Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Turn-on Fluorescence Sensor for Detection of Cyanide based a novel dicyanovinyl phenylacetylene

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Contents

1. Spectroscopic data (^{1}H and ^{13}C-NMR) and Mass spectrum.

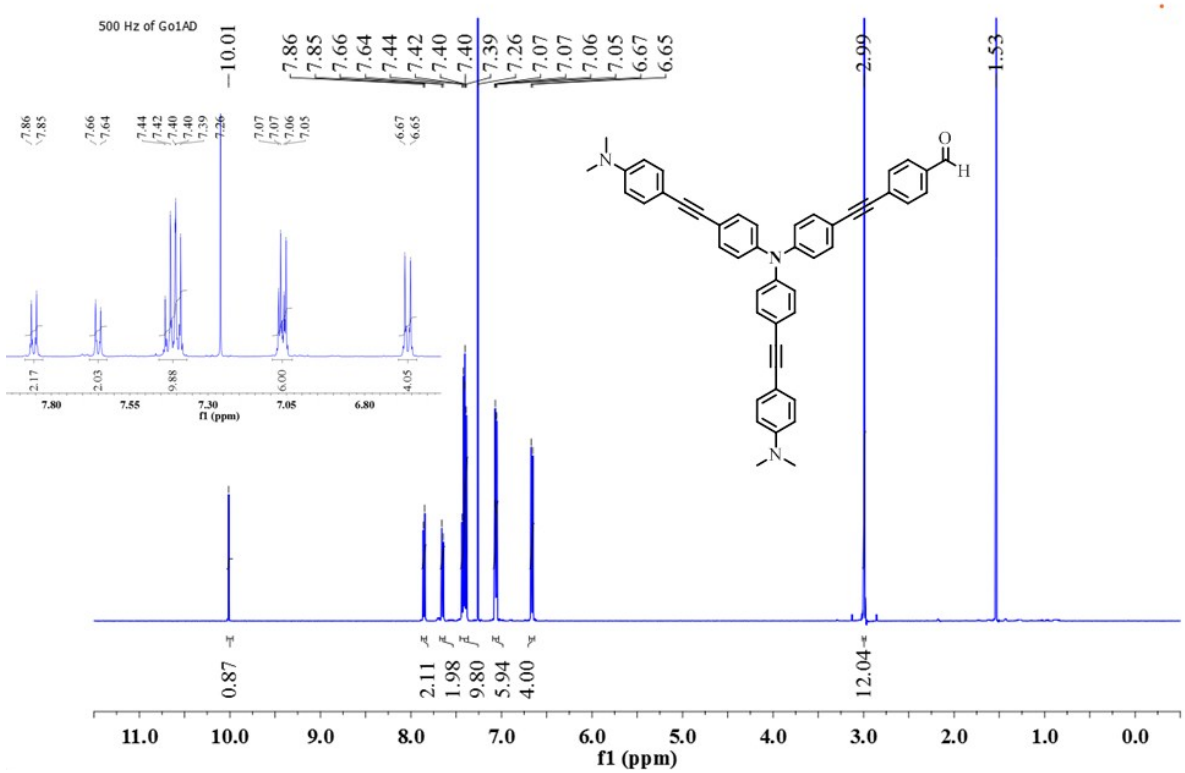


Figure S1. ^{1}H-NMR spectrum of **2** in $CDCl_3$ (500 MHz).

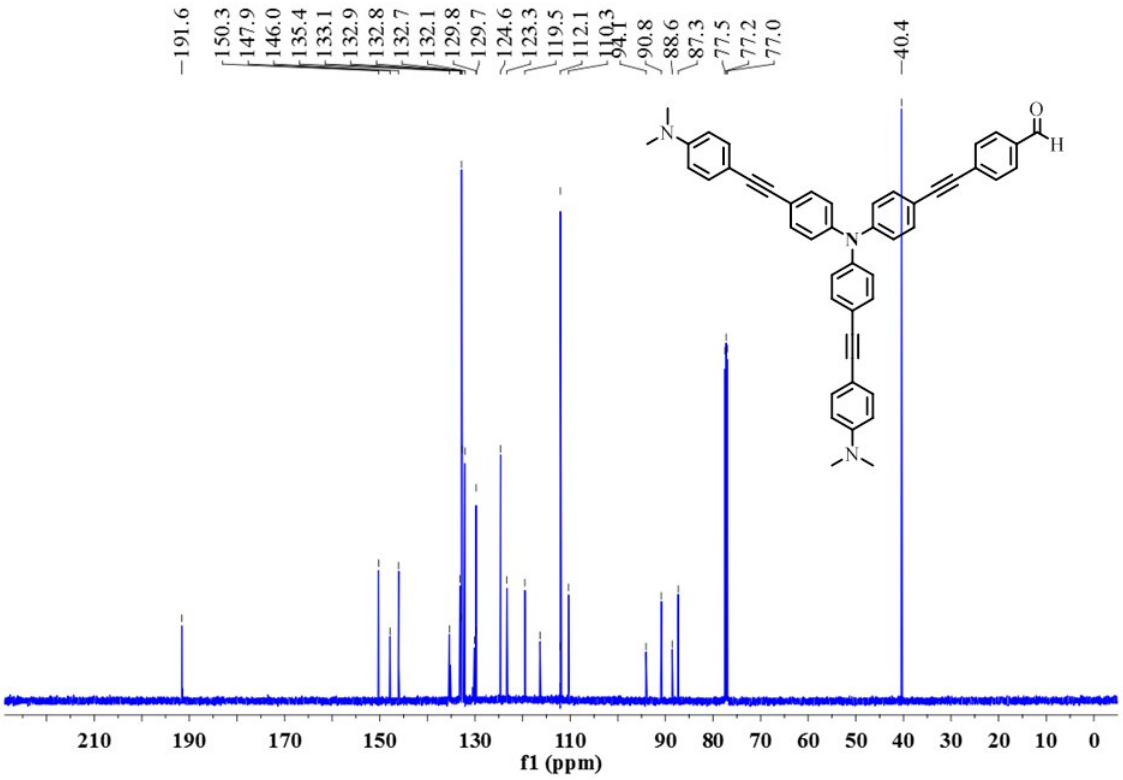


Figure S2. ^{13}C-NMR spectrum of **2** in $CDCl_3$ (125 MHz).

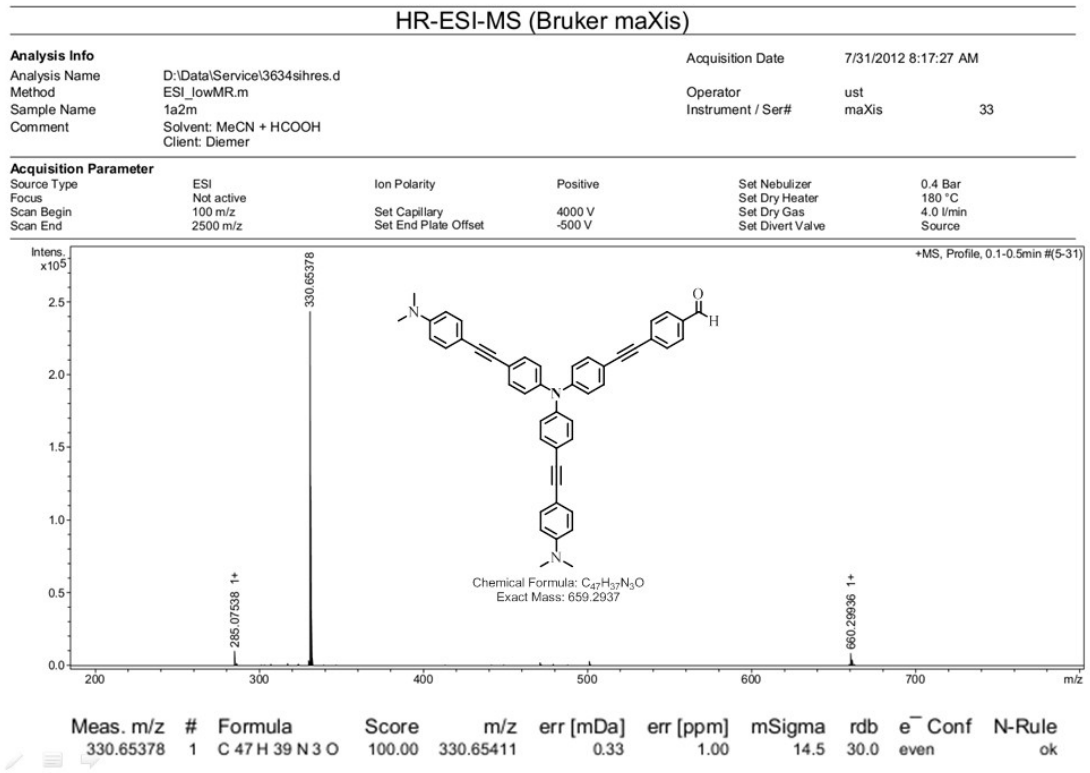


Figure S3. HRMS spectrum of **2**.

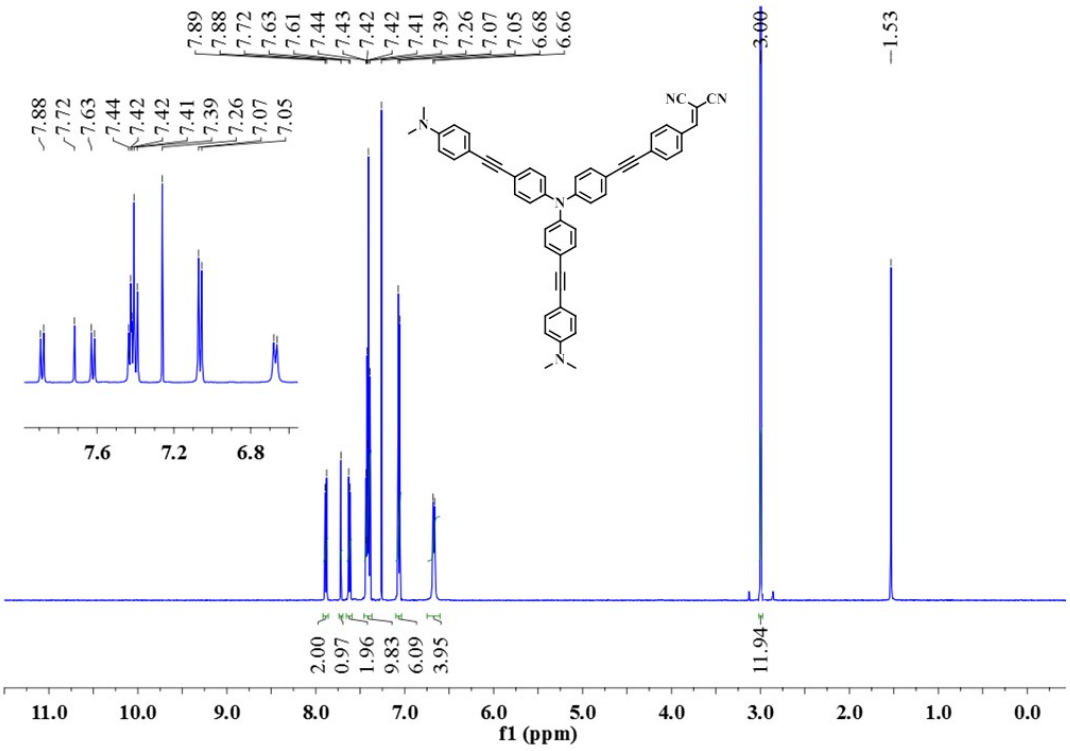


Figure S4. ^{1}H-NMR spectrum of **3** in $CDCl_3$ (500 MHz).

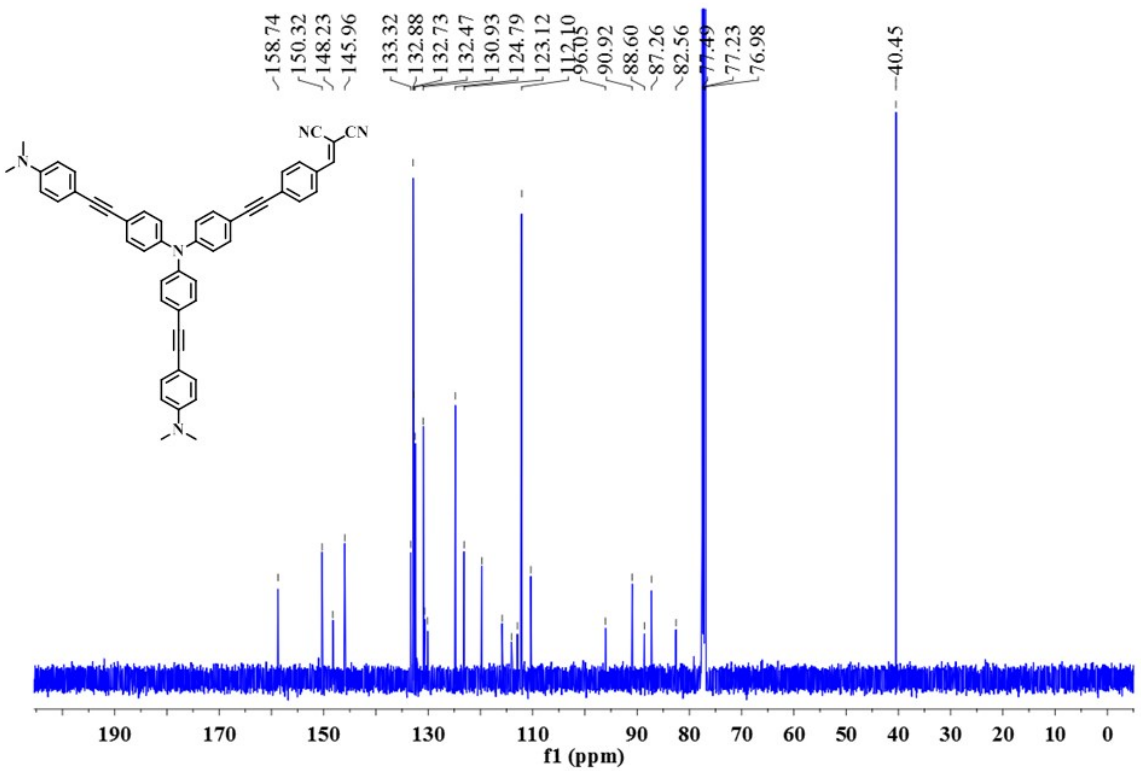
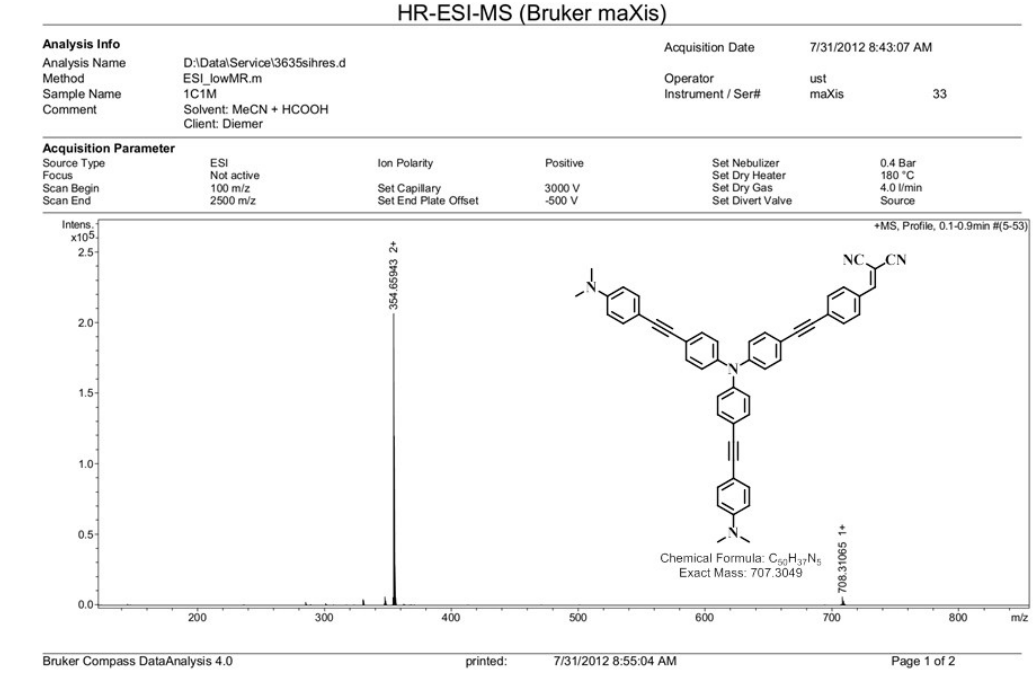


Figure S5. ^{13}C-NMR spectrum of **3** in in $CDCl_3$ (125 MHz).



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
354.65943	1	C 50 H 39 N 5	100.00	354.65972	0.30	0.84	18.2	34.0	even	ok
	2	C 49 H 43 N O 4	81.89	354.65906	-0.37	-1.05	25.8	29.0	even	ok

Figure S6. HRMS spectrum of **3**.

2. Suitable condition of compound 3.

2.1. Various solvent.

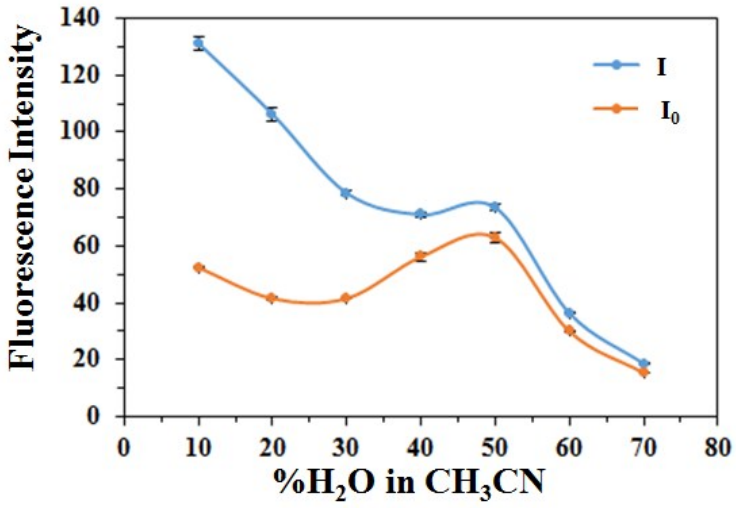


Figure S7. Emission spectra of **3** (10 μM) by various % H_2O in CH_3CN (v/v) before (orange line) and after (blue line) the addition of cyanide ion (100 μM) in HEPES buffer pH 7.4 (λ_{ex} = 368 nm and λ_{em} = 460 nm).

2.2. Various pH

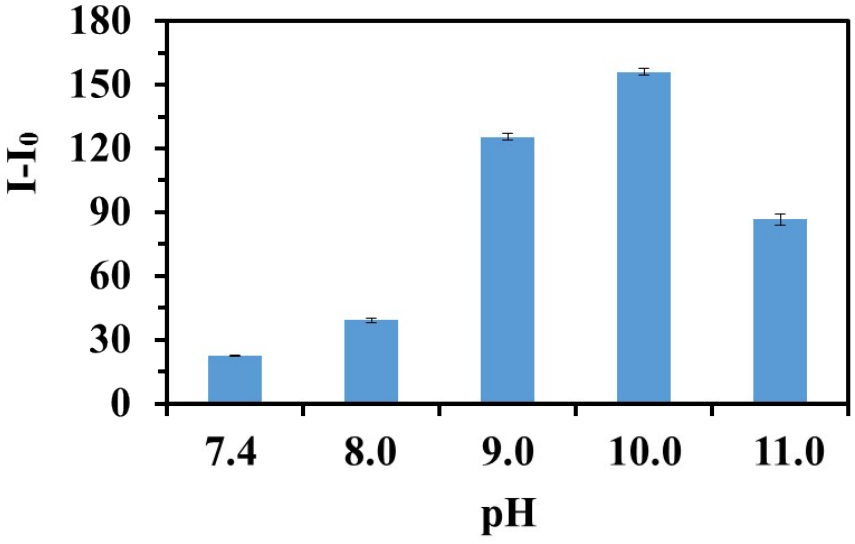


Figure S8. Difference of fluorescent emission intensity ($I-I_0$) of **3** (10 μM) by various pH (7-12) in 10% (v/v) H_2O (100 mM HEPES buffer pH 7-12 in CH_3CN before and after the addition 100 μM cyanide ion (λ_{ex} = 368 nm and λ_{em} = 460 nm).

* At pH 12.0, precipitate was occurred in the solution.

3. Absorption spectra of compound 3 before and after the addition of CN^-.

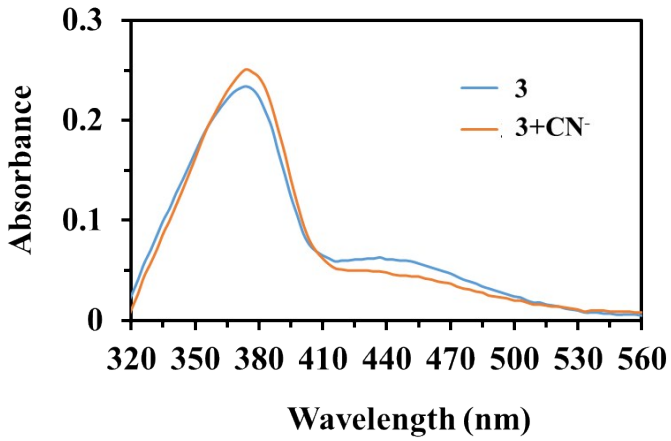


Figure S9. Absorption spectra of **3** (10 μM) in CH_3CN/100 mM HEPES buffer pH 10.0 (9:1 v/v) before and after the addition of CN^- (10 μM).

4. The photophysical properties of compound 3.

Compound	Absorption		Emission	
	λ_{max} (nm)	ε ($\times 10^6$ $M^{-1}cm^{-1}$)	λ_{em} (nm)	Φ_F [a]
3	368	84,600	460	0.008
3 + CN^-	368	86,900	460	0.016

Quinine sulfate in 0.1 M H_2SO_4 (Φ_F = 0.54) was used as standard.

Table S1. Photophysical properties of **3** in 10% H_2O (100 mM HEPES buffer pH 10.0) in CH_3CN before and after the addition of cyanide ion.

5. Calibration curve of compound 3 for CN^- detection.

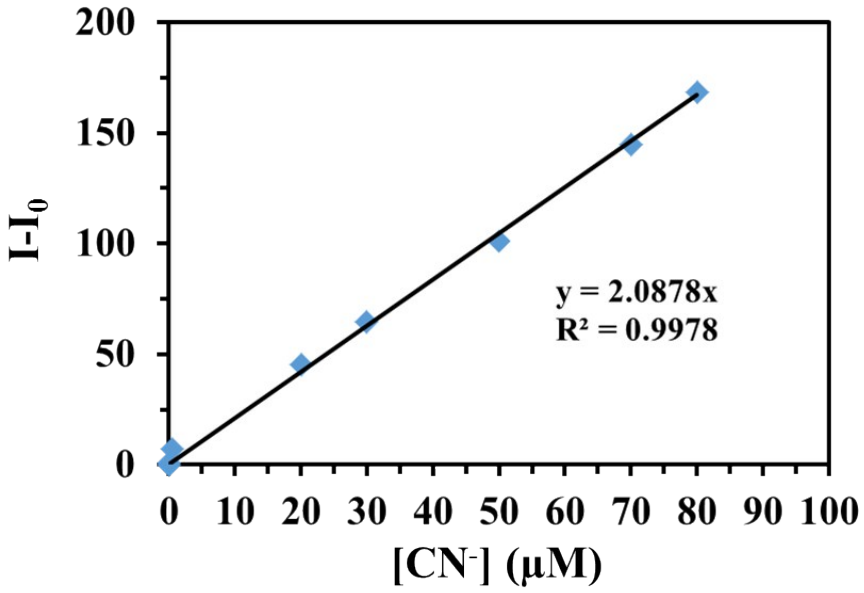


Figure S10. Fluorescence emission spectra of 3 (10 μM) in CH_3CN/ 100 mM HEPES buffer pH 10.0 (9:1 v/v) response to the addition of CN^- at various concentration 0-80 μM (λ_{ex} = 368 nm).

6. Fluorescence intensity of compound 3 under different temperature.

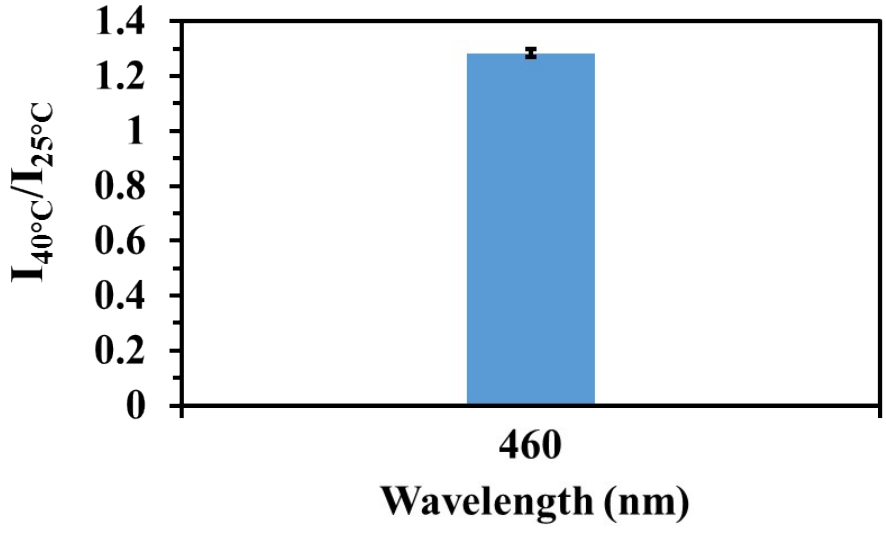


Figure S11. Fluorescence intensity of **3** (10 μM) in a mixture of solvents (CH_3CN : 100 mM HEPES buffer, 9 : 1) after the addition of CN^- at temperature 25°C and 40°C (λ_{ex} = 368 nm and λ_{em} = 460 nm).

7. CN^- distillation set.

Figure S12. CN^- distillation glassware set by following AOAC 28.1.47.