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 (Φr = 0.58 in 1N H2SO4) as standard. The quantum yield was calculated using the following equation:

\[
Φ_x = Φ_s \left( \frac{A_x F_x}{A_s F_s} \right) \left( \frac{n_s^2}{n_x^2} \right)
\]

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

![Graphs showing UV-vis and fluorescent kinetics](Fig. S1)

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 \mu M \text{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 \([\text{CN}^-]\) from 0-200 \mu M. Spectra data were recorded 10 min after the addition of \text{CN}^- with \lambda_{ex} = 480 nm, \text{d}_{ex} = 10 nm, \text{d}_{em} = 10 nm.

Fig. S5 (a) Color changes and (b) fluorescence color changes under a 365 nm UV light of probe 1 (20 \mu M) with 100 \mu M of different anions (from left to right: none, \text{CN}^-, \text{S}^{2-}, \text{Cys}, \text{F}^-, \Gamma, \text{SCN}^-, \text{SO}_4^{2-}, \text{NO}_2^-, \text{HSO}_4^-, \text{N}_3^-, \text{Cl}^-, \text{NO}_3^-, \text{Br}^-, \text{N}_3^-, \text{H}_2\text{PO}_4^-, \text{HCO}_3^-, \text{PO}_4^{3-}, \text{CO}_3^{2-} \text{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 \text{CN}^-\). Total concentration of 1 + \text{CN}^- was kept constant at 50 \mu M.
3. Enlarged $^1$H NMR spectra changes of probe 1 with addition of CN$^-$

![Diagram of molecular structure and NMR spectra changes](image)

(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 1-CN adduct in DMSO-d$_6$ (400 MHz)

Fig. S9 IR spectrum of the probe 1-CN adduct
5. Structure characterizations for probe 1

![EI-MS of 1-CN adduct](image)

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

![1H NMR spectrum of probe 1](image)

**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$_3$COOD and CDCl$_3$

Fig. S13 HR-MS spectrum of probe 1
Fig. S14 IR spectrum of probe 1