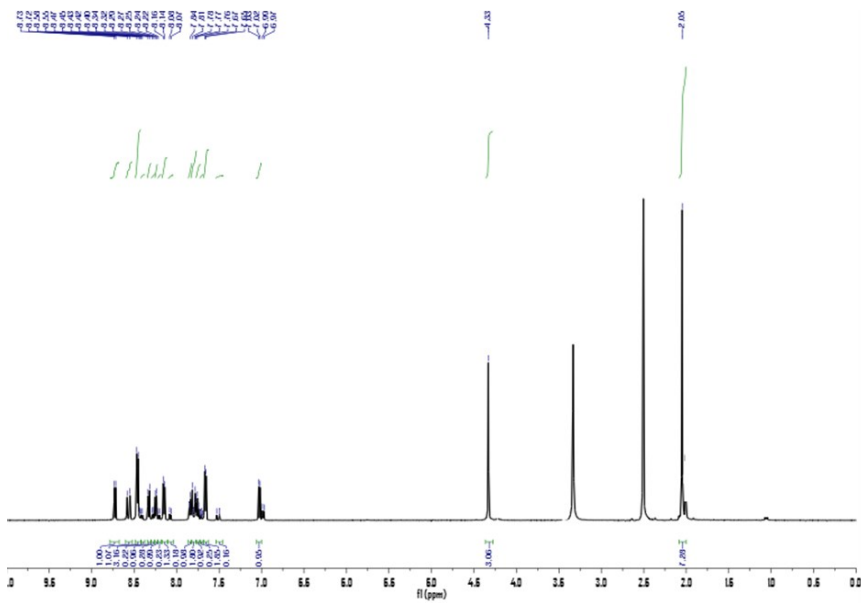
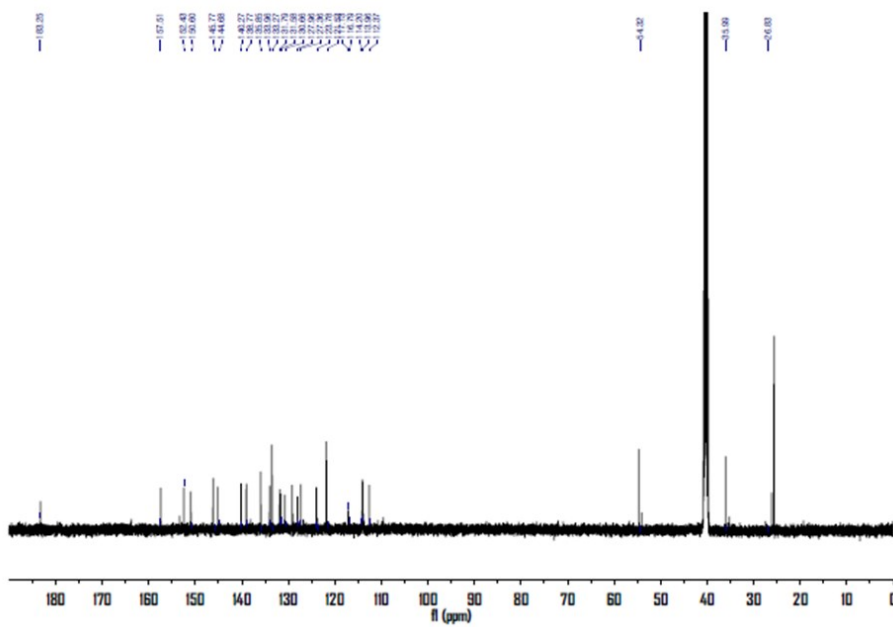


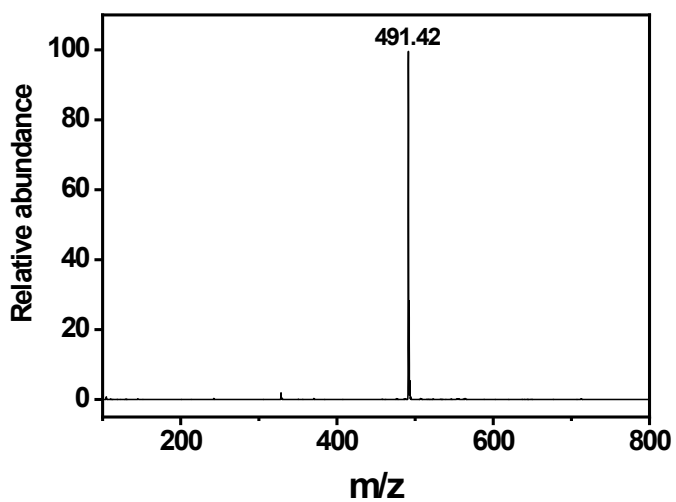
Figure S2.  $^1\text{H-NMR}$  of compound **1b** in  $\text{DMSO-}d_6$ .



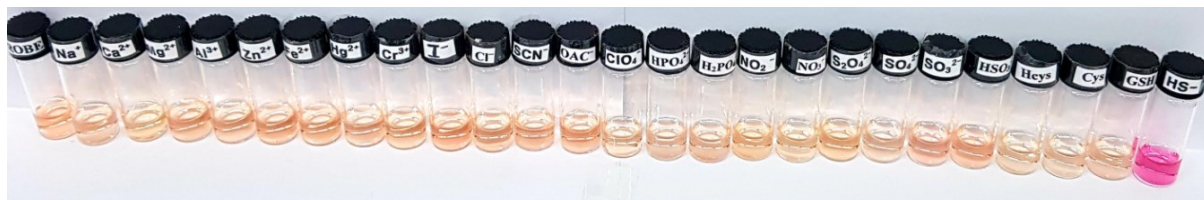
**Figure S3.**  $^1\text{H}$ -NMR of probe **1** in  $\text{DMSO-}d_6$ . The solvent peaks appeared at ppm.



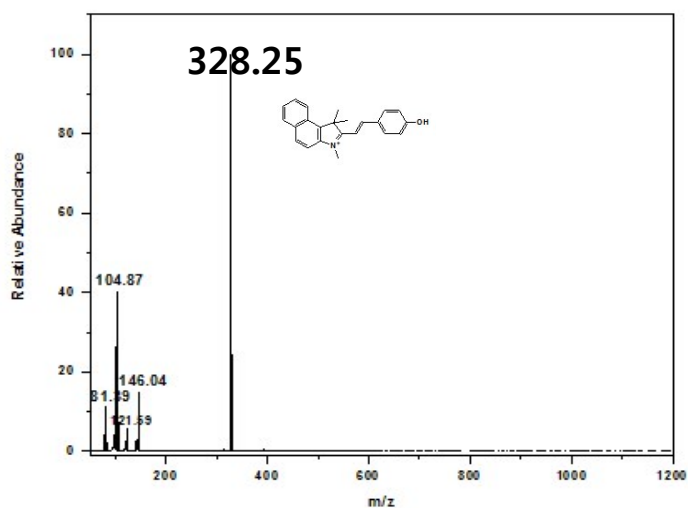
**Figure S4.**  $^{13}\text{C}$ -NMR of probe **1** in  $\text{DMSO-}d_6$ . The peaks at 40 ppm derived from solvent.



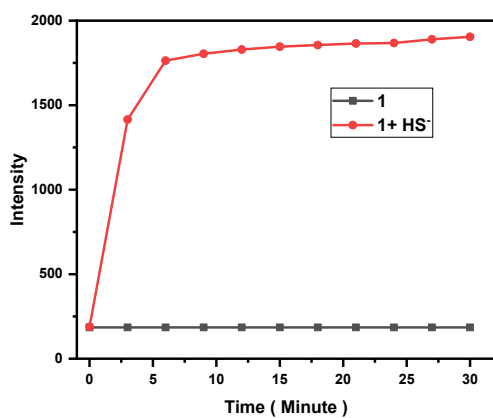
**Figure S5.** The electrospray ionization spectrum of probe **1** affords the peaks at  $m/z = 491.42$ , indicating  $[1 - I]^+$ . The calculated mass of  $[1 - I]^+$  is 491.52.



**Figure S6.** Colorimetric changes of probe **1** upon the addition of various analytes and NaHS



**Figure S7.** The electrospray ionization spectrum of probe **1** after treatment with hydrogen sulfide. It affords the peaks at  $m/z = 328.25$ , indicating  $[\mathbf{1b} - \text{I}]^+$ .



**Figure S8.** Time course experiment of probe **1** (10  $\mu\text{M}$ ) reacting with NaHS (100  $\mu\text{M}$ ) at 25  $^{\circ}\text{C}$  in PBS (10 mM, pH 7.4)/CH<sub>3</sub>CN (v/v, 99/1).  $\lambda_{\text{ex}} = 545 \text{ nm}$ .