

Fluorescence light-up detection of cyanide in water based on cyclization reaction followed by ESIPT and AIEE

Chunshuang Liang and Shimei Jiang

Fig. S1 Time-dependent absorption spectra changes of **1** (50 μM , DMSO) in the presence of 100 equiv. of cyanide. The arrows indicate the changes over time. Inset: the time-dependent changes of absorbance at 332 nm and 455 nm.

Fig. S2 Time-dependent fluorescence ($\lambda_{\text{ex}} = 398 \text{ nm}$) spectra changes of **1** (50 μM , DMSO) in the presence of 100 equiv. of cyanide. The arrow indicates the changes over time. Inset: the time-dependent changes of emission intensity at 476 nm.

Fig. S3. (a) Absorption spectra and (b) colorimetric responses of **1** (50 μM) before and after addition of various anions (100 equiv.) in DMSO. The spectra and pictures were obtained immediately.

Fig. S4. (a) Fluorescence spectra ($\lambda_{\text{ex}} = 398 \text{ nm}$) and (b) fluorimetric (excitation at 365 nm) responses of **1** (50 μM) before and after addition of various anions (100 equiv.) in DMSO. The spectra were obtained after 120 min.

Fig. S5. The (a) absorption and (b) fluorescence intensity ($\lambda_{\text{ex}} = 398 \text{ nm}$) changes of **1** (50 μM) in the presence of 100 equiv. of CN^- at 25 $^\circ\text{C}$, 50 $^\circ\text{C}$ and 70 $^\circ\text{C}$ were recorded in DMSO.

Fig. S6. ESI mass spectrometry of **1** after the addition of TBACN (5 equiv).

Fig. S7. ^{13}C NMR spectra of (a) **1** (2.5 mM, $\text{DMSO-}d_6$) after the addition of TBACN ($\text{DMSO-}d_6$ solution, 5 equiv) and (b) the synthetic product **2**.

Fig. S8. ^1H NMR spectra of **1** (2.5 mM, $\text{DMSO-}d_6$) before (a) and after (b) the addition of TBACN ($\text{DMSO-}d_6$ solution, 15 equiv). (c) ^1H NMR spectra of the synthetic product **2**.

Fig. S9. Time-dependent UV-Vis spectral changes of **1** (50 μM) upon the addition of 100 equiv. of CN^- in water with CTAB (a) 1 min to 15 min (b) 15 min to 150 min.

Fig. S10. Time-dependent fluorescence changes of **1** (50 μM) upon the addition of 100 equiv. of CN^- in water with CTAB ($\lambda_{\text{ex}} = 347$ nm) from 1 min (yellow line) to 15 min (blue line) and 150 min (green line). Inset: Time-dependent changes of emission intensity at 508 nm.

Fig. S11. Colorimetric responses of **1** (50 μM) before and after addition of various anions (5 equiv., immediately) in water with CTAB.

Fig. S12. Colorimetric response of **1** (50 μM) to CN^- (5 equiv.) in the presence of various anions (5 equiv.) in water with CTAB. The spectra were obtained immediately.

Table. S1. Chemodosimeters for cyanide determination in water.

Fig. S13. Fluorescence intensity spectra of **1** (50 μM) in the presence of different concentration of CN^- (0-100 equiv.) in water with CTAB ($\lambda_{\text{ex}} = 347$ nm). Inset: fluorescence intensities at 508 nm as a function of CN^- concentration. The spectra were obtained after 150 min.

Fig. S14. Fluorescent response of **1** (50 μM) to CN^- (100 equiv.) in the presence of various anions (100 equiv.) in water with CTAB ($\lambda_{\text{ex}} = 347$ nm). The spectra were obtained after 150 min.

Fig. S15. pH dependence of fluorescence intensity at 510 nm of **1** with or without CN^- (100 equiv.).

Fig. S16. ^1H NMR spectrum of **2** in CDCl_3 .

Fig. S17. ^{13}C NMR spectrum of **2** in DMSO.

Fig. S18. ESI-MS spectrum of **2** in DMSO/MeOH.

Fig. S19. FT-IR spectrum of **2**.

Fig. S1 Time-dependent absorption spectra changes of **1** (50 μM , DMSO) in the presence of 100 equiv. of cyanide. The arrows indicate the changes over time. Inset: the time-dependent changes of absorbance at 332 nm and 455 nm.

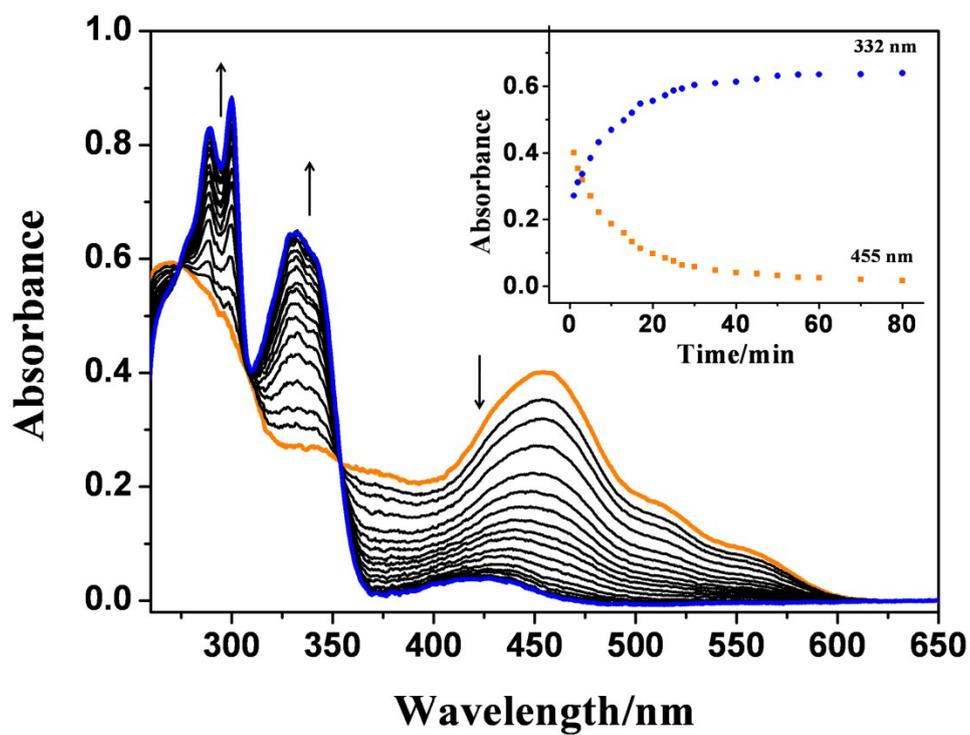


Fig. S2 Time-dependent fluorescence ($\lambda_{\text{ex}} = 398 \text{ nm}$) spectra changes of **1** ($50 \mu\text{M}$, DMSO) in the presence of 100 equiv. of cyanide. The arrow indicates the changes over time. Inset: the time-dependent changes of emission intensity at 476 nm.

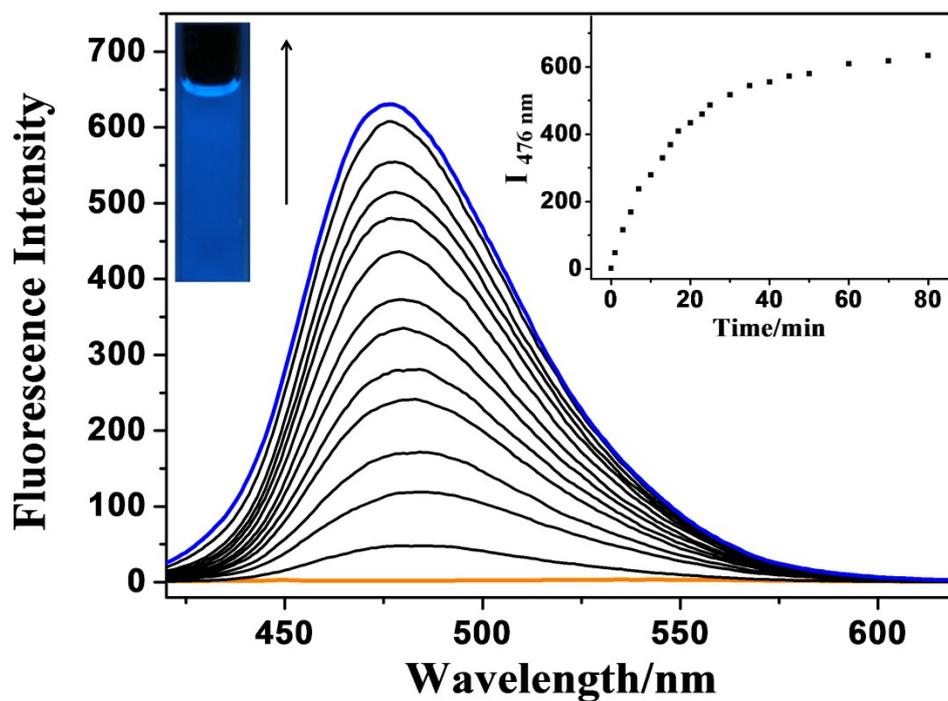


Fig. S3. (a) Absorption spectra and (b) colorimetric responses of **1** (50 μM) before and after addition of various anions (100 equiv.) in DMSO. The spectra and pictures were obtained immediately.

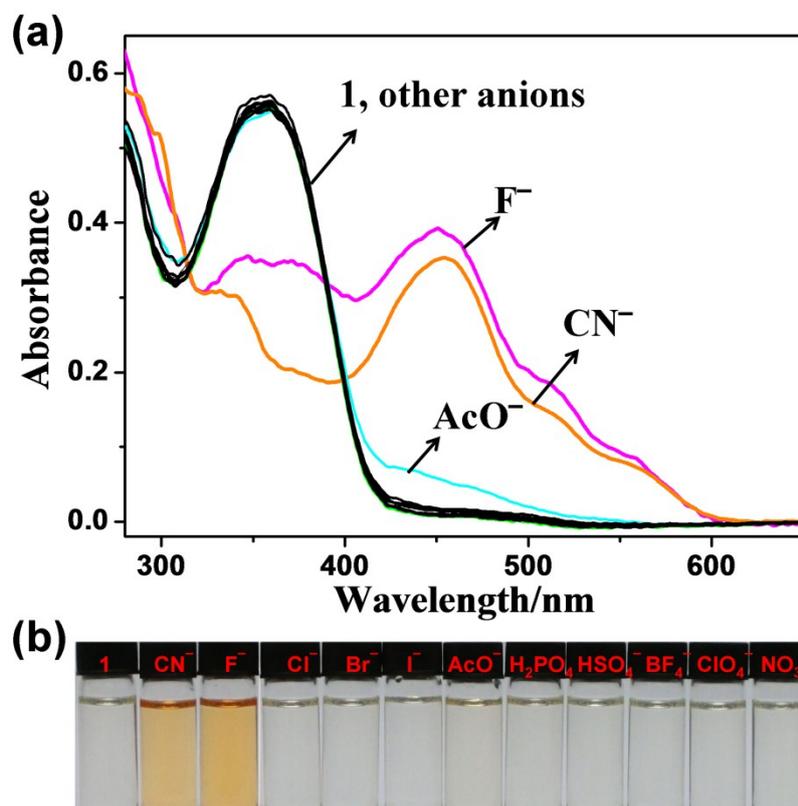


Fig. S4. (a) Fluorescence spectra ($\lambda_{\text{ex}} = 398 \text{ nm}$) and (b) fluorimetric (excitation at 365 nm) responses of **1** ($50 \mu\text{M}$) before and after addition of various anions (100 equiv.) in DMSO. The spectra were obtained after 120 min.

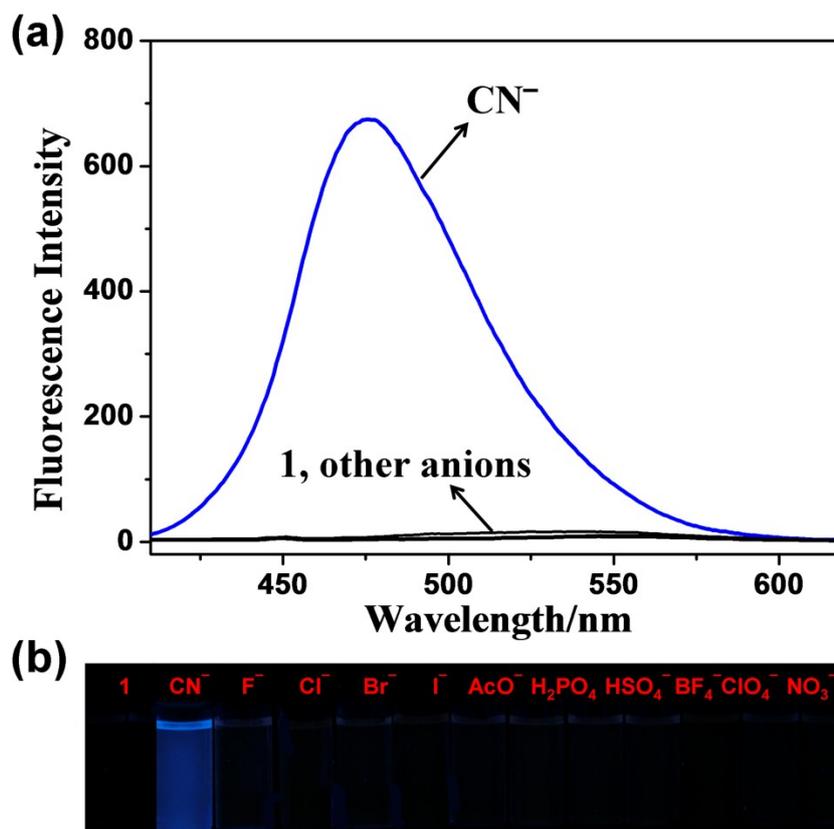


Fig. S5. The (a) absorption and (b) fluorescence intensity ($\lambda_{\text{ex}} = 398 \text{ nm}$) changes of **1** ($50 \mu\text{M}$) in the presence of 100 equiv. of CN^- at $25 \text{ }^\circ\text{C}$, $50 \text{ }^\circ\text{C}$ and $70 \text{ }^\circ\text{C}$ were recorded in DMSO.

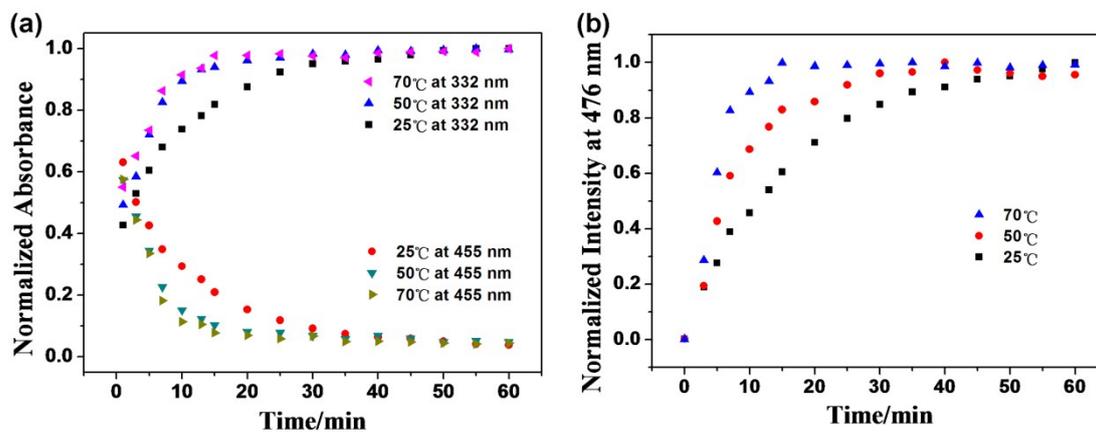


Fig. S6. ESI-MS spectrum of **1** after the addition of TBACN (5 equiv).

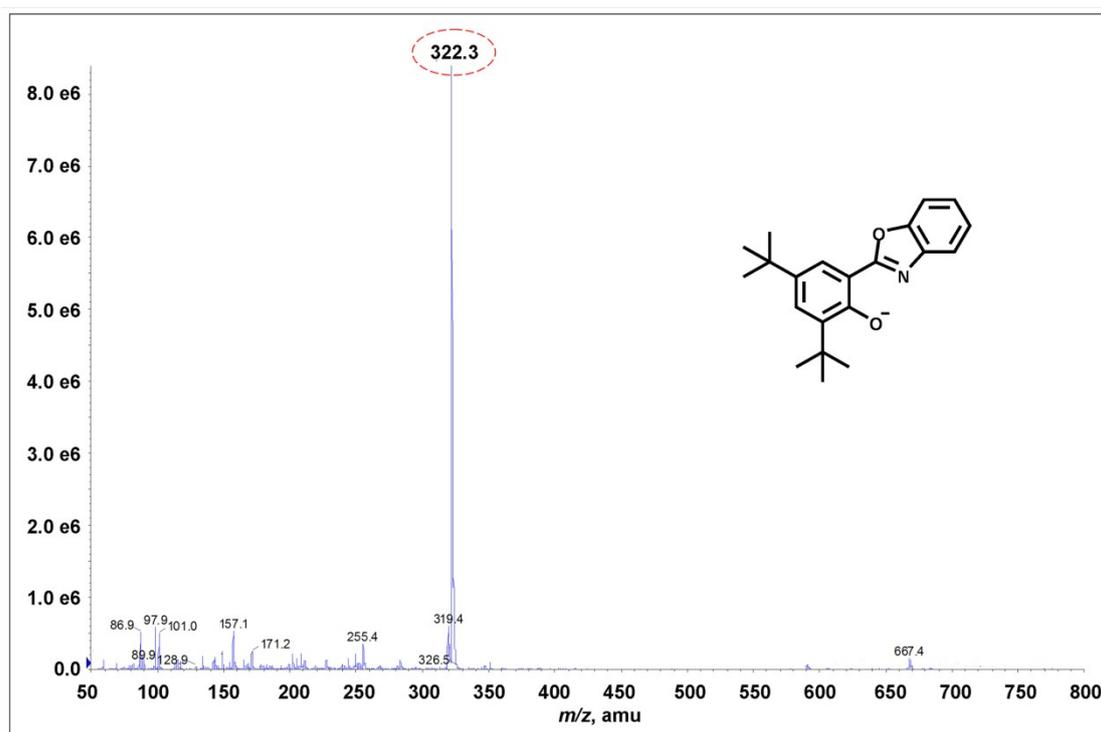


Fig. S7. ^{13}C NMR spectra of (a) **1** (2.5 mM, $\text{DMSO-}d_6$) after the addition of TBACN ($\text{DMSO-}d_6$ solution, 5 equiv) and (b) the synthetic product **2**.

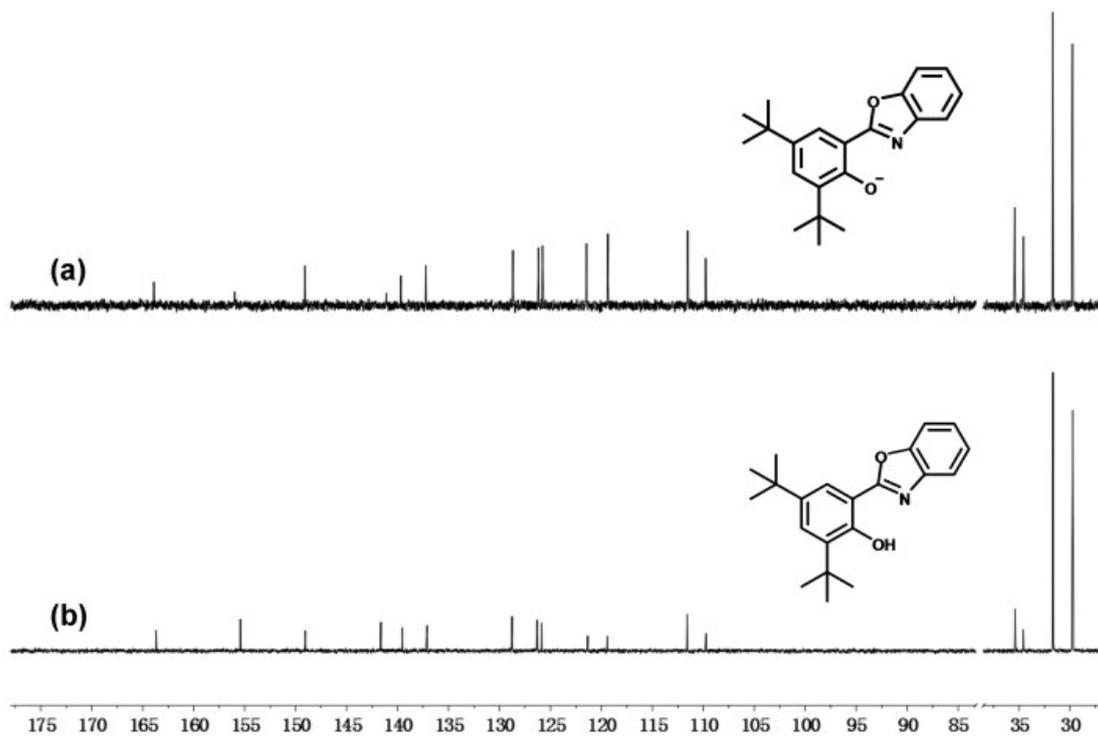


Fig. S8. ^1H NMR spectra of **1** (2.5 mM, $\text{DMSO-}d_6$) before (a) and after (b) the addition of TBACN ($\text{DMSO-}d_6$ solution, 15 equiv). (c) ^1H NMR spectra of the synthetic product

2.

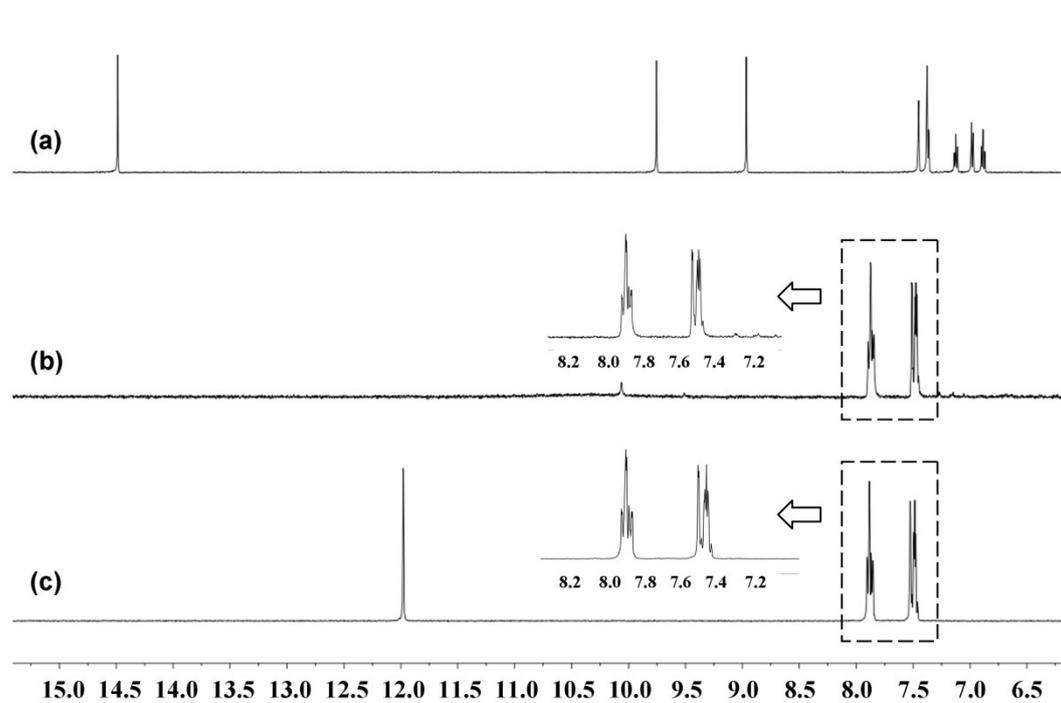


Fig. S9. Time-dependent UV-Vis spectral changes of **1** (50 μM) upon the addition of 100 equiv. of CN^- in water with CTAB (a) 1 min to 15 min (b) 15 min to 150 min.

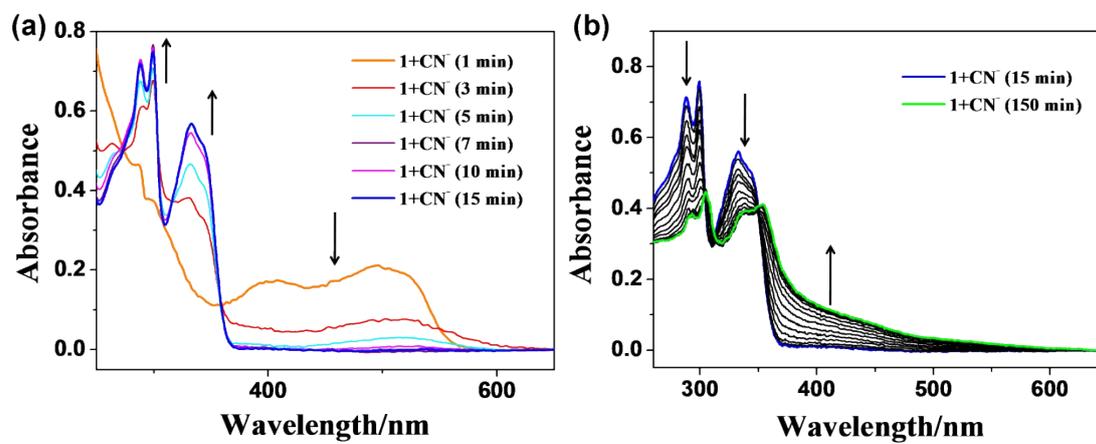


Fig. S10. Time-dependent fluorescence changes of **1** (50 μM) upon the addition of 100 equiv. of CN^- in water with CTAB ($\lambda_{\text{ex}} = 347 \text{ nm}$) from 1 min (yellow line) to 15 min (blue line) and 150 min (green line). Inset: Time-dependent changes of emission intensity at 508 nm.

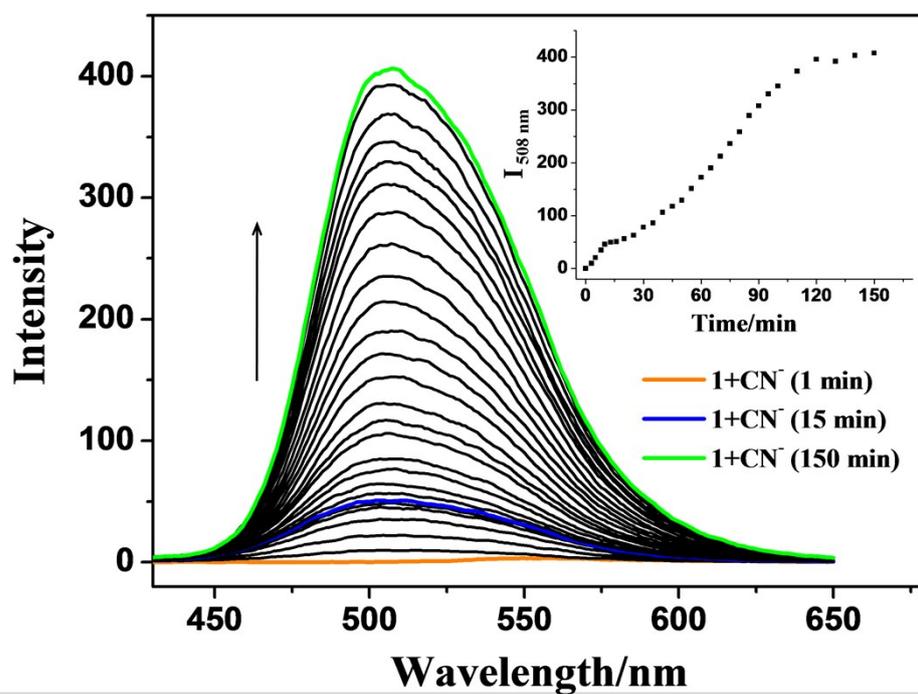


Fig. S11. Colorimetric responses of **1** (50 μM) before and after addition of various anions (5 equiv., immediately) in water with CTAB.



Fig. S12. Colorimetric response of **1** (50 μM) to CN^- (5 equiv.) in the presence of various anions (5 equiv.) in water with CTAB. The spectra were obtained immediately.

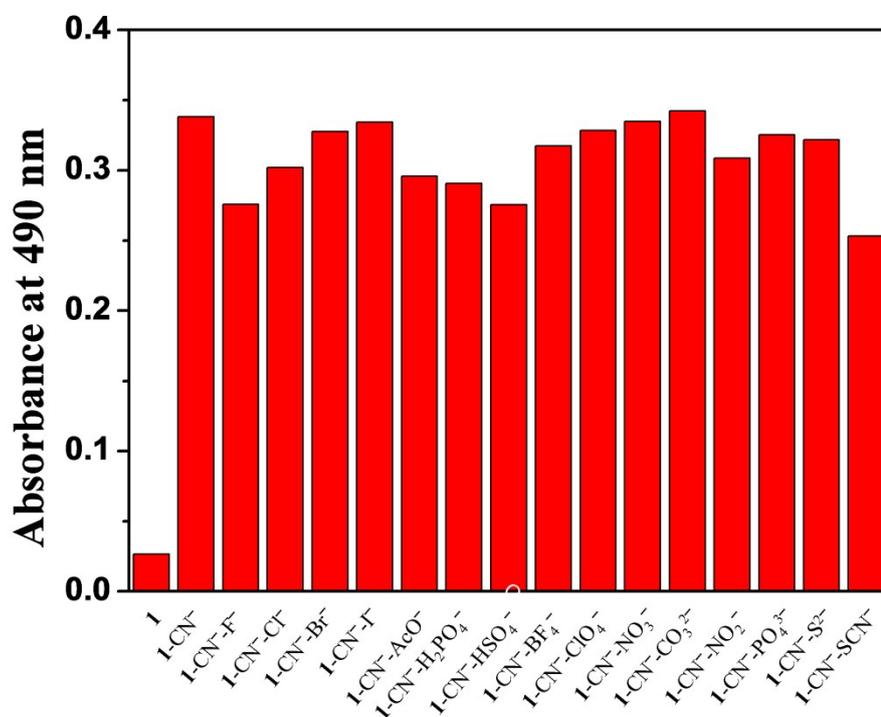


Table. S1. Chemodosimeters for cyanide determination in water.

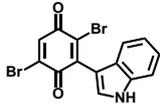
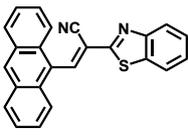
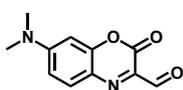
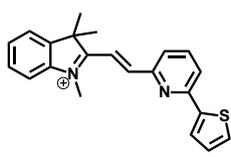
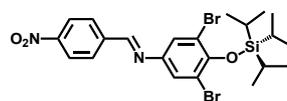
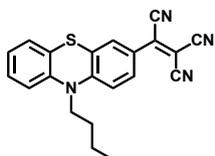
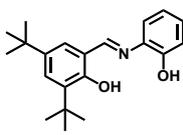
Chemodosimeter	Medium	LOD (M)	Reference in maintext
	HEPES buffer	1.9×10^{-8} M	65
	HEPES buffer	5.52×10^{-8} M	66
	HEPES-DMSO (250 : 1, v/v)	2.86×10^{-7} M.	67
	DMSO-H ₂ O (5 : 95 v/v)	1.5×10^{-6} M	68
	Aqueous CTABr	4.93×10^{-5} M	69
	Water with Triton X-100	1.56×10^{-6} M	70
	Water with CTAB	5.92×10^{-7} M	Our work

Fig. S13. Fluorescence intensity spectra of **1** (50 μM) in the presence of different concentration of CN^- (0-100 equiv.) in water with CTAB ($\lambda_{\text{ex}} = 347 \text{ nm}$). Inset: fluorescence intensities at 508 nm as a function of CN^- concentration. The spectra were obtained after 150 min.

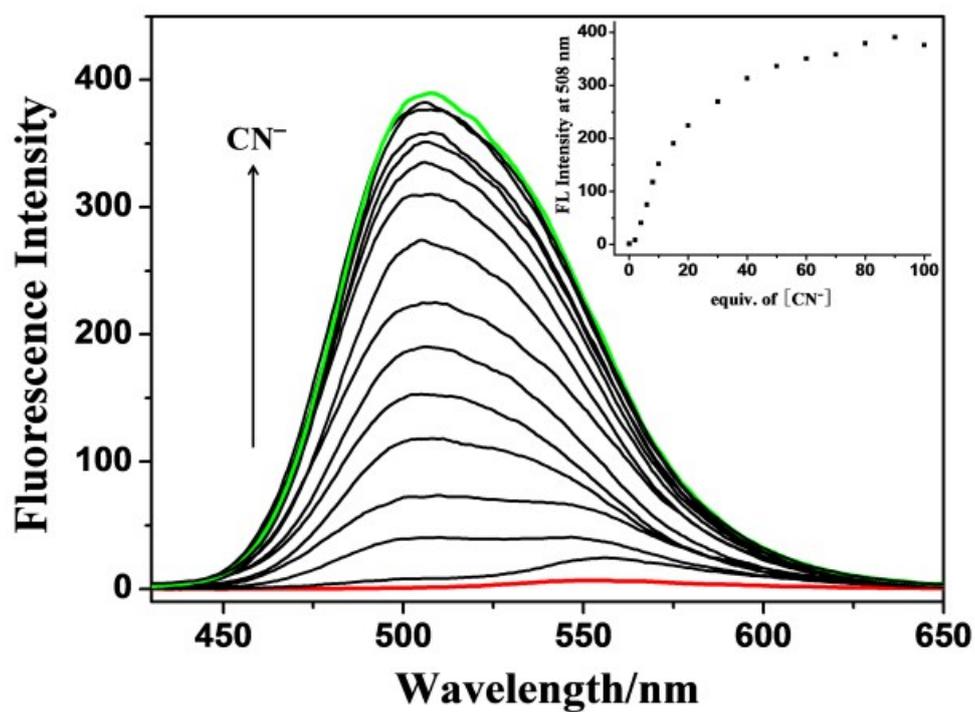


Fig. S14. Fluorescent response of **1** (50 μM) to CN^- (100 equiv.) in the presence of various anions (100 equiv.) in water with CTAB ($\lambda_{\text{ex}} = 347 \text{ nm}$). The spectra were obtained after 150 min.

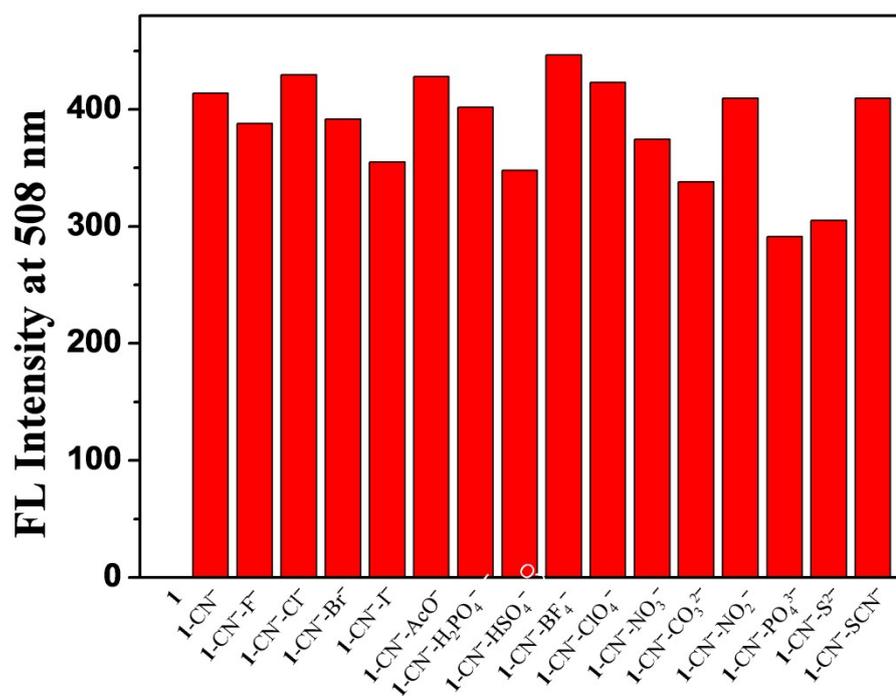


Fig. S15. pH dependence of fluorescence intensity at 510 nm of **1** with or without CN^- (100 equiv.).

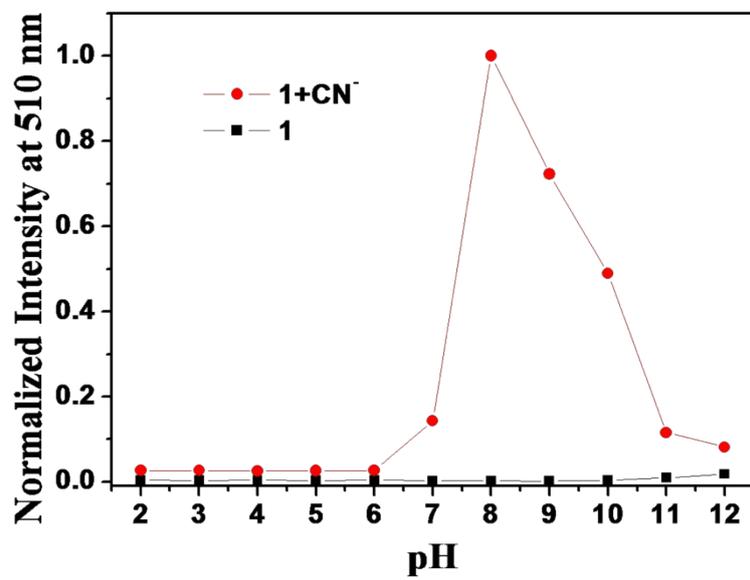


Fig. S16. ^1H NMR spectrum of **2** in CDCl_3 .

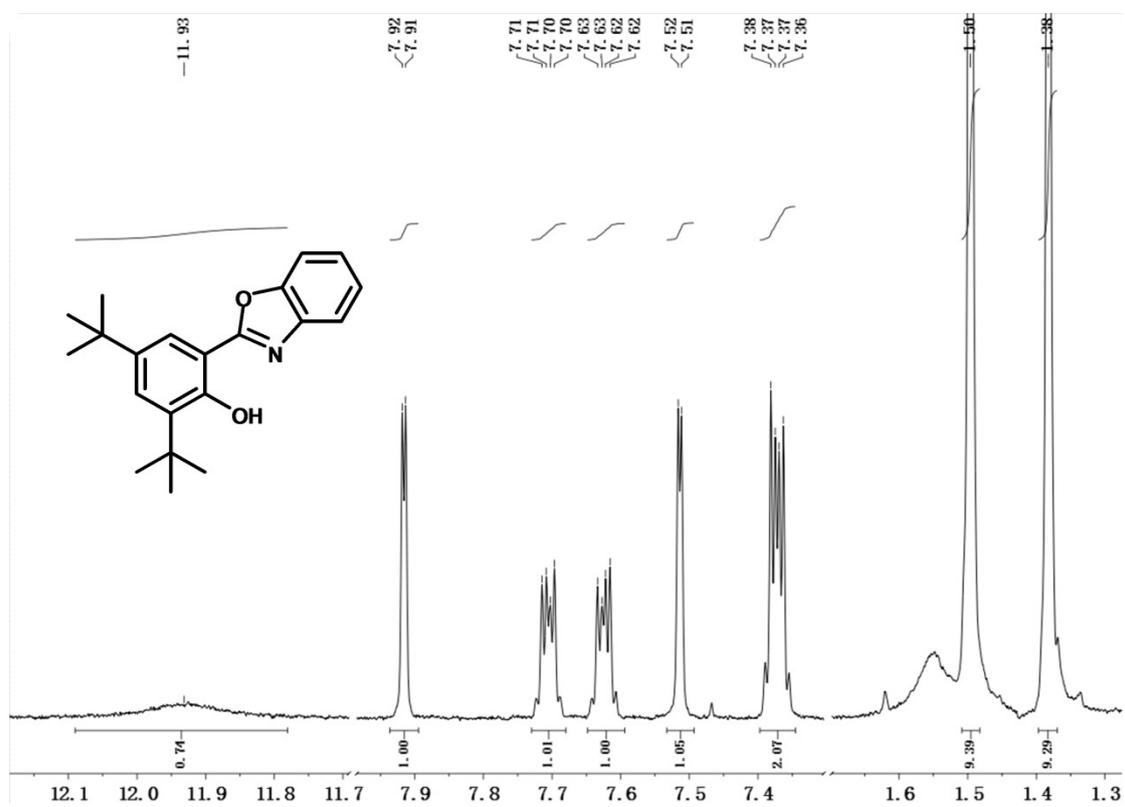


Fig. S17. ^{13}C NMR spectrum of **2** in DMSO.

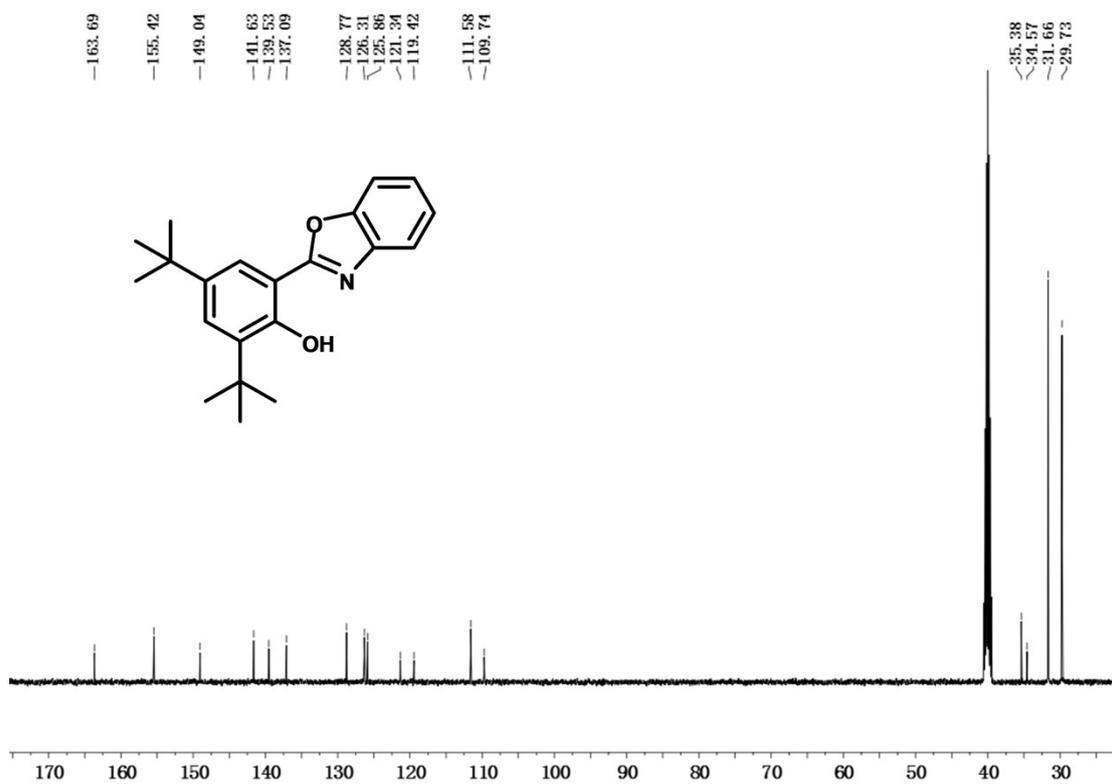


Fig. S18. ESI-MS spectrum of **2** in DMSO/MeOH.

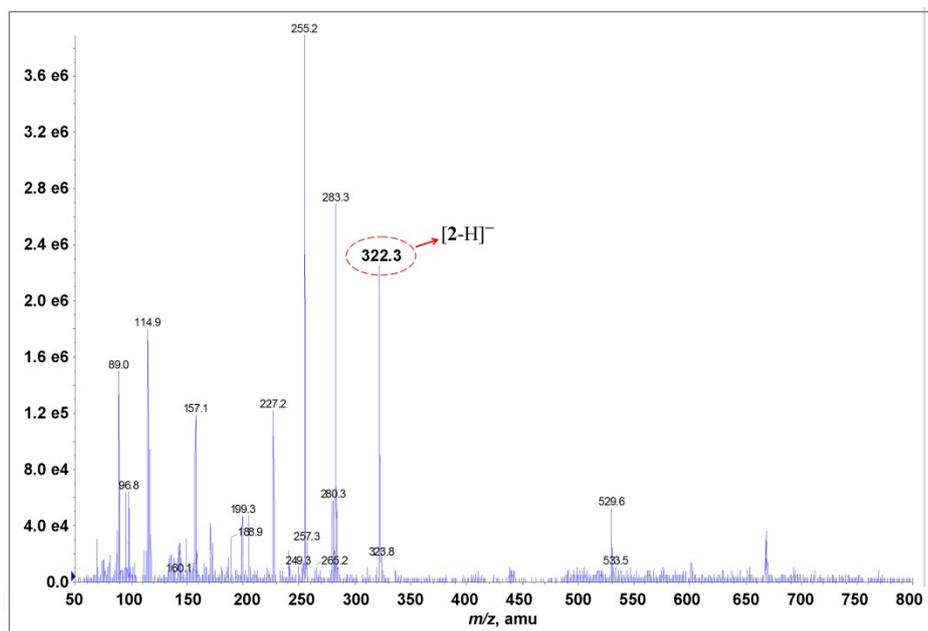


Fig. S19. FT-IR spectrum of 2.

