

## Supporting Information

# Novel phenylacetylene-indolium fluorophore for naked eye detection of cyanide

Nakorn Niamnont<sup>a,\*</sup>, Apiwat Promchat<sup>b</sup>, Chutima Siangma<sup>a</sup>,

Chuenjai Pramaulpornsatit<sup>a</sup>, Mongkol Sukwattanasinitt<sup>b</sup>

<sup>a</sup> *Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand.*

<sup>b</sup> *Organic Synthesis Unit, Department of Chemistry, Faculty of Science and Nanotec-CU Center of Excellence on Food and Agriculture, Chulalongkorn University, Bangkok 10330, Thailand.*

[nakorn.nia@kmutt.ac.th](mailto:nakorn.nia@kmutt.ac.th)

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

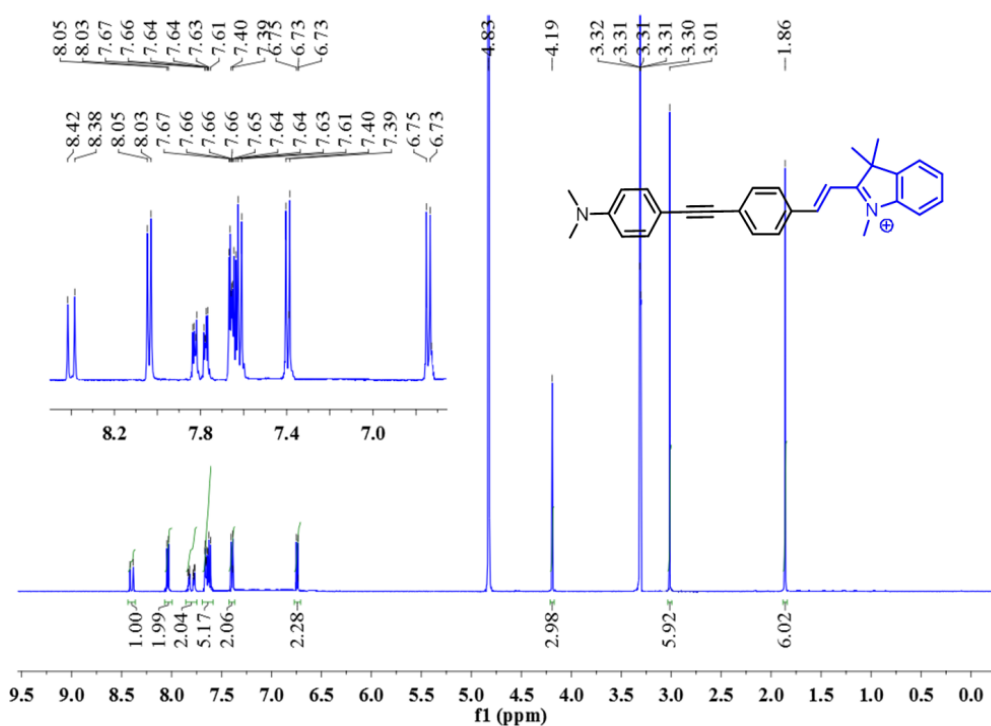


Figure S1.  $^1\text{H}$ -NMR spectrum of **2** in Acetone- $d_6$  (500 MHz).

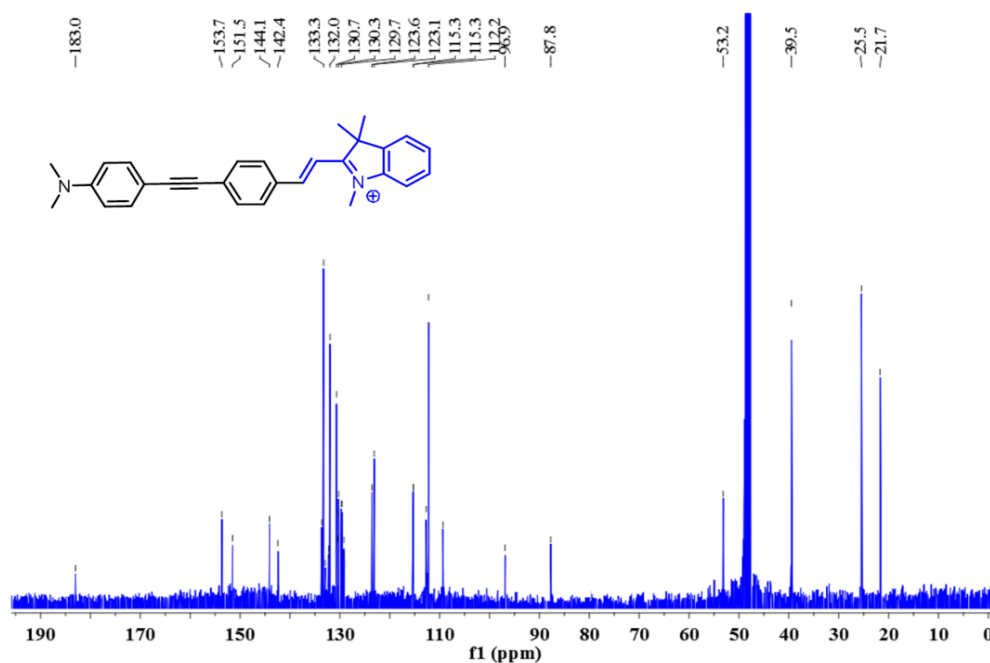
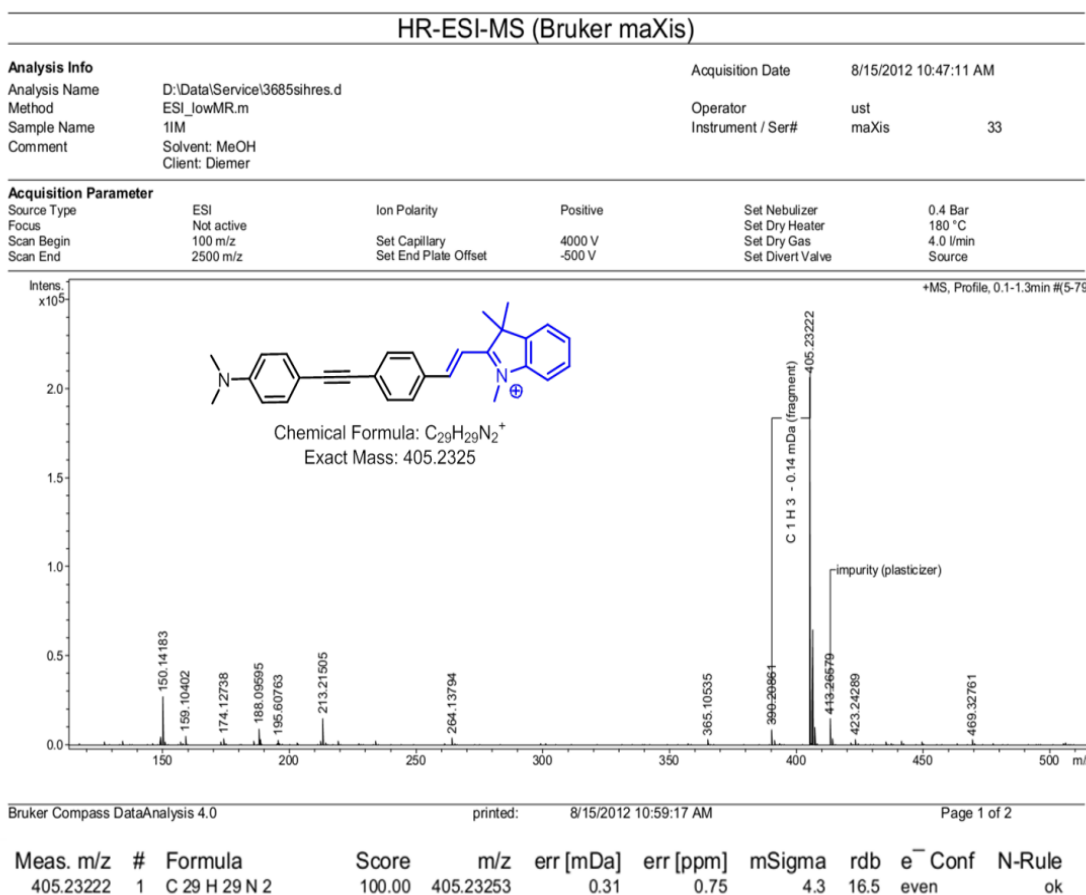


Figure S2.  $^{13}\text{C}$ -NMR spectrum of **2** in Acetone- $d_6$  (500 MHz).



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

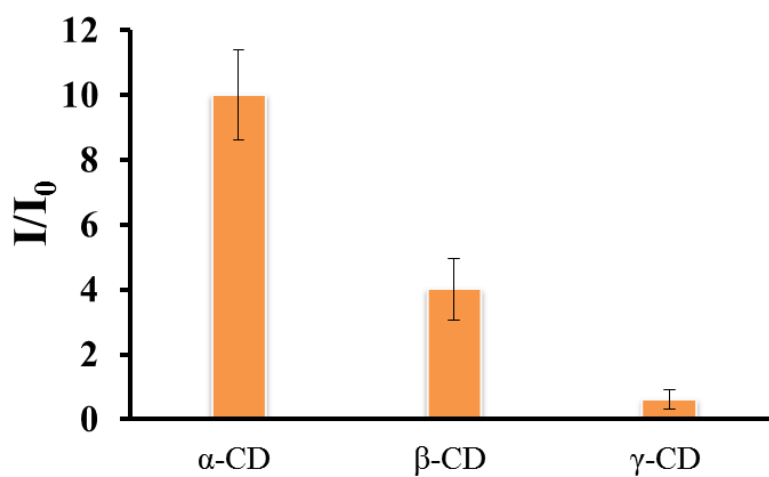
Compound	Absorption		Emission	
	$\lambda_{\max}$ (nm)	$\log \epsilon$ (M <sup>-1</sup> cm <sup>-1</sup> )	$\lambda_{\text{em}}$ (nm)	$\Phi_{\text{F}}^{\text{a}}$
<b>2</b>	450	4.29	595	0.025
<b>2 + CN<sup>-</sup></b>	360	2.58	450	0.34

Quinine sulfate in 0.1 M H<sub>2</sub>SO<sub>4</sub> ( $\Phi_{\text{F}} = 0.54$ ) was used as standard

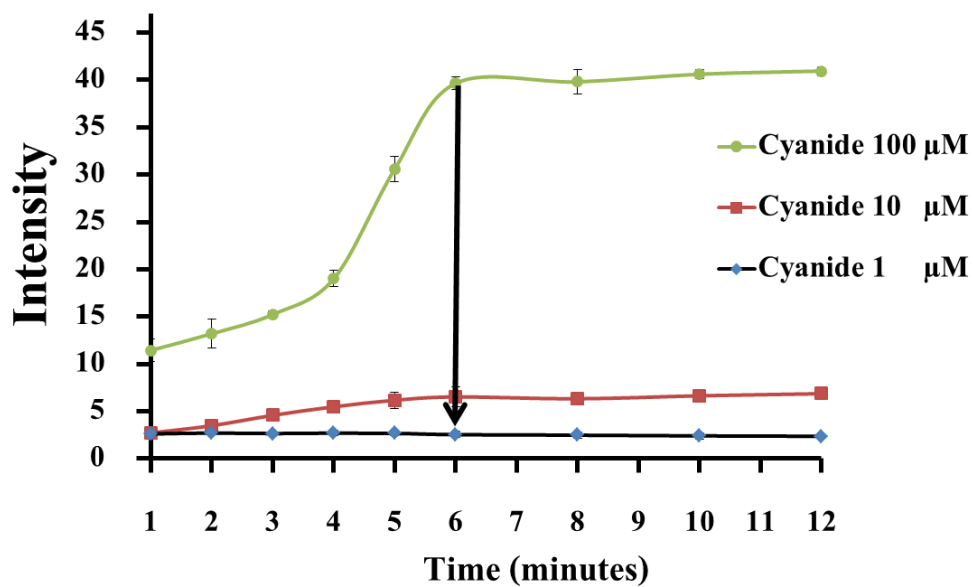
**Table S1.** Photophysical properties of **2** mixed cyclodextrins (400  $\mu\text{M}$ ) in HEPES (10 mM, pH 7.4)



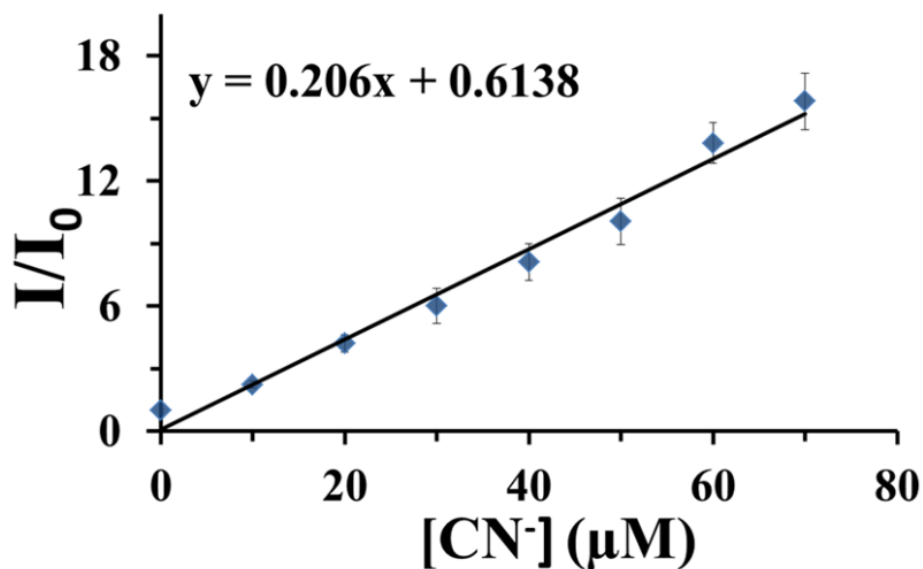
**Figure S4.** Image of **2** only (100  $\mu\text{M}$ ) (left) and **2** mixed  $\alpha$ -cyclodextrins (800  $\mu\text{M}$ ) in HEPES buffer pH 7.4.



**Figure S5.** Emission spectra ratios ( $I/I_0$ ) of **2** (10  $\mu\text{M}$ ) in the presence of  $\alpha$ -,  $\beta$ -, and  $\gamma$  cyclodextrins (400  $\mu\text{M}$ ) and cyanide ion (100  $\mu\text{M}$ ) in HEPES buffer pH 7.4, excited at 360 nm.



**Figure S6.** Reaction-time profile of probe **2** (50  $\mu\text{M}$ ) mixed cyclodextrins (400  $\mu\text{M}$ ) in HEPES buffer pH 7.4 in the presence of different concentrations of  $\text{CN}^-$ .



**Figure S7.** The corresponding calibration curve of **2** (50  $\mu\text{M}$ ) mixed cyclodextrins (400  $\mu\text{M}$ ) in the presence of cyanide ions at various concentrations.

## Mass Spectrum List Report

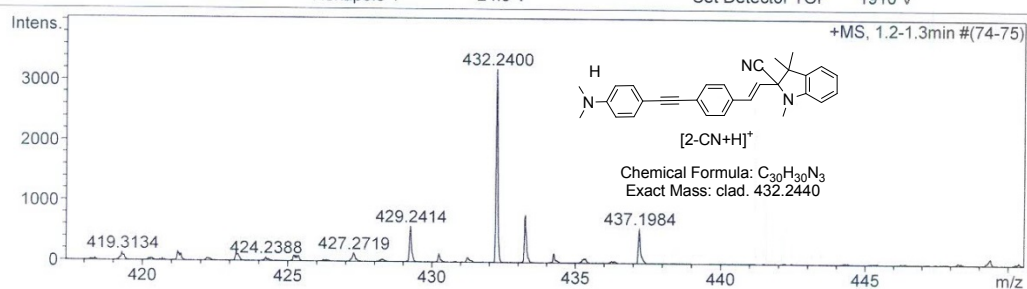
### Analysis Info

Analysis Name OSNN580708002.d  
 Method Tune\_low\_POS\_Natee20130403.m  
 Sample Name N2  
 N2

Acquisition Date 7/8/2015 3:02:07 PM  
 Operator Administrator  
 Instrument micrOTOF 72

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	79 V
Scan Range	n/a	Capillary Exit	180.0 V	Set Pulsar Pull	406 V
Scan Begin	50 m/z	Hexapole RF	150.0 V	Set Pulsar Push	388 V
Scan End	3000 m/z	Skimmer 1	45.0 V	Set Reflector	1300 V
		Hexapole 1	24.3 V	Set Flight Tube	9000 V
				Set Detector TOF	1910 V



#	m/z	I	I %	S/N	FWHM	Res.
1	418.3732	34	1.1	4.0	0.0539	7755
2	419.3134	125	3.9	15.8	0.0747	5616
3	420.6841	40	1.3	5.1	0.0131	32077
4	421.2404	115	3.6	14.6	0.1354	3110
5	421.2404	115	3.6	14.6	0.1354	3110
6	424.2388	57	1.8	7.2	0.0527	8049
7	426.2377	19	0.6	2.4	0.0651	6545
8	426.3377	20	0.6	2.5	0.1069	3987
9	427.2719	131	4.1	16.7	0.1068	4000
10	428.2637	39	1.2	5.0	0.1185	3614
11	429.2414	584	18.3	74.1	0.0679	6321
12	430.2406	132	4.1	16.7	0.0675	6374
13	431.2400	73	2.3	9.3	0.1116	3865
14	432.2400	3198	100.0	406.4	0.0650	6650
15	433.2454	781	24.4	99.3	0.0739	5866
16	434.2461	141	4.4	17.9	0.0594	7307
17	435.3062	69	2.2	8.8	0.1516	2872
18	436.3295	29	0.9	3.7	0.1310	3331
19	437.1984	574	17.9	73.1	0.0692	6314

**Figure S8.** The cross checked cyanide addition to probe 2 by using EI-HRMS.