Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

A novel colorimetric and ratiometric fluorescent probe for sensing SO_2 derivatives and its bio-imaging in living cells

Tingting Niu[a,1], Ting Yu[b,1], Guoxing Yin[b], Haimin Chen*[a], Peng Yin*[b] and Haitao Li[b]

[a]*Key Laboratory of Marine Biotechnology of Zhejiang Province, Ningbo University, Ningbo, Zhejiang 315211, China*

[b]*Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research (Ministry of Education), Key Laboratory of the Assembly and Application of Organic Functional Molecules of Hunan Province, Hunan Normal University, Changsha 410081, China.*

* Corresponding author. Tel.: (+86) 73188865515; fax: (+86) 73188872531.

E-mail: chenhaimin@nbu.edu.cn; yinpeng@hunnu.edu.cn;

[1] T. Niu and T. Yu contributed equally to this work.

Calculation of the detection limit (LOD)

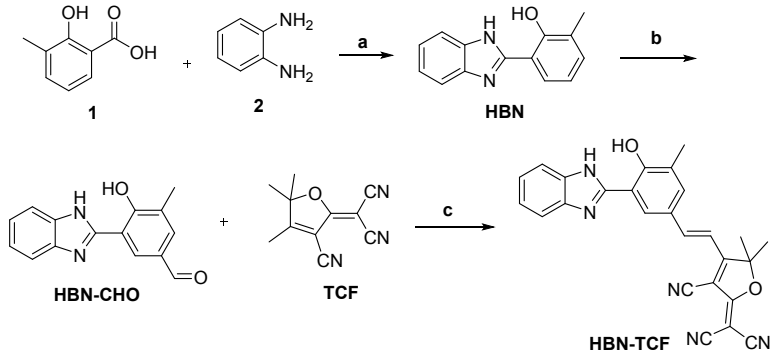
$$LOD = K \times Sb_1/S$$

$$Sb_1 = \sqrt{\frac{\sum(\bar{x} - x_i)^2}{n-1}}$$

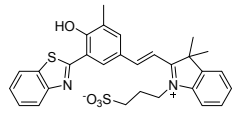
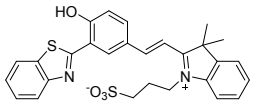
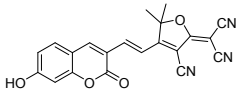
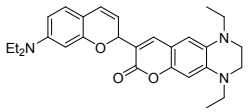
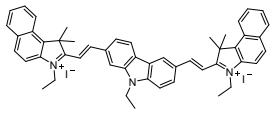
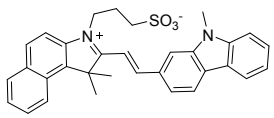
K=2 or 3

Sb_1: the standard deviation of the blank solution.

S: the slope of the linear calibration plot between the fluorescence emission intensity and the concentration of Na_2SO_3



Scheme S1. Synthetic scheme for probe **HBN-TCF**.

Probes	Emission Wavelength/nm	Emission distance/nm	Limit/nM	Ref.
	**485/610**	**125**	**56**	[1]
	**450/590**	**140**	**340**	[2]
	**523/663**	**140**	**0.27**	[3]
	**585**	**-**	**8.3**	[4]
	**465/600**	**135**	**25**	[5]
	**463/625**	**162**	**58**	[6]

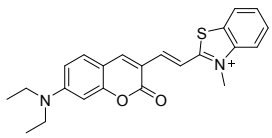
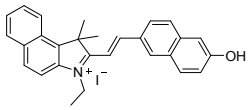
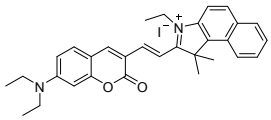
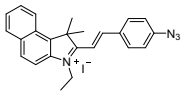
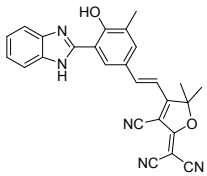
	**478/633**	**155**	**380**	[7]
	**467/593**	**126**	**3.6**	[8]
	**560/650**	**90**	**2.67**	[9]
	**467/580**	**113**	**27.6**	[10]
	**482/664**	**182**	**82**	**This Work**

Table S1. Comparison of different fluorescent probes for SO_2 derivatives.

Absorbption and fluorescence spectra

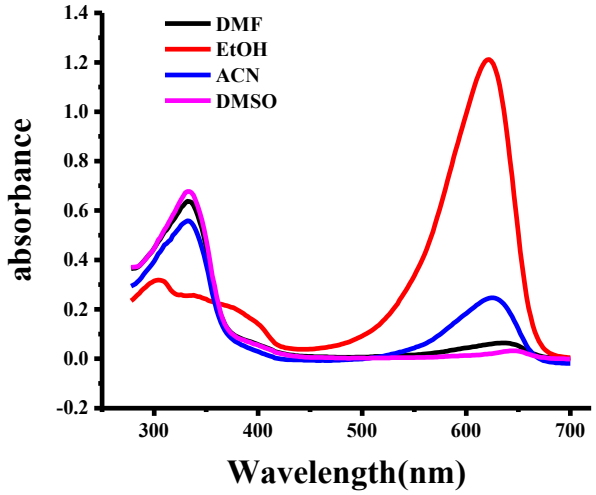


Fig. S1 Absorption spectra of probe HBN-TCF (10 μM) in presence of 10 equiv. of SO_3^{2-} in different solvents.

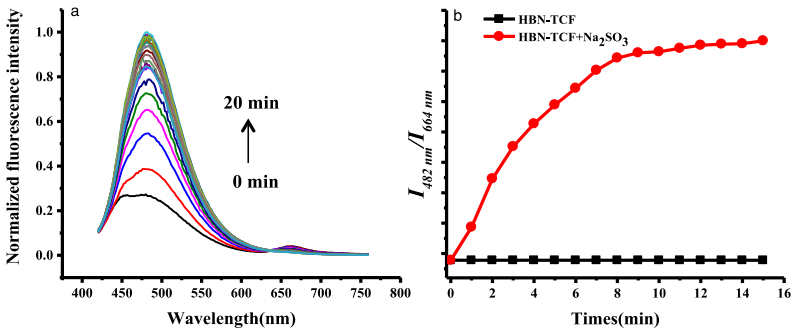


Fig. S2 (a) The time-dependence normalized fluorescence intensity spectrum of probe HBN-TCF (10 μM) towards to Na_2SO_3 (0.1 mM) in DMF-PBS (10 mM, pH = 7.4, v/v, 5:5). λ_{Ex} = 400 nm, λ_{Em} = 482 nm. Slit: 10.0 nm/10.0 nm. (b) The plot of normalized fluorescence intensity of probe HBN-TCF as a function of time.

Selectivity and interference

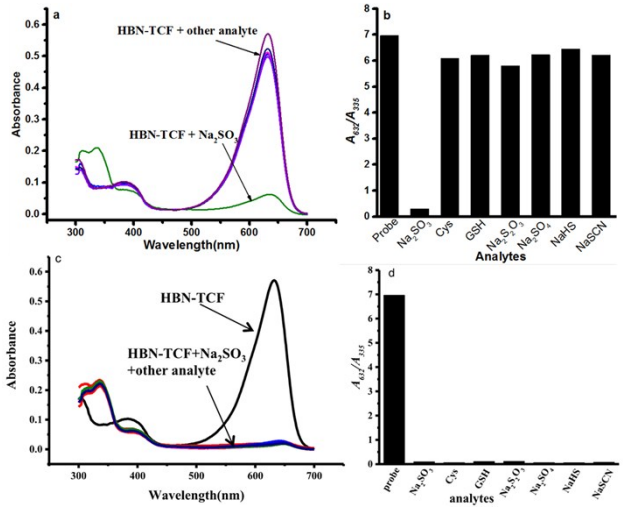


Fig. S3 Absorption spectra of (a) probe HBN-TCF (10 μM) and (c) probe HBN-TCF (10 μM) with Na_2SO_3 (0.1 mM) in the presence of 0.1 mM of different sulfur-containing analytes including SO_4^{2-}, SCN^-, $S_2O_3^-$, HS^-, Cys, GSH in DMF-PBS buffer(10 mM, pH 7.4, v/v, 5:5). (b) and (d) are the histogram representing the ratio changes of absorbance at 335 nm and 632 nm of (a) and (c), respectively.

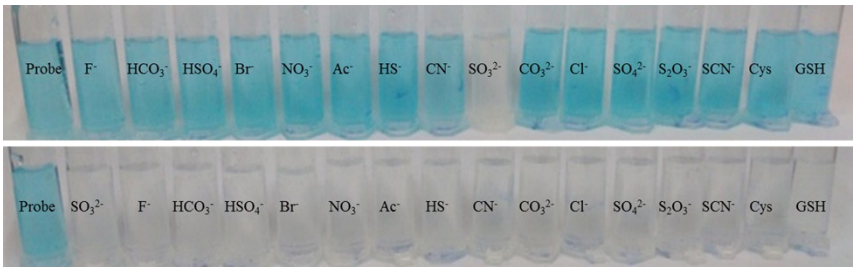


Figure S4. The top row is the photograph of probe HBN-TCF (10 μM) in the presence of various anions (10.0 equiv.). The down row is the photograph of probe HBN-TCF (10 μM) in the presence of 10.0 equiv. of Na_2SO_3 upon the addition of other sodium salts. From left to right, (10 equiv.) of probe HBN-TCF alone, F^-, HCO_3^-, HSO_4^-, Br^-, NO_3^-, Ac^-, HS^-, CN^-, CO_3^{2-}, Cl^-, SO_4^{2-}, $S_2O_3^{2-}$, SCN^-, Cys and GSH in DMF-PBS buffer (10 mM, pH 7.4, v/v, 5:5).

Cytotoxicity of HBN-TCF

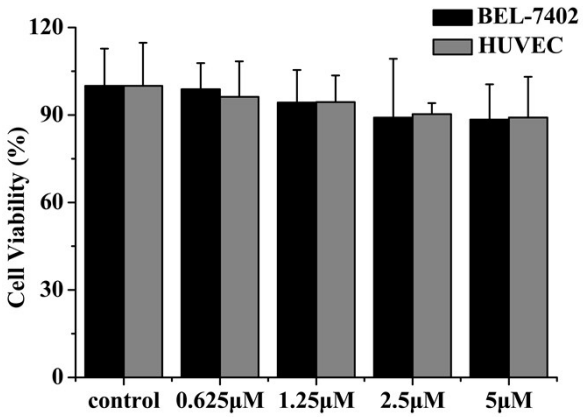


Fig. S5 MTT assay for the survival rate of BEL-7402 and HUVEC cells treated with various concentrations of probe HBN-TCF for 24 h.

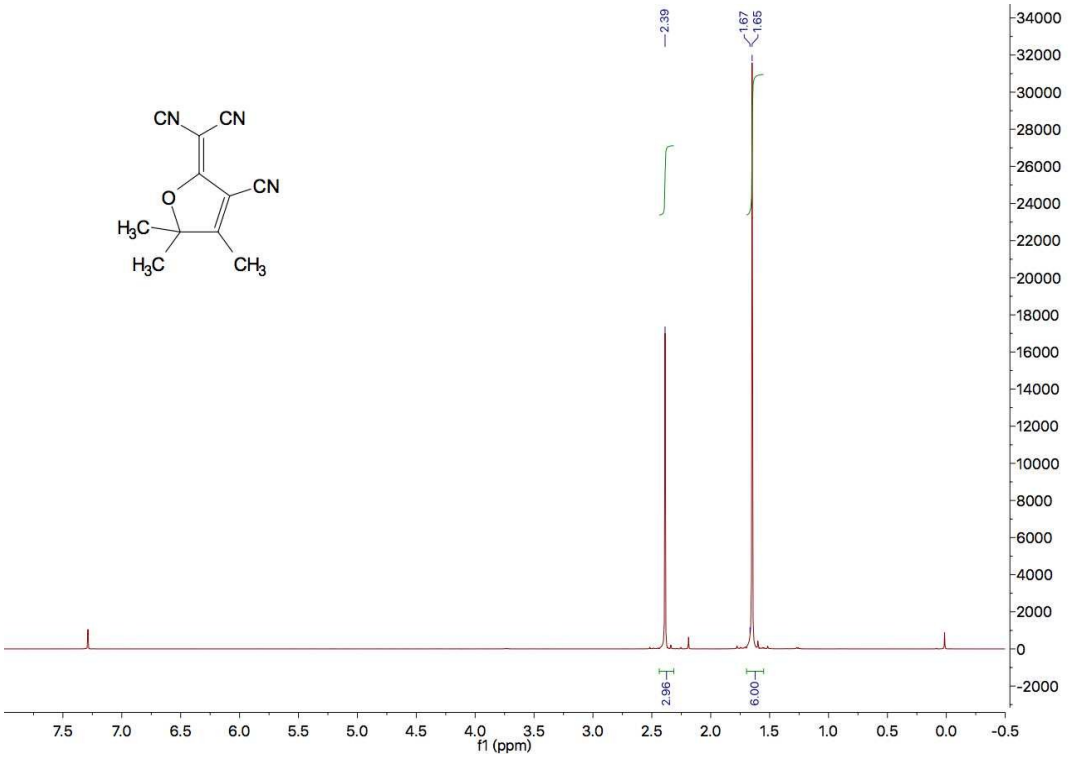


Fig. S6 ^{1}H NMR spectrum of compound **TCF** in $CDCl_3$.

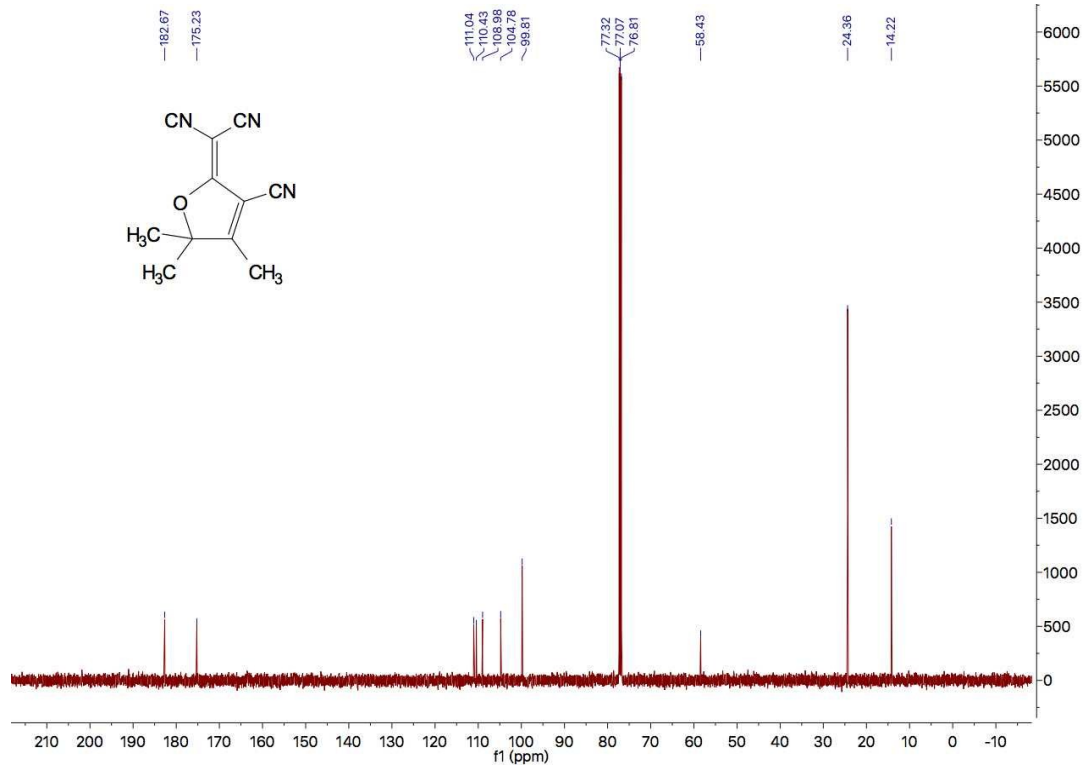


Fig. S7 ^{13}C NMR spectrum of compound **TCF** in $CDCl_3$.

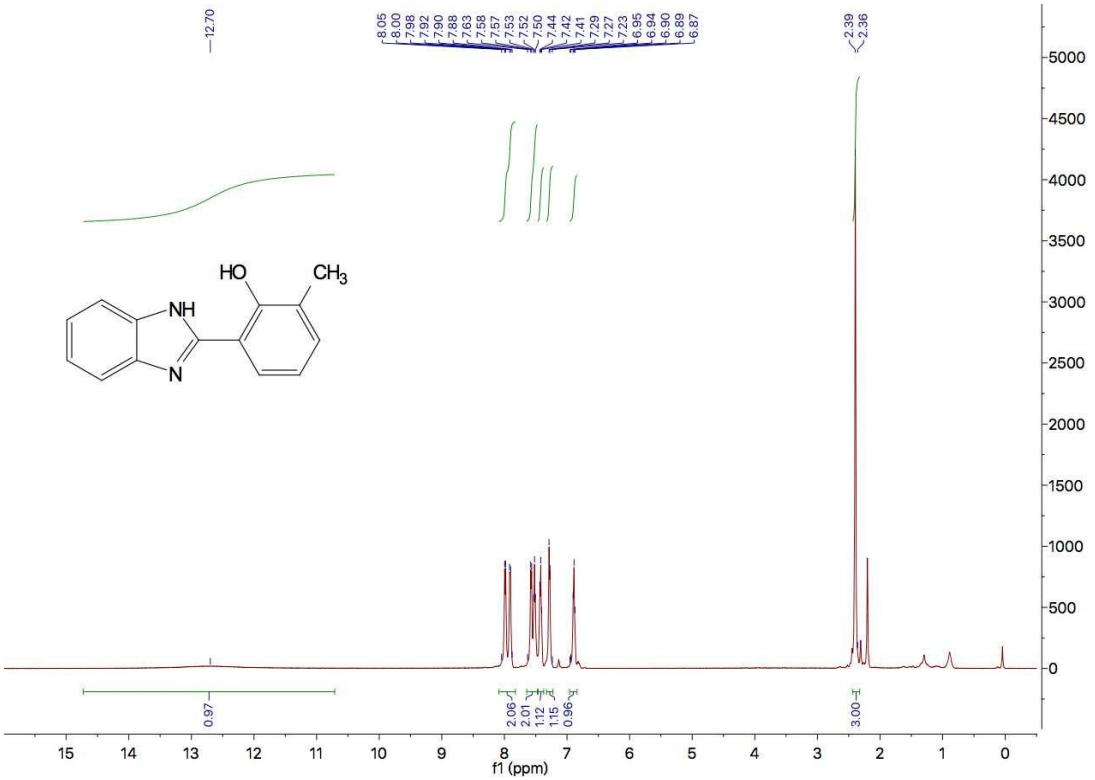


Fig. S8 ^{1}H NMR spectrum of compound **HBN** in $CDCl_3$.

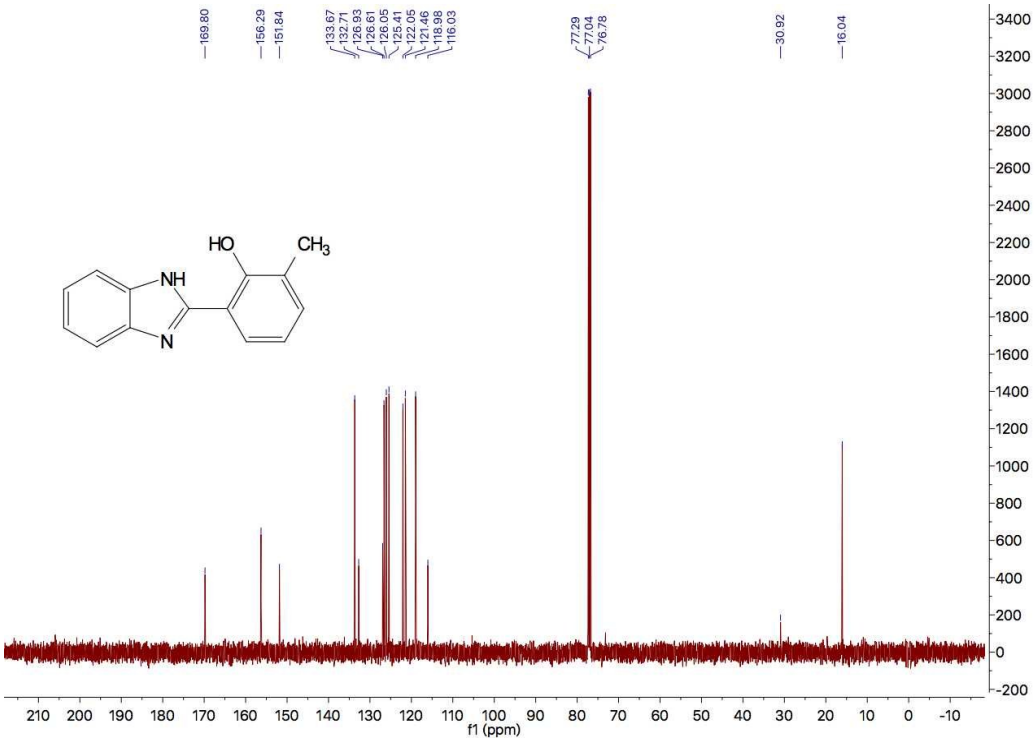


Fig. S9 ^{13}C NMR spectrum of compound **HBN** in $CDCl_3$.

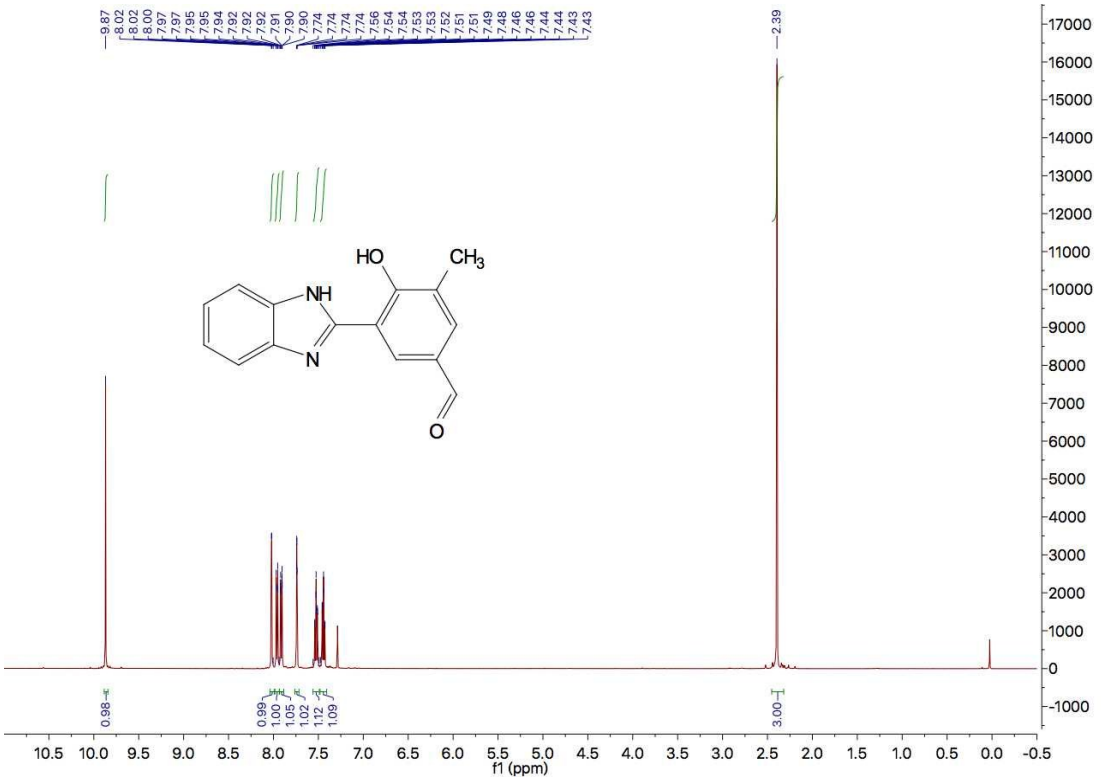


Fig. S10 ^{1}H NMR spectrum of compound **HBN-CHO** in $CDCl_3$.

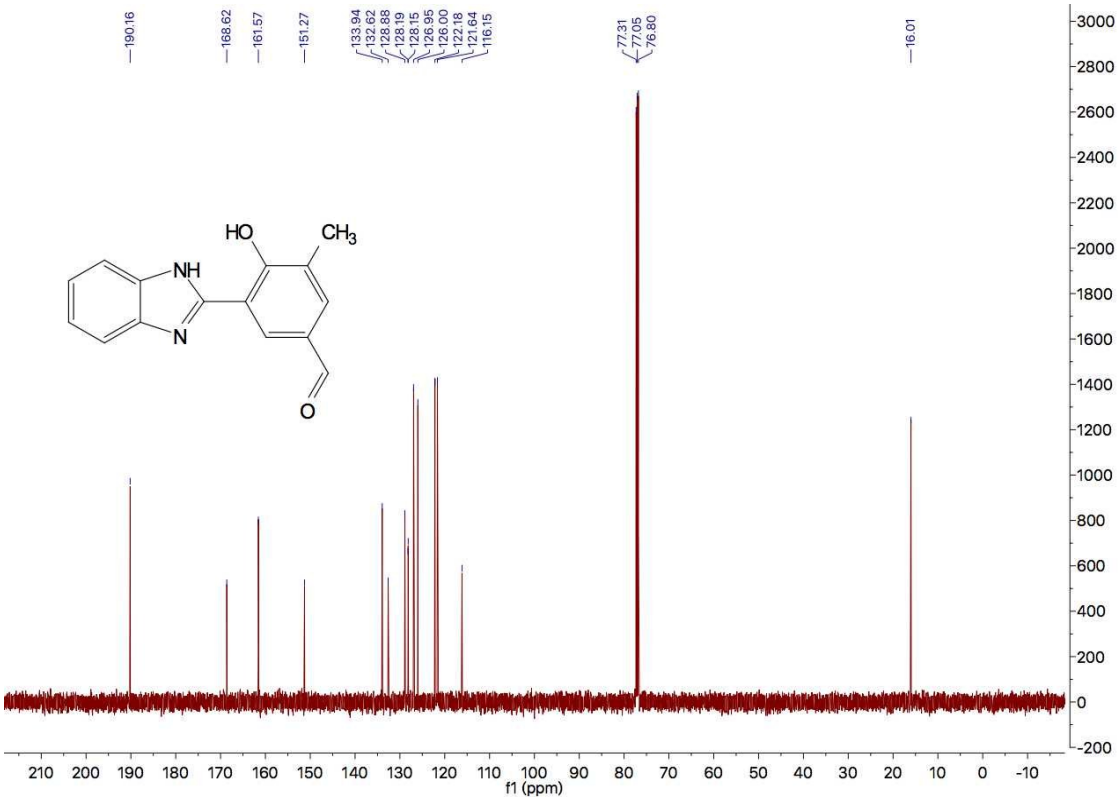


Fig. S11 ^{13}C NMR spectrum of compound **HBN-CHO** in $CDCl_3$.

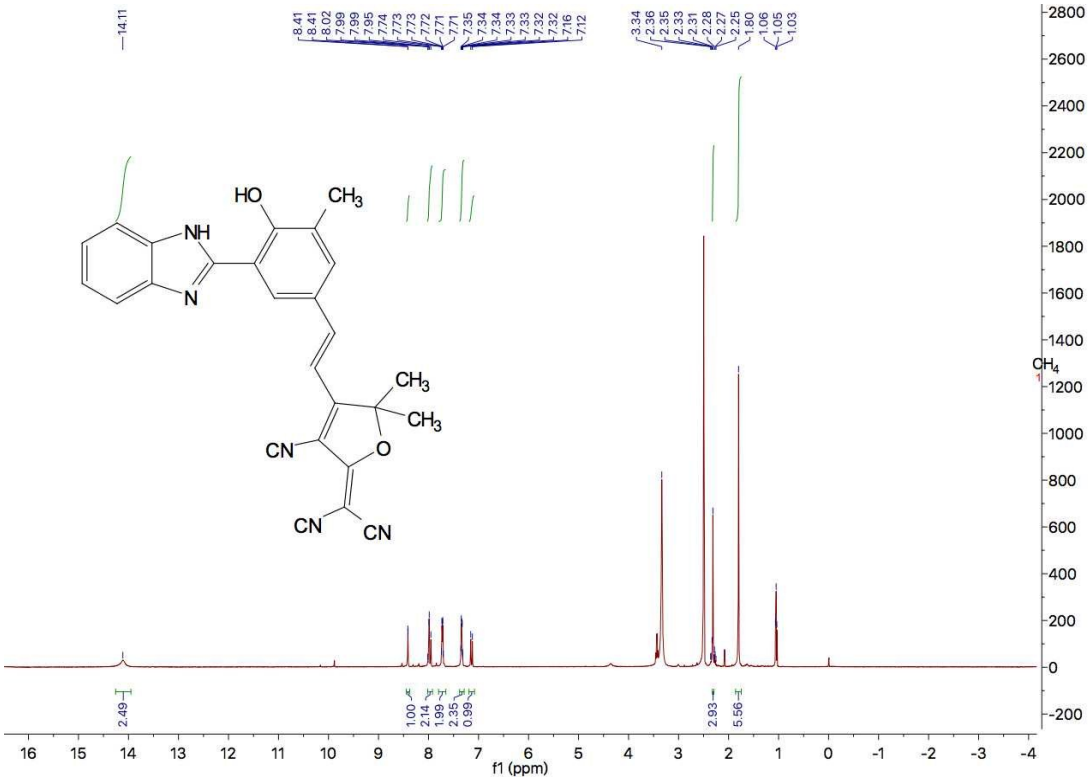


Fig. S12 [1]H NMR spectrum of probe **HBN-TCF** in DMSO-d_6.

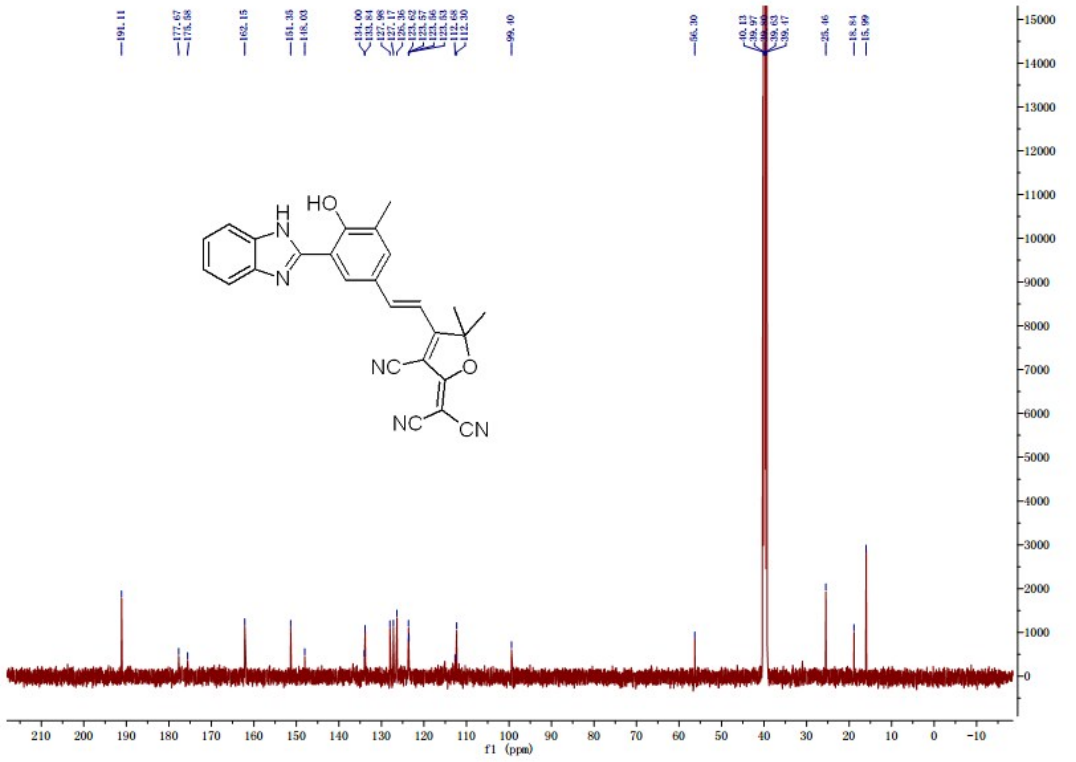


Fig. S13 [13]C NMR spectrum of probe **HBN-TCF** in DMSO-d_6.

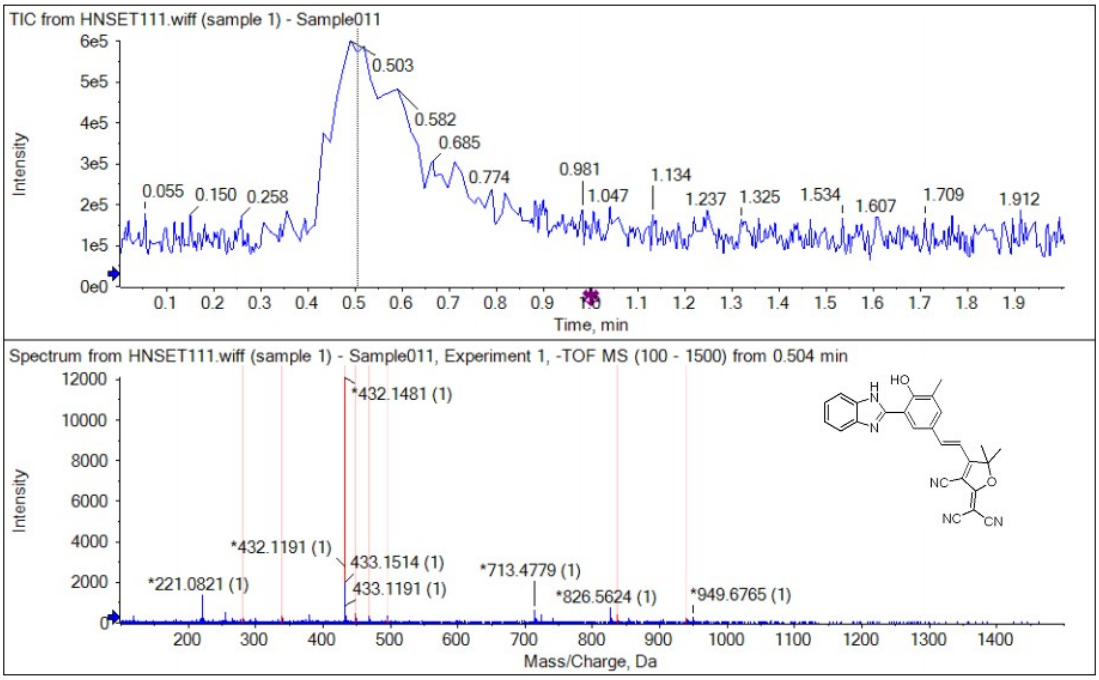


Fig. S14 HRMS spectrum of probe **HBN-TCF**.

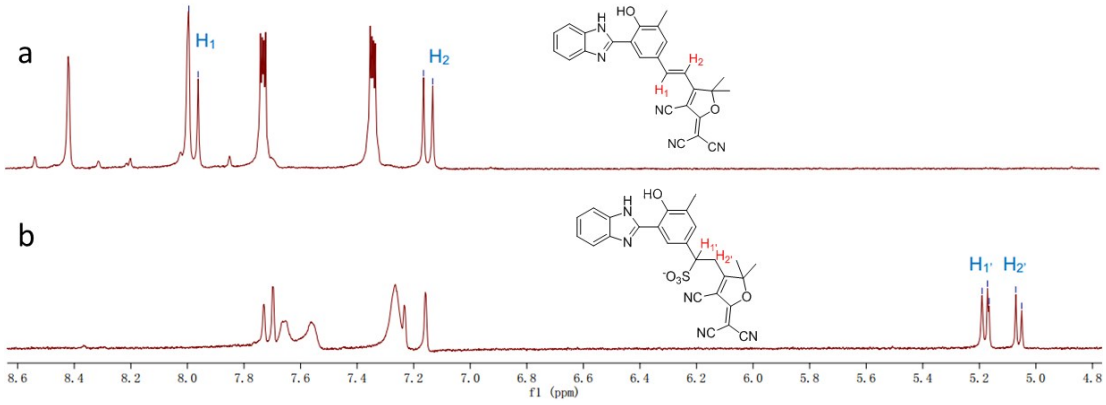


Fig. S15 (a) ^{1}H NMR spectrum of probe **HBN-TCF** in DMSO-d_6. (b) ^{1}H NMR spectrum of probe **HBN-TCF** with 5 equiv. of Na_2SO_3 in DMSO-d_6 and D_2O.

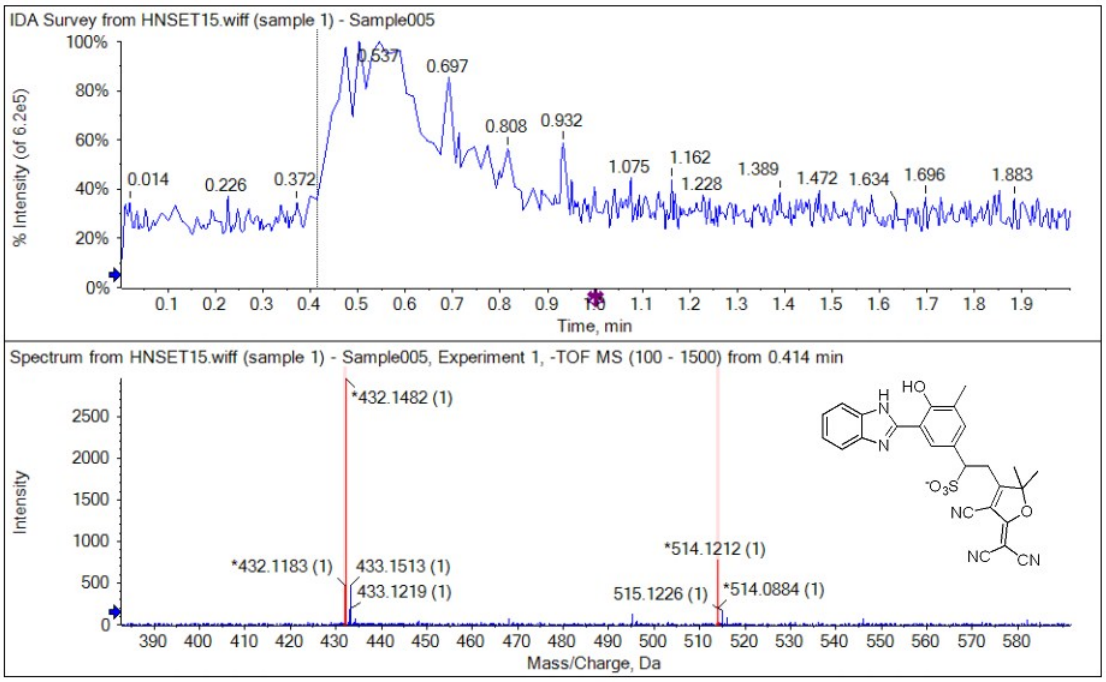


Fig. S16 HRMS spectrum of the reaction mixture of probe **HBN-TCF** with Na_2SO_3.

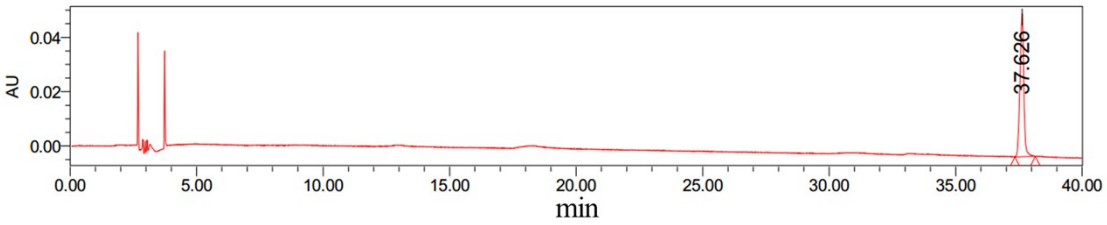


Fig. S17 HPLC chromatogram of probe HBN-TCF.

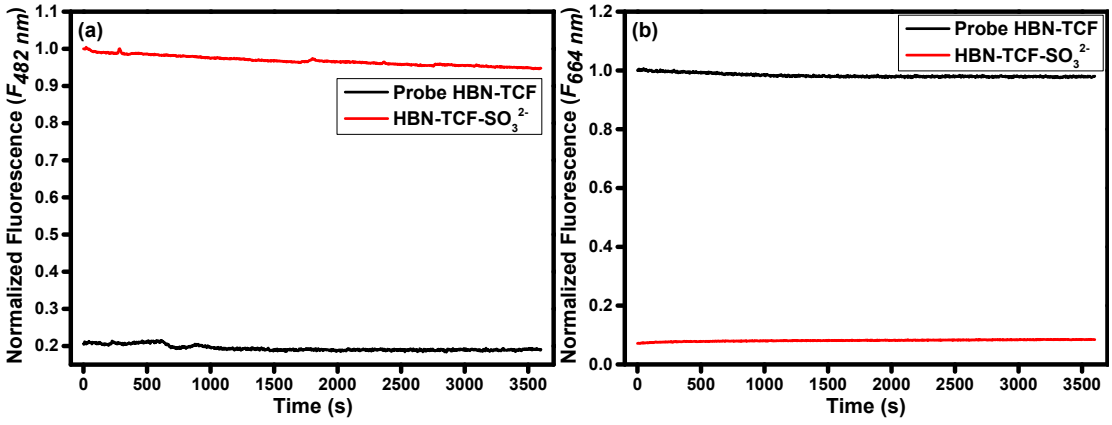


Fig. S18 Time-dependent fluorescence intensity changes at (a) 482 nm and (b) 664 nm for Probe HBN-TCF and HBN-TCF-SO_3^{2-} (10.0 μM) at room temperature for 1 h, respectively. Conditions: DMF - PBS (pH 7.4, 10 mM, v/v, 5/5), λ_{ex} = 400 nm, slit (nm): 2.5/5.

References

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