Electronic Supplementary Information

Boron fluoride regulated "naked eye" and ratiometric fluorescent detection of CN^- as a test strip and its bioimaging

Sha Li,[a] Fangjun Huo, [b] Kaiqing Ma, [b] Yongbin Zhang,[b] Caixia Yin*[a]

[a]*Institute of Molecular Science, Key Laboratory of Chemical Biology and Molecular Engineering of Ministry of Education, Shanxi University, Taiyuan, 030006, China.*

[b] *Research Institute of Applied Chemistry, Shanxi University, Taiyuan, 030006, China*.

*Corresponding author:

C.X. Yin, E-mail: yincx@sxu.edu.cn,Tel/Fax: +86-351-7011022

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Experimental Section

1.1. Materials and instruments

Drugs and solvents used are analytical pure are purchased from suppliers in the experiments and do not need further purification. All the water used in the experiment is deionized water. Silica gel GF254 plates and glass capillary with an inner diameter of 0.3 mm and a length of 100 mm were used in TLC analysis. The pH value of the solution was measured by the FE20-Five Easy Plus^{TM} pH meter (Mettler Toledo, Switzerland). UV-Vis absorption spectra and fluorescence emission spectra (λ_{ex} = 500 nm, slit: 5 nm/2 nm) were respectively measured by Hitachi U-3900 UV-visible spectrophotometer and Hitachi F-7000 fluorescence spectrophotometer. Standard quartz cuvettes (1 cm) for all-optical spectra measurements were purchased from Shanghai Huamei Experiment Instrument Plants, China. ^{1}H NMR and ^{13}C NMR experimental data were obtained by a Bruker AVANCE-600 MHz NMR spectrometer (Bruker, Billerica, MA). The MS spectra were performed on LTQ-MS (Thermo) Electrospray ionization mass spectrometry. The fluorescence images of **B-2** reacting to CN^- in HepG-2 cells were collected on a Zeiss LSM880 Airyscan confocal laser scanning microscope (λ_{ex}=488 nm). The main synthetic method of compound **2** is based on literature reports [S1, S2].

1.2. Solution preparation and optical measurement

Dissolve the probe **B-2** (2 mM) in DMSO as a stock solution. CN^- (2 mM) solution was prepared by dissolved KCN in deionized water. Stock solutions (2 mM) of F^-, Cl^-, Br^-, I^-, NO_3^-, SO_3^{2-}, SCN^-, CH_3COO^-, HPO_4^{2-}, $H_2PO_4^-$, $P_2O_7^{4-}$, CO_3^{2-}, were prepared by direct dissolution of proper amounts of sodium salts. UV-vis and fluorescence

spectra were detected in acetonitrile: hepes (3: 2 v/v, Hepes buffer, pH 7.4) solutions. Fluorescence measurements were carried out with a slit width of 5 nm/2 nm (λ_{ex}=500 nm).

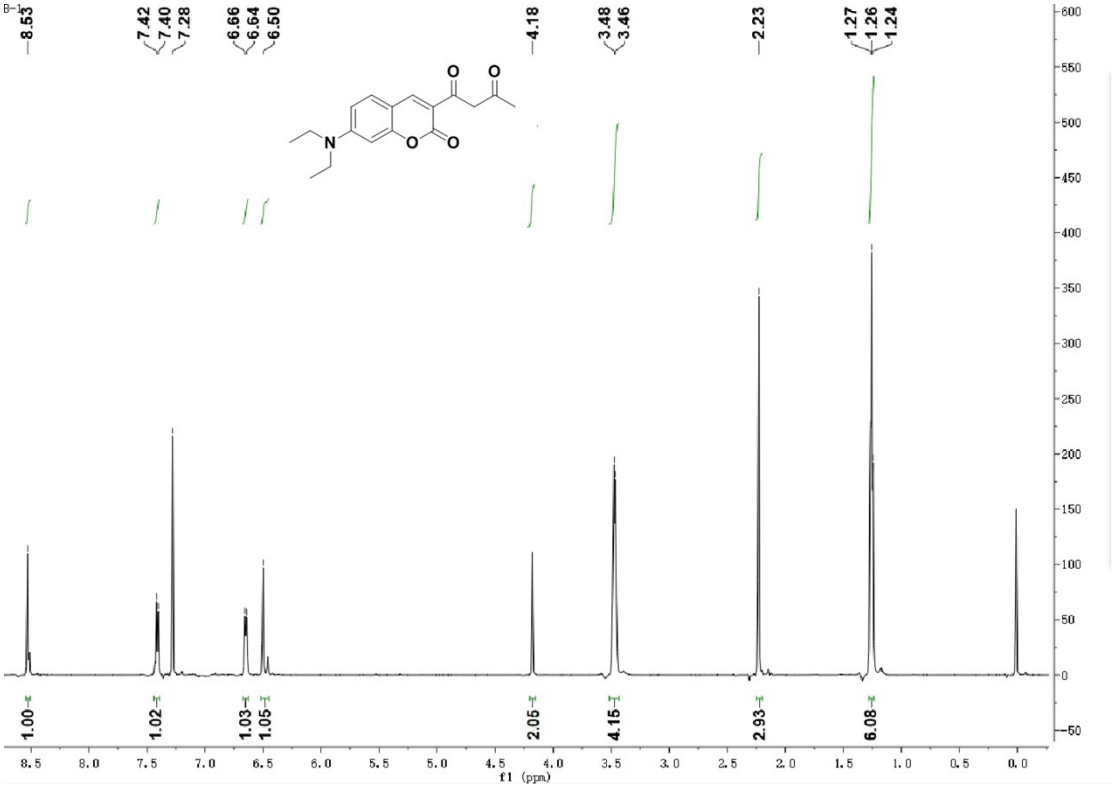
1.3. Cell imaging experiments

The HepG-2 cells were cultured in DMEM medium (12% FBS and 1% antibiotics) in an incubator at 37°C and 5% CO_2. The cells were laid on 6-well plates and incubated overnight. Cells were plated in 6-well plates, and cultured overnight. The cells were washed with PBS three times before being imaged with a confocal laser scanning microscope. DMSO-soluble **B-2** was added to the cell medium (2 mL) at a final concentration of 5 μM. After incubating for 15 minutes, gently wash the excess **B-2** with PBS (10mM, pH=7.4) for 3 times. Meanwhile, another portion of HepG-2 cells pretreated with 5 μM **B-2** was treated with 10 μM CN^- and incubated at 37°C for 10 min. Before imaging, the stained HepG-2 cells were washed with PBS once. The **B-2** enables the yellow channel (λ_{ex}=488 nm) recognition and fluorescence imaging on the Zeiss LSM880 Airyscan confocal laser scanning microscope.

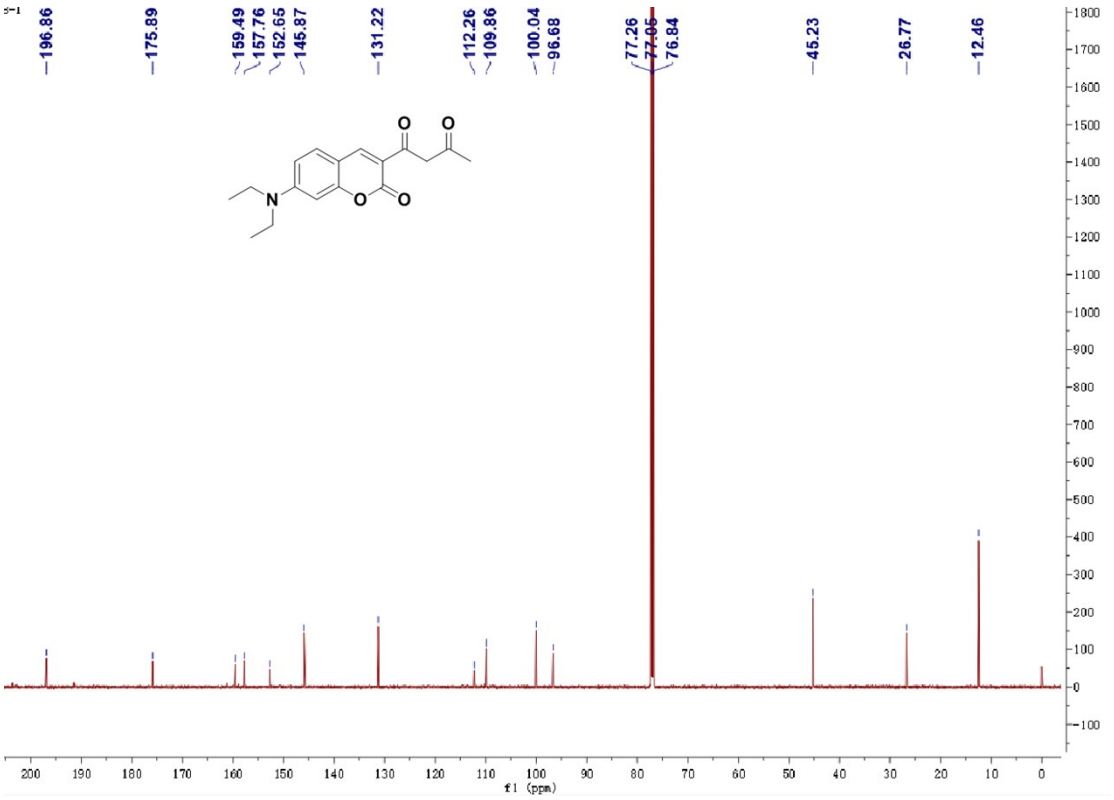
References

[S1] S. Y. Zhu, M. J. Li, L. Sheng, P. Chen, Y. M. Zhang, Analyst, 2012, **137**, 5581.
[S2] Y. Wen, F.J. Huo, C.X. Yin, Chin. Chem. Lett. 2019, **30**, 1834.

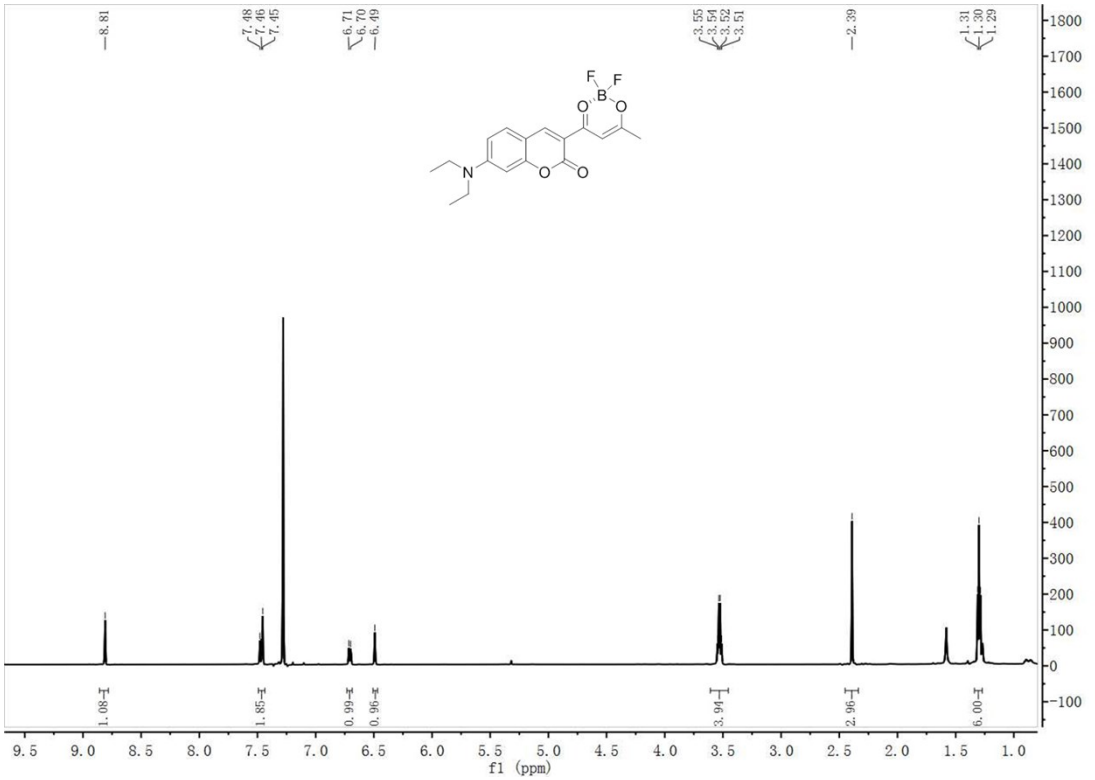
Fig. S1 : ^{1}H NMR and ^{13}C NMR of compound 2 and **B-2**.



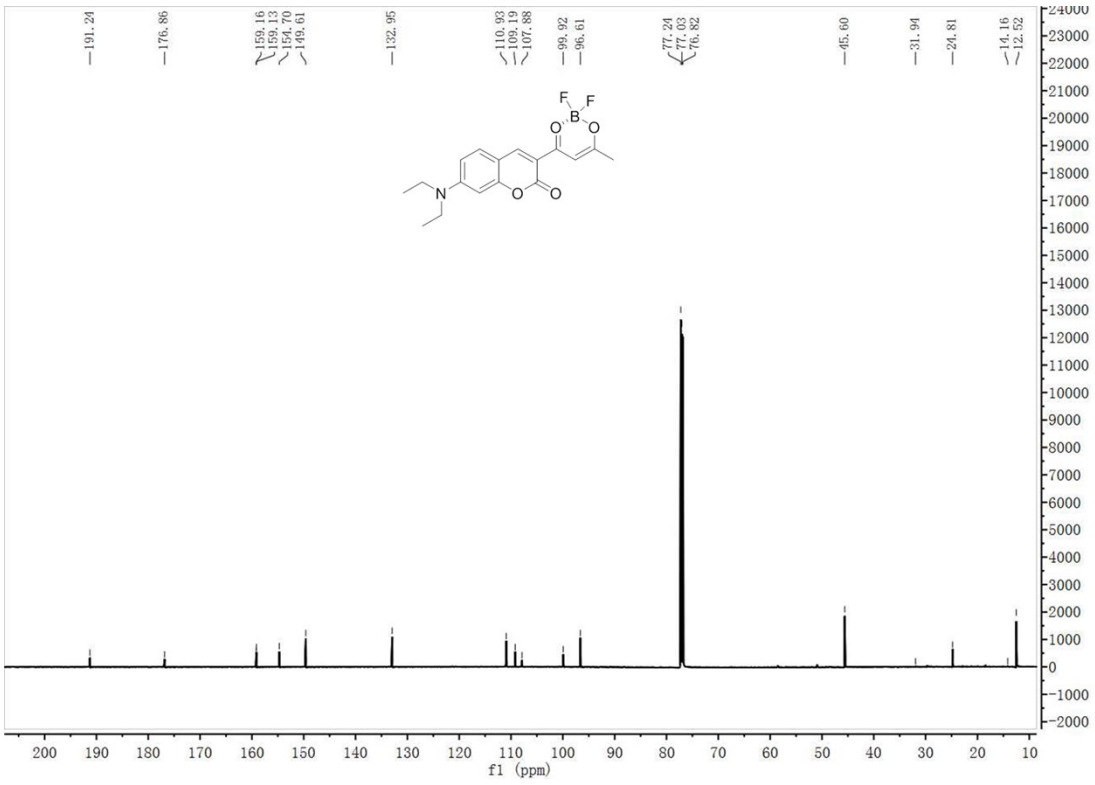
The ^{1}H NMR (600MHz) spectra of Compound 2 in $CDCl_3$.



The ^{13}C NMR (150 MHz) spectra of Compound 2 in $CDCl_3$.



The ^{1}H NMR (600MHz) spectra of **B-2** in $CDCl_3$.



The ^{13}C NMR (150 MHz) spectra of **B-2** in $CDCl_3$.

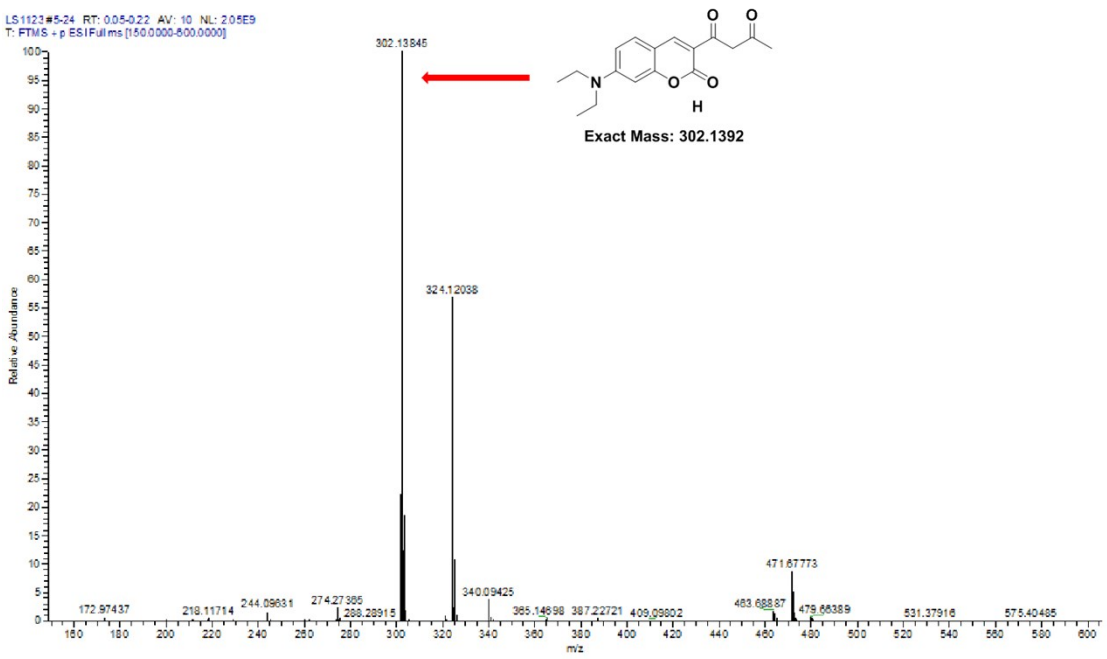


Fig. S2 (A) The ESI-MS of Compound 2.

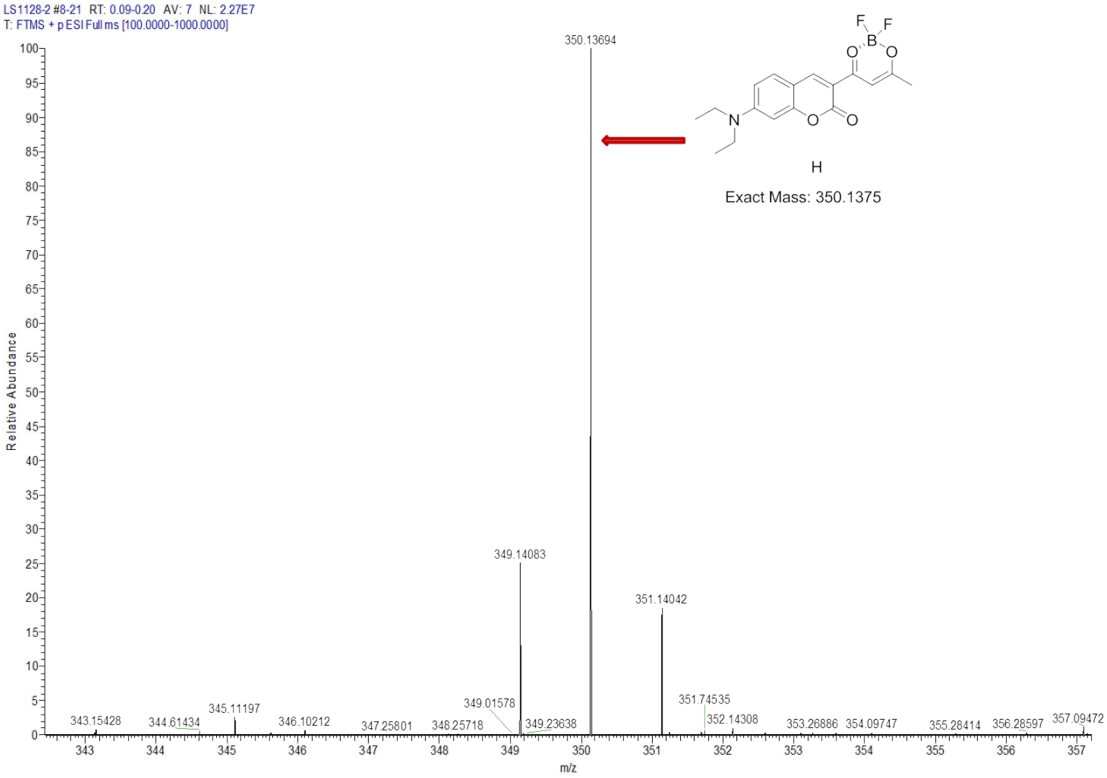


Fig. S2 (B) The ESI-MS of **B-2**.

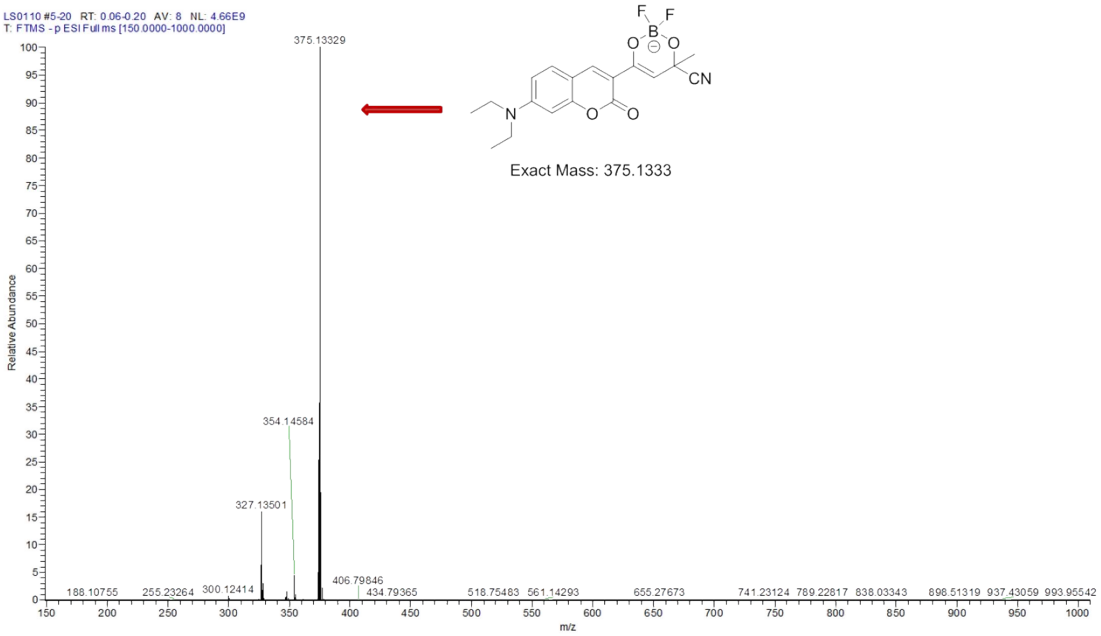


Fig. S3 The ESI-MS of product obtained by reaction of **B-2** with CN^-.

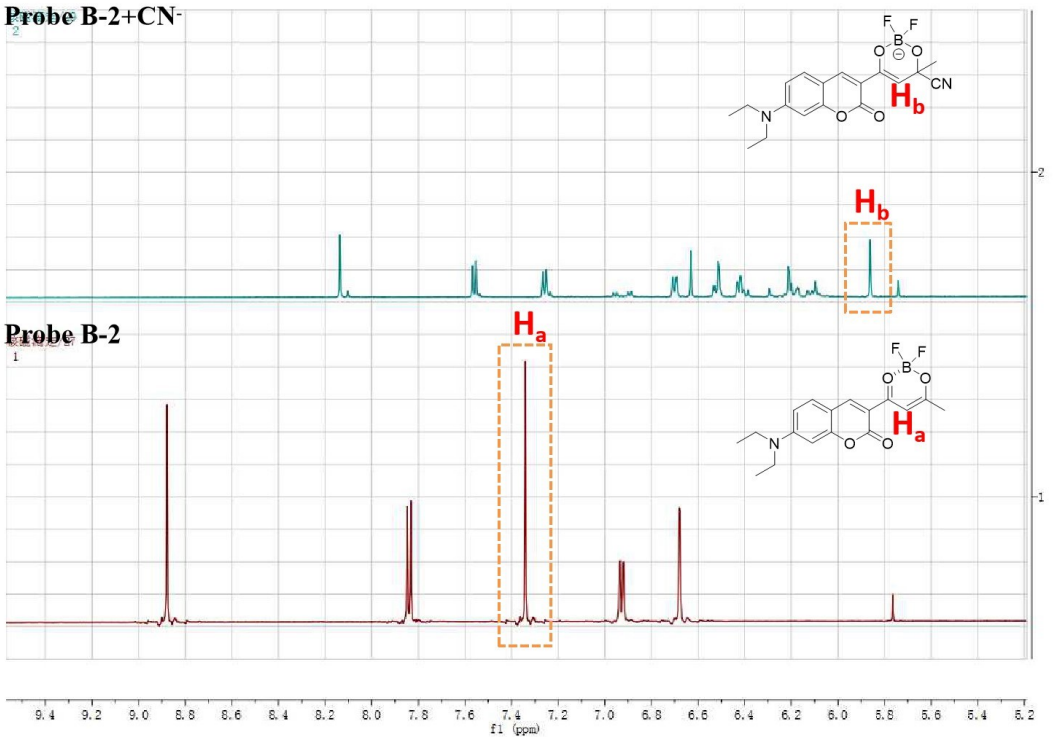


Fig. S4 ^1H NMR spectra of **B-2** in $CDCl_3$ and after addition of 2.0 eq. CN^- in $CDCl_3$.

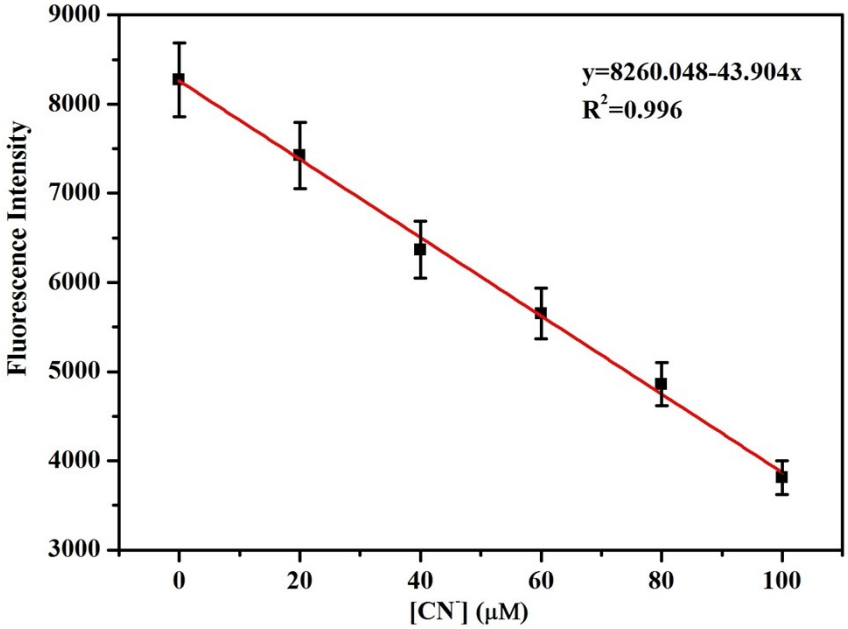
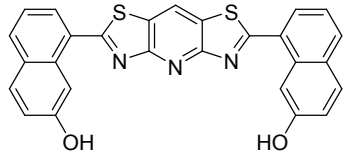
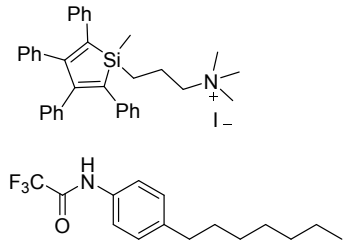
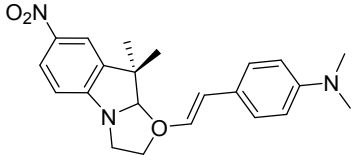
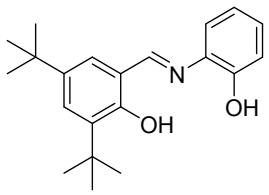
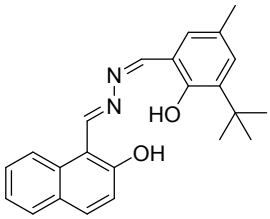
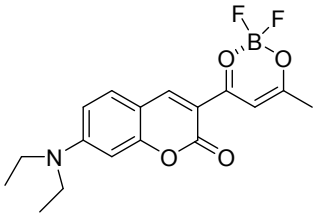


Fig. S5 The Plot of fluorescence intensity as a function of the concentrations of CN^-.

Table S1. Summarize the reported fluorescent probes for detecting CN^-.

Probes	Distinguishing targets for detection	λem (nm)	detection limit (μM)	Ref.
	Ag^+ CN^-	515	0.24	8
	CN^-	476	7.74	18
	CN^-	564	0.4	26

	CN^-	476	0.59	33
	CN^-	557	0.81	37
	CN^-	560	0.072	This work

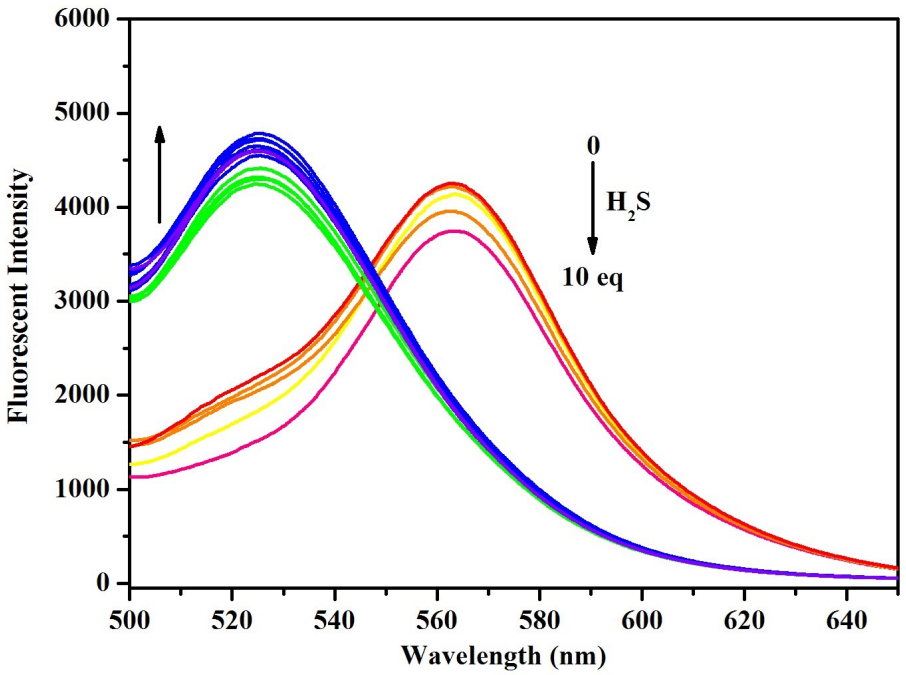


Fig. S6 Fluorescence spectra of **B-2** (10.0 μM) in the presence of various concentrations of H_2S in PBS-DMSO (3/2, v/v, PH 7.4) (λ_{ex}=480 nm, slit width: 5 nm/2 nm).

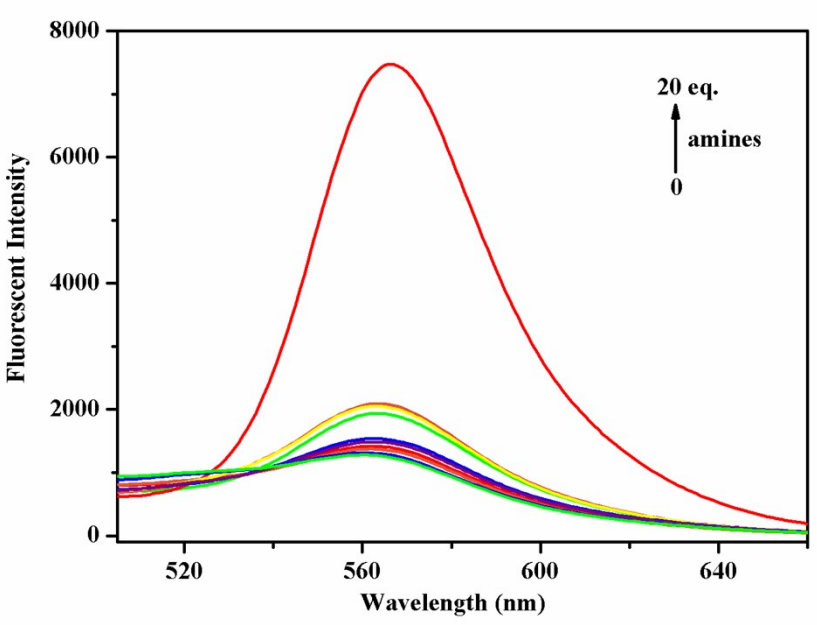


Fig. S7 Fluorescence spectra of **B-2** (10.0 μM) in the presence of various concentrations of amines in PBS-DMSO (3/2, v/v, PH 7.4) (λ_{ex}=480 nm, slit width: 5 nm/2 nm).

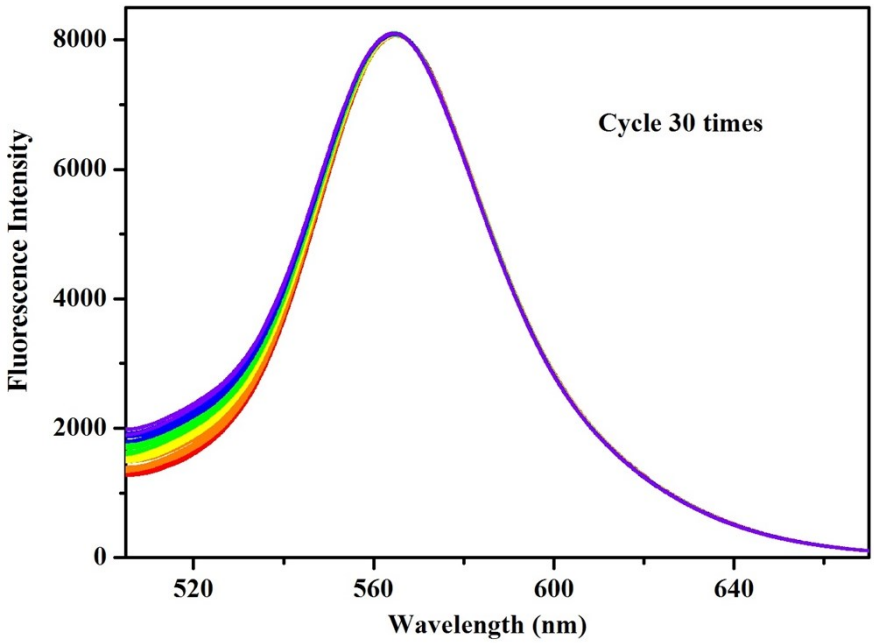


Fig. S8 Fluorescence spectra of **B-2** (10.0 μM) was cycled 30 times in PBS-DMSO (3/2, v/v, PH 7.4) (λ_{ex}=480 nm, slit width: 5 nm/2 nm).