

Supporting information

A novel near-infrared fluorescent hydrogen sulfide probe for live cells and tissues imaging

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1. The characterization of the REDCP and NIR-NP

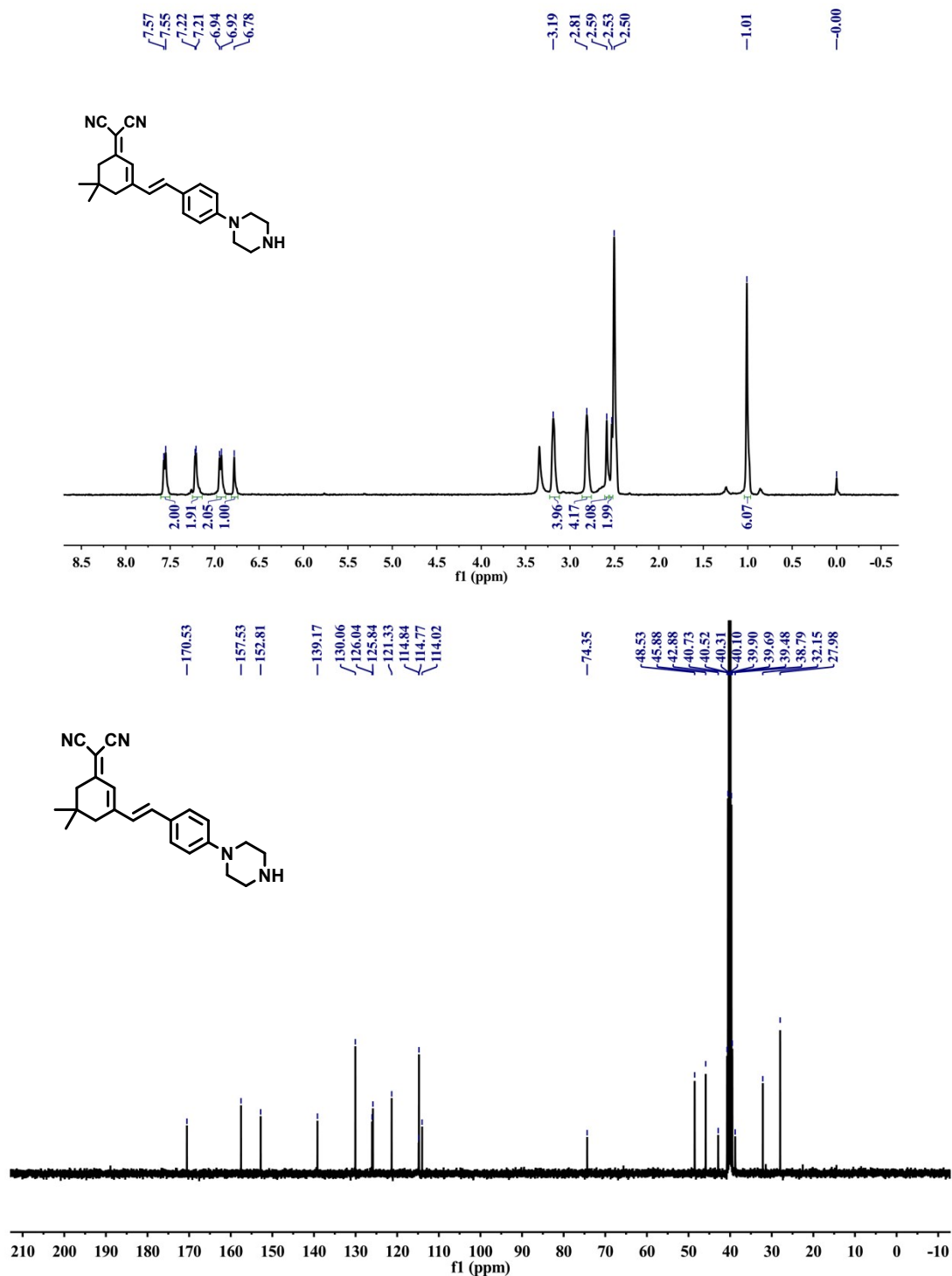


Fig.S1. ¹H NMR and ¹³C NMR spectrum of REDCP (DMSO-D₆, 400 MHz)

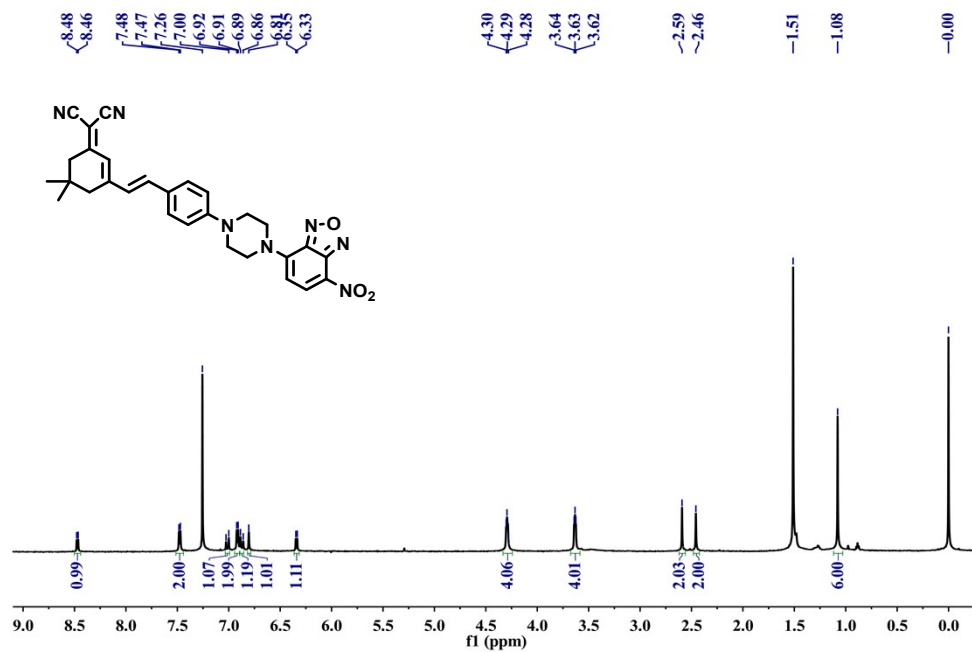


Fig.S2. ¹H NMR spectrum of NIR-NP (CDCl₃-D₆, 600 MHz)

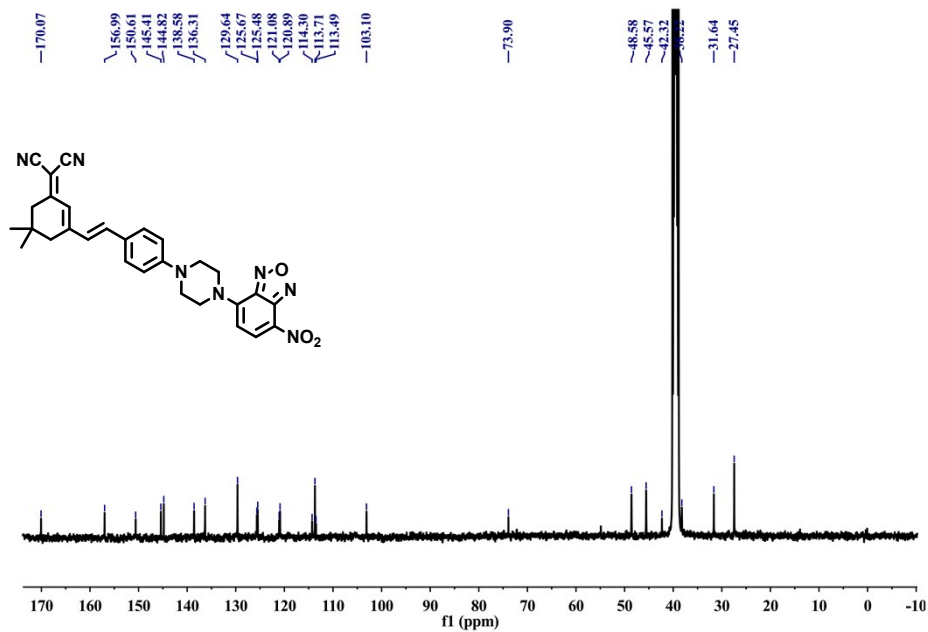


Fig.S3. ¹³C NMR spectrum of NIR-NP (DMSO-D₆, 400 MHz)

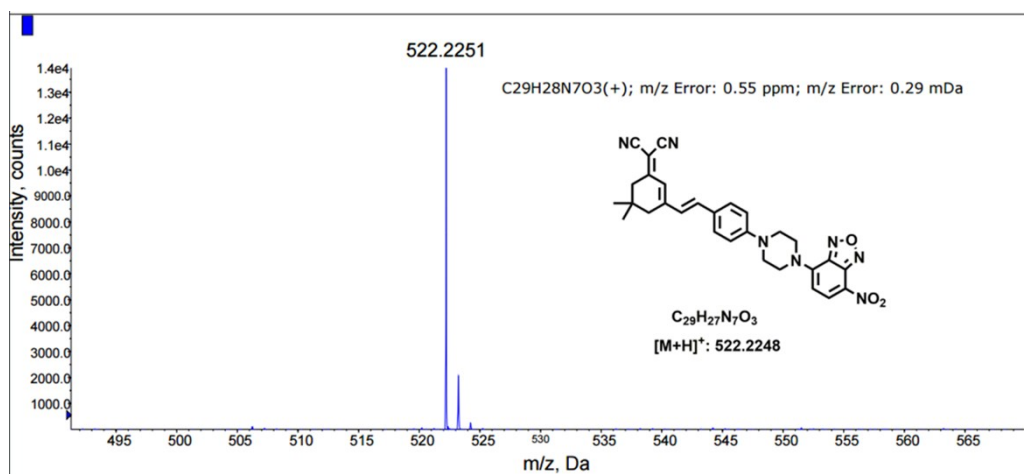
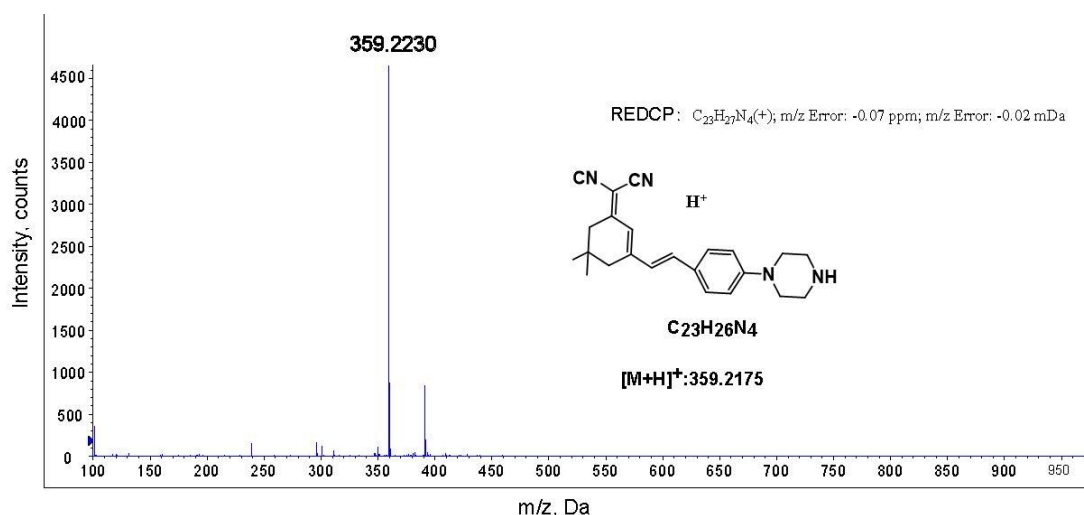


Fig.S4. HRMS of REDCP m/z Calcd. .for $C_{23}H_{26}N_4$: 359.2175 $[M+H]^+$, found: 359.2230 and NIR-NP m/z Calcd. .for $C_{29}H_{28}N_7O_3$: 522.2248 $[M+H]^+$, found: 522.2251.

2. The UV and fluorescence properties of the NIR-NP probe

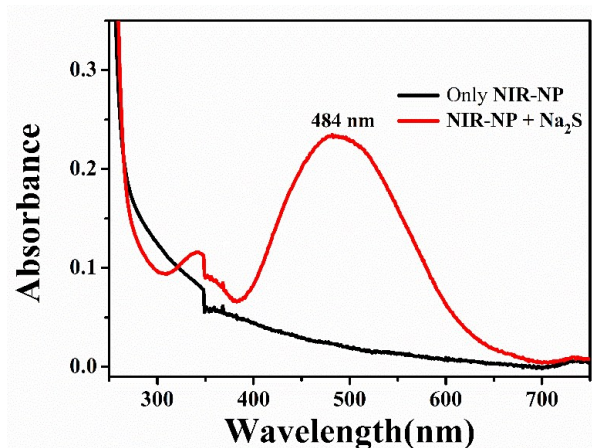


Fig.S5. The change of ultraviolet visible light absorption NIR-NP (10 μM) was analyzed in the absence (black) and presence (red) of 100 μM Na_2S .

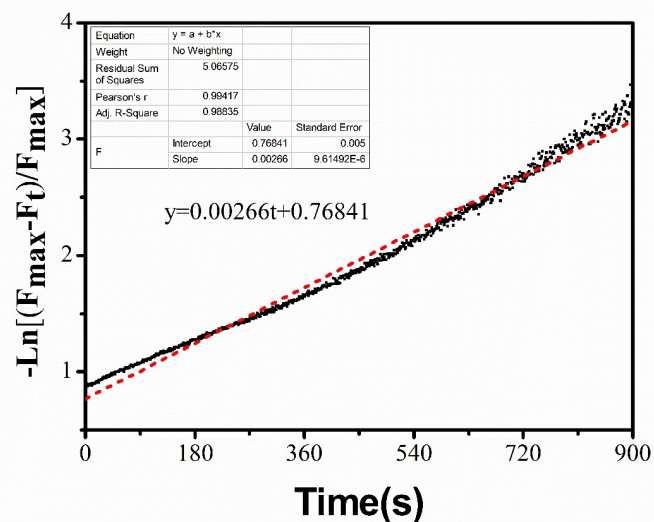


Fig. S6. Pseudo first-order kinetic plot of the reaction of NIR-NP (10 μM) with Na_2S (100 μM), slope = 0.00266×10^{-3} , so $k' = 2.7 \times 10^{-3} \text{ s}^{-1}$.

3. The probe properties was analyzed in biological systems

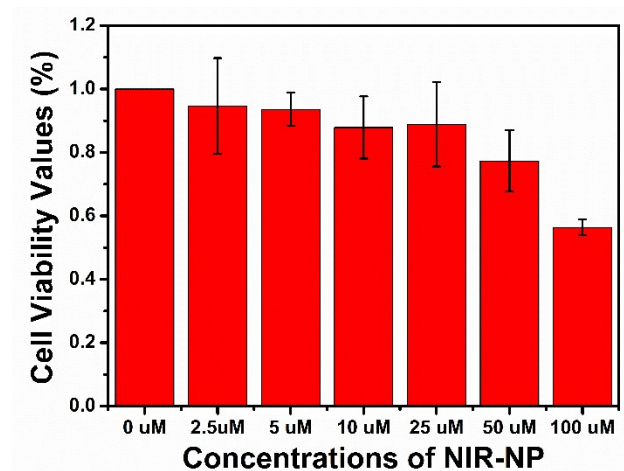


Fig.S7. Cell viability of HeLa cells after 24 hours by CCK-8 assay, and the experiment was repeated three times and the data are shown as mean ($\pm\text{SD}$).

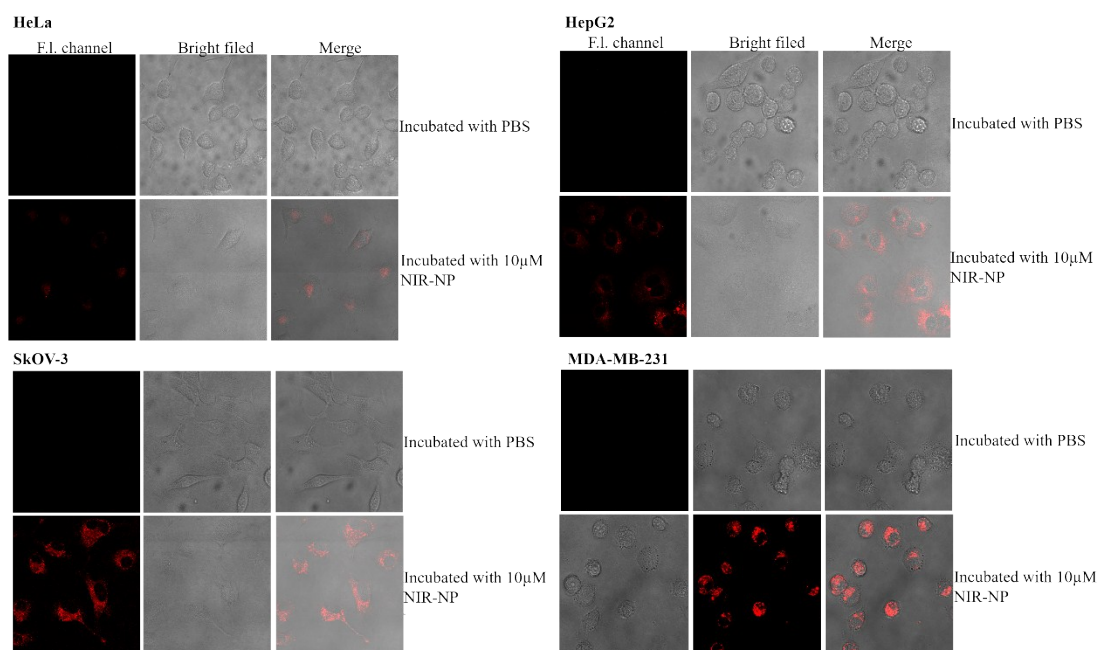


Fig.S8. The confocal imaging of different tumor cells. The cells was incubated with PBS as control (above) and incubation with 10 μM probe **NIR-NP** for 30min (below). Confocal images was performed by confocal microscopy: λ_{ex} : 440 nm / λ_{em} : 600-700 nm.

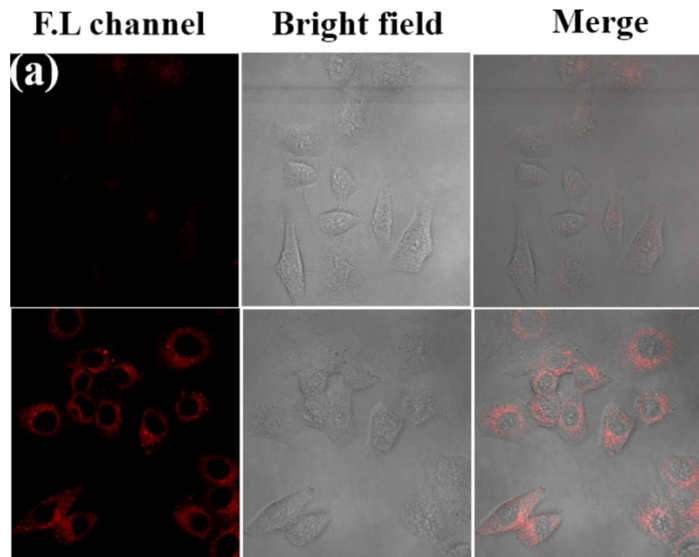


Fig.S9. (a) HepG2 cells were pre-treated with 1mM PAG for 1 h and then incubated with 10 μM **NIR-NP**; **(b)** pre-treated with 1 mM PAG for 1 h and incubated 10 μM **NIR-NP**, then incubated with 100 μM Na_2S for 30 min; confocal image was performed by confocal microscopy: λ_{ex} : 440 nm / λ_{em} : 600-700 nm.

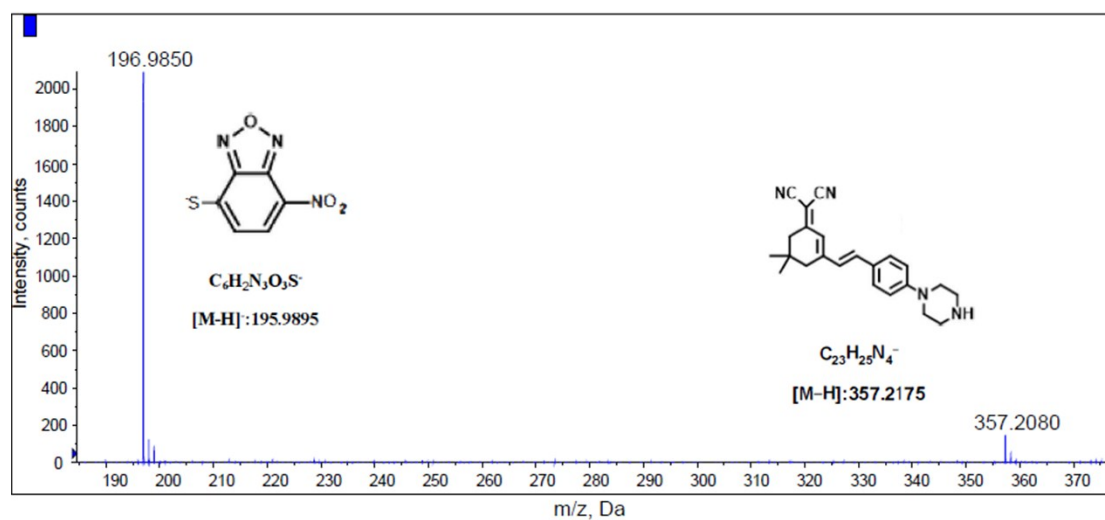
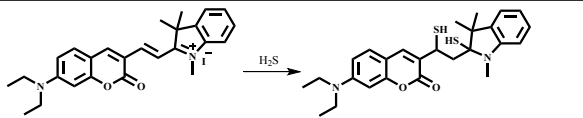
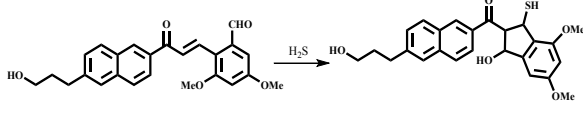
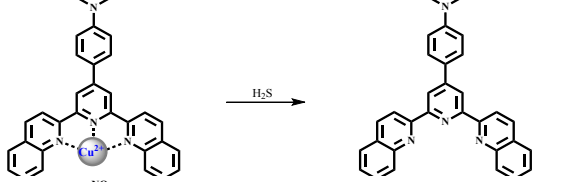
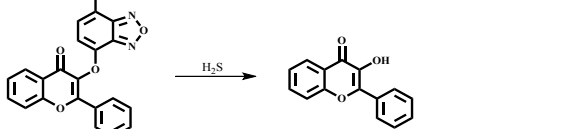
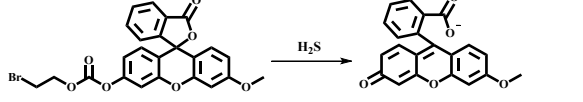
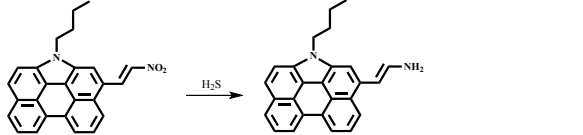
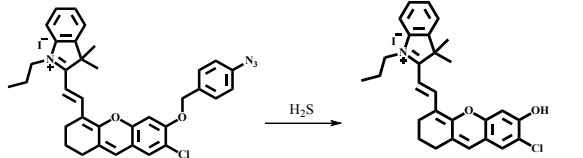
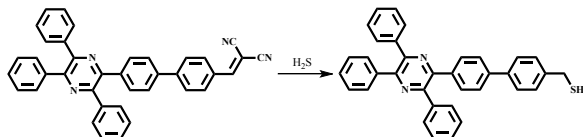
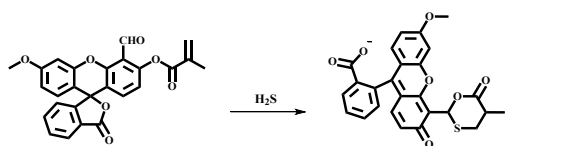
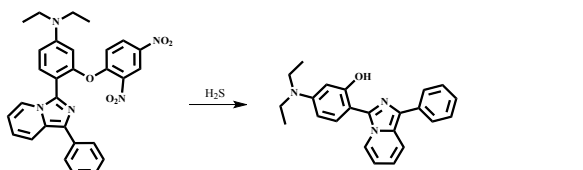
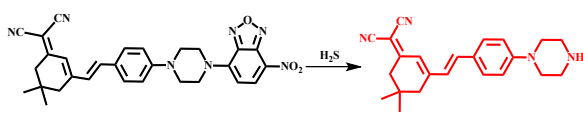


Fig.S10. HRMS spectra for analyzing the reaction mechanism of NIR-NP and Na_2S , and the REDCP-H whose m/z Calcd.for $C_{23}H_{25}N_4^-$: 357.2175 $[M-H]$, found: 357.2080 and NBD-SH, m/z Calcd.for $C_6H_2N_3O_3S^-$: 195.9895 $[M-H]$, found 195.9850 with negative mode.

Table S1 Comparison of **NIR-NP** with recently reported probes for detection of H_2S

Recognition process	LOD	Stokes Shift	Fluorescence signal	Ref.
	0.014 μM	no data	Turn-Off	1
	0.050 μM	135 nm	Turn-On	2
	2.240 μM	146 nm	Turn-On	3
	0.020 μM	170 nm	Turn-On	4
	0.130 μM	47 nm	Turn-On	5
	0.139 μM	73 nm	Blue-Shift	6
	0.260 μM	40 nm	Turn-On	7
	0.500 μM	57 nm	Blue-Shift	8
	0.037 μM	22 nm	Turn-On	9
	0.360 μM	193 nm	Turn-On	10
	0.030 μM	186 nm	Turn-On	This work

Reference

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