Supporting Information

A fast-response near-infrared fluorescent probe for detection of H₂S in living cells

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Figure S1. Probe **1** solubility test shows linearity from abs at 620 nm vs concentration (1-20 μM).



Figure S2. HRMS spectrum of probe 1 (1 mM) in the presence of H₂S (5 mM).



Figure S3. Time-dependent fluorescence intensities change of probe **1** (2 μ M) at 660 nm, when treated with different concentrations of Na₂S (100 μ M; 150 μ M; 200 μ M; 250 μ M; 300 μ M) in PBS buffer.



Figure S4. Time-dependent HPLC traces of the reaction of **1** (200 μ M) with Na₂S (2 mM) to give 4. Conditions: Venusil MP C18 column with 4.6 mm x 250 mm; wavelength: 274 nm; flow 1 mL / min; buffer A: 0.1% (v / v) trifluoroacetic acid in water; buffer B: Methanol; elution condition: 0-3





Figure S5. The emission intensity at 660 nm of **1** (2 μ M) at the indicated pH values in the absence or presence of H₂S (200 μ M).



Figure S6. Concentration-dependent normalized cell viability in the presence of probe 1 (5-25 μ M) for 24 h.

8.493 8.470 8.167 8.167 8.167 8.167 8.167 8.175 7.7.75 7.7.747 7.7.740 7.7.740 7.7.740 7.7.740 7.7.740 7.7.740 7.7.709 7.7.091 7.7.091 7.7.095 7.7.095 7.7.095 7.7.095 7.7.095 7.7.095 7.7.055 6.6903 6.6903 6.6569 6.5569



Figure S7. Real time ¹HNMR spectra, showing thiolysis reaction by the formation of NBD-SH.

| Probe | λex/λem (nm) | Fluorescence enhancement | ф | LOD/µ M | Rate/K ₂ | Ref |
|---|-----------------|-----------------------------|------|------------|--------------------------------------|--------------|
| | 620/660 | ~10 | 0.29 | 0.27 | 29.8 M ⁻¹ s ⁻¹ | This work |
| $ \begin{array}{c} NO_2 \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$ | 730/796 | ~87 | ND | 0.04 | 14.9 M ⁻¹ s ⁻¹ | 1 |
| | 565/585 | ~19 | 0.77 | 0.36 | 27.8 M ⁻¹ s ⁻¹ | 2 |
| | 567/589 | ~4.5 | 0.36 | 0.58 | 113 M ⁻¹ s ⁻¹ | 3 |
| $HO \longrightarrow O \longrightarrow O$ | 502/530 | ~65 | 0.64 | 0.057 | 28 M ⁻¹ s ⁻¹ | 3 |
| | 449/496 | ~200 | 0.81 | 0.9 | 7.6 M ⁻¹ s ⁻¹ | 4 |
| | 394/532 | ~68 | ND | 2.46 | 20.4 M ⁻¹ s ⁻¹ | 5 |

Table S1 comparison of properties of our probe with other probes operating

| \mathbf{r}_{0}^{0} | 415/560 | ~273 | ND | 0.43 | 6.8 M ⁻¹ s ⁻¹ | 6 |
|---|---------|------|----|-------|-------------------------------------|---|
| $ \begin{array}{c} & & \\ & & $ | 480/510 | ~150 | ND | 2.6 | ND | 7 |
| N N N N N N N N N N N N N N N N N N N | 330/468 | ~29 | ND | 0.024 | ND | 8 |





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 17-OCT-2019

 Scans:
 1
 Time:
 08:42:08

 Scale:
 16.8418





Date: 17-OCT-2019 Time: 08:35:53 Scale: 10.2697







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