

Supporting Information for

**A Nile Red-based Near-infrared Fluorescent Probe for Endogenous Hydrogen
Polysulfides in Living Cells**

Kai-Bin Li,[#] Feng-Zao Chen,[#] Siqi Zhang, Wei Shi, De-Man Han*, Chen Cai, Cai-Xia Chen

Department of Chemistry, Taizhou University, Jiaojiang, 318000, China

Contents list:

- S1. Additional Figures
- S2. Generation of reactive nitrogen and oxygen species (RNS / ROS)
- S3. Original spectral copy of new compounds
- S4. The procedure for the preparation of Na₂S₂ and Na₂S₄

S1. Additional Figures

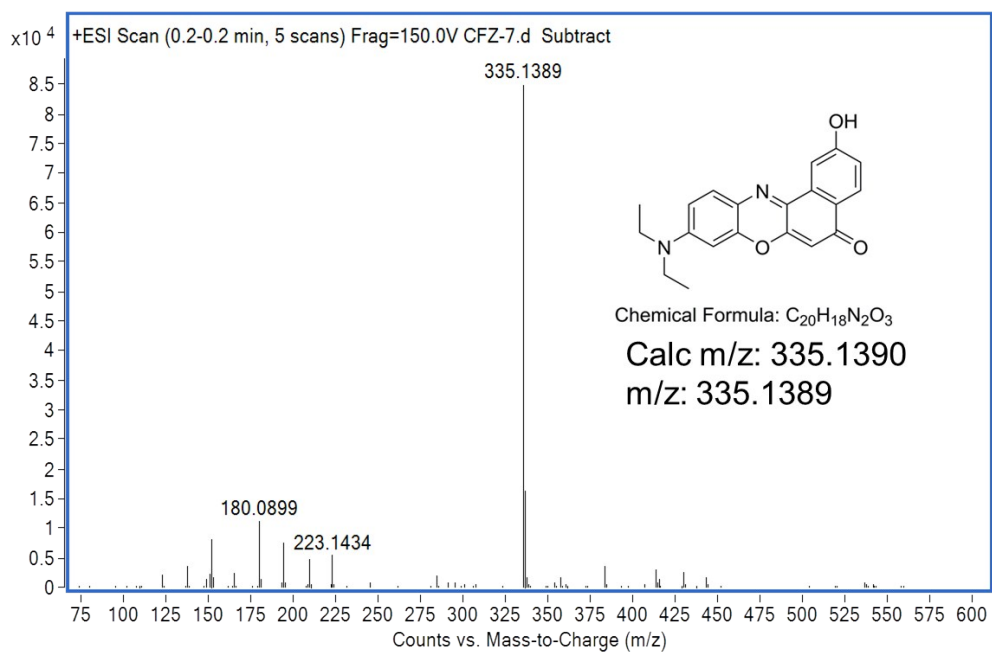


Fig. S1. HR-MS of the product of KB1+Na₂S₂

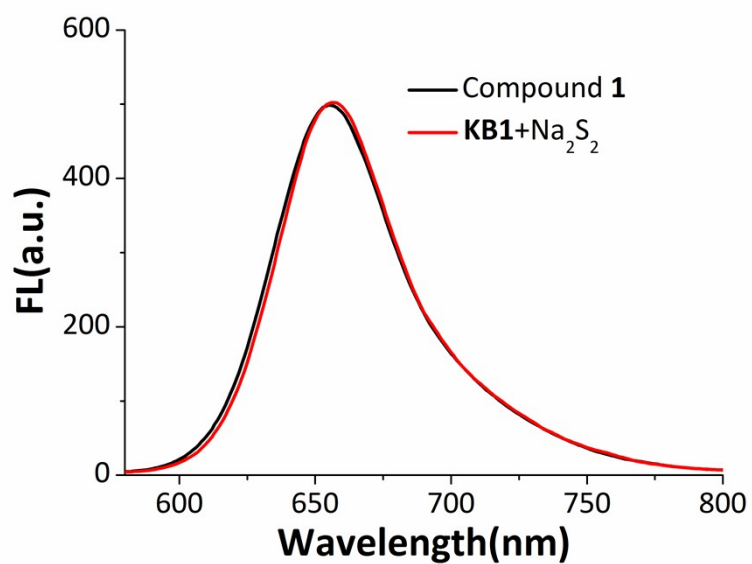


Fig. S2. Fluorescence spectra of compound **1** (5 μ M) and KB1+Na₂S₂ (5 μ M)

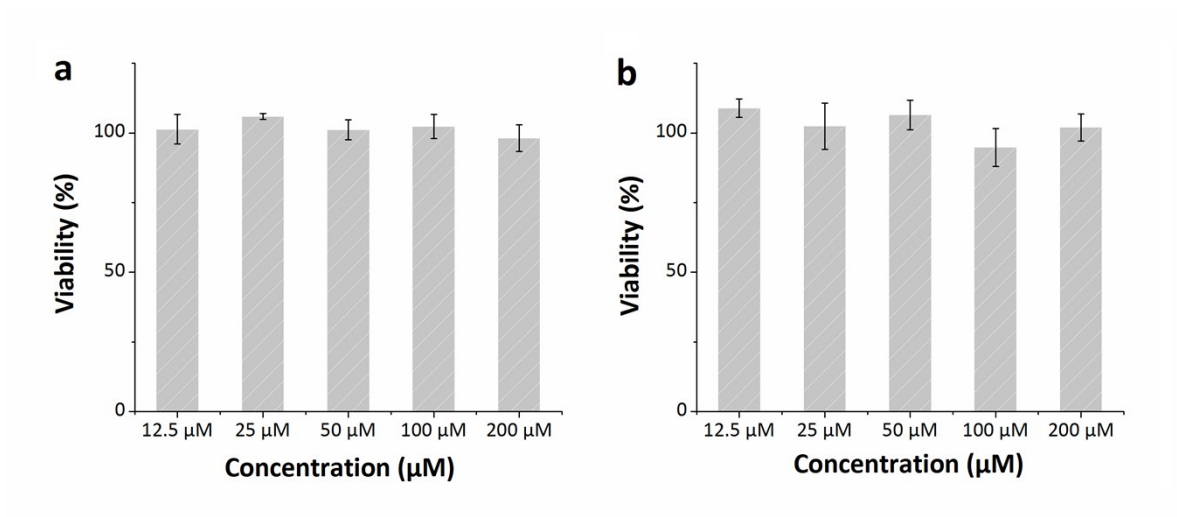


Fig. S3. Cell viability of (a) MCF-7 and (b) HeLa cells in the presence of **KB1** with indicated concentration determined by MTS

S2. Generation of reactive nitrogen and oxygen species (RNS / ROS)

ONOO⁻: The synthesis of peroxynitrite involved nitrosation of H₂O₂ at pH ≥12.0 by isoamyl nitrite (CAS: 110-46-3).

NO: Nitric oxide was generated from SNP (Sodium Nitroferricyanide (III) Dihydrate, CAS: 13755-38-9).

ClO⁻: NaClO was dissolved in deionized water.

H₂O₂: H₂O₂ was dissolved in deionized water.

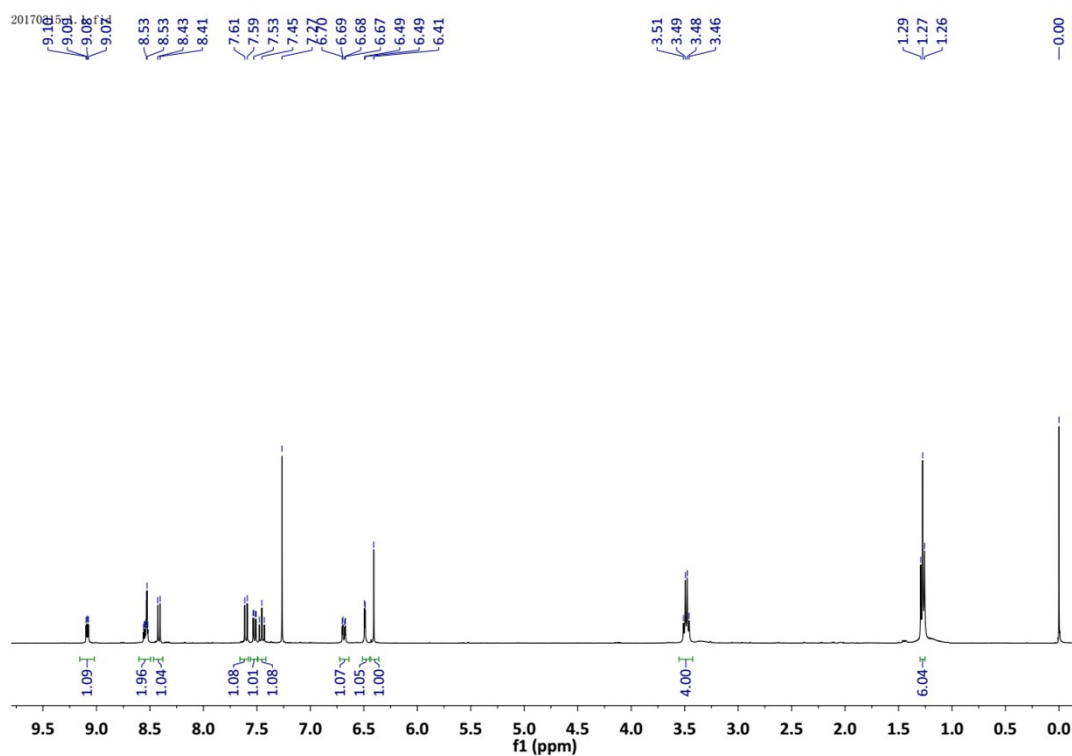
·OH: Hydroxyl radicals were generated by the addition of Fe²⁺ and H₂O₂ in 10 mM HEPES buffer (pH 7.4).

¹O₂: ¹O₂ was generated by hydrogen peroxide/sodium hypochlorite system.

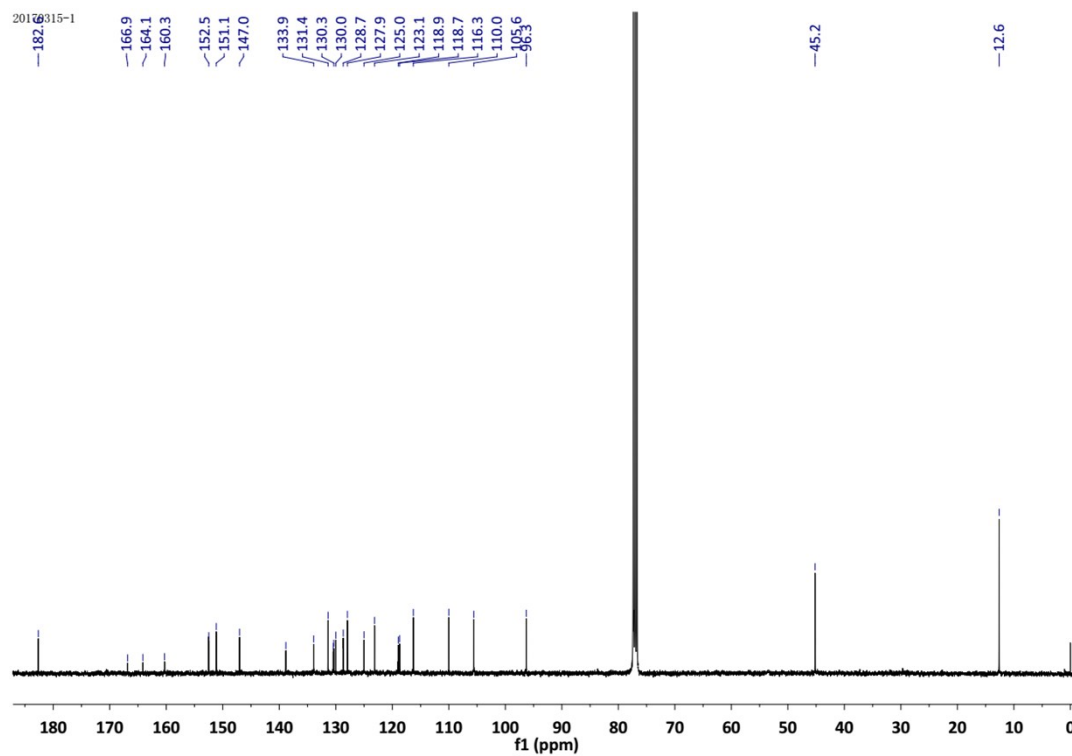
O₂⁻: O₂⁻ was generated by xanthine and xanthine oxidase. Xanthine oxidase was added first. After xanthine oxidase was dissolved, xanthine was added and the mixtures were stirred at 25 °C for 1 h.

S3. Original spectral copy of new compounds

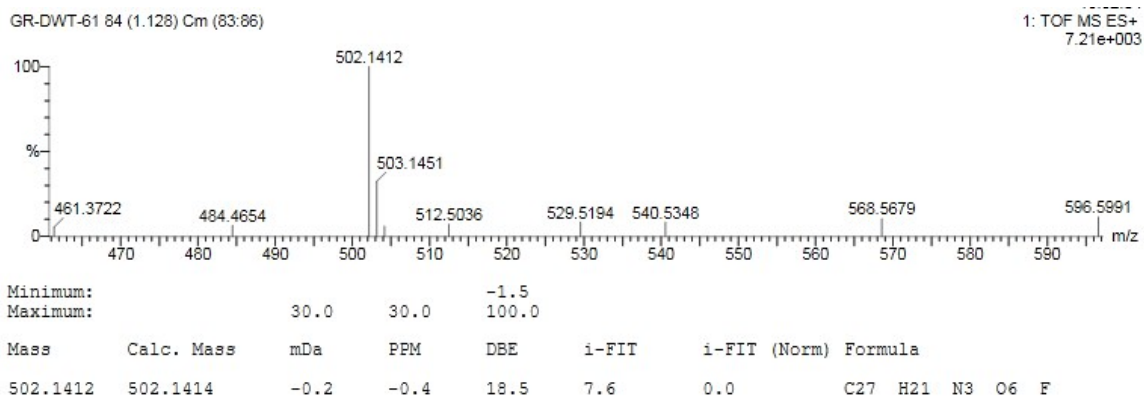
¹H NMR of KB1:



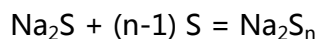
¹³C NMR of KB1:



HR-ESI-MS of KB1



S4. The procedure for the preparation of Na₂S₂ and Na₂S₄



To a solution of sodium sulfide (0.78 g, 0.01 mmol) and sulfur (0.32 g, 0.01 mmol) in distilled water (100 mL), the mixture was refluxed for 1h, then 0.1 mol/L of Na₂S₂ solution was obtained. Na₂S₄ solution was obtained by using the same method with 3 equivalents of sulfur.