Electronic Supplementary Material (ESI) for RSC Advances.

A near-infrared BODIPY-based fluorescent probe for the detection of hydrogen sulfide in fetal bovine serum and living cells

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1. Additional Absorption and Emission Spectra

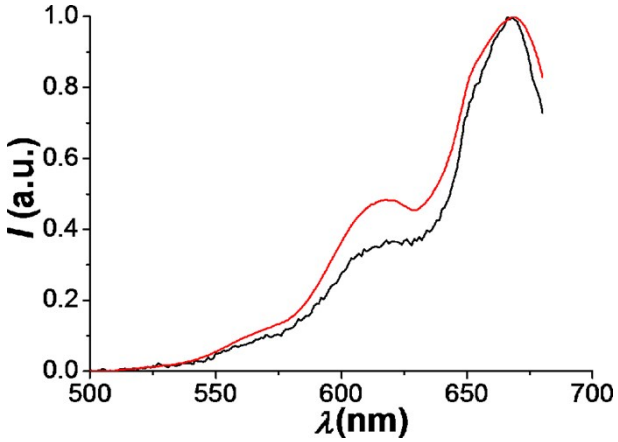


Figure S1 Normalized excitation spectra (λ_{em} = 683 nm) of **BDP-680** (10 μM) prior to (black curve) and after (red curve) addition of NaSH (500 μM) for 0.5 h in MeCN/H_2O (8/2, v/v; pH = 7.2) at 25 °C.

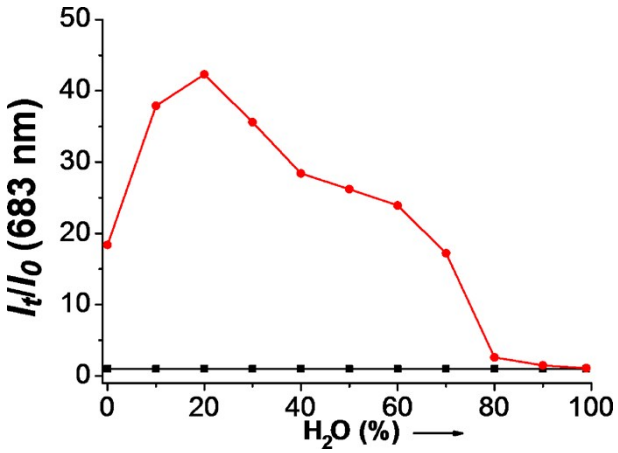


Figure S2 The effect of water content on the relative fluorescence intensity of **BDP-680** (10 μM) upon addition of 500 μM NaSH in MeCN/H_2O. All the data was measured at 683 nm (λ_{ex} = 610 nm) at 25 °C 30 min after addition of NaSH (black square: **BDP-680**; red circle: **BDP-680** + NaSH).

2. **MTT assays**

MTT experiment was performed in 96-well plate to assess the cytotoxicity of the probe. The MTT assays in Human Hepatoma SMMC-7721 cells with probe concentrations from 2.5 to 80 μM in comparison with the blank and negative control. Cells were plated on cell plates at 4×10^3 cells per well and allowed to incubate for 24 hr. The **BDP-680** in various concentrations was added to the well and incubated for 24 hr followed by classical MTT treatment and data acquiring.

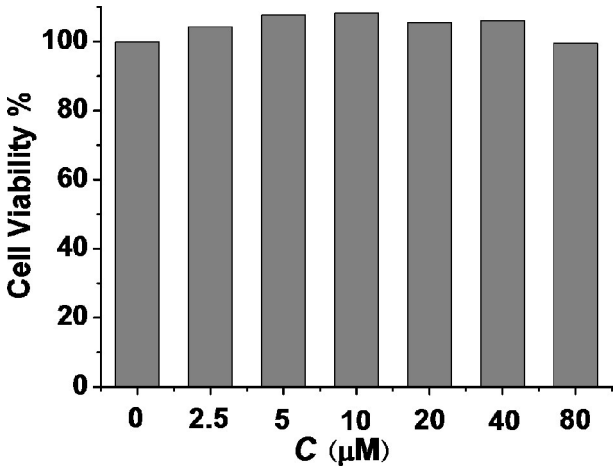
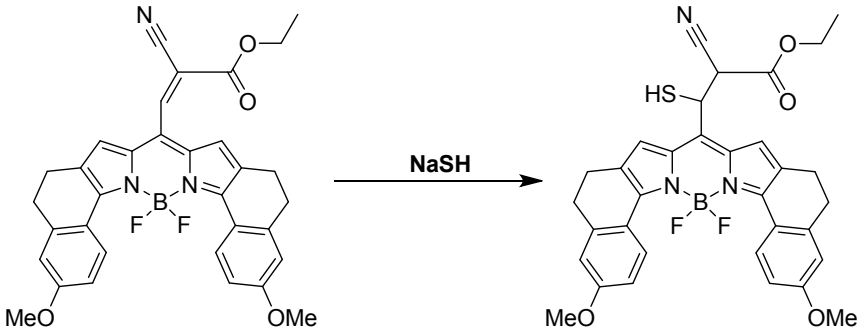


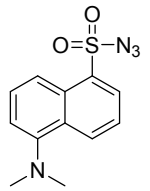
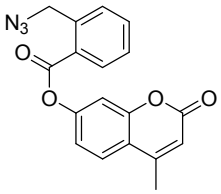
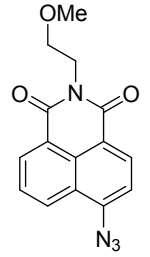
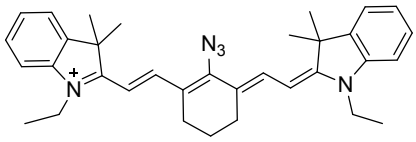
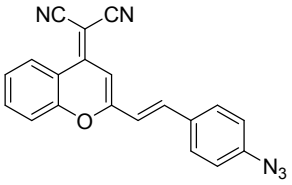
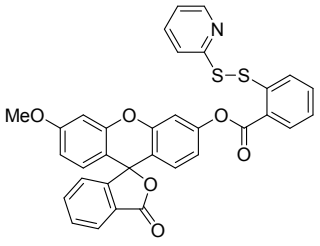
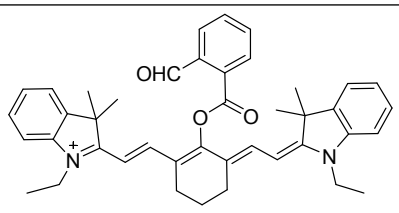
Figure S3. Cell viability assay of **BDP-680** in 7721 Cell, all compounds were incubated with the cells for 24 hr, and the cell viability was observed via MTT assays.

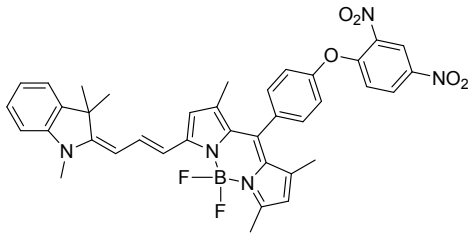
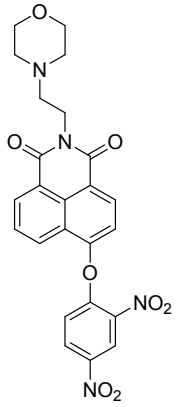
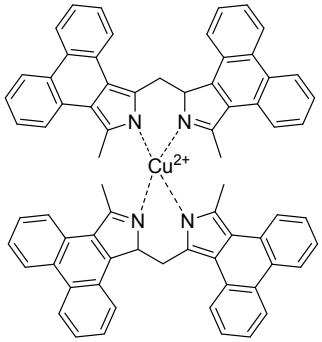
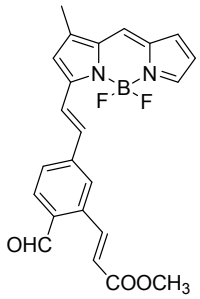
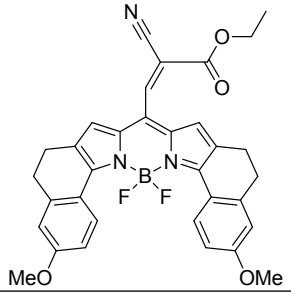
3. The plausible mechanism for selective reaction of BDP-680 to NaSH



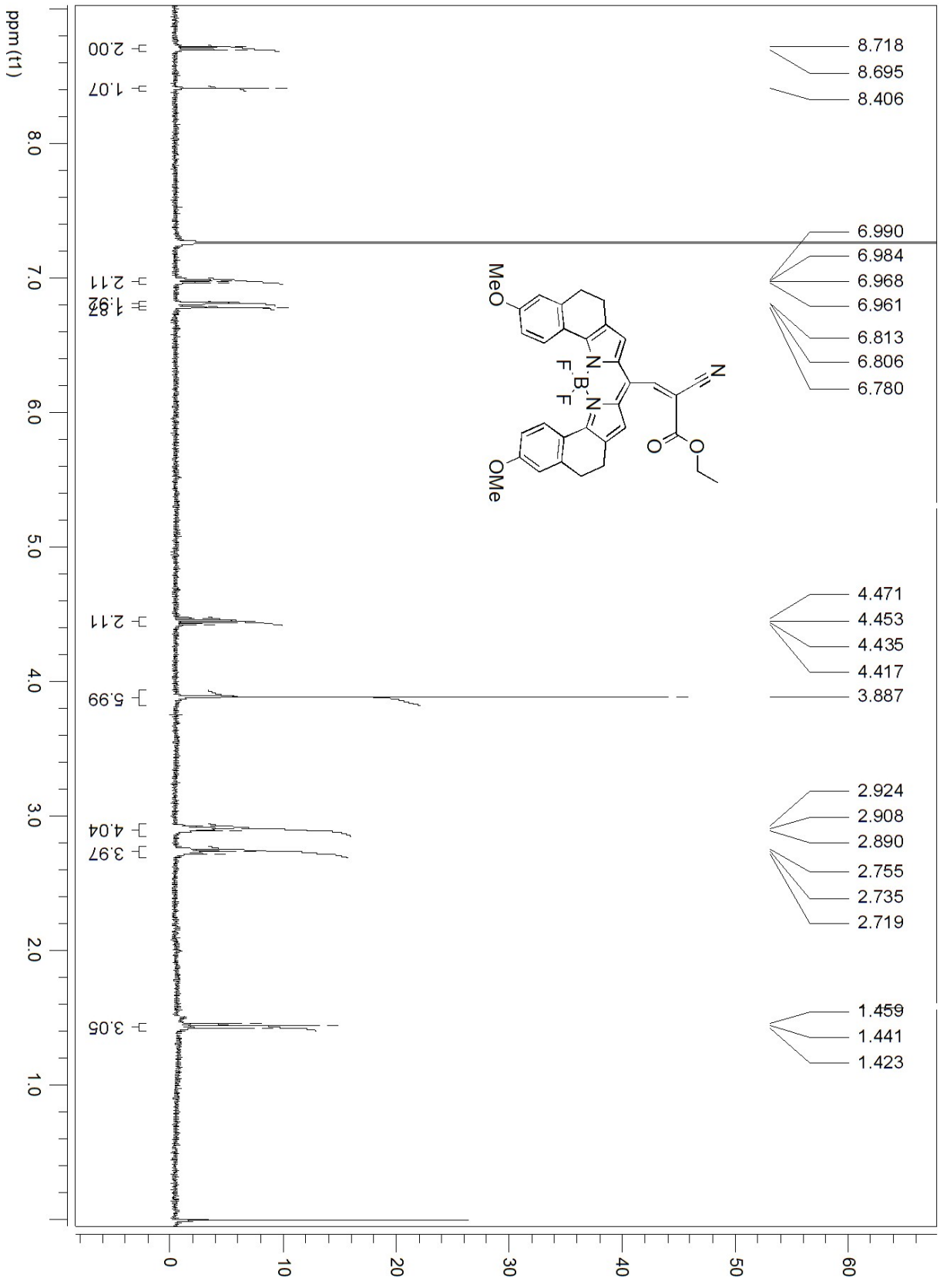
Scheme S1 The plausible mechanism for selective reaction of **BDP-680** to NaSH

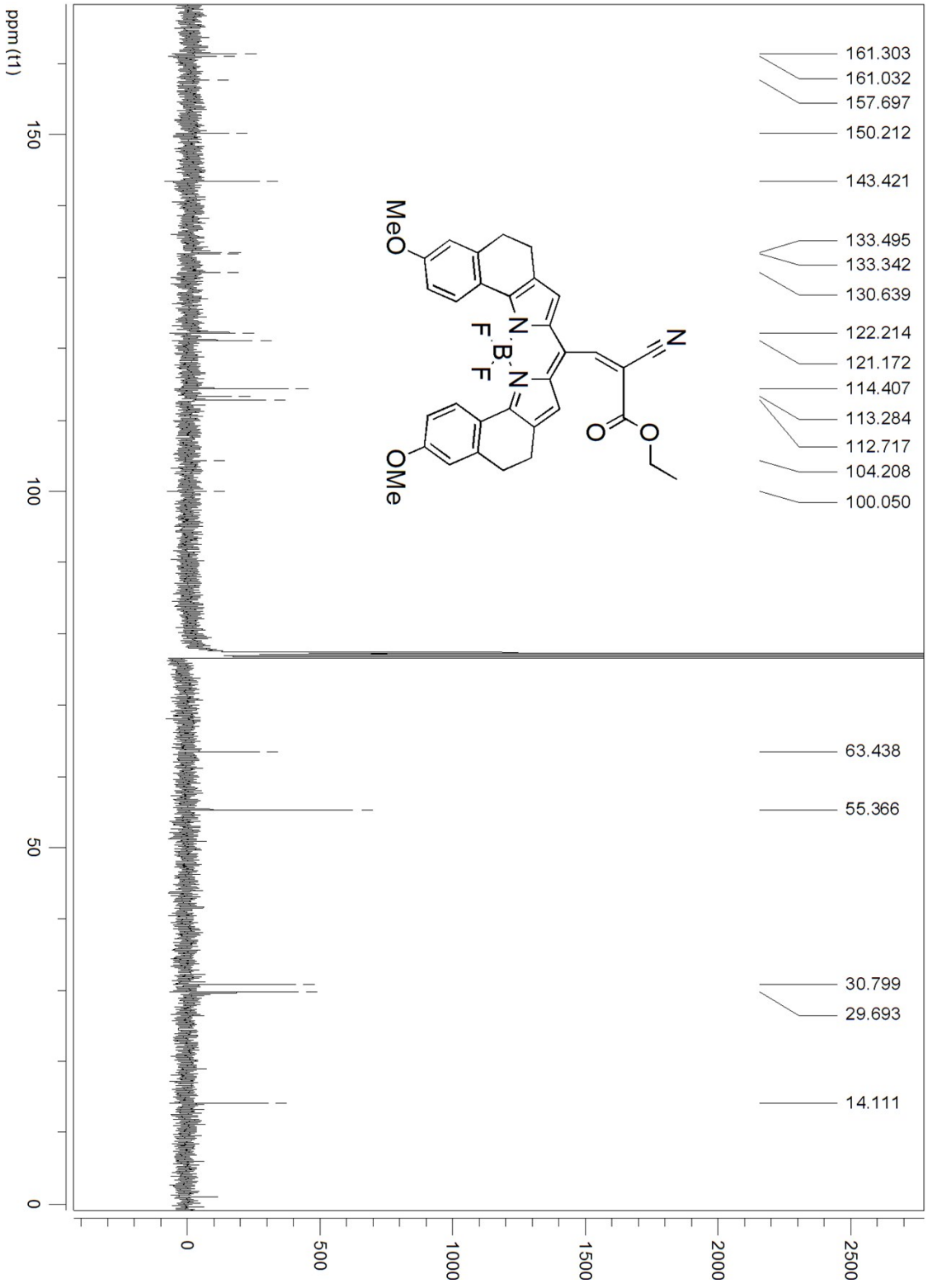
4. Table S1. Comparison of fluorescent probes for H_2S.

Probes	λex/λem [nm]	Linear response range	Detection limit	Ref.
	340/535	1–100 μM	1 μM	23
	365/450	——	10 μM	25
	435/545	——	1-5 μM	26
	625/710	1–100 μM	0.08 μM	27
	520/670	25–250 μM	3.05 μM	28
	465/—	0–10 μM	——	32
	700/780	0–70 μM	5.0–10 nM	34

	650/780	0–10 μM	0.05 μM	38
	450/555	0–100 μM	0.48 μM	39
	—/600	——	1 μM	42
	520/561	0–350 μM	2.5 μM	45
	610/683	0–100 μM	0.5 μM	This work

5. Spectroscopic data




ppm (t1)
150
100
50
0
0
500
1000
1500
2000
2500
MeO
OMe
N
B
F
F
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N
O
O
161.303
161.032
157.697
150.212
143.421
133.495
133.342
130.639
122.214
121.172
114.407
113.284
112.717
104.208
100.050
63.438
55.366
30.799
29.693
14.111

6. X-ray crystal structure determinations of BDP-680

Crystals suitable for the X-ray structural determination were mounted on a Mac Science DIP2030 imaging plate diffractometer and irradiated with graphite monochromated Mo-*K*α radiation (λ = 0.71073 Å) for the data collection. The unit cell parameters were determined by separately autoindexing several images in each data set using the DENZO program (MAC Science).[1] For each data set, the rotation images were collected in 3° increments with a total rotation of 180° about the ϕ axis. The data were processed using SCALEPACK. The structures were solved by a direct method with the SHELX-97 program.[2] Refinement on F^1 was carried out using the full-matrix least-squares by the SHELX-97 program.[2] All non-hydrogen atoms were refined using the anisotropic thermal parameters. The hydrogen atoms were included in the refinement along with the isotropic thermal parameters.

Crystal data for **BDP-680**. $C_{33}H_{28}BF_2N_3O_4$, M = 579.40, triclinic, a = 8.0202(2), b = 14.3300(2), c = 16.5784(3) Å, α = 112.088(1), β = 101.887(2), γ = 90.329(3)°, V = 1720.36(6) Å^3, T = 296(2) K, space group P-1, Z = 2, F(000) = 728, D_{calc} = 1.352 g cm^{-3}, μ = 0.25 mm^{-1}, R_{int} = 0.022, R_1 = 0.080 ($I > 2\sigma(I)$), wR_2 (all data) = 0.228, *GOF* = 1.17. CCDC reference number 1023076 for **BDP-680.**

CCDC reference number 1023076 for **BDP-680** contains the supplementary crystallographic data. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336033; or **deposit@ccdc.cam.uk).**

7. References

1 Z. Otwinowski and W. Minor, *Methods Enzymol.* 1997, **276**, 307.

2 G. M. Sheldrick, *SHELX-97*, University of Göttingen, Göttingen, Germany, 1997.