Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

Colorimetric and near infrared fluorescent detection of cyanide by a new phenanthroimidazole–indolium conjugated probe

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1. Determination of the fluorescence quantum yield

The fluorescence quantum yields of probe **1** (Φ = 0.014) and **1-CN** adduct (Φ = 0.034) were determined in Tris·HCl buffer (10 mM, pH = 9.3, containing 50% MeOH, v/v) at 25°C, using quinine sulfate (Φ_f = 0.58 in 1N H_2SO_4) as standard. The quantum yield was calculated using the following equation:

$$\Phi_x = \Phi_s(A_s F_x / A_x F_s)(n_x^2/n_s^2)$$

where, A_x and A_s are the absorbance of the sample and the reference, respectively, at the same excitation wavelength, F_x and F_s are the corresponding relative integrated fluorescence intensities, and n is the refractive index of the solvent.

2. Additional data for sensing cyanide by probe 1

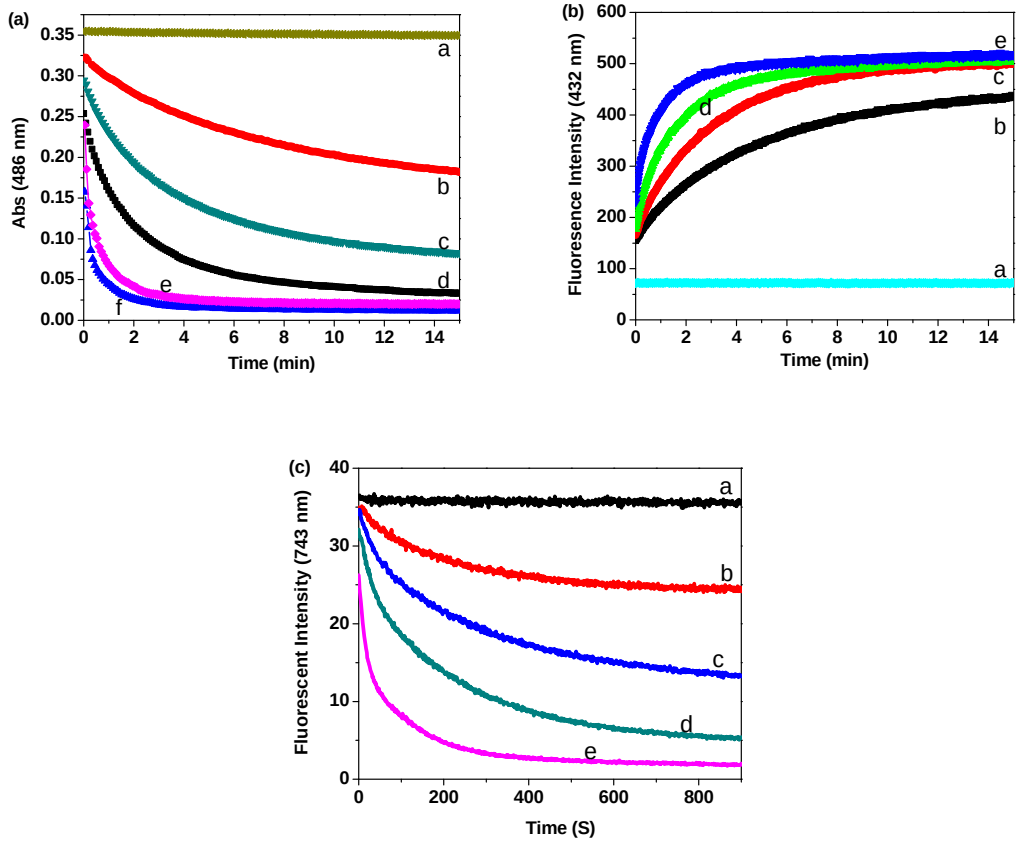


Fig. S1 (a) UV-vis kinetics of probe **1** (20 μM) monitored at 486 nm with different concentration of CN^- (a. 0 μM, b. 10 μM, c. 20 μM, d. 40 μM, e. 100 μM, f. 200 μM). (b) Fluorescent kinetics of probe **1** (20 μM) monitored at 432 nm (λ_{ex}: 380 nm) with different concentration of CN^- (a. 0 μM, b. 20 μM, c. 40 μM, d. 100 μM, e. 200 μM). (c) Fluorescent kinetics of probe **1** (20 μM) monitored at 743 nm (λ_{ex}: 480 nm) with different concentration of CN^- (a. 0 μM, b. 10 μM, c. 20 μM, d. 40 μM, e. 100 μM). All reactions were investigated in MeOH–Tris·HCl buffer (10 mM, pH = 9.3, 1 : 1, v/v) at 25 °C.

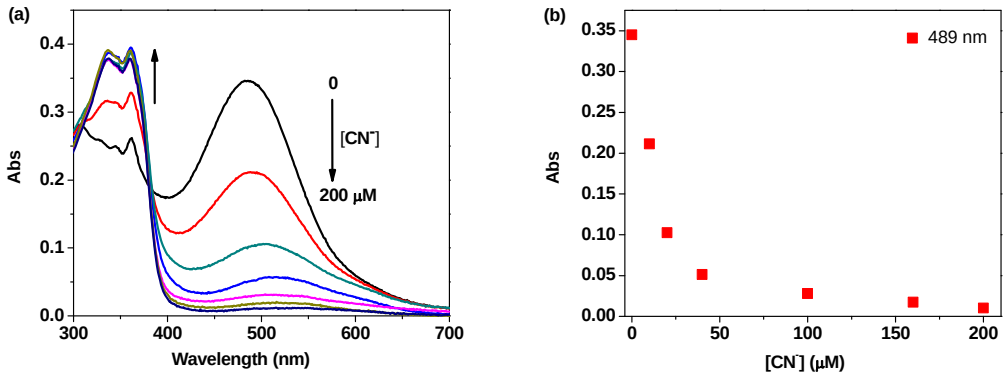


Fig. S2 (a) UV-vis spectra of probe **1** (20 μM) upon addition of 0, 10, 20, 40, 100, 160, 200 μM CN^- in MeOH–Tris·HCl buffer (10 mM, pH = 9.3, 1 : 1, v/v) at 25°C. (b) The absorbance intensity changes of probe **1** at 489 nm as a function of CN^- concentrations. Each spectrum were recorded 10 min after the addition of CN^-.

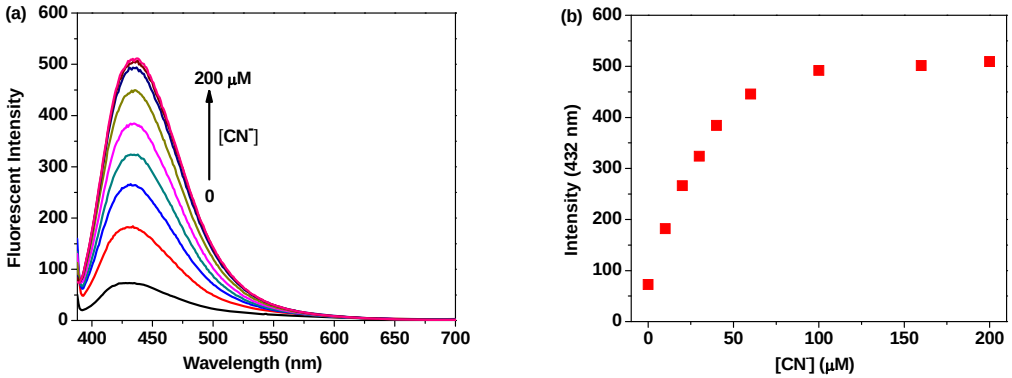


Fig. S3 (a) Fluorescence spectra changes of probe **1** (20 μM) upon addition of 0, 10, 20, 30, 40, 60, 100, 160, 200 μM of CN^- in MeOH–Tris·HCl buffer (10 mM, pH = 9.3, 1 : 1, v/v) at 25 °C. (b) Fluorescence intensity changes of probe **1** at 432 nm against [CN^-] from 0-200 μM. Spectra data were recorded 10 min after the addition of CN^- with λ_{ex} = 380 nm, d_{ex} = 5 nm, d_{em} = 10 nm.

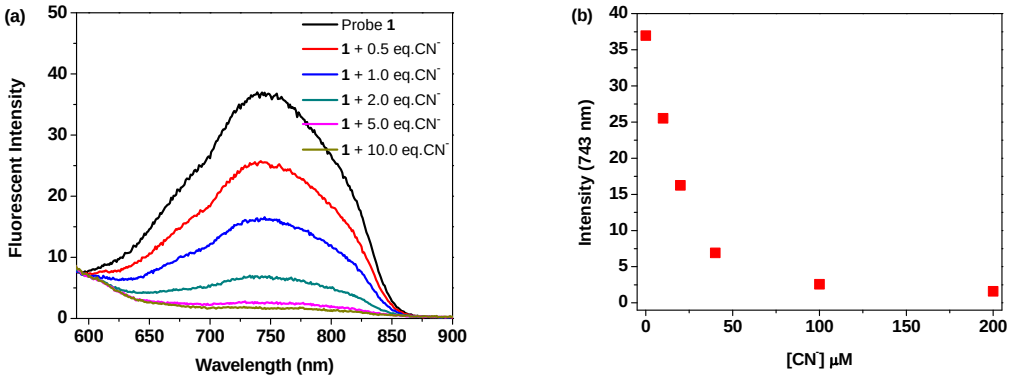


Fig. S4 (a) Fluorescence spectra changes of probe **1** (20 μM) upon addition of 0, 10, 20, 40, 100,

200 μM CN^- in MeOH–Tris·HCl buffer (10 mM, pH = 9.3, 1 : 1, v/v) at 25 °C. (b) Fluorescence intensity changes of probe **1** at 743 nm against [CN^-] from 0-200 μM. Spectra data were recorded 10 min after the addition of CN^- with λ_{ex} = 480 nm, d_{ex} = 10 nm, d_{em} = 10 nm.

Fig. S5 (a) Color changes and (b) fluorescence color changes under a 365 nm UV light of probe **1** (20 μM) with 100 μM of different anions (from left to right: none, CN^-, S^{2-}, Cys, F^-, I^-, SCN^-, SO_4^{2-}, NO_3^-, HSO_4^-, N_3^-, Cl^-, NO_2^-, Br^-, N_3^-, $H_2PO_4^-$, HCO_3^-, PO_4^{3-}, CO_3^{2-} and ClO_4^- MeOH–Tris·HCl buffer (10 mM, pH = 9.3, 1 : 1, v/v) at room temperature.

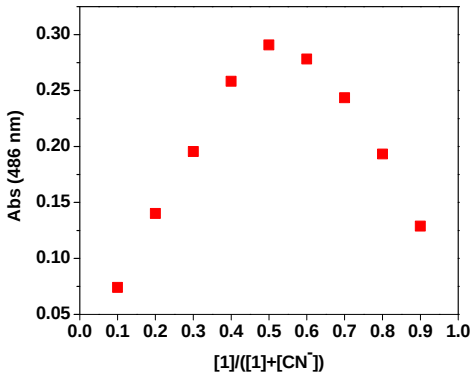
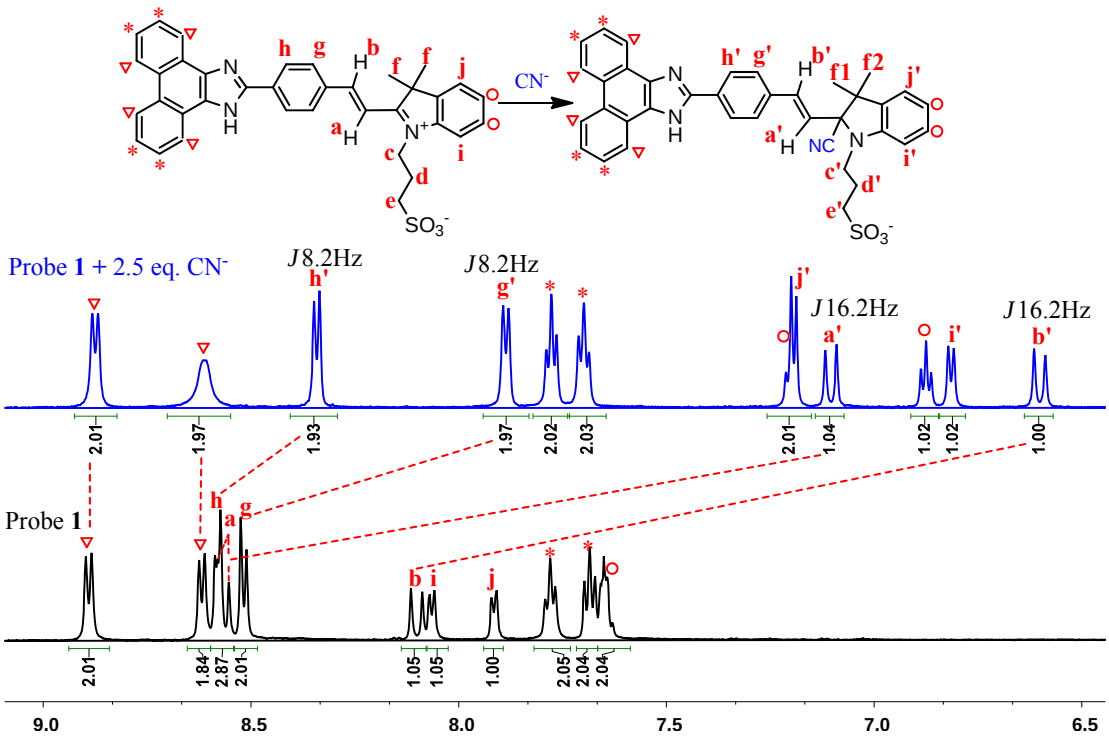
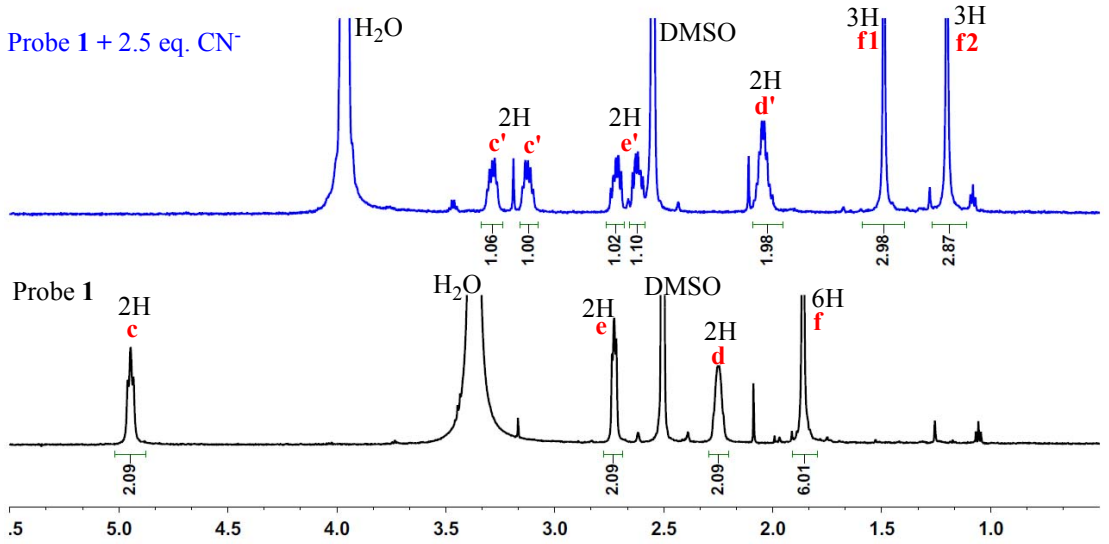


Fig. S6 Job's plot examined between probe **1** and CN^-. Total concentration of **1** + CN^- was kept constant at 50 μM.

3. Enlarged ^{1}H NMR spectra changes of probe 1 with addition of CN^-



(1) Aromatic protons signal change of probe **1** with addition of CN^-



(2) Aliphatic protons signal change of probe **1** with addition of CN^-

Fig S7. Enlarged ^{1}H NMR (600 MHz) spectra changes of probe **1** with addition of CN^-.

4. Structure characterizations for the isolated 1-CN adduct

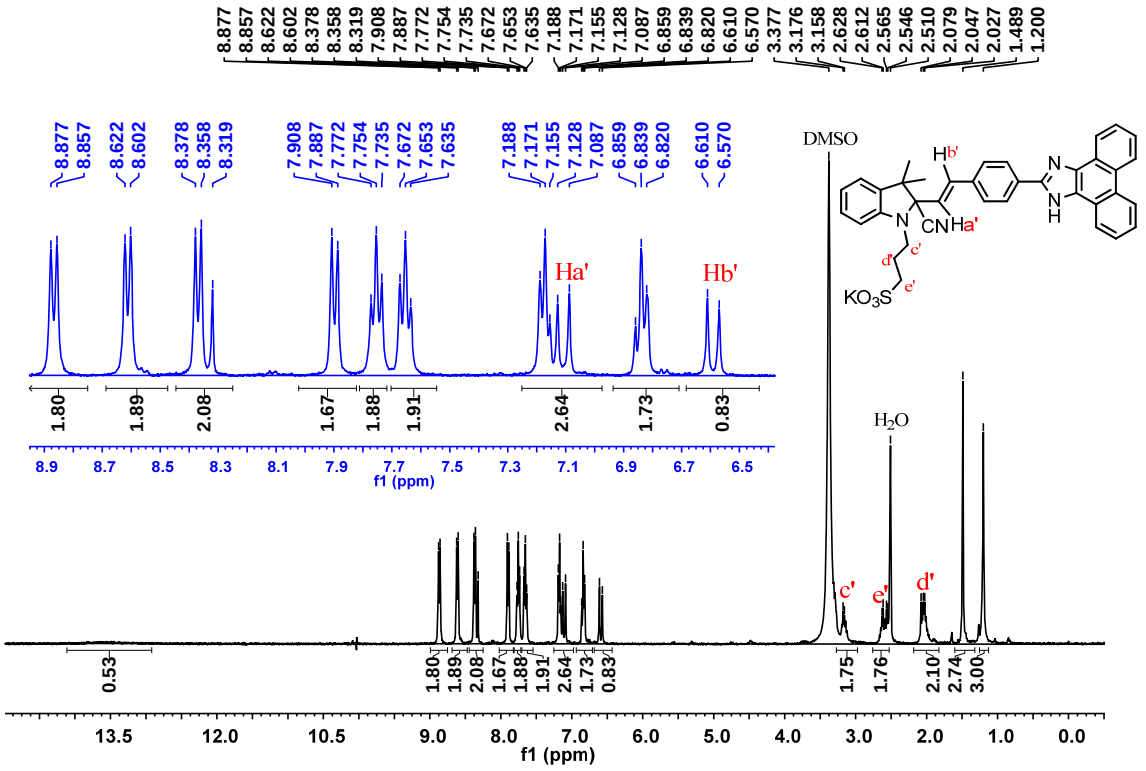


Fig. S8 ^{1}H NMR spectrum of the isolated probe **1**-CN adduct in DMSO-d_6 (400 MHz)

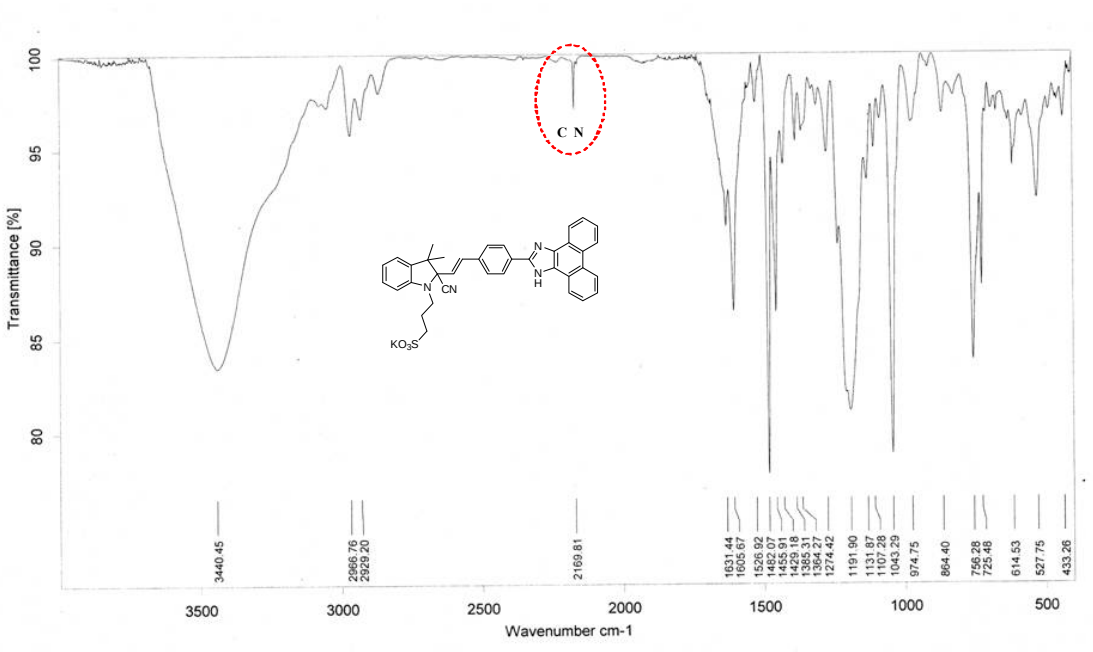


Fig. S9 IR spectrum of the probe **1**-CN adduct

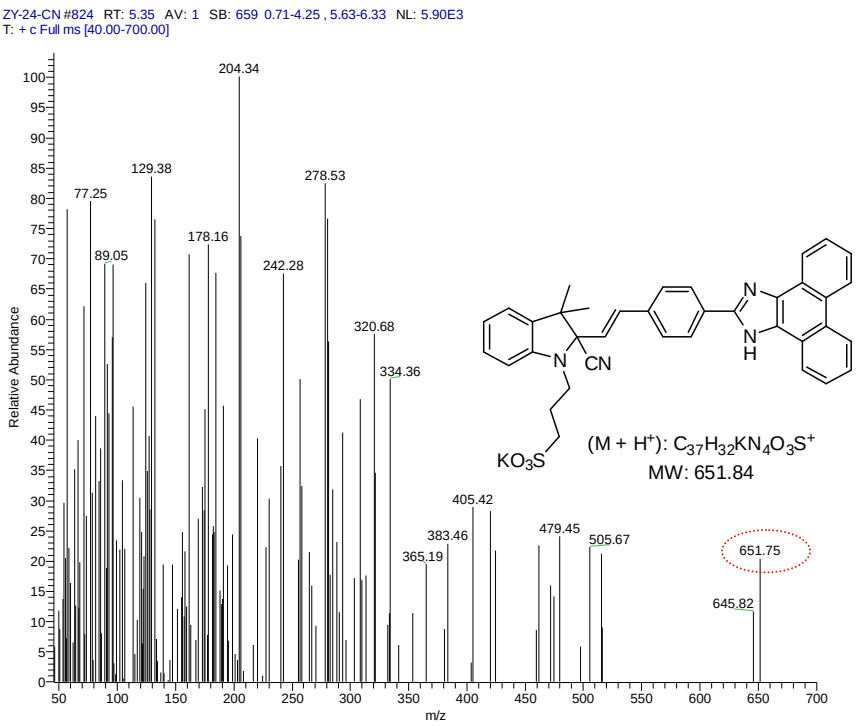


Fig. S10 EI-MS of **1**-CN adduct.

5. Structure characterizations for probe 1

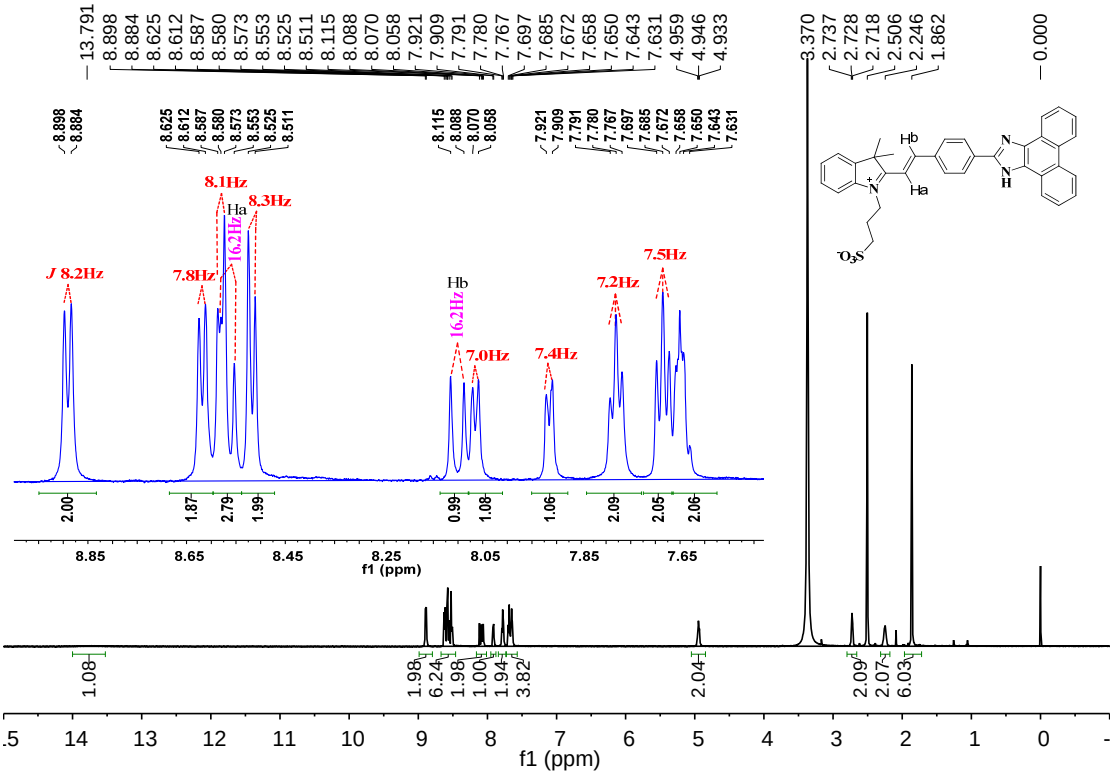


Fig. S11 ^{1}H NMR spectrum of probe **1** in DMSO-d_6 (600 MHz);

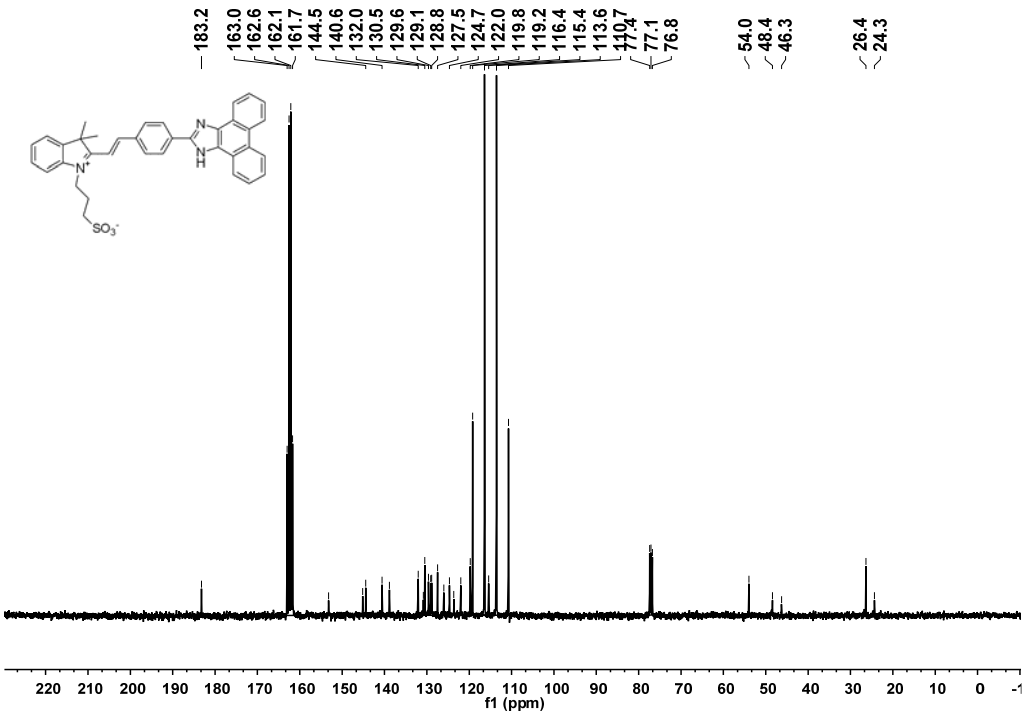


Fig. S12 ^{13}C NMR spectrum of probe **1** in a mixture of CF_3COOD and $CDCl_3$

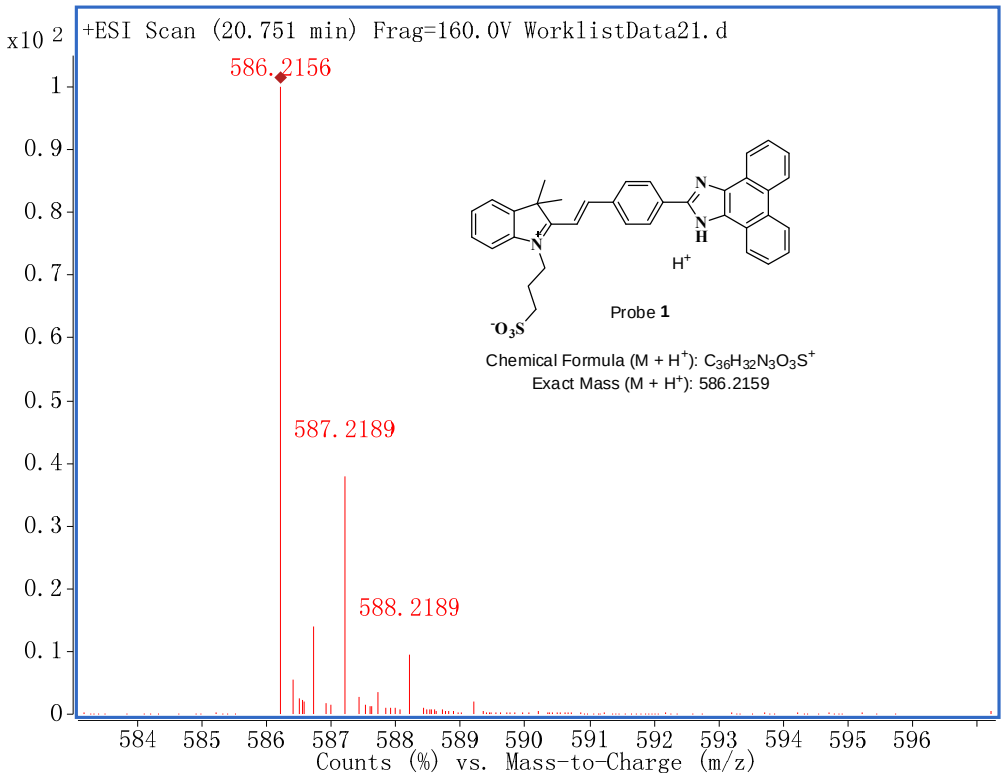


Fig. S13 HR-MS spectrum of probe **1**

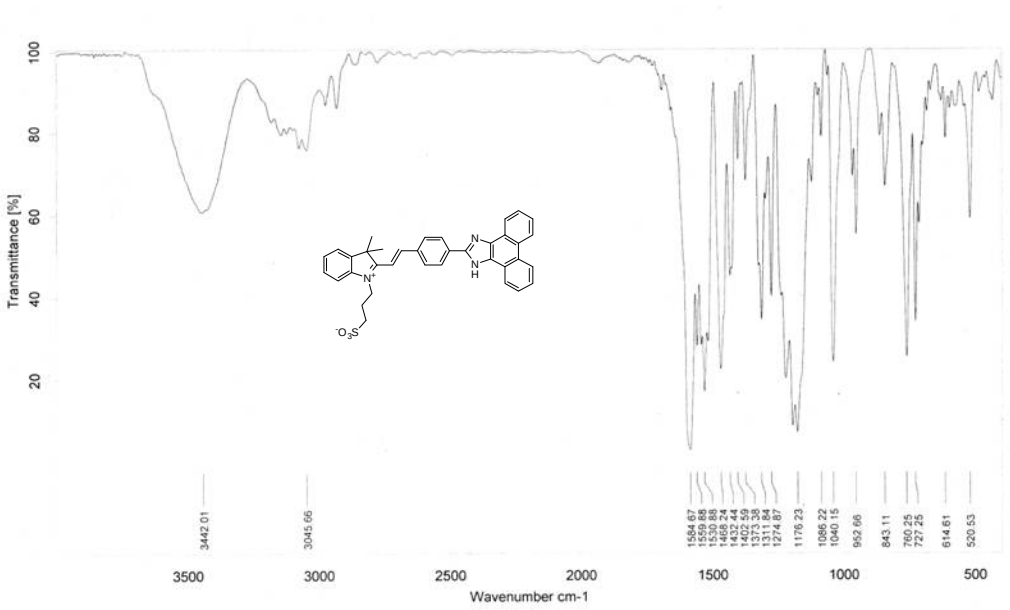


Fig. S14 IR spectrum of probe **1**