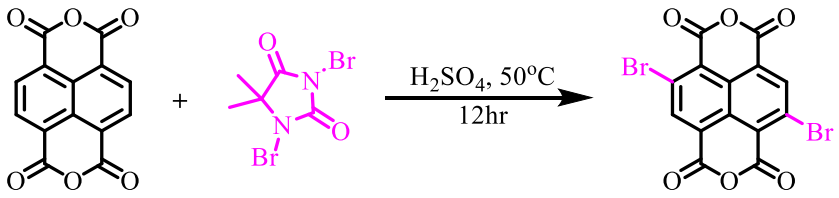
Electronic Supporting Information

Experimental procedures:

Synthesis of 2,6-Dibromo-1,4,5,8-naphthalenetetracarboxylic Dianhydride (4):

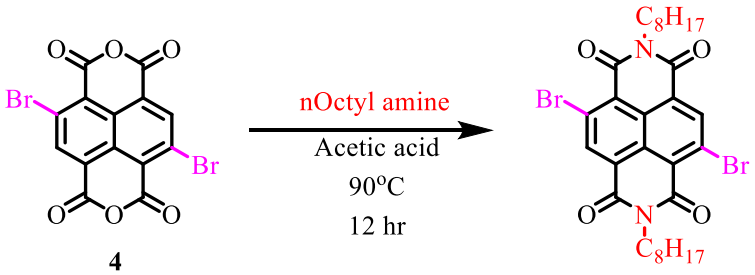


2 3 4

Synthesized using reported literature procedure[1]

In single-necked RB flask, NDA (**2**) (2.68 g, 10 mmol) was stirred in concentrated sulfuric acid (25 mL) at ambident temperature, the mixture was stirred at room temperature for 5 min to obtain a solution. DBH (**3**) (4.28 g, 15 mmol) was added in 8 portions over a period of 2h at room temperature (without escaping bromine from solution). The resulting brown solution was stirred at 50°C for 12 h. The mixture was poured into crushed ice to precipitate solid. The precipitated solid was filtered, washed with water then with methanol, and finally dried under vacuum to obtain crude product. (3.49 g, 82%); 1H NMR (400 MHz, [D_6]DMSO): 8.78 (s, 2H); ^{13}C NMR (100 MHz, [D_6]DMSO): 157.9, 156.4, 137.5, 129.4, 127.4, 124.2, 123.4

Synthesis of 4,9-dibromo-2,7-dioctylbenzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetraone (5)



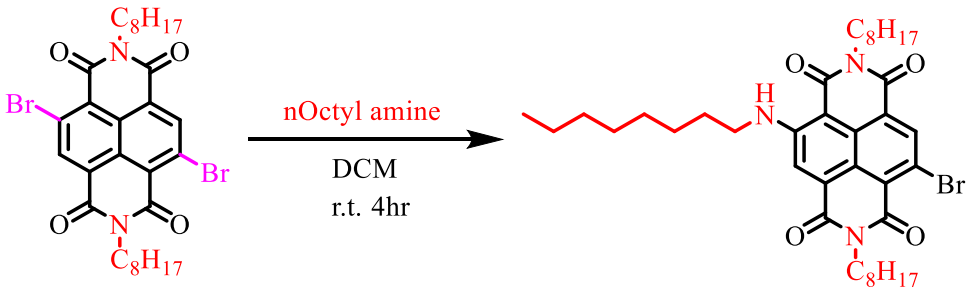
4 5

Synthesized using reported literature procedure[1]

Dibromo-NDA (**4**) (1.06 g, 2.5 mmol), n-octylamine (1.24 mL, 7.5 mmol), and acetic acid (80 mL) was stirred under nitrogen atmosphere at 90°C for 12 h. The mixture was cooled to room

temperature. The precipitate was separated by filtration, washed with methanol and dried under vacuum to obtain 4,9-dibromo-2,7-dioctylbenzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetraone (**5**) as a yellow crystalline solid (1.21g, 75%); ^{1}H NMR (400 MHz, $CDCl_3$): 8.99 (s, 1H, Ar-H), 4.20-4.16 (t, 4H), 1.77-1.69 (quin, 4H), 1.42-1.27 (m, 20H), 0.89-0.86 (t, 6H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 160.9, 160.8, 139.2, 128.4, 127.8, 125.5, 124.2, 41.7, 31.9, 29.4, 29.3, 28.0, 27.2, 22.7, 14.2

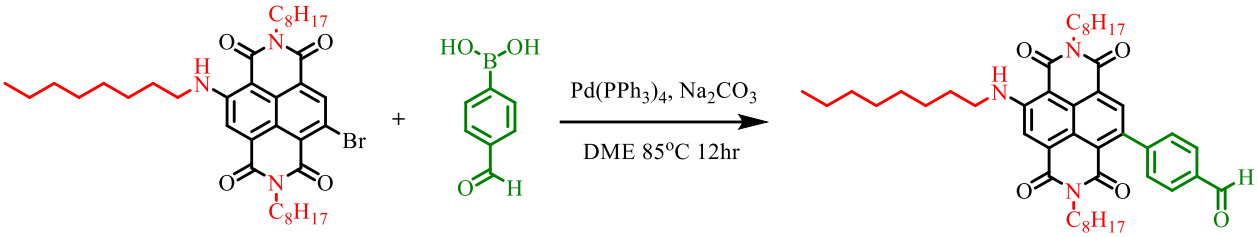
Synthesis of 4-bromo-2,7-dioctyl-9-(octylamino)benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetraone (6)



5 **6**

In a 100 mL dried oven RB flask take dibromo NDI (**5**) (0.5g, 0.00077 mol) and add 30 mL of dry DCM to it, stir the reaction mixture for 5 min then add n-octyl amine (0.119g/0.153 ml, 0.00092) to it stirred the reaction mixture for 4 h under nitrogen atmosphere. The resulting reaction mixture was extracted with DCM and followed by washing of 6N HCl repeatedly, then with saturated NaCl, organic layer was collected and dried over sodium sulphate then evaporated on rota evaporator. The crude product was purified by silica gel column chromatography. The yield of isolated product (70% yield); ^{1}H NMR (400 MHz, $CDCl_3$) 10.05 (s, 1H), 8.79 (s, 1H), 8.21 (s, 1H), 4.14 (t, 4H), 3.55 (t, 2H), 1.83 (t, 2H), 1.71-1.28(m, 34H), 0.88 (m, 9H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 165.8, 161.9, 161.7, 161.3, 151.7, 138.2, 128.6, 127.2, 123.3, 123.2, 121.3, 120.4, 120.1, 99.8, 43.3, 41.4, 40.5, 31.8, 29.7, 29.3, 29.2, 29.1, 28.0, 27.9, 27.1, 27.0, 22.6, 14.0

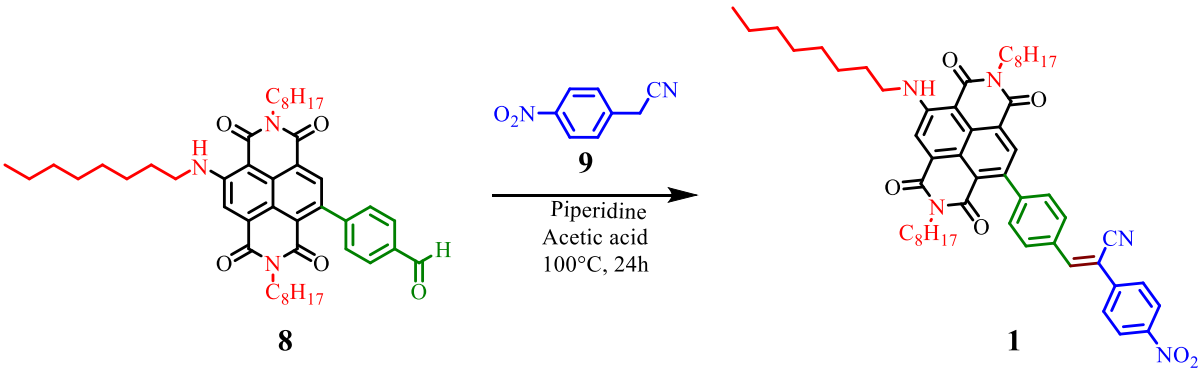
Synthesis of 4-(2,7-dioctyl-9-(octylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn] [3,8]phenanthrolin-4-yl)benzaldehyde (8)



6 7 8

Charge 100 mL reaction RB flask with compound NDI (**6**) (0.5 g, 0.00072 mol) and add 30 mL dimethoxyethane (DME) degassed it for 3 times and then 2M sodium carbonate 10 mL added to it, degassed it for several times then (4-formylphenyl)boronic acid (**7**)(0.13g, 0.009 mole) was added again degassed it for 2 times, catalyst $Pd(PPh_3)_4$ (10 mole%) were added at rt under nitrogen atmosphere. After 24h refluxing solvent evaporated on rota evaporator the residue remained in flask extracted in DCM (100 mL × 3 times). Then crude product washed with saturated NaCl. The organic layer was dried on sodium sulphate and crude product was purified using silica gel column chromatography. The yield of isolated product (63.83% yield) ; ^{1}H NMR (400 MHz, $CDCl_3$) 10.15 (s, 1H), 10.11 (s,1H), 8.45 (s, 1H), 8.31 (s, 1H), 8.10 (d, 2H), 7.51 (d, 2H), 4.18 (t, 2H), 4.02 (t, 2H), 3.61 (q, 2H), 1.86 (q, 2H), 1.75 (m, 2H), 1.61-1.20 (m, 35H), 0.9 (m, 10H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 191.9, 166.2, 162.7, 162.6, 152.1, 147.7, 139.7, 135.4, 134.4, 129.6, 129.3, 129.1, 128.2, 122.9, 122.6, 120.6, 120.2, 99.7, 43.3, 41.0, 40.4, 31.8, 31.7, 29.4, 29.3, 29.2, 29.1, 28.0, 27.1, 27.0, 22.6, 12.0

Synthesis of (Z)-3-(4-(2,7-dioctyl-9-(octylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthrolin-4-yl)phenyl)-2-(4-nitrophenyl)acrylonitrile (1).



8 1

In an oven dried 50 mL RB, the reaction mixture of 2-(4-nitrophenyl)acetonitrile (**9**) (0.022 gm, 0.00014 mole) in 10 mL acetic acid was stirred followed by the addition of 1.5 mL of piperidine in a nitrogen atmosphere. The colour of the mixture changed immediately to a transparent pink. The mixture was stirred further for 30 min. then compound NDI aldehyde (**8**)

(0.1 gm, 0.00014 mole) was added and the reaction mixture was heated to 100°C. The completion reaction was monitored using TLC. After completion of reaction (24 h), the mixture was cooled to room temperature and poured into ice water. The prepared compound was extracted using DCM (100 mL×3 times). Then the crude product was washed with sodium bicarbonate followed by saturated NaCl. The obtained organic layer was dried on sodium sulfate and the crude product was purified using silica gel column chromatography. The yield of isolated product (29.16% yield) ; ^{1}H NMR (400 MHz, $CDCl_3$) 10.16 (s, 1H), 8.50 (s, 1H), 8.35 (d, 3H), 8.08 (d, 2H), 7.85 (d, 2H), 7.74 (s, 1H), 7.50 (d, 2H), 4.20 (t, 2H), 4.04 (t, 2H), 3.61 (q, 2H), 1.84 (q, 2H) 1.73-0.84(m, 43H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 162.7, 152.1, 147.9, 145.1, 134.7, 129.7, 129.3, 126.8, 124.4, 122.7, 120.6, 117.3, 43.4, 41.1, 31.8, 31.7, 29.7, 29.5, 29.4, 29.3, 29.2, 29.1, 28.0, 27.2, 27.1, 27.08, 27.02, 22.6, 14.1

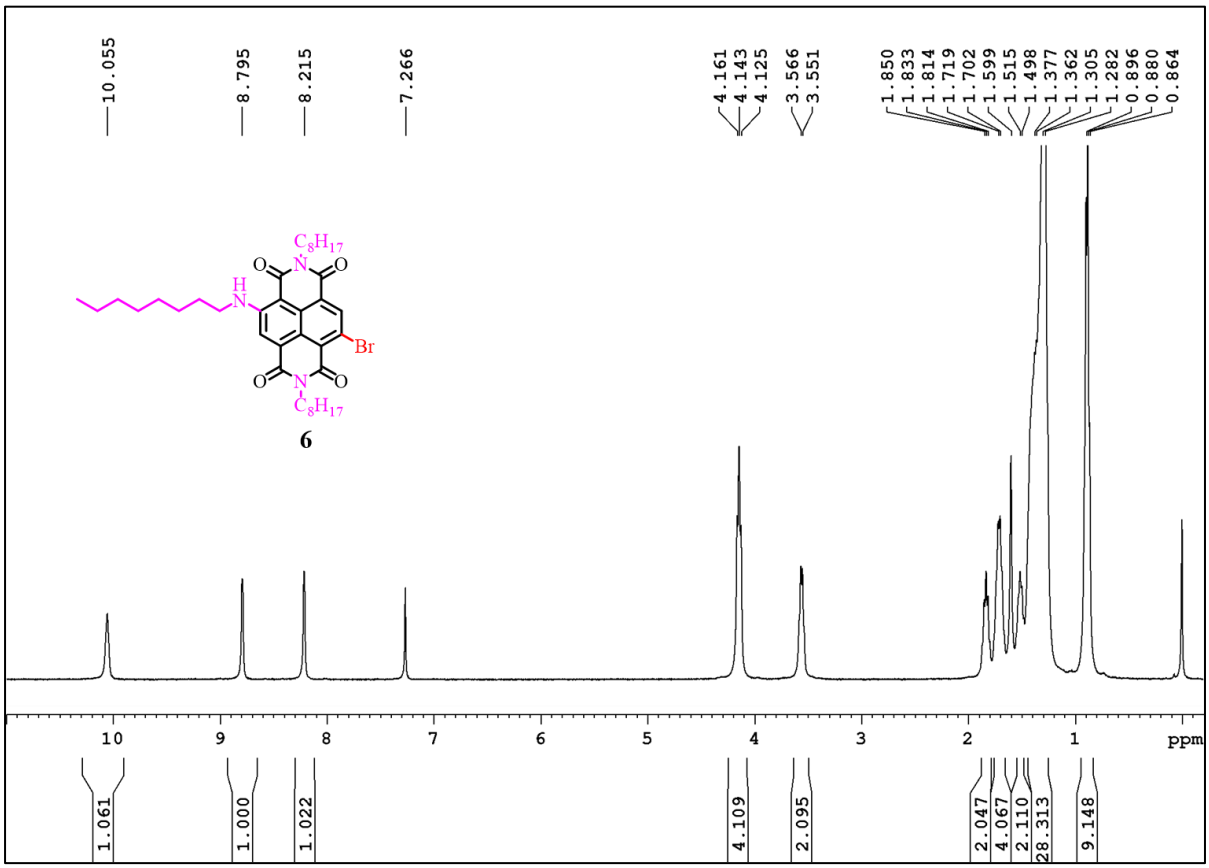


Figure S1. ^{1}H NMR spectra of Compound **6**

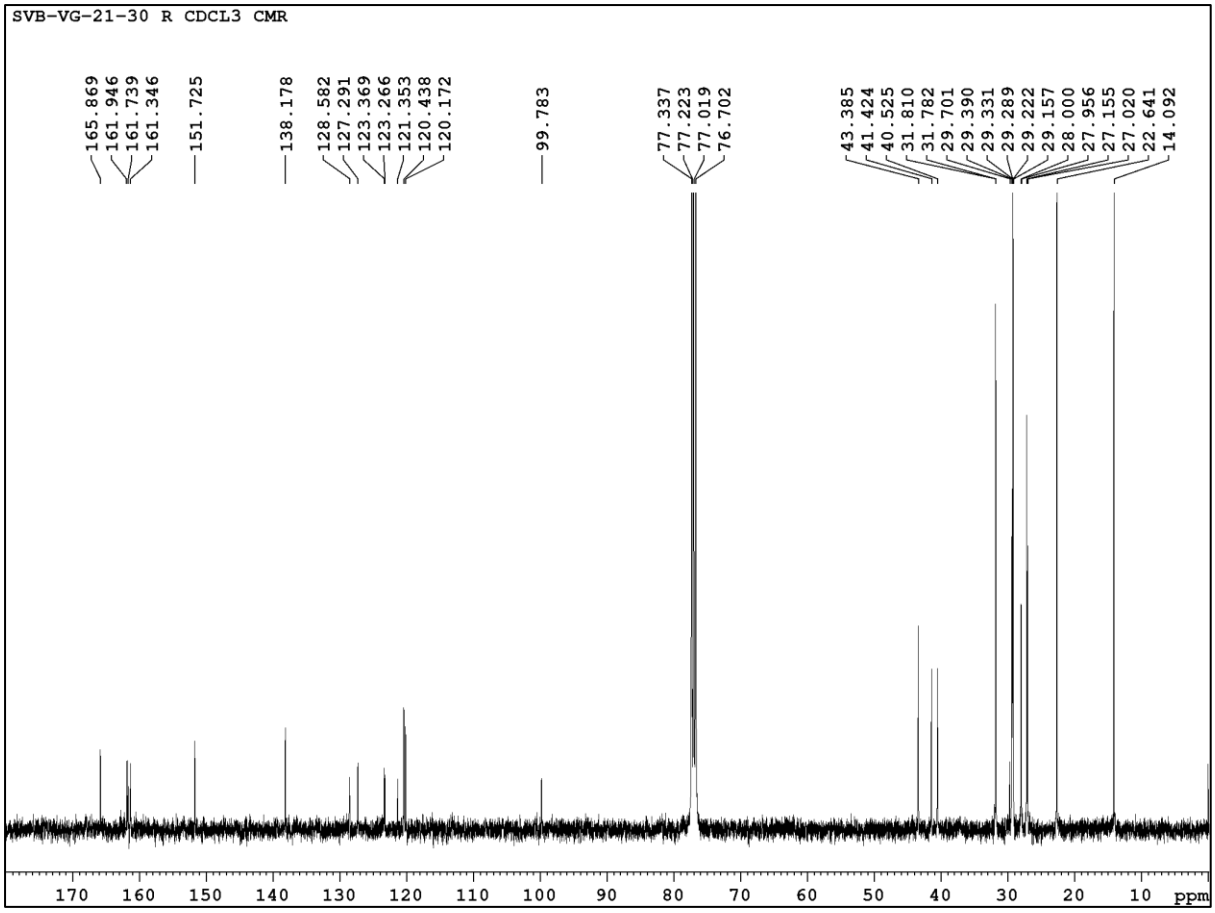


Figure S2. ^{13}C NMR spectra of Compound **6**

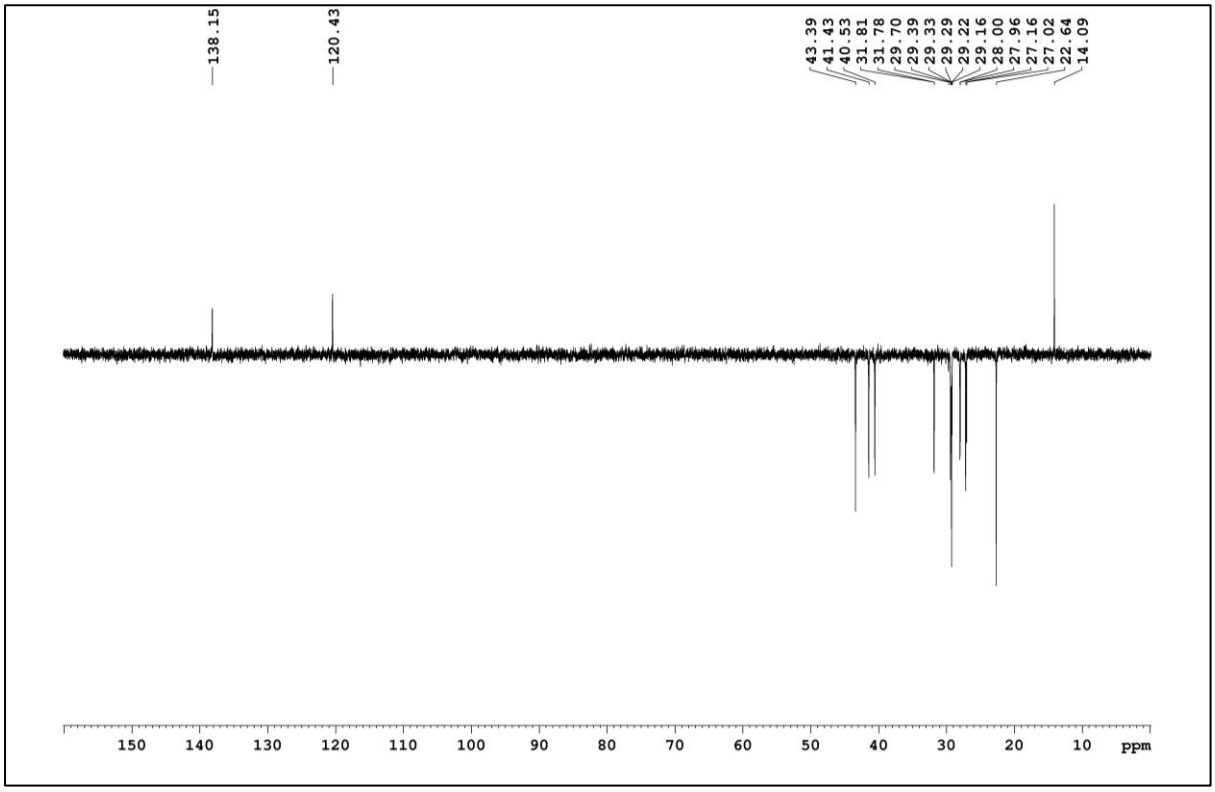
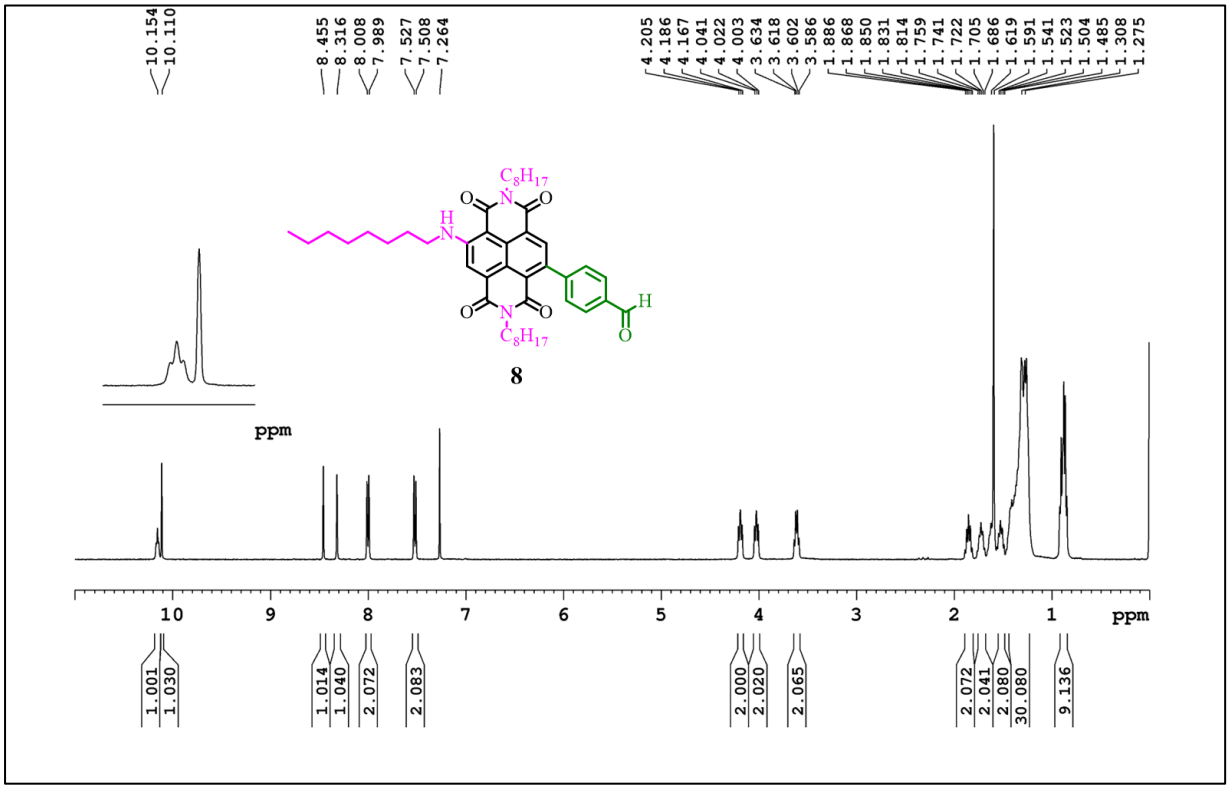


Figure S3. DEPT spectra of Compound **6**



8

Figure S4. ^{1}H NMR spectra of Compound **8**

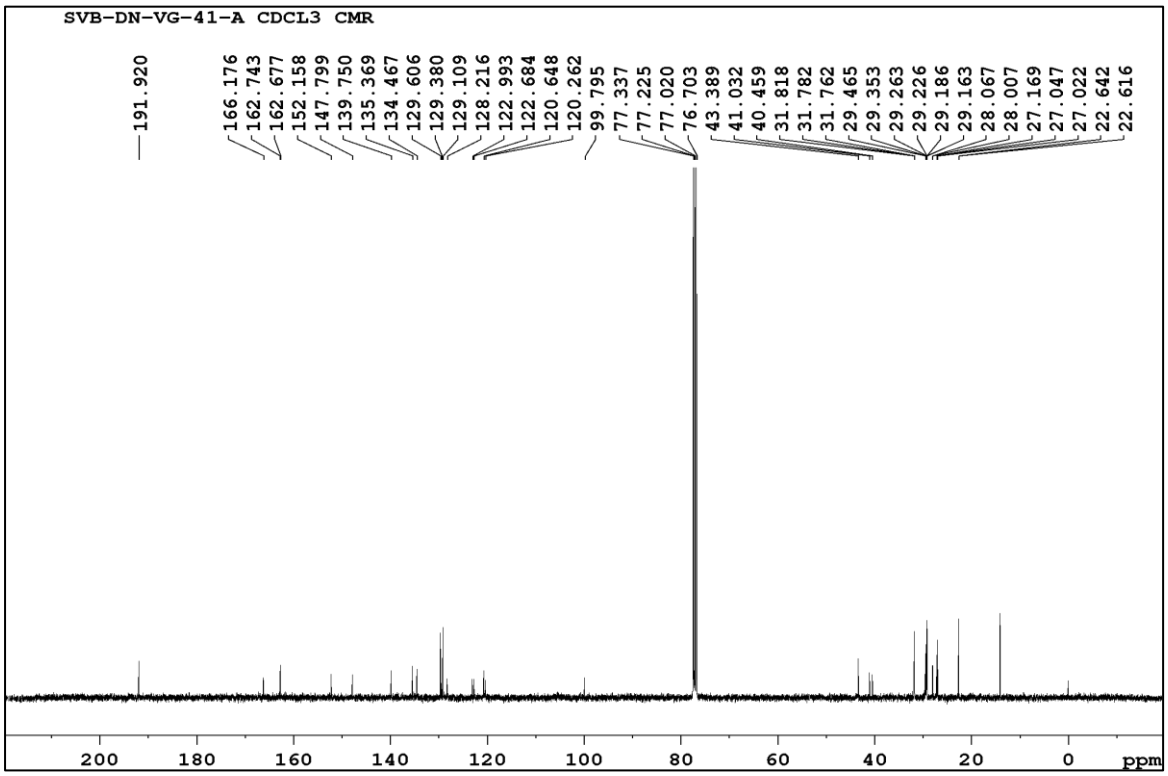


Figure S5. ^{13}C NMR spectra of Compound **8**

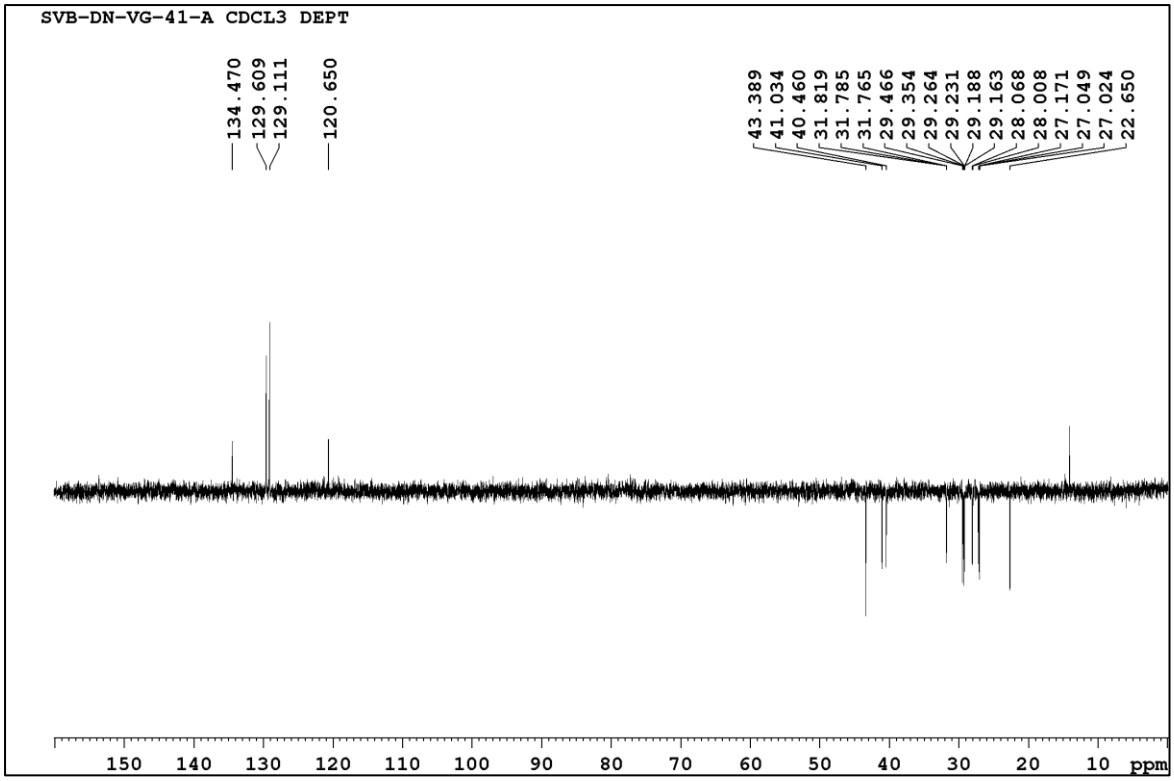


Figure S6. DEPT NMR spectra of Compound **8**

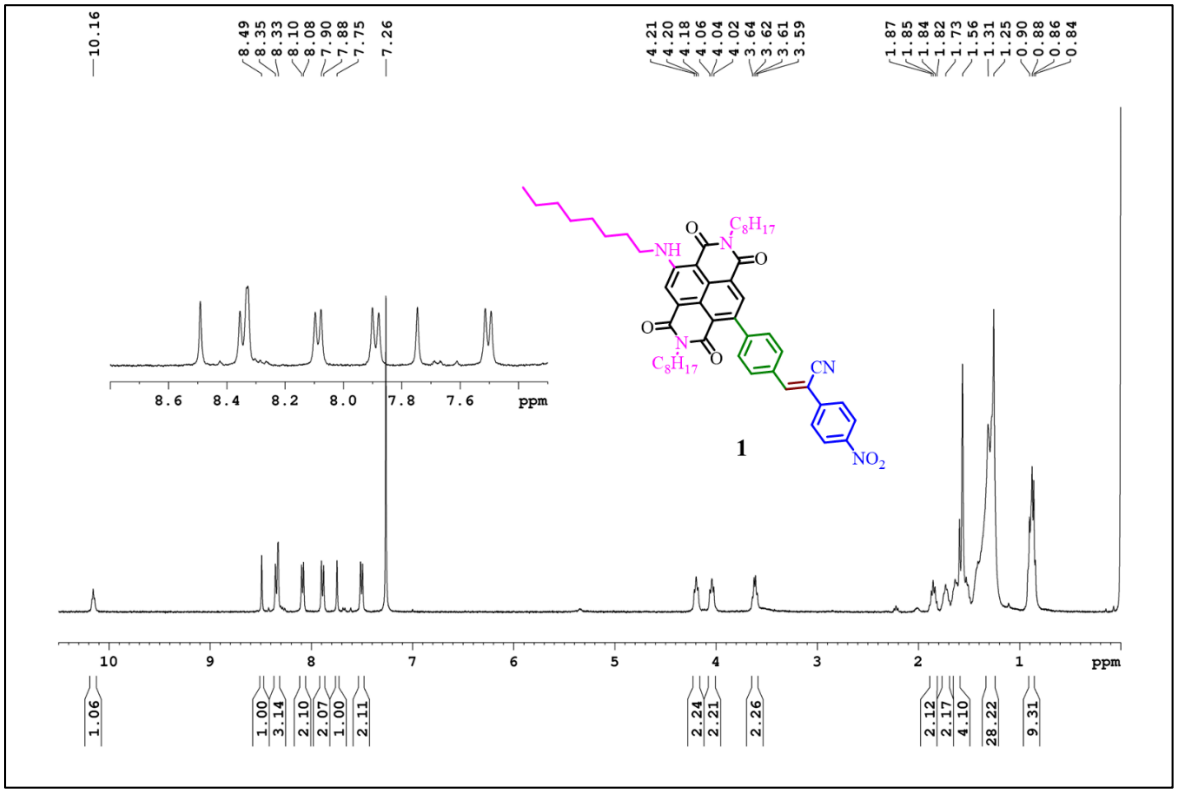


Figure S7. ^{1}H NMR spectra of Compound **1**

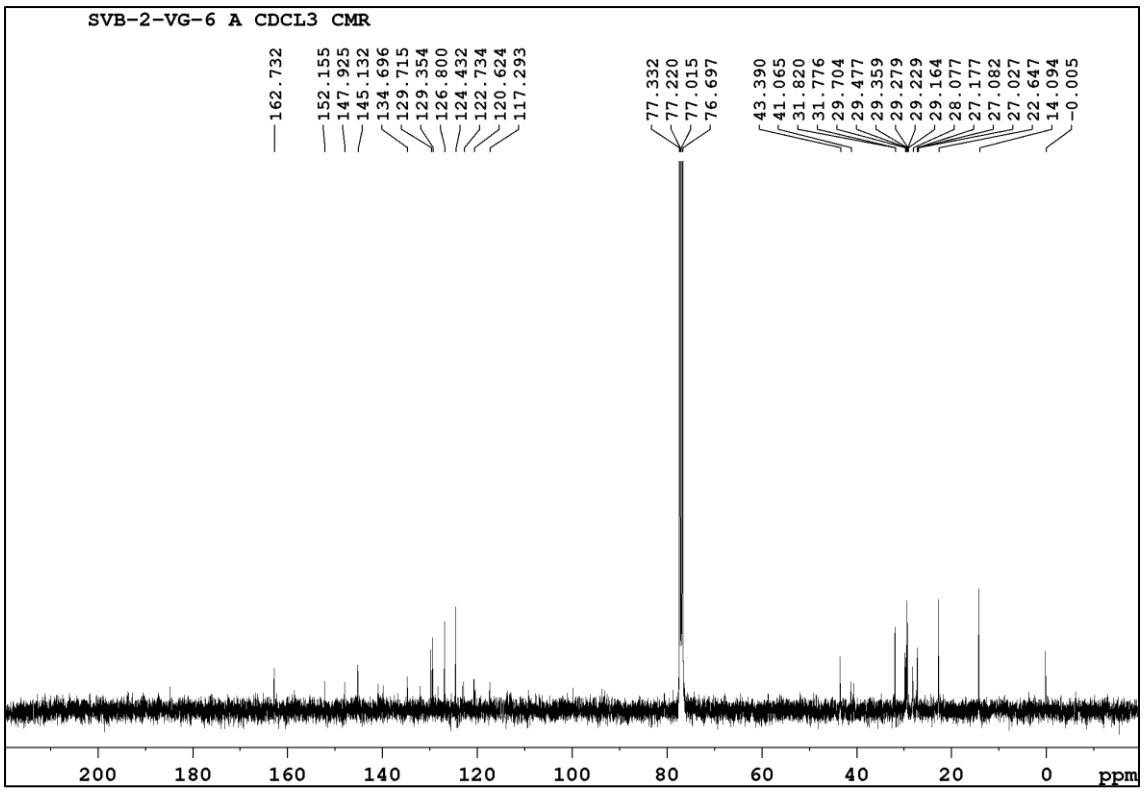


Figure S8. ^{13}C NMR spectra of Compound **1**

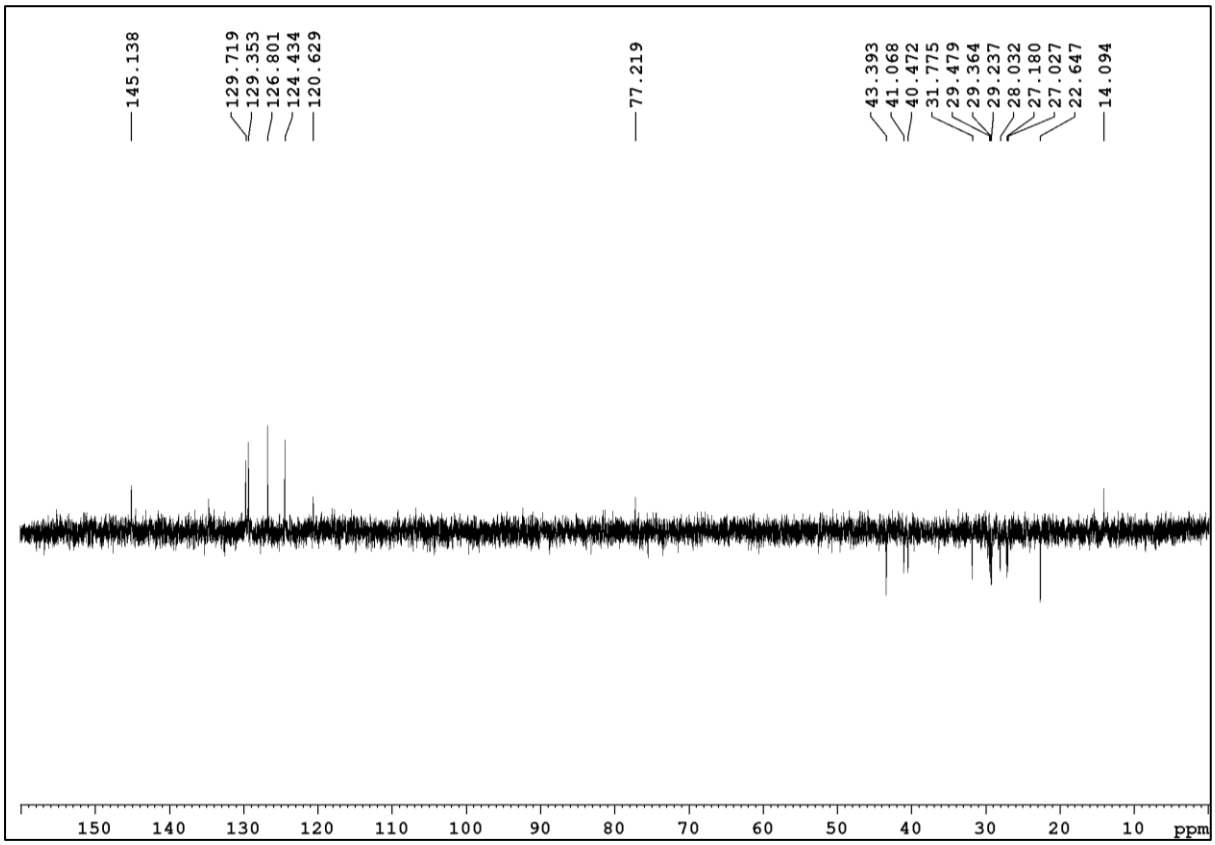


Figure S9. DEPT spectra of Compound **1**

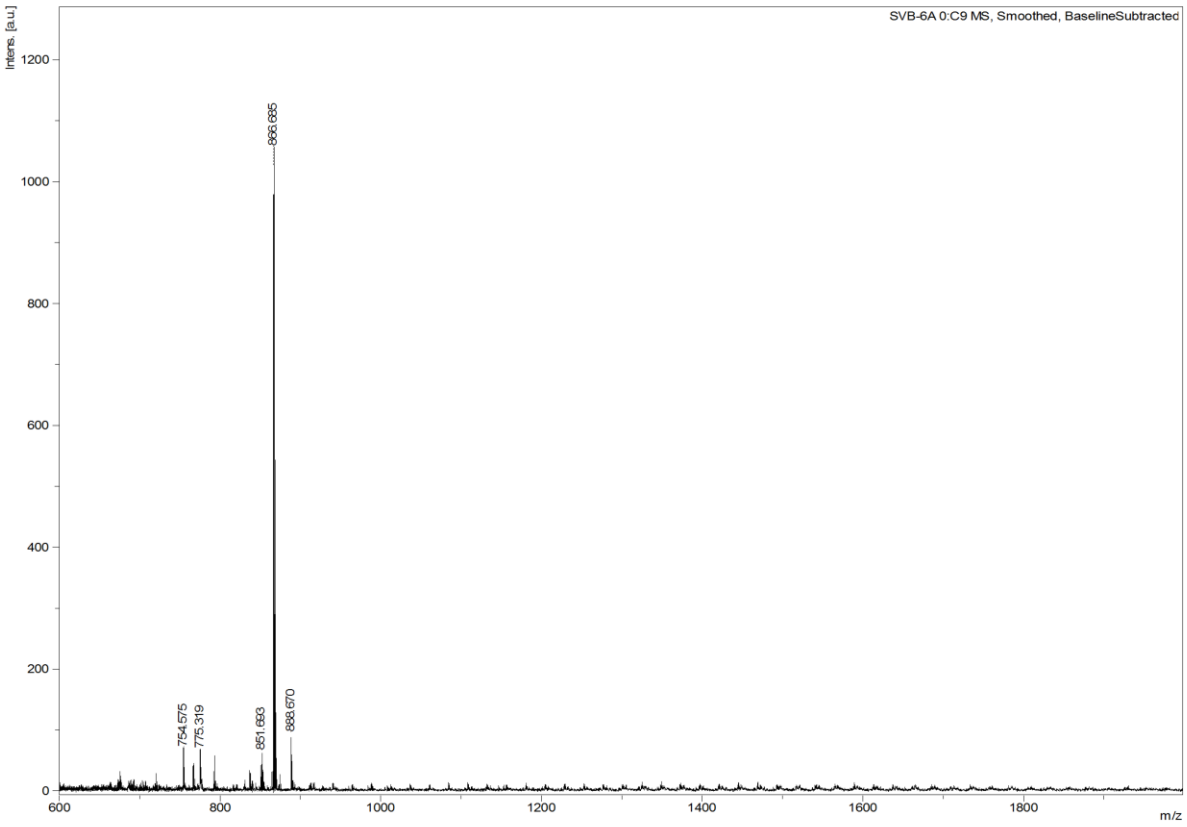


Figure S10. HRMS of Compound **1**

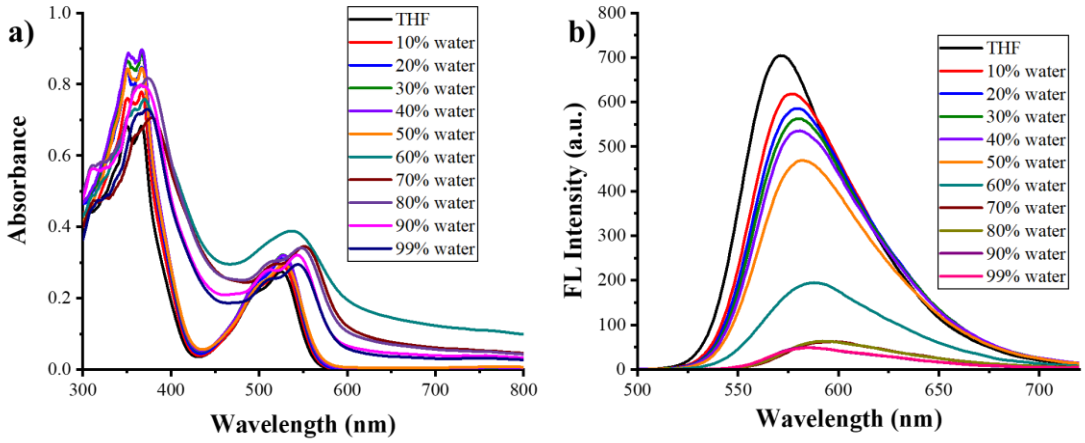


Figure S11. (a) UV−vis absorption spectra in THF/H_2O f_w (0 to 99%). (b) Fluorescence emission spectra of the NDI **1** in THF/H_2O (v/v) mixtures with different water fractions at λ_{ex} = 369 nm

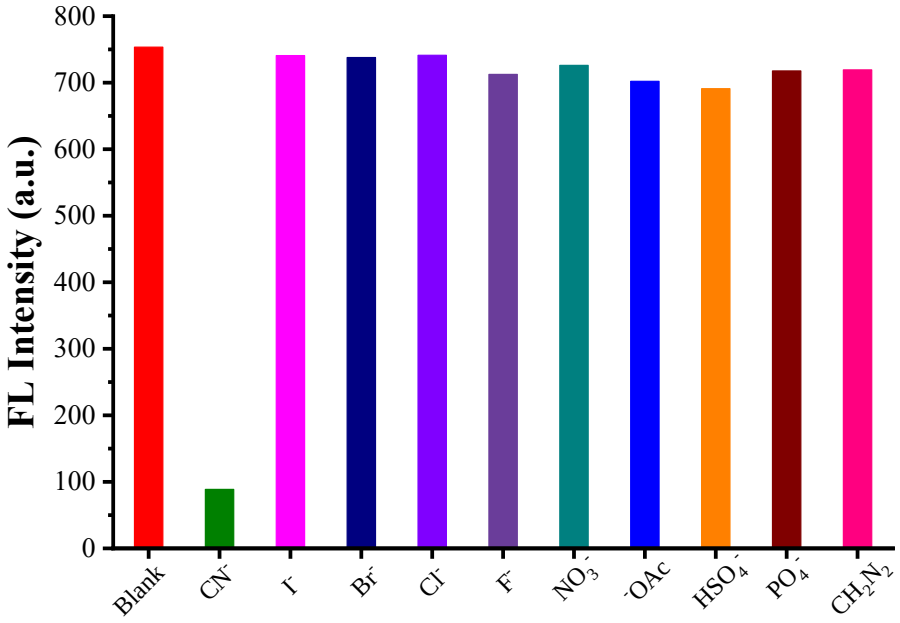


Figure S12. (a) Fluorescence responses of probe **1** toward 2 equiv. of CN^-, I^-, Br^-, Cl^-, F^-, NO_3^-, ^-OAc, HSO_4^-, $H_2PO_4^-$, and ClO_4^- at 575 nm wavelength in chloroform,

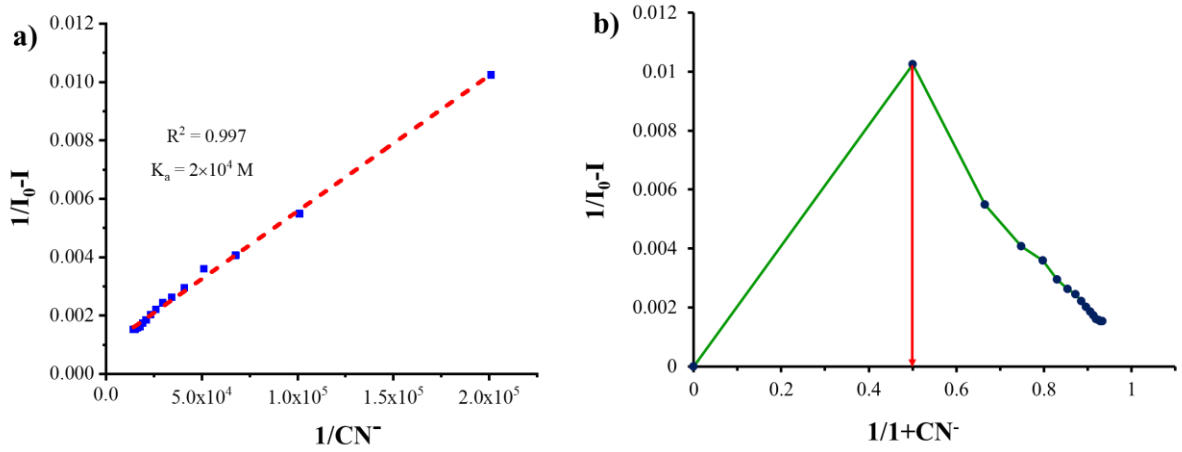


Figure S13. a) B-H plot b) Jobs plot

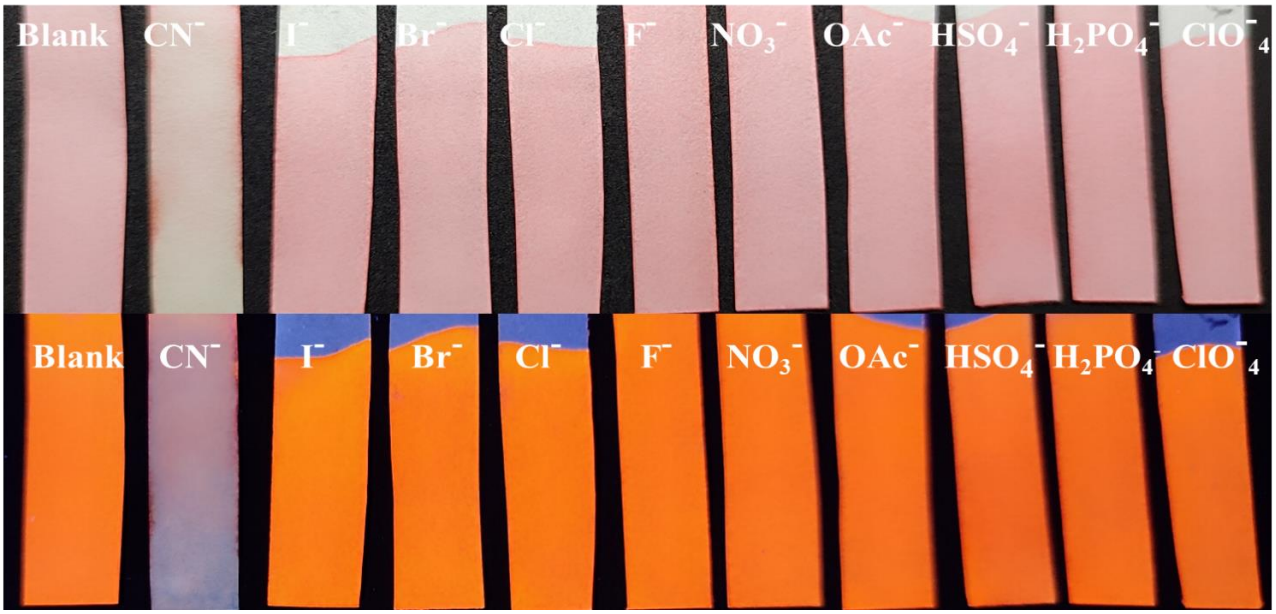


Figure S14. Paper strip based selectively detection of CN^- ion with the probe NDI **1**, over other anions used by naked eyes a) under visible light and b) under 365 nm UV light.

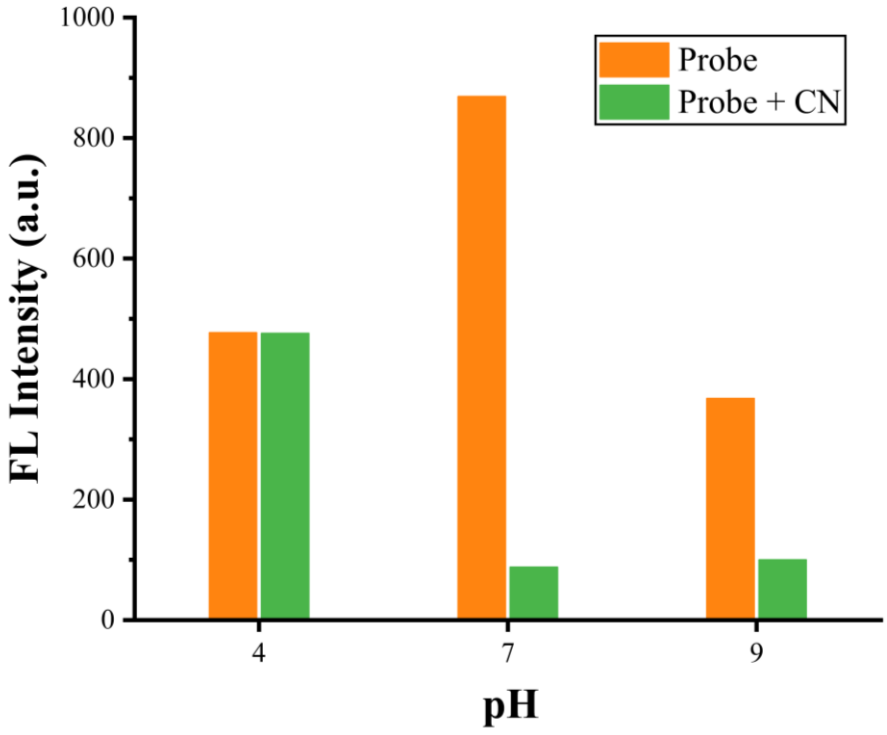


Figure S15. pH dependence study of probe **1** with CN

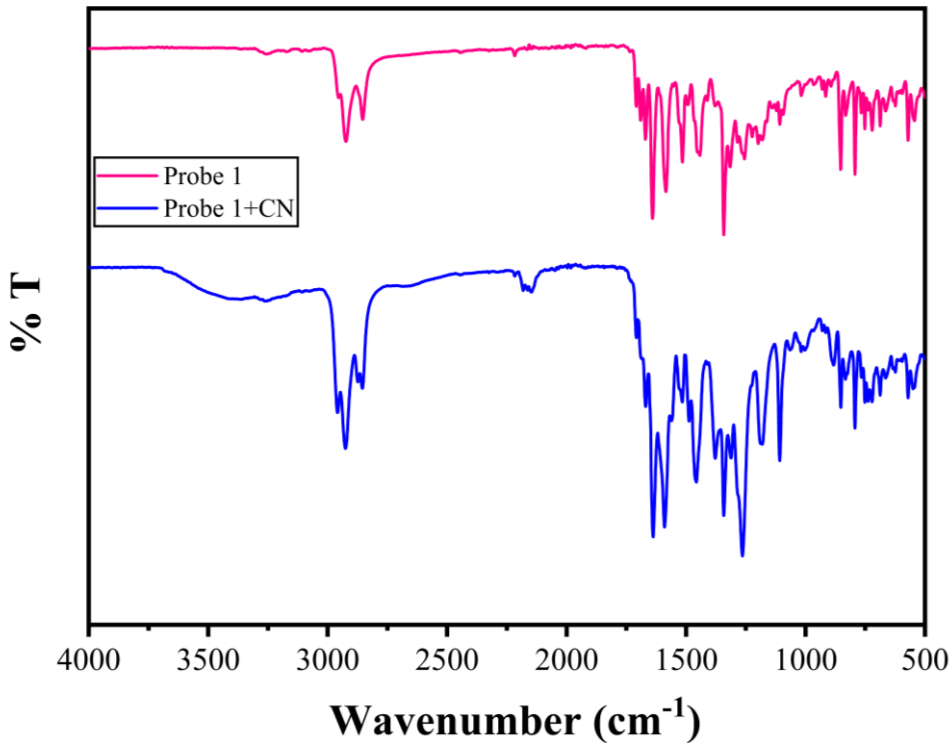


Figure S16. IR spectra of probe 1 with and without CN

Table S1. Fluorescence life time of **probe 1** and **probe 1+CN** in chloroform

Sample Code	Solvent	τ_1 (ns)	Contribution (%)
NDI-1	$CHCl_3$	7.58	100%
NDI-1 + CN	$CHCl_3$	7.88	-

Table S2: HOMO & LUMO of probe **1** and $1+CN^-$

1	**Orbital number**	**Orbital energy (eV)**	**Orbital picture**

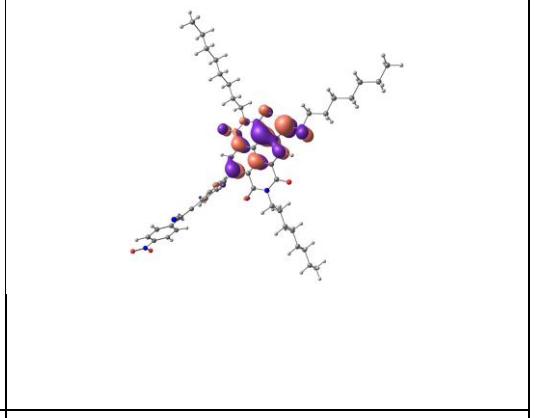
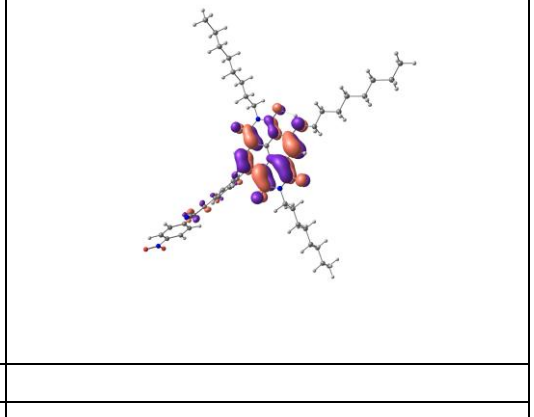
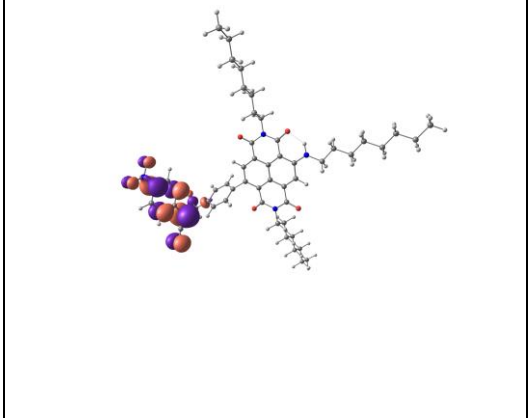
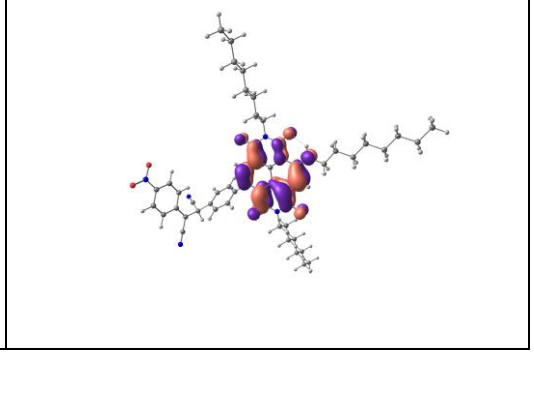
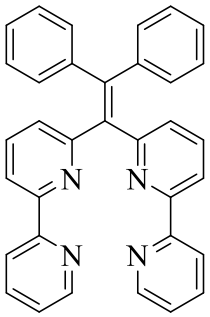
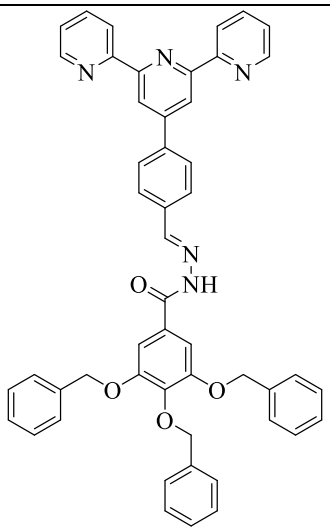
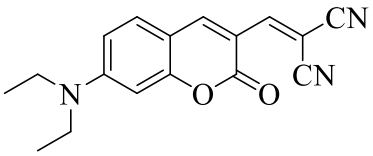
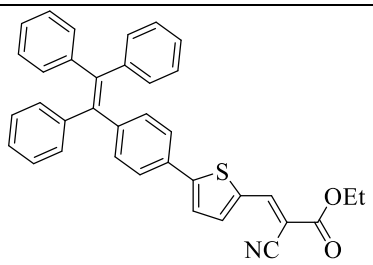
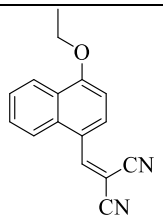
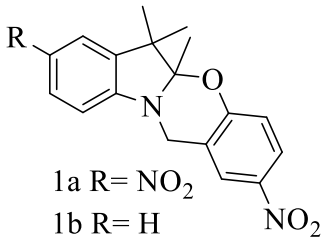
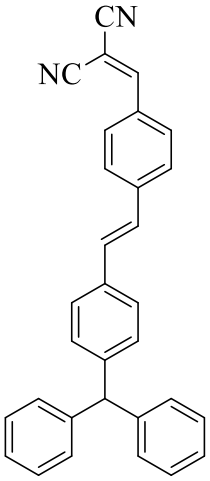
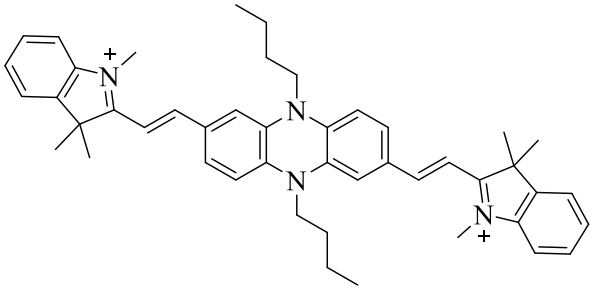
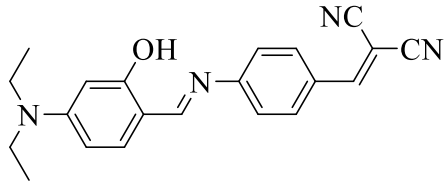
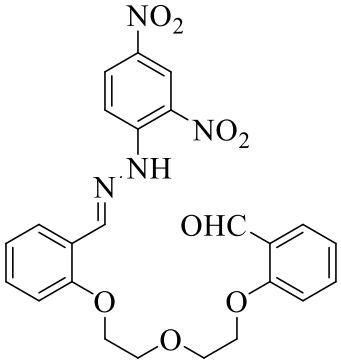
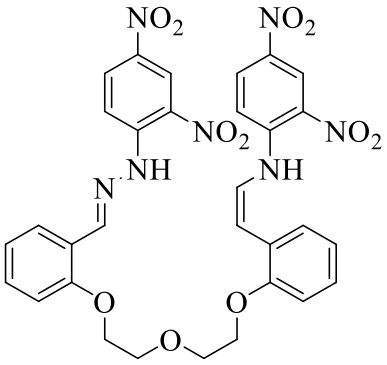
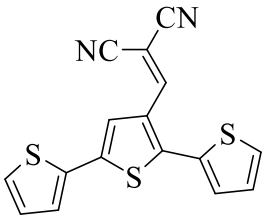
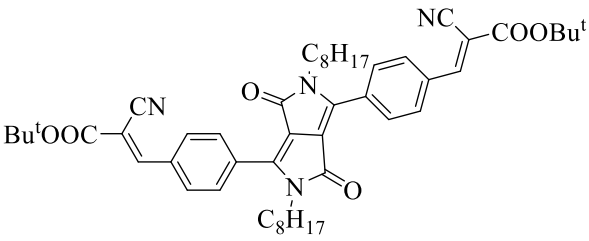
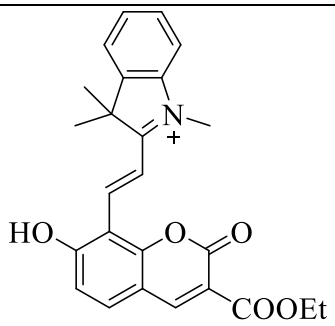
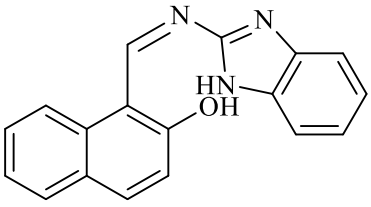
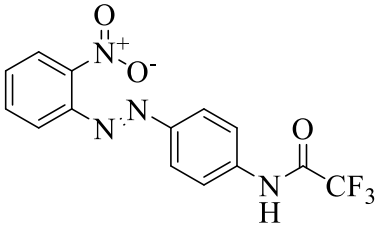
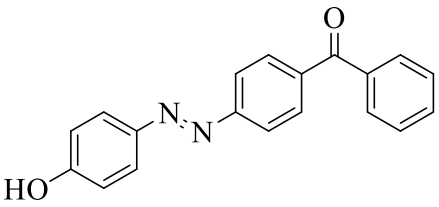
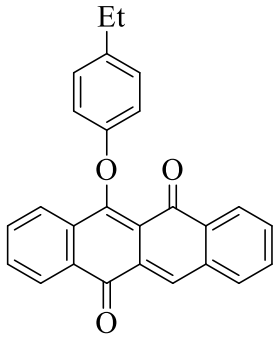
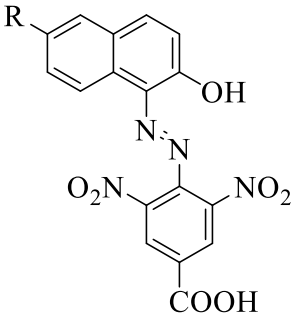
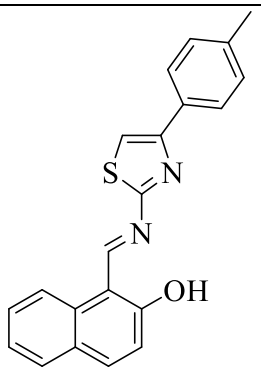
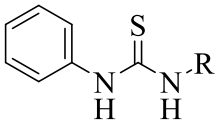
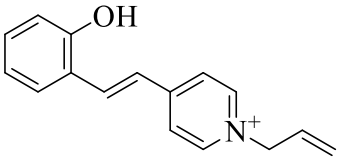
HOMO	232	-6.20	
LUMO	233	-3.45	
1+CN^-			
HOMO	239	-4.45	
LUMO	240	-3.12	

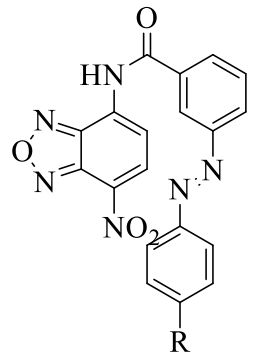
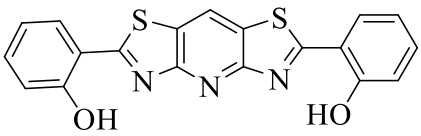
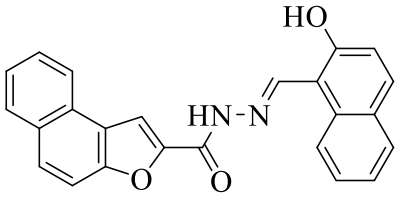
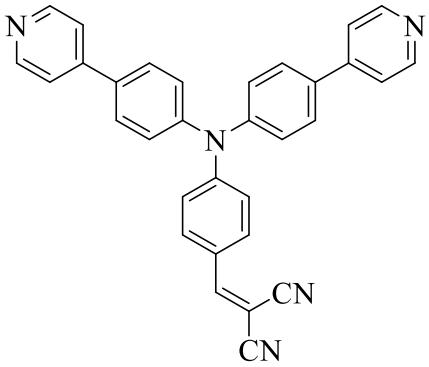
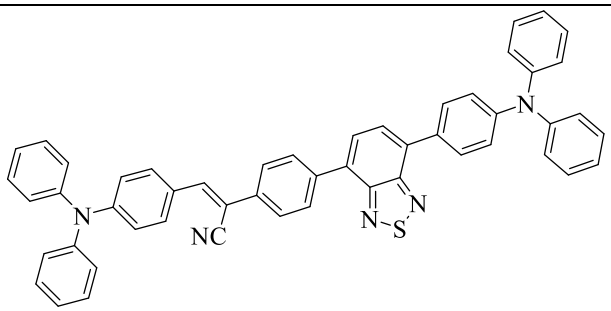
Table S3. Comparison of CN^- sensing with literature

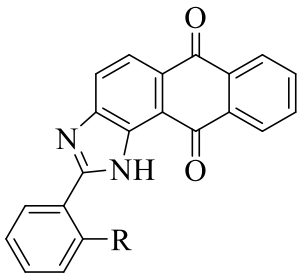
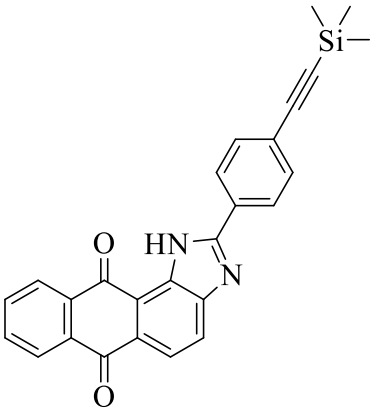
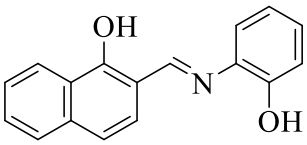
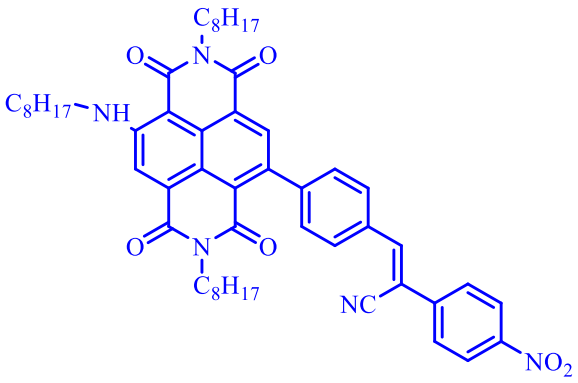
Compound	**Sensing method**	**LOD (μM)**	**Test strip**	**Ref.**
	Fluorescence turn-on	0.59	No	S[2]
	Fluorescence turn-on	1.09	No	S[3]
	Colorimetric Probe	1.5	No	S[4]
	Fluorescence turn-Off	0.67	Yes	S[5]
	Colorimetric Probe	1.1	Yes	S[6]

	Chemosensor	1	No	S[7]
	Fluorescence turn-on and colorimetric	66	No	S[8]
	Fluorescence turn-on	1.4	No	S[9]
	Fluorescence turn-off	2.4	yes	S[10]
	Colorimetric	3	yes	S[11]

	Colorimetric	1	yes	S[11]
	Fluorescence turn-on	6	No	S[12]
	Fluorescence turn-off	0.75	yes	S[13]
	Colorimetric chemosensor	9.8	yes	S[14]
	Fluorescence turn-on	14	yes	S[15]
	–	5	No	S[16]

	Colorimetric chemosensor	20	No	S[17]
	Photochromic sensor	5.26	No	S[18]
	Colorimetric sensor	0.744	No	S[19]
	Colorimetric chemosensor	19.4	No	S[20]
	Colorimetric sensor	1.27	Yes	S[21]
	Colorimetric sensor	8.0	Yes	S[22]

	Fluorescence sensor	1.5	No	S[23]
	Fluorescence turn-on	0.46	Yes	S[24]
	Fluorescence sensor	20.0	Yes	S[25]
	Fluorescence sensor	6	No	S[26]
	Fluorescence turn-on	5	Yes	S[27]

	Fluorescence turn-on	0.6	No	S[28]
	Colorimetric and Fluorescence	1.30	No	S[29]
	Fluorescence sensor	1.5	No	S[30]
	Naked eye, Colorimetric, Fluorescence sensor	0.41	Yes	This Work

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