Supporting Information

Catalytic cyanation of aryl iodides using DMF and ammonium bicarbonate as the combined source of cyanide: A dual role of copper catalyst

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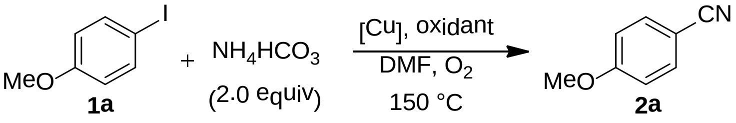
1. General Methods

Unless otherwise stated, all commercial reagents and solvents were used as purchased without additional purification. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F254 plates. Visualization on TLC was achieved by the use of UV light (254 nm) and treatment with *p*-anisaldehyde, phosphomolybdic acid or ceric ammonium molybdate stain followed by heating. Flash column chromatography was undertaken on silica gel (Merck Kieselgel 60 F254 400-630 mesh). ^{1}H NMR was recorded on Bruker FT AM 400 (400 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = double of doublet, dt = double of triplet, td = triple of doublet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR and inverse gated decoupled ^{13}C NMR spectra were recorded on Brucker FT AM 400 (100 MHz) and were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-d. Infrared (IR) spectra were recorded neat in 0.5 mm path length using a sodium chloride cell. Frequencies are given in reciprocal centimeters (cm-1) and only selected absorbance is reported. High resolution mass spectra were obtained from the Korea Basic Science Institute (Daegu) by using EI method. Unless otherwise stated, all commercial reagents and solvents were used without additional puri fication.

2. Optimization for the Copper-Catalyzed Cyanation of 4-Iodoanisole

An oven-dried round bottom Schlenk flask (10 mL) equipped with a magnetic stir bar were charged with 4-iodoanisole (70.2 mg, 0.3 mmol), NH_4HCO_3 (2.0 equiv), Cu source (10 - 20 mol %), oxidant (if solid at room temperature; 0.4 - 4.0 equiv). Then it was evacuated and backfilled with oxygen (this process was repeated 3 times). Oxidant (if liquid at room temperature, 40 mol % - 4.0 equiv) and DMF (1.5 mL) were added. The reaction mixture was stirred for given time at 150 ^{o}C, cooled to room temperature, and diluted with EtOAc and aqueous NH_3 solution (3 M). The reaction mixture was filtered through a short pad of celite and washed with EtOAc (in case of using Ag_2CO_3 as a oxidant). Then two layers were separated, and the aqueous layer was extracted with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The NMR yield of product **(2a)** was determined by integration using an internal standard (1,1,2,2-tetrachloroethane).

Table S1: Optimization of Reaction Conditions[a]



entry	[Cu] (mol %)	oxidant (equiv.)	time (h)	yield (%)[b]
1	$Cu(NO_3)_2·3H_2O$ (20)	TBHP in decane (4.0)	48	42
2	$Cu(NO_3)_2·3H_2O$ (20)	TBHP in H_2O (4.0)	48	38
3	$Cu(NO_3)_2·3H_2O$ (20)	^{t}BuOO^{t}Bu (4.0)	48	12
4	$Cu(NO_3)_2·3H_2O$ (20)	H_2O_2 (4.0)	48	7
5	$Cu(NO_3)_2·3H_2O$ (20)	PIDA (1.2)	48	21
6	$Cu(NO_3)_2·3H_2O$ (20)	DDQ (2.0)	48	0[c]
7	$Cu(NO_3)_2·3H_2O$ (20)	TEMPO (1.0)	24	50
8	$Cu(NO_3)_2·3H_2O$ (20)	NMO (1.0)	24	9
9	$Cu(NO_3)_2·3H_2O$ (20)	Ag_2CO_3 (1.5)	24	85
10	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (0.4)	24	80(76)[d]
11	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (0.4)	24	66[e]
12	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2O (0.4)	24	67
13	$Cu(NO_3)_2·3H_2O$ (10)	AgOTf (0.4)	24	62
14	$Cu(NO_3)_2·3H_2O$ (10)	AgOAc (0.4)	24	44
15	CuI (10)	Ag_2CO_3 (0.4)	24	26
16	$CuSO_4$ (10)	Ag_2CO_3 (0.4)	24	16
17	$CuBr_2$ (10)	Ag_2CO_3 (0.4)	24	<5
18	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (0.4)	24	50[f]
19	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (0.4)	24	9[g]
20	–	Ag_2CO_3 (0.4)	24	0
21	$Cu(NO_3)_2·3H_2O$ (10)	–	24	16
22	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (1.0)	24	<5[h]
23	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (1.0)	24	22[i]
24	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (1.0)	24	11[j]
25	$Cu(NO_3)_2·3H_2O$ (10)	Ag_2CO_3 (1.0)	24	27[k]

[a] Reaction conditions: **1a** (0.3 mmol), NH_4HCO_3 (2.0 equiv), oxidant, and [Cu] in DMF (1.5 mL) under O_2 balloon at 150 °C for indicated time. [b] ^{1}H NMR yield (internal standard: 1,1,2,2 tetrachloroethane). [c] Decomposition. [d] Isolated yield in the parenthesis. [e] Run at 140 °C. [f] Under air atmosphere. [g] Under N_2 atmosphere. Instead of DMF [h] DMSO. [i] DMA. [j] NMP. [k] DMPU.

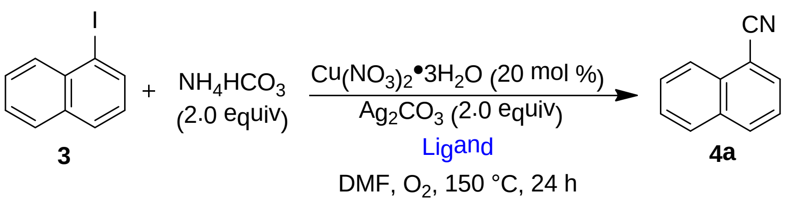
3. General Procedure for the Copper-Catalyzed Cyanation of Electron-rich Aryl Iodides

An oven-dried 10 mL round bottom Schlenk flask equipped with a magnetic stir bar were charged with aryl iodides (0.3 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (10 - 20 mol %), NH_4HCO_3 (2.0 equiv, 0.6 mmol), and Ag_2CO_3 (0.4 - 1.0 equiv). Then it was evacuated and backfilled with oxygen (this process was repeated 3 times). Then DMF (1.5 mL) was added and the reaction mixture was stirred for 24 h at 150 ^oC, cooled to room temperature, and diluted by adding EtOAc and 3 M aqueous NH_3 solution. The reaction mixture was filtered through a short pad of celite and was washed with EtOAc. Two layers were separated, and the aqueous layer was extracted with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated in *vacuo*. The residue was purified by column chromatography to give the cyanated product.

4. Optimization Study for Ligand Effects in the Copper-Catalyzed Cyanation of 1-Iodonaphthalene

An oven-dried round bottom Schlenk flask (10 mL) equipped with a magnetic stir bar were charged with $Cu(NO_3)_2 \cdot 3H_2O$ (20 mol %), Ag_2CO_3 (2.0 equiv, 0.6 mmol), NH_4HCO_3 (2.0 equiv) and ligand (if solid at room temperature; 20 mol %). Then it was evacuated and backfilled with oxygen (this process was repeated 3 times). 1-Iodonaphthalene (**3**) and ligand (if liquid at room temperature, 20 mol %) and DMF (1.5 mL) were added to reaction mixture. The reaction mixture was stirred for 24 h at 150 ^oC, cooled to room temperature, and diluted with EtOAc and aqueous NH_3 solution (3 M). The reaction mixture was filtered through a short pad of celite and washed with EtOAc. Then two layers were separated, and the aqueous layer was extracted with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The NMR yield of the product **4a** was determined by integration using an internal standard (1,1,2,2-tetrachloroethane).

***Table S2*:** Ligand Effect in the Copper-Catalyzed Cyanation of 1-Iodonaphthalene[a]



entry	Ligand (20 mol %)	Yield (%)[b]	Remained **3** (%)[b]
1	1,10-Phenanthroline	61	11
2	Bathocuproine	43	49
3	4,7-Dihydroxy-1,10-phenanthroline	45	43
4	2,2'-Bipyridine	54	14
5	4,4'-Dimethoxy-2,2'-bipyridine	47	38

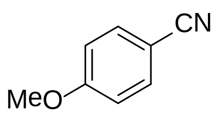
6	4,4'-Di-*tert*-butyl-2,2'-bipyridyl	42	47
7	L-Proline	35	53
8	Dipiperidinomethane	59	27
9	1,4-Diazabicyclo[2.2.2]octane	55	20
10	2-Picolinic acid	52	30
11	2-(Methylamino)pyridine	59	21
12	*N*,*N*,*N′*,*N′*-Tetramethylethylenediamine	75	0
13	*N*-Methylpiperazine	73	0
14	(±)-*trans*-1,2-Diaminocyclohexane	72	12
15	2-Aminopyridine	85	0

[a] Reaction conditions: **3** (0.3 mmol), NH_4HCO_3 (2.0 equiv), $Cu(NO_3)_2{\cdot}3H_2O$ (20 mol %), Ag_2CO_3 (2.0 equiv) and ligand (20 mol %) in DMF (1.5 mL) under O_2 balloon at 150 °C for 24 h. [b] ^{1}H NMR yield (internal standard:1,1,2,2 tetrachloroethane)

5. General Procedure for the Copper-Catalyzed Cyanation Using 2-Aminopyridine as a Ligand

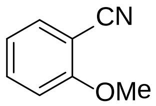
An oven-dried 10 mL round bottom Schlenk flask equipped with a magnetic stir bar and charged with aryl iodides (0.3 mmol), $Cu(NO_3)_2{\cdot}3H_2O$ (20 mol %, 0.06 mmol), NH_4HCO_3 (2.0 equiv, 0.6 mmol), Ag_2CO_3 (2.0 equiv, 0.6 mmol) and 2-aminopyridine (20 mol %, 0.06 mmol) was evacuated and backfilled with oxygen (this process was repeated 3 times). Then DMF (1.5 mL) was added. The reaction mixture was stirred for 24 h at 150 °C, and cooled to room temperature, diluted by adding EtOAc and 3 M aqueous NH_3 solution. The reaction mixture was filtered through a short pad of celite, and washed with EtOAc. Two layers were separated, and the aqueous layer was extracted with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated in *vacuo*. The residue was purified by column chromatography to give the cyanated product.

6. Characterization Data of Cyanated Products



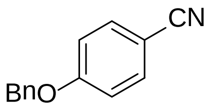
2a

4-Methoxybenzonitrile[1] **(2a)**; Eluents (EtOAc/hexane = 3:7, R_f = 0.6), white solid; m.p. 58-59 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 6.8, 2.1 Hz, 2H), 6.95 (dd, *J* = 6.8, 2.1 Hz, 2H), 3.86(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 133.9, 119.2, 114.7, 103.9, 55.5.



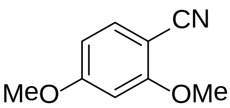
2b

2-Methoxybenzonitrile[1] **(2b)**; Eluents (EtOAc/hexane = 3:7, R_f = 0.5), yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.50 (m, 2H), 7.06-6.94 (m, 2H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 134.3, 133.7, 120.7, 116.4, 111.2, 101.8, 55.9.



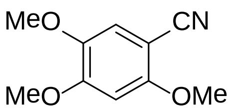
2c

4-(Benzyloxy)benzonitrile[1] **(2c)**; Eluents (EtOAc/hexane = 1:4, R_f = 0.5), white solid; m.p. 93-94 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 6.8, 2.1 Hz, 2H), 7.42-7.30 (m, 5H), 7.00 (dd, *J* = 6.8, 2.1 Hz, 2H), 5.10 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 135.7, 134.0, 128.7, 128.4, 127.4, 119.1, 115.6, 104.2, 70.3.



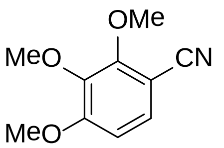
2d

2,4-Dimethoxybenzonitrile[1] **(2d)**; Eluents (EtOAc/hexane = 3:7, R_f = 0.5), pale-yellow solid; m.p. 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.6 Hz, 1H), 6.51 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.46 (d, *J* = 2.3 Hz, 1H), 3.90 (s, 3H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 162.8, 134.9, 116.9 105.7, 98.5, 94.1 55.9, 55.7.



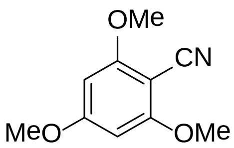
2e

2,4,5-Trimethoxybenzonitrile[1,2] **(2e)**; Eluents (EtOAc/hexane = 2:3, R_f = 0.4), yellow solid; m.p. 106-107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 (s, 1H), 6.48 (s, 1H), 3.92 (s, 3H), 3.89 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 154.1, 143.0, 116.9, 114.8, 96.5, 91.5, 56.5, 56.1.



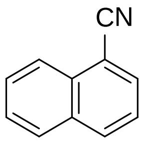
2f

2,3,4-Trimethoxybenzonitrile[2] **(2f)**; Eluents (EtOAc/hexane = 2:3, R_f = 0.5), Pale-yellow solid; m.p. 55-56 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.8 Hz, 1H), 6.69 (d, *J* = 8.8 Hz, 1H), 4.06 (s, 3H), 3.91 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 155.9, 141.9, 128.7, 116.5, 107.5, 99.2, 61.7, 61.1, 56.2.



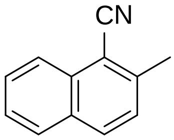
2g

2,4,6-Trimethoxybenzonitrile[1] **(2g)**; Eluents (EtOAc/hexane = 2:3, R_f = 0.4), white solid; m.p. 137-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.05 (s, 2H), 3.86 (s, 6H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 163.7, 114.5, 90.3, 84.0, 56.0, 55.6.



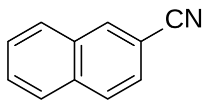
4a

1-Naphthonitrile[1] **(4a)**; Eluents (EtOAc/hexane = 1:9, R_f = 0.5), yellow liquid; ^{1}H NMR (400 MHz, CDC13) δ 8.23 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.95 – 7.86 (m, 2H), 7.74-7.65 (m, 1H), 7.64 – 7.58 (m, 1H), 7.51 (dd, *J* = 8.4, 7.2 Hz, 1H); ^{13}C NMR (100 MHz, CDC13) δ 133.2, 132.9, 132.6, 132.3, 128.6, 128.5, 127.5, 125.1, 124.9, 117.7, 110.2.



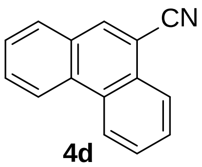
4b

2-Methyl-1-naphthonitrile[3] **(4b)**; Eluents (EtOAc/hexane = 1:9, R_f = 0.5), colourless solid; m.p. 84-85 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.3 Hz, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.64 (dd, *J* = 8.2, 7.0 Hz, 1H), 7.53 (dd, *J* = 8.0, 7.0 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 2.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 132.7, 132.5, 131.1, 128.5, 128.3, 127.6, 126.5, 124.8, 117.0, 109.2, 21.2.



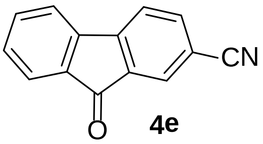
4c

2-Naphthonitrile[1] **(4c)**; Eluents (EtOAc/hexane = 1:9, R_f = 0.5), white solid; m.p. 63-64 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.88 (t, *J* = 8.4 Hz, 3H), 7.68 – 7.55 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.6, 134.1, 132.2, 129.1, 129.0, 128.3, 128.0, 127.6, 126.3, 119.2, 109.3.



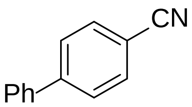
4d

Phenanthrene-9-carbonitrile[1] **(4d)**; Eluents (EtOAc/hexane = 1:9, R_f = 0.6), white solid; m.p. 108-109 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 – 8.65 (m, 2H), 8.30 (d, *J* = 9.6 Hz, 1H), 8.24 (s, 1H), 7.93 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.84 – 7.72 (m, 3H), 7.68 (td, *J* = 8.0, 1.1 Hz, 1H); ^{13}C NMR (100 MHz, CDCl3) δ 135.6, 131.7, 130.0, 129.8, 129.7, 129.4, 128.8, 128.2, 128.1, 127.6, 126.1, 123.0, 122.8, 117.9, 109.4.



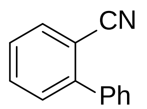
4e

2-Cyano-9*H*-fluoren-9-one[4] **(4e)**; Eluents (CH_2Cl_2/hexane = 3:2, R_f = 0.4), orange solid; m.p. 171-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ δ 7.87 (s, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.4 Hz, 1H), 7.68 – 7.54 (m, 3H), 7.42 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ δ 191.2, 148.0, 142.6, 138.4, 135.3, 134.5, 134.1, 130.8, 127.4, 124.9, 121.4, 120.9, 118.0, 112.6; HRMS (EI) m/z calcd. for $C_{14}H_7NO$ $[M]^+$: 205.0528, found: 205.0526.



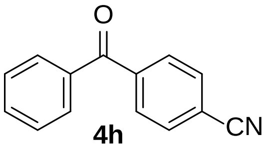
4f

4-Phenylbenzonitrile[1] (4f); Eluents (EtOAc/hexane = 1:4, R_f = 0.6), pale-yellow solid; m.p. 83-84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.65 (m, 4H), 7.62 – 7.56 (m, 2H), 7.53 – 7.40 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 139.1, 132.5, 129.1, 128.6, 127.7, 127.2, 118.9, 110.9.



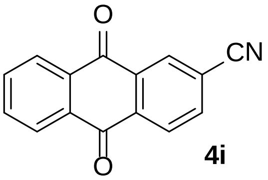
4g

2-Phenylbenzonitrile[5] (4g); Eluents (EtOAc/hexane = 1:4, R_f = 0.5), yellow solid; m.p. 38-39 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.57 (td, *J* = 7.7, 1.4 Hz, 1H), 7.60 – 7.38 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 138.1, 133.7, 132.7, 130.0, 128.71, 128.68, 127.5, 118.7, 111.3.



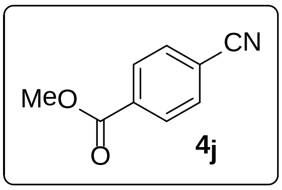
4h

4-Cyanobenzophenone[6] (4h); Eluents (EtOAc/hexane = 1:4, R_f = 0.4), white solid; m.p. 113-114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.84 (m, 2H), 7.82 – 7.75 (m, 4H), 7.64 (tt, *J* = 7.5, 1.4 Hz, 1H), 7.56 – 7.46 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 141.2, 136.3, 133.3, 132.1, 130.2, 130.0, 128.6, 117.9, 115.6; HRMS (EI) m/z calcd. for $C_{14}H_9NO$ $[M]^+$: 207.0684, found: 204.0685.

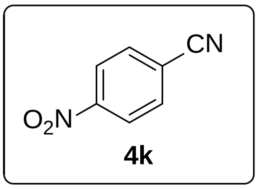


4i

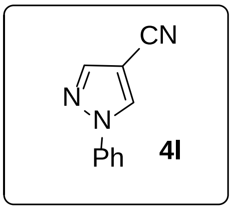
9,10-Dioxo-9,10-dihydroanthracene-2-carbonitrile (4i); Eluents (CH_2Cl_2/hexane = 3:2, R_f = 0.4), yellow solid; m.p. 210-211 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (dd, *J* = 1.7, 0.6 Hz, 1H), 8.43 (dd, *J* = 8.0, 0.6 Hz, 1H), 8.38 – 8.30 (m, 2H), 8.05 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.90 – 7.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.7, 181.2 136.6, 135.6, 134.85, 134.82, 133.8, 133.1, 133.0, 131.3, 128.0, 127.61, 127.60, 117.8, 117.2, IR (neat) 3075, 3039, 2922, 2852, 2233, 1672, 1586, 1287, 1198, 931, 814, 707 cm^{-1}; HRMS (EI) m/z calcd. for $C_{15}H_7NO_2$ $[M]^+$: 233.0477, found: 233.0478.



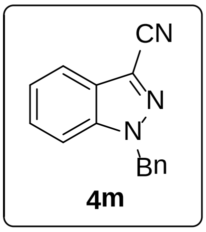
Methyl 4-cyanobenzoate[7] (4j); Eluents (EtOAc/hexane = 1:4, R_f = 0.5), white solid; m.p. 66-67 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.8 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 2H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 133.9, 132.2, 130.1, 117.9, 116.4, 52.7.



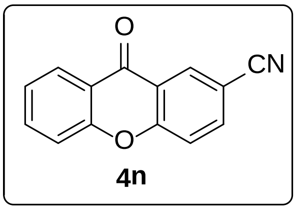
4-Nitrobenzonitrile[1] (4k); Eluents (EtOAc/hexane = 3:7, R_f = 0.6), yellow solid; m.p. 140-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 6.9, 2.0 Hz, 2H), 7.87 (dd, *J* = 6.9, 2.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 133.4, 124.3, 118.3, 116.7.



1-Phenyl-1*H*-pyrazole-4-carbonitrile[8] (4l); Eluents (EtOAc/hexane = 3:7, R_f = 0.5), pale-yellow solid; m.p. 91-92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.98 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.54 – 7.45 (m, 2H), 7.44 – 7.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 138.7, 131.8, 129.7, 128.2, 119.8, 113.0, 94.3; HRMS (EI) m/z calcd. for $C_7H_7N_3$ [*M*]+: 169.0640, found: 169.0643.



1-Benzyl-1*H*-indazole-3-carbonitrile (4m); Eluents (EtOAc/hexane = 3:7, R_f = 0.5), white solid; m.p. 94-95 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.44 – 7.38 (m, 2H), 7.32 – 7.23 (m, 4H), 7.21 – 7.16 (m, 2H), 5.60 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 134.9, 128.9, 128.4, 127.9, 127.4, 125.7, 123.6, 119.7, 118.0, 113.5, 110.4, 54.3, IR (neat) 2230, 1672, 1495, 1459, 1444, 1351, 1323, 1307, 1156, 1111, 740, 698 cm^{-1}; HRMS (EI) m/z calcd. for $C_{15}H_{11}N_3$ [*M*]+: 233.0953, found: 233.0955.



2-Cyano-9*H*-xanthen-9-one[9] **(4n);** Eluents (CH_2Cl_2/hexane = 4:1, R_f = 0.5), white solid; m.p. 219-220 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 2.1 Hz, 1H), 8.32 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.93 (dd, *J* = 8.8, 2.1 Hz,1H), 7.79 (td, *J* = 7.0 Hz, 1.8 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.46 (td, *J* = 8.0, 1,1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 158.0, 155.8, 136.8, 135.7, 132.3, 126.9, 125.0, 122.1, 121.6, 119.7, 118.1, 117.7, 108.1.

7. References

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Appendix I

Spectral Copies of ^{1}H and ^{13}C NMR of Compounds Obtained in this study

Electronic Supplementary Material (ESI) for Chemical Communications
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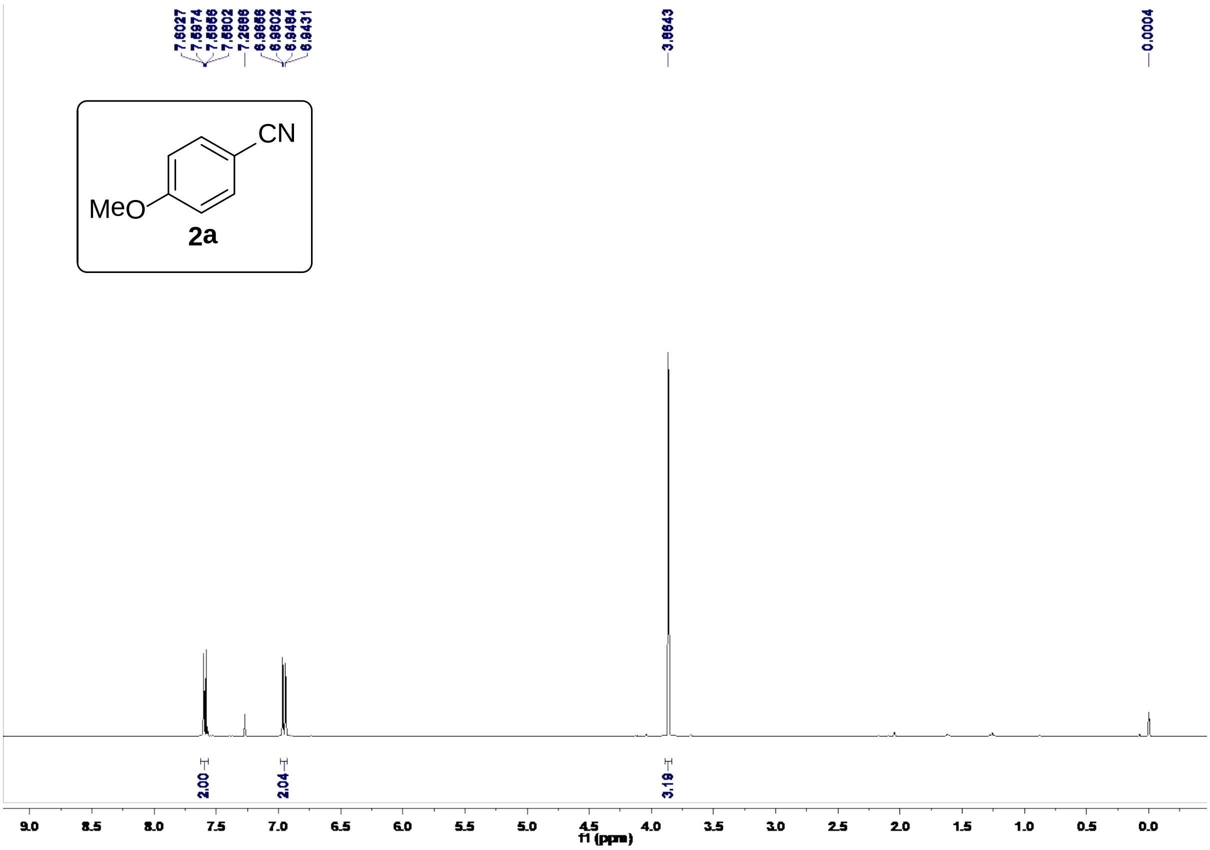
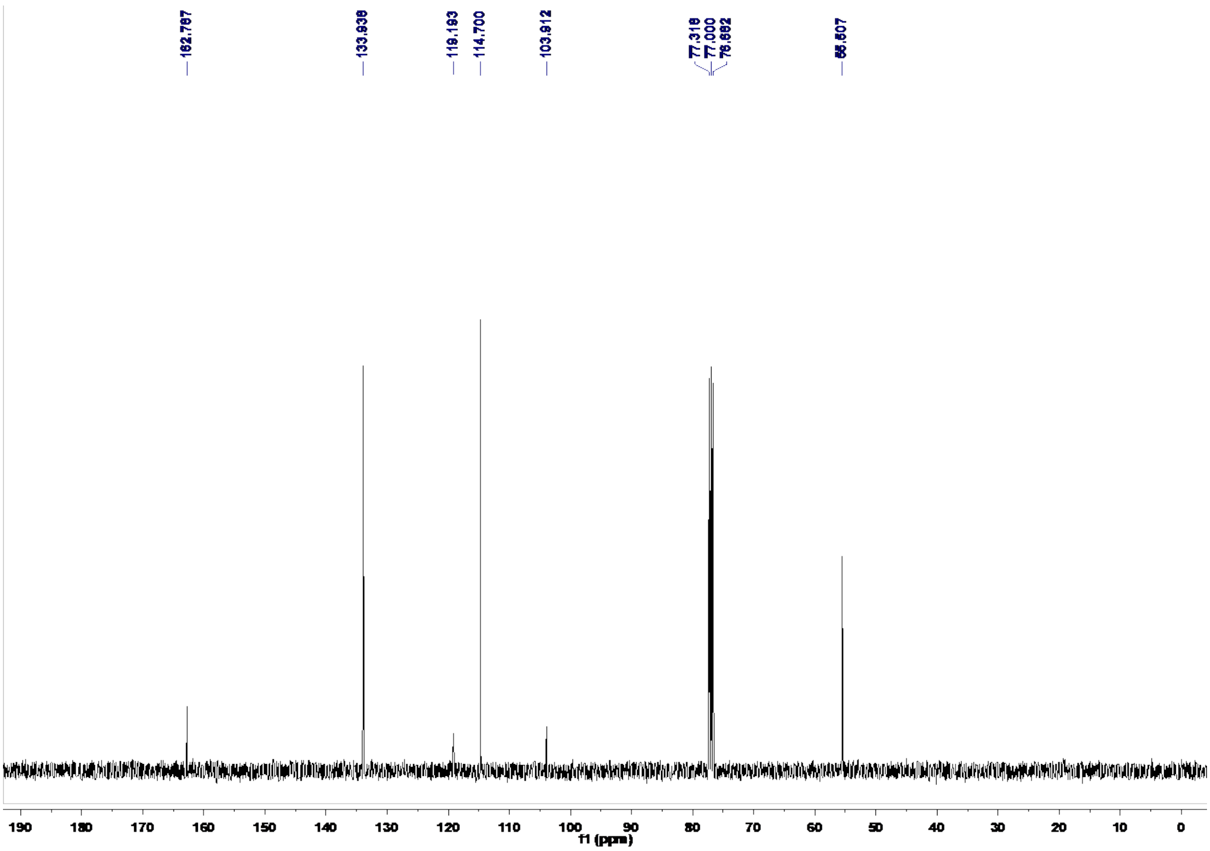
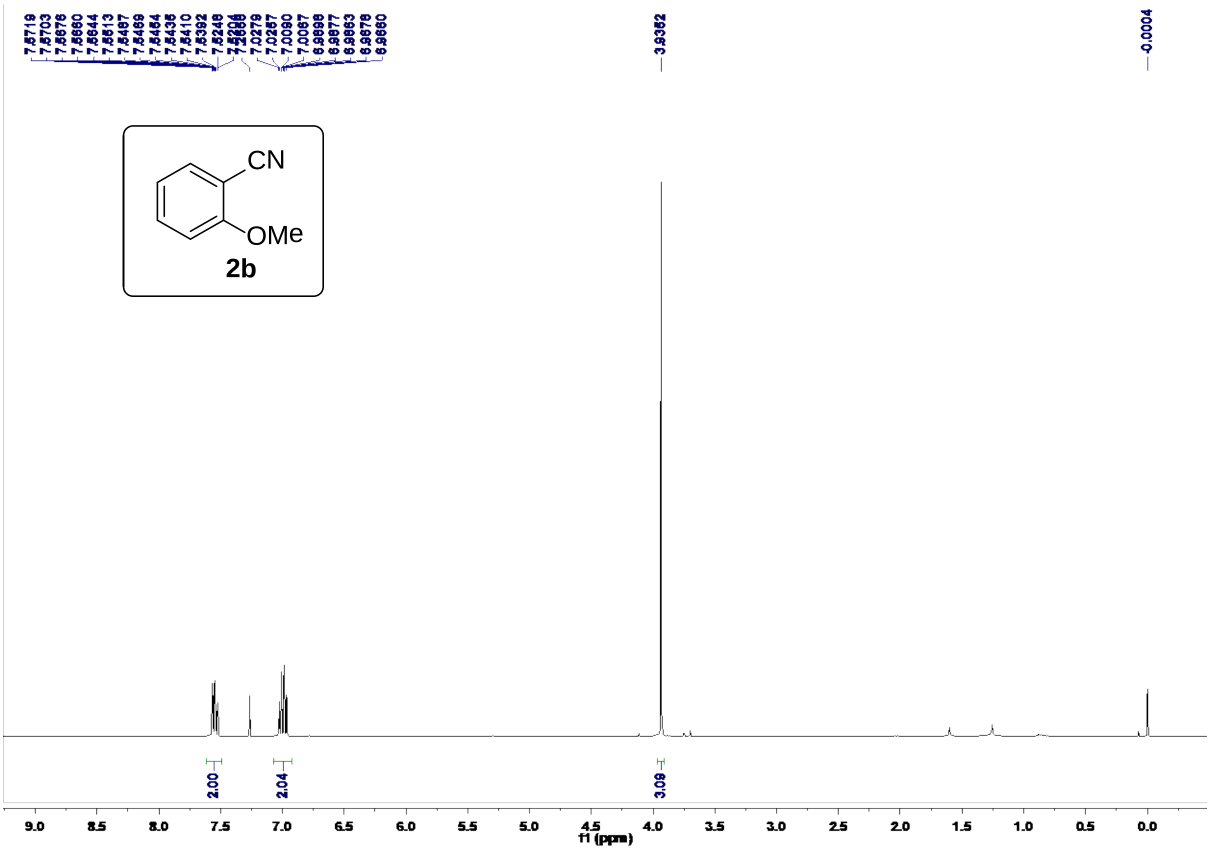
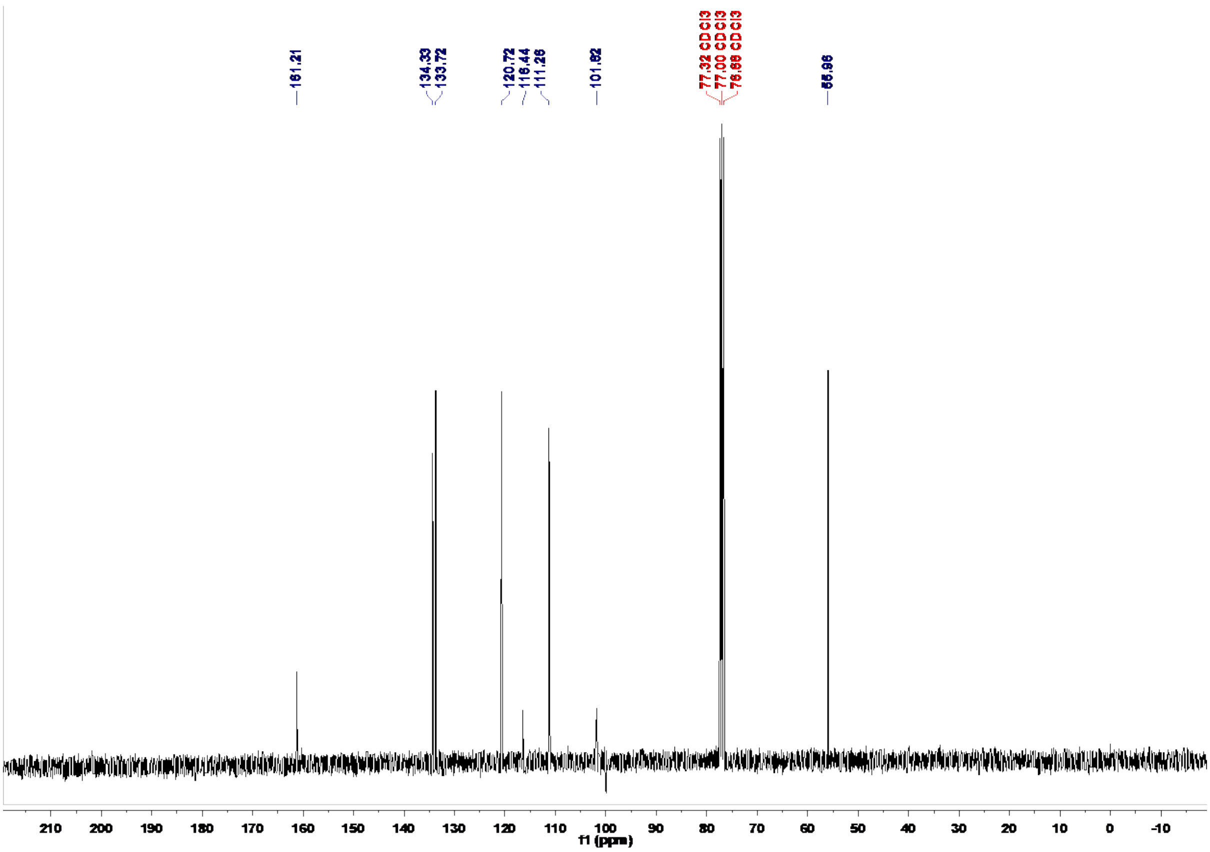
4-Methoxybenzonitrile (2a)



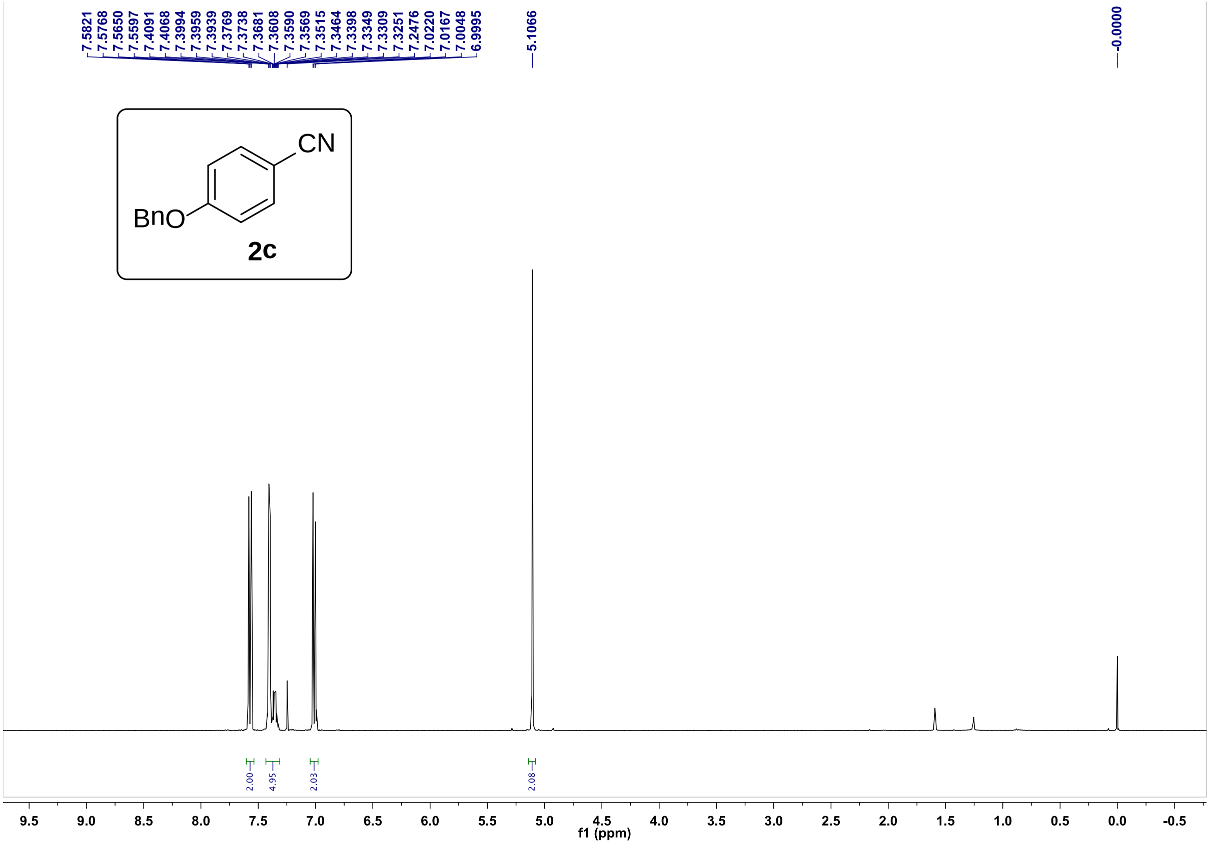


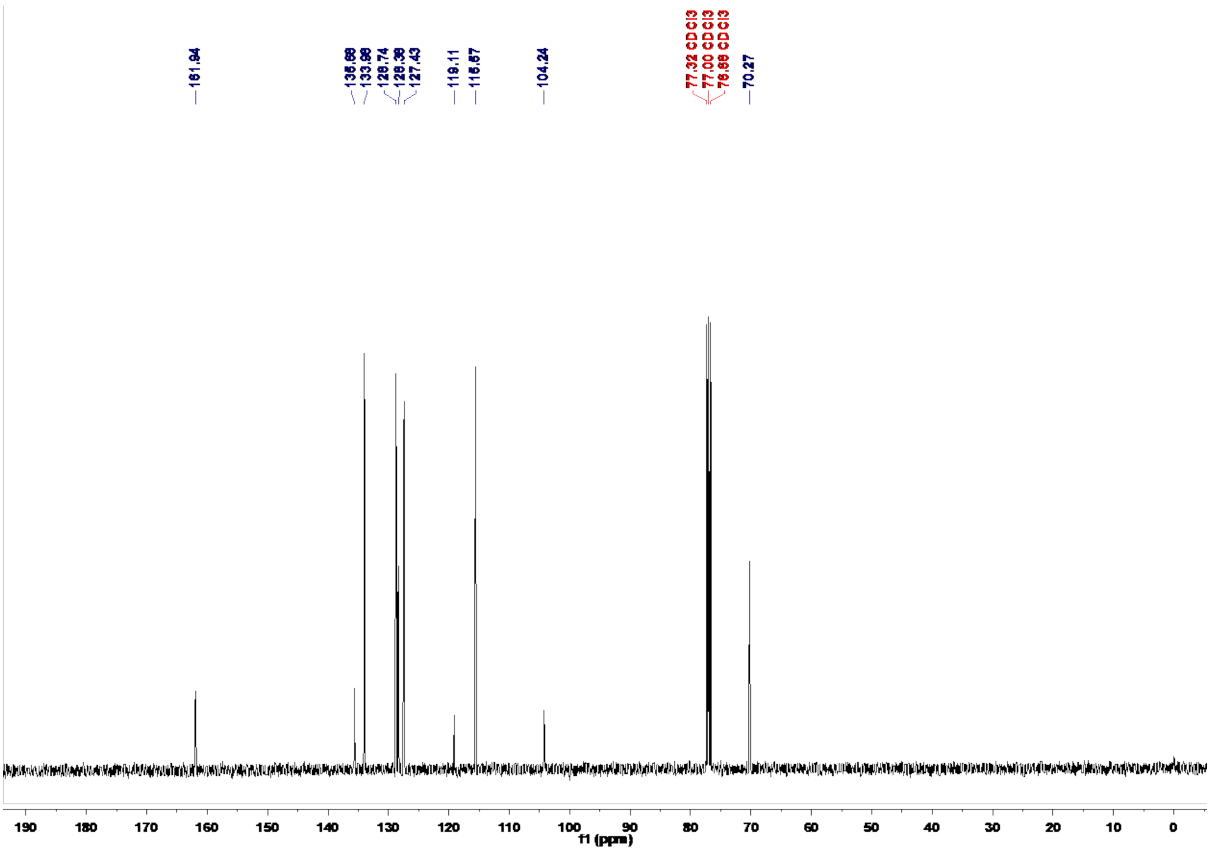
2-Methoxybenzonitrile (2b)



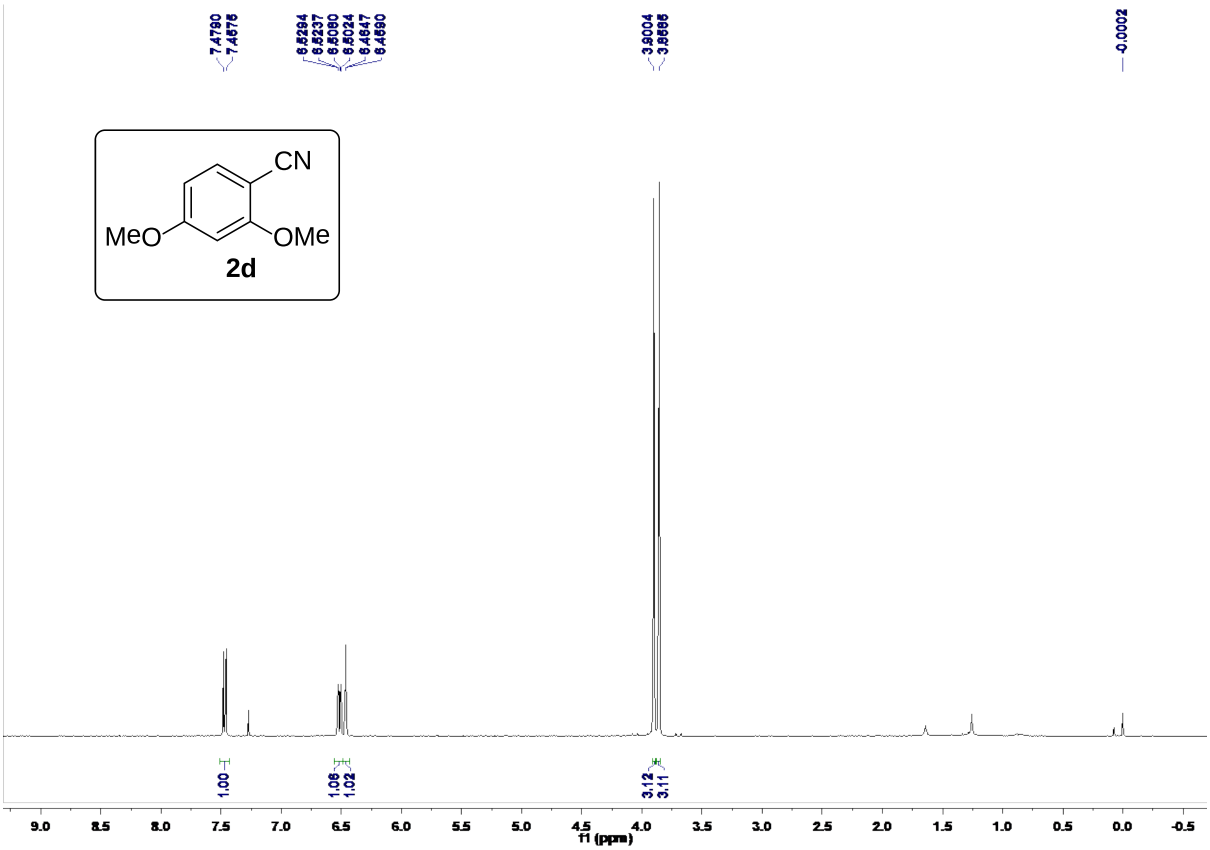


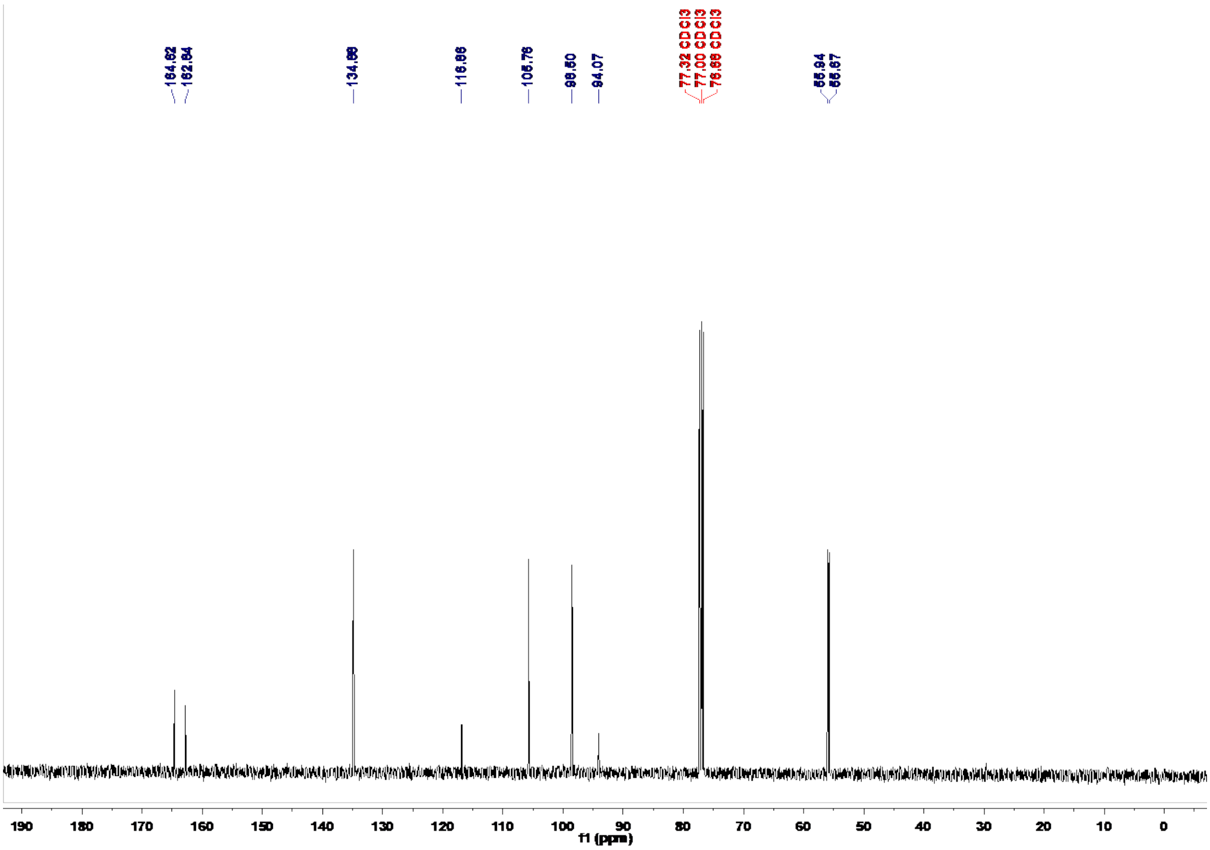
4-(Benzyloxy)benzonitrile (2c)



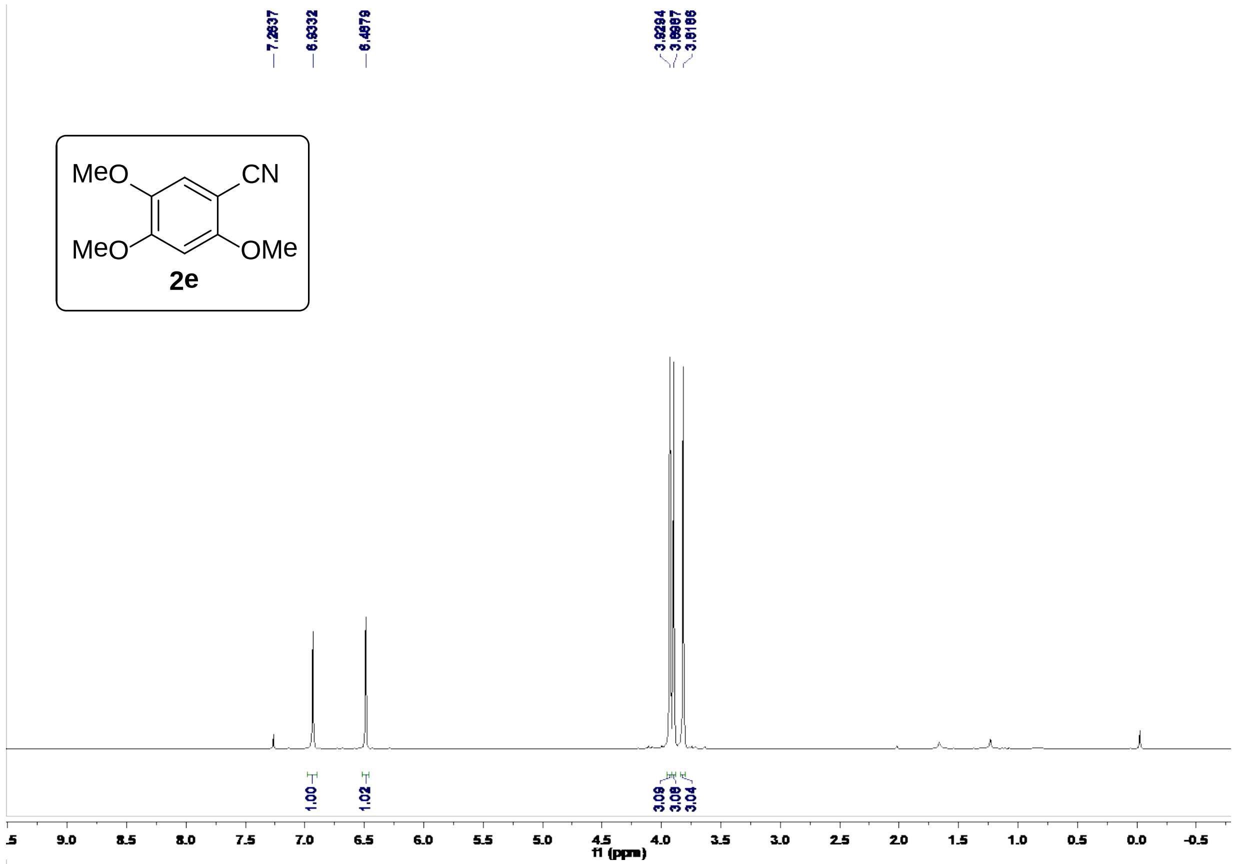


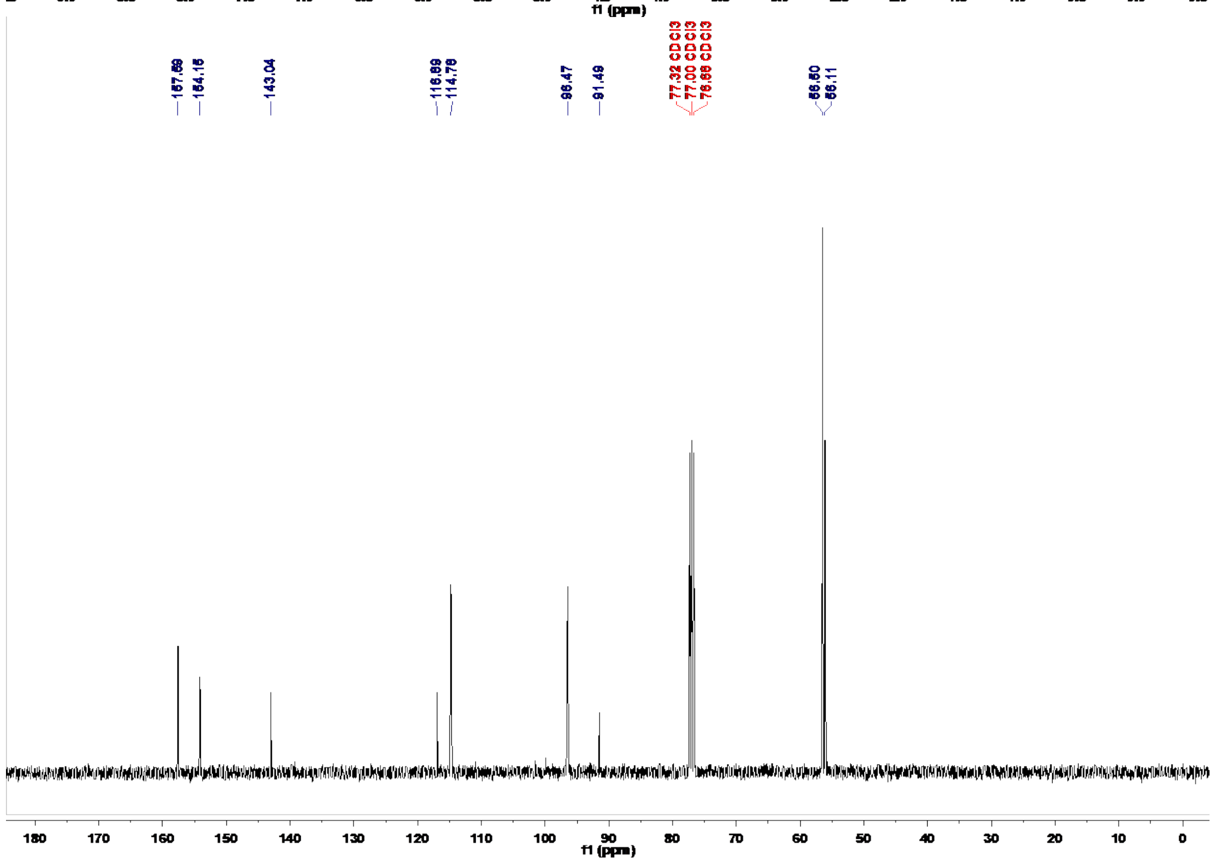
2,4-Dimethoxybenzonitrile (2d)





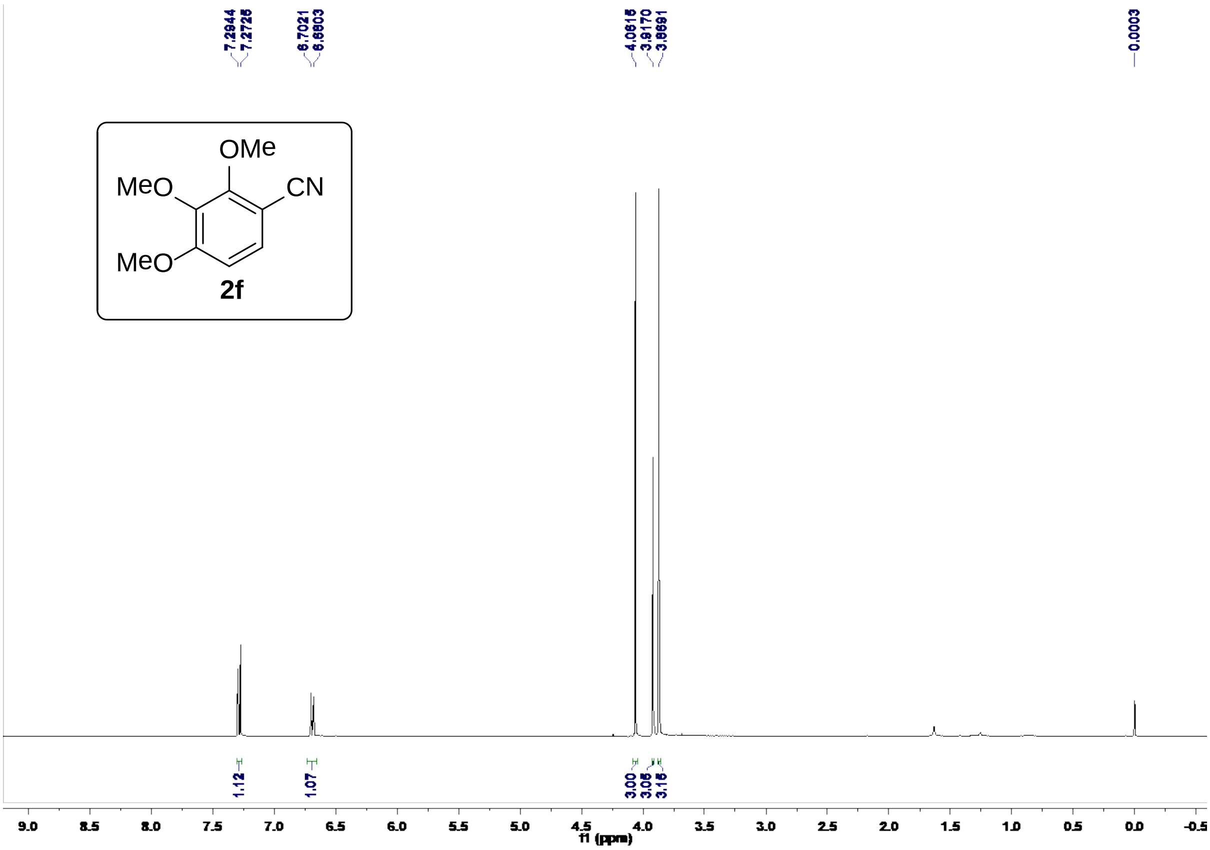
2,4,5-Trimethoxybenzonitrile (2e)

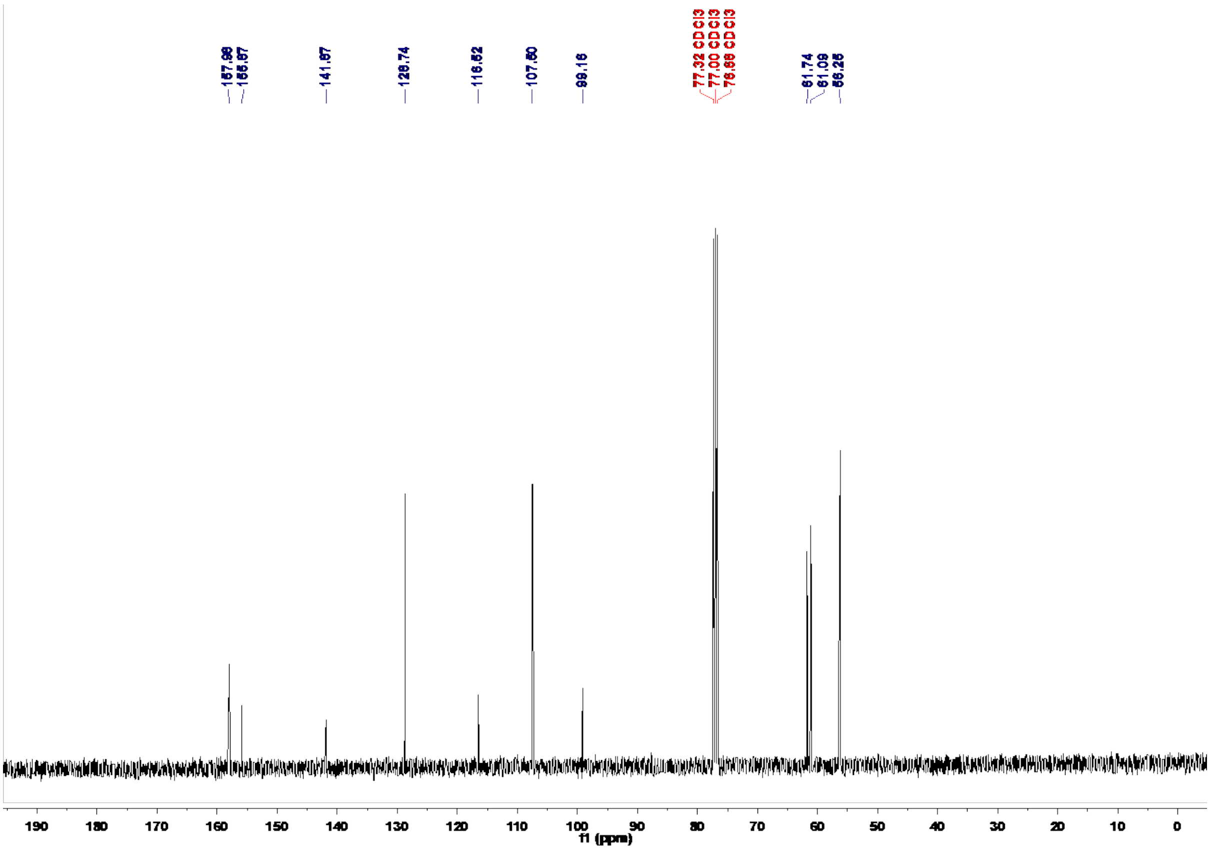




Electronic Supplementary Material (ESI) for Chemical Communications

2,3,4-Trimethoxybenzonitrile (2f)





Electronic Supplementary Material (ESI) for Chemical Communications

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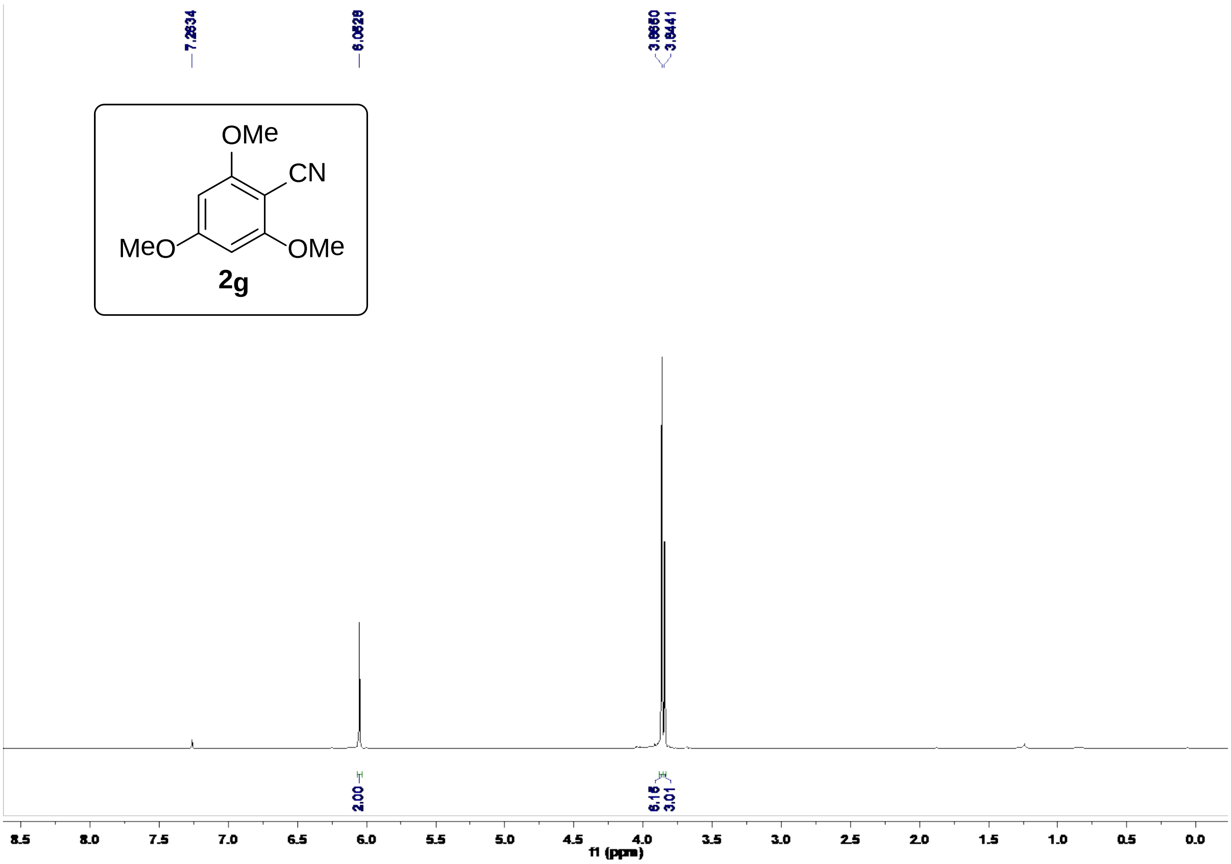
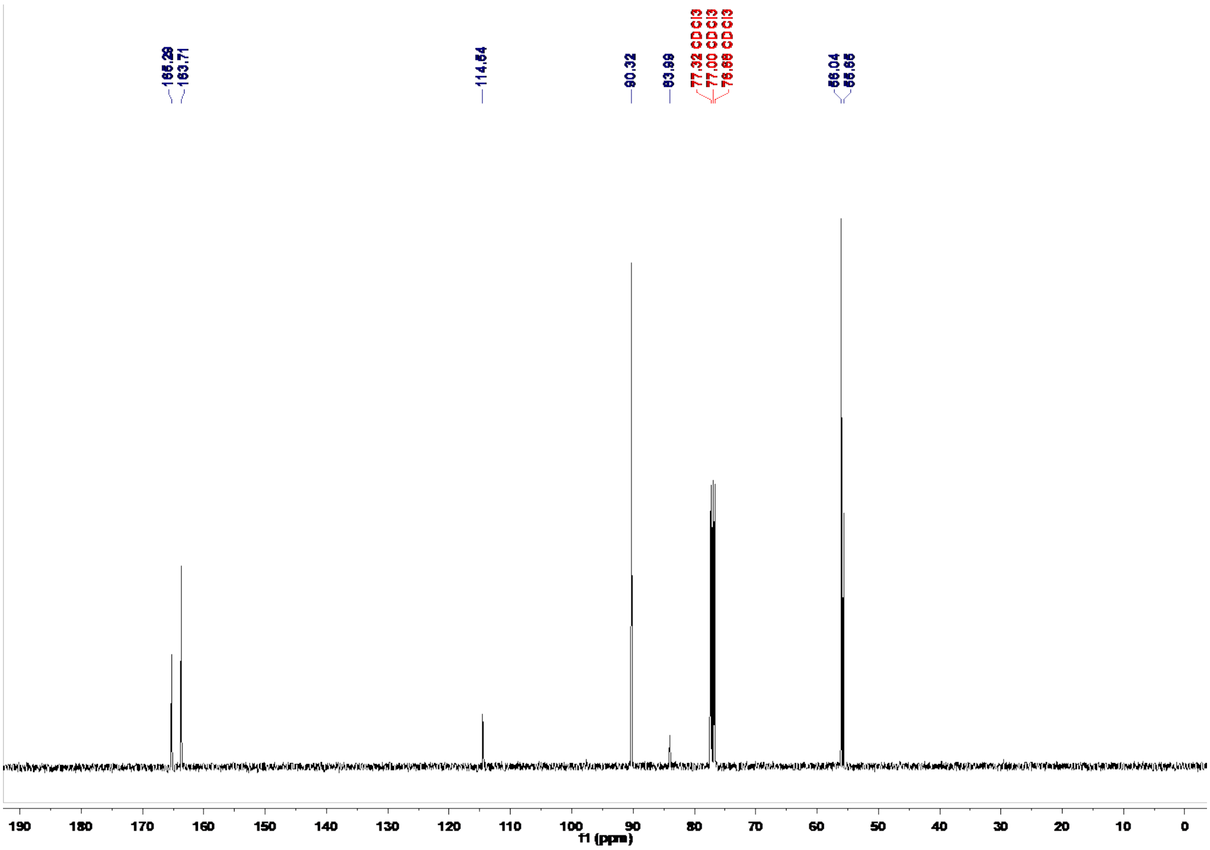
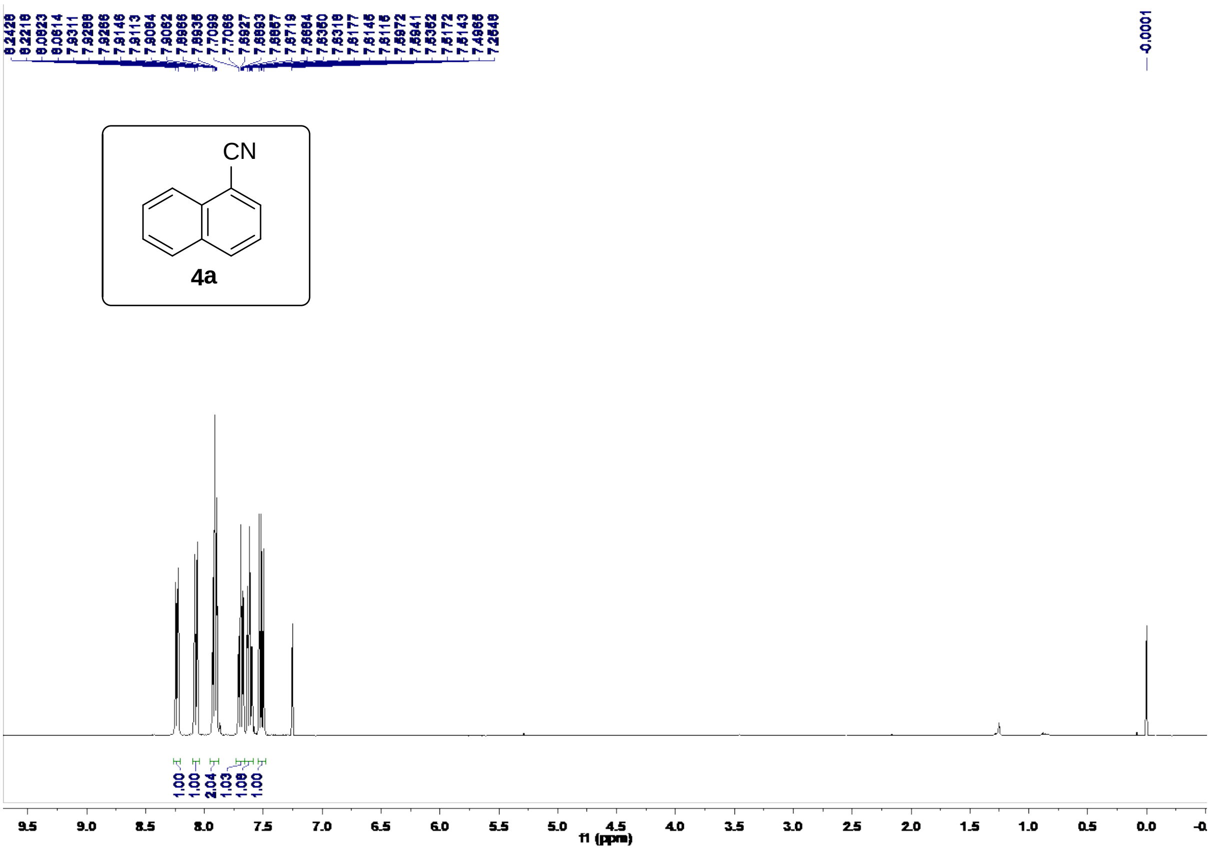
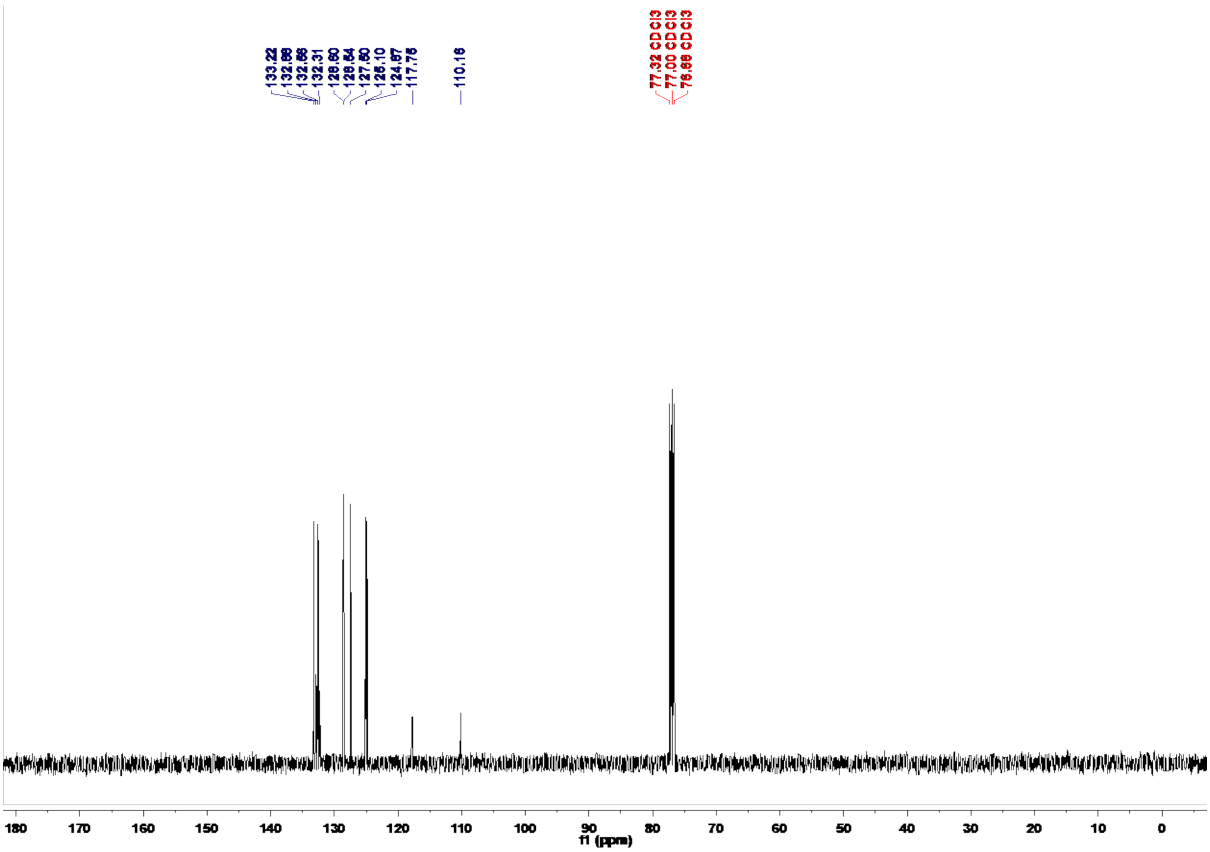


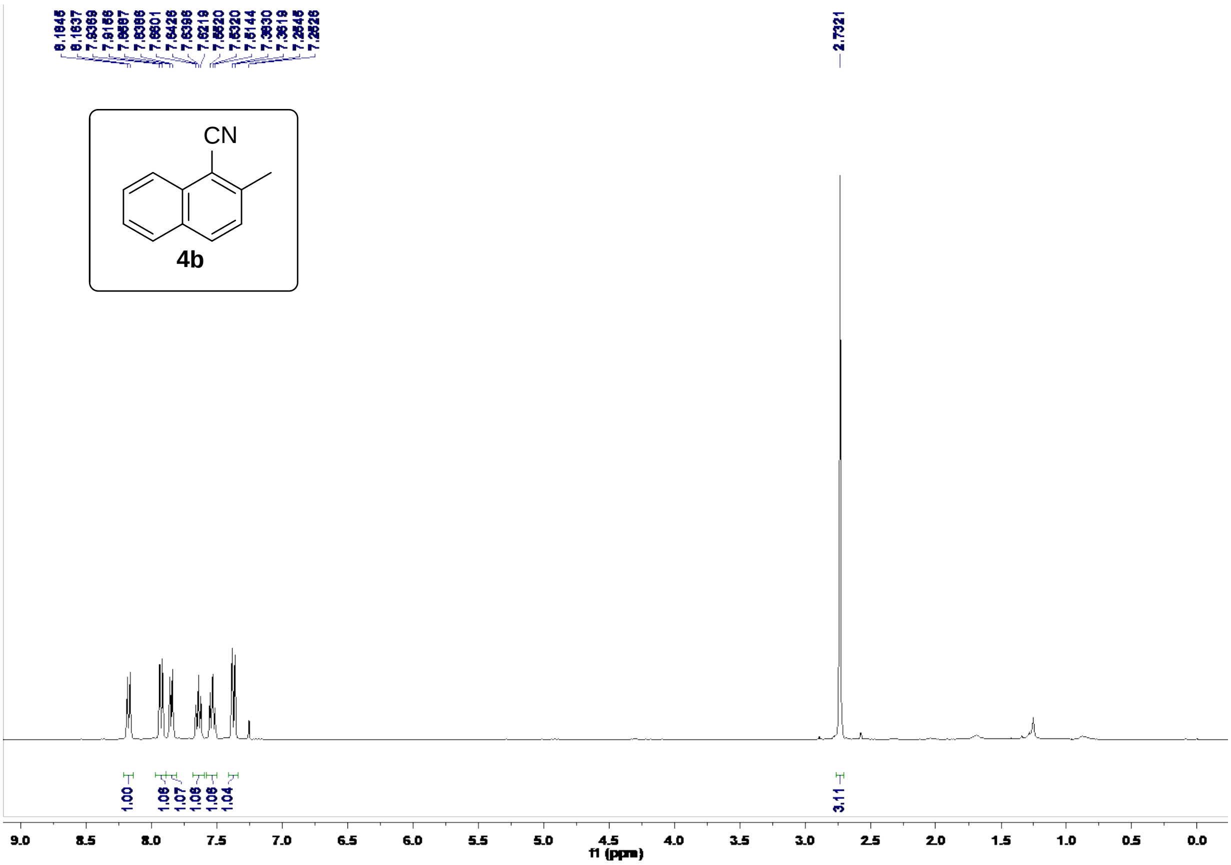


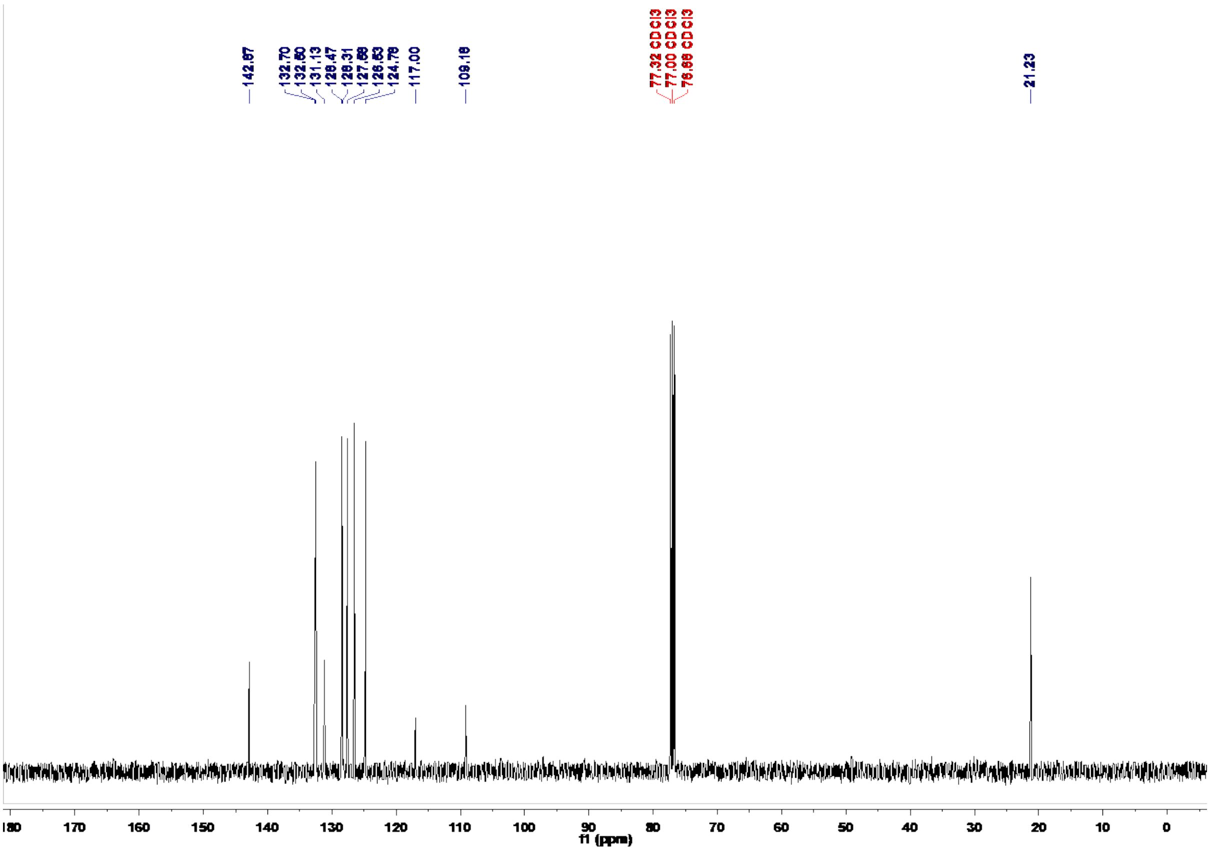
1-Naphthonitrile (4a)



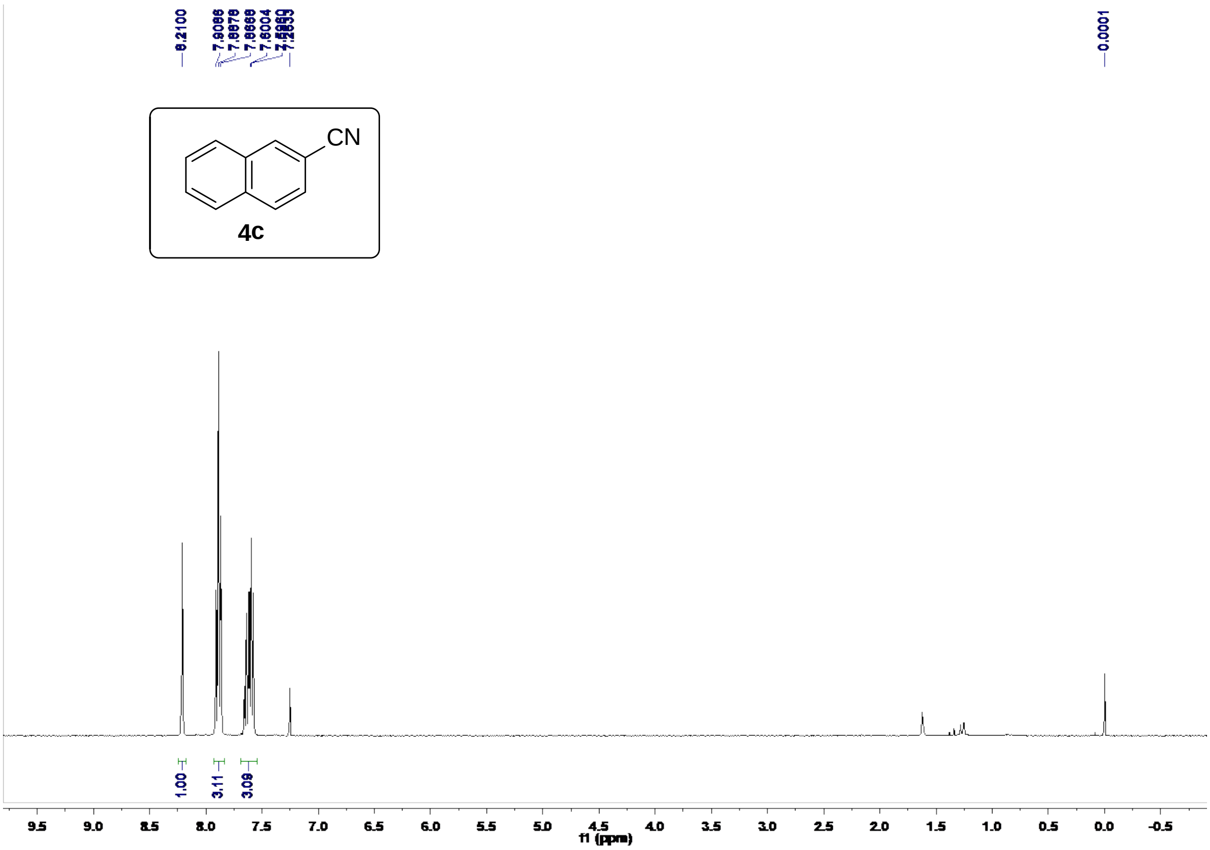


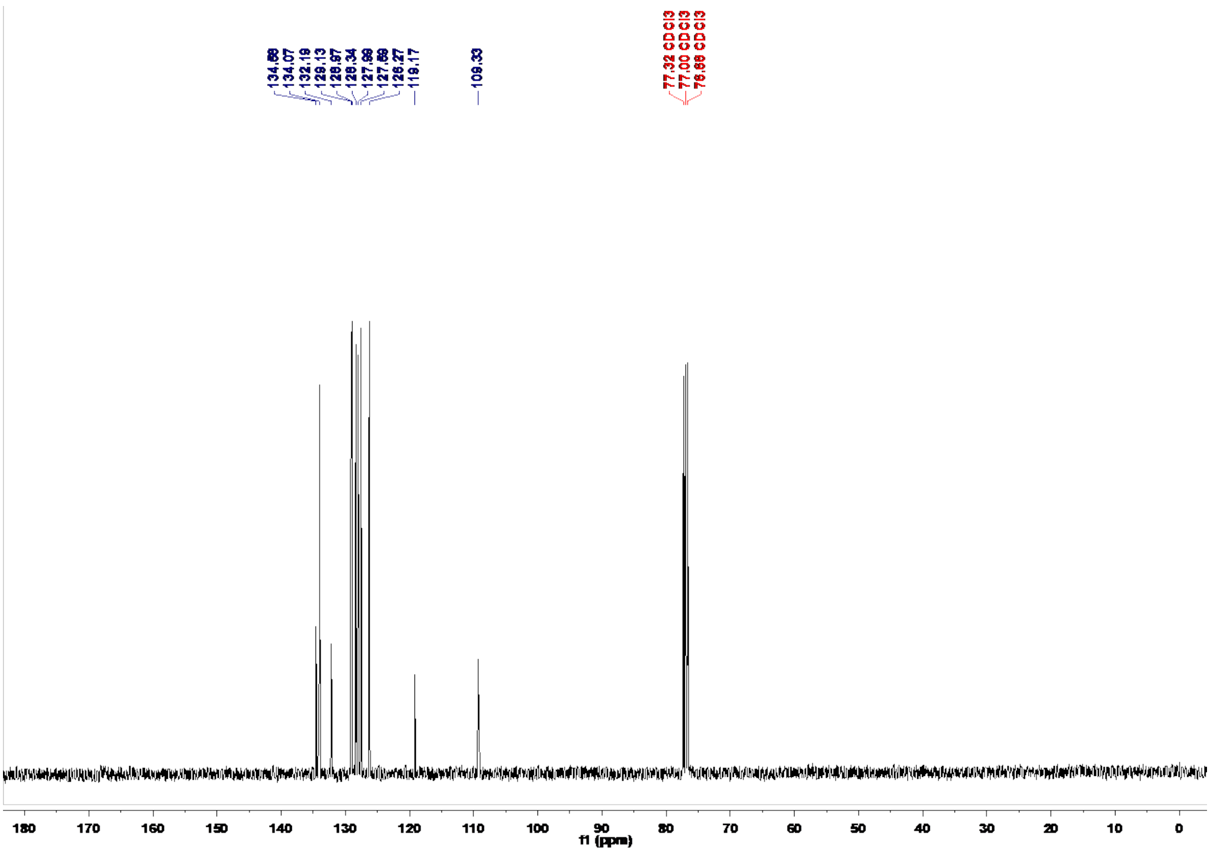
2-Methyl-1-naphthonitrile (4b)



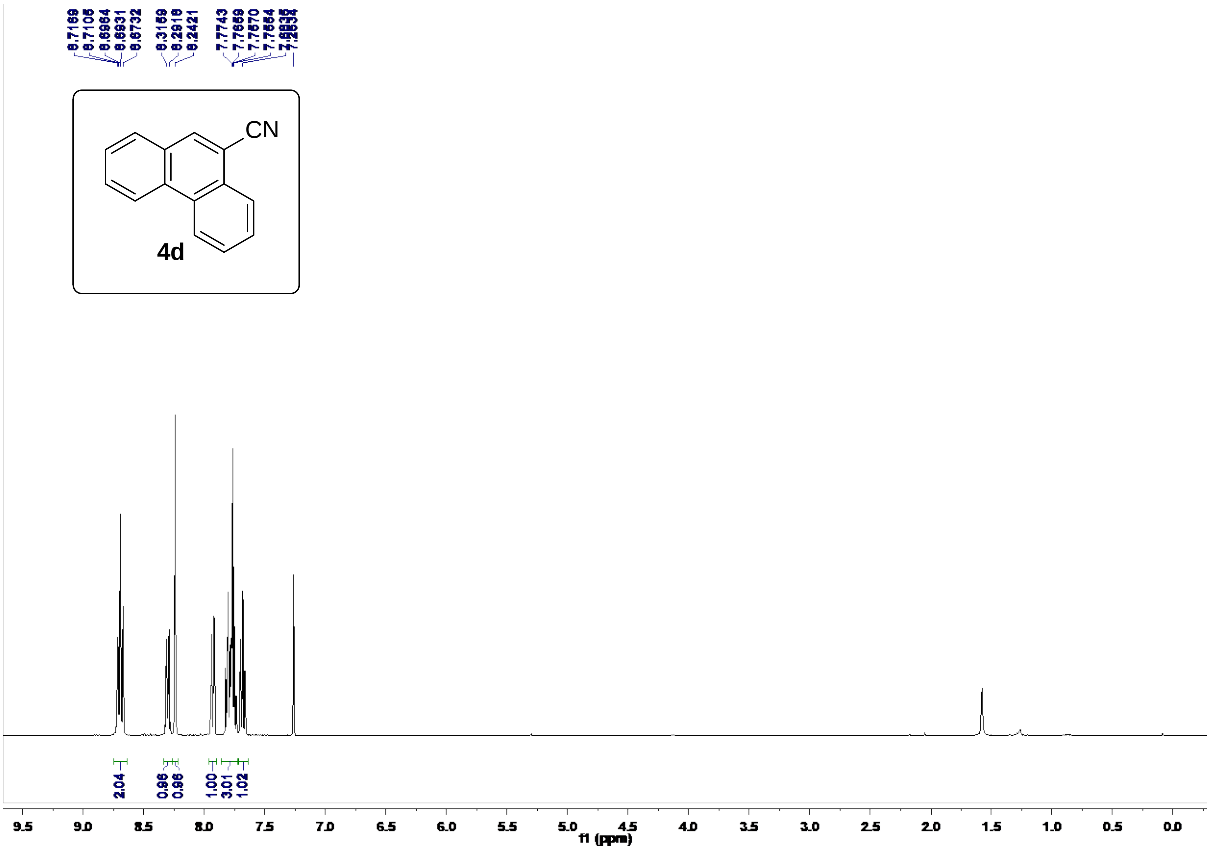


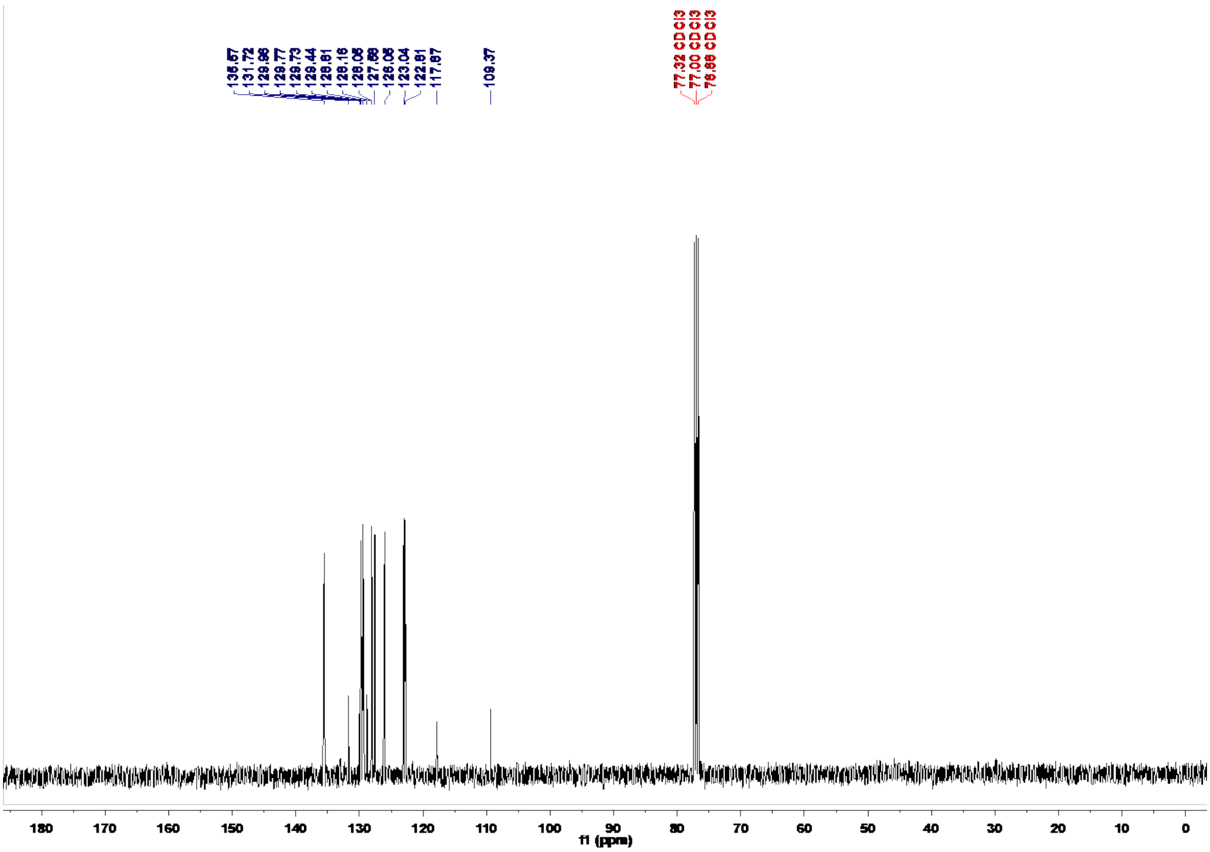
2-Naphthonitrile (4c)



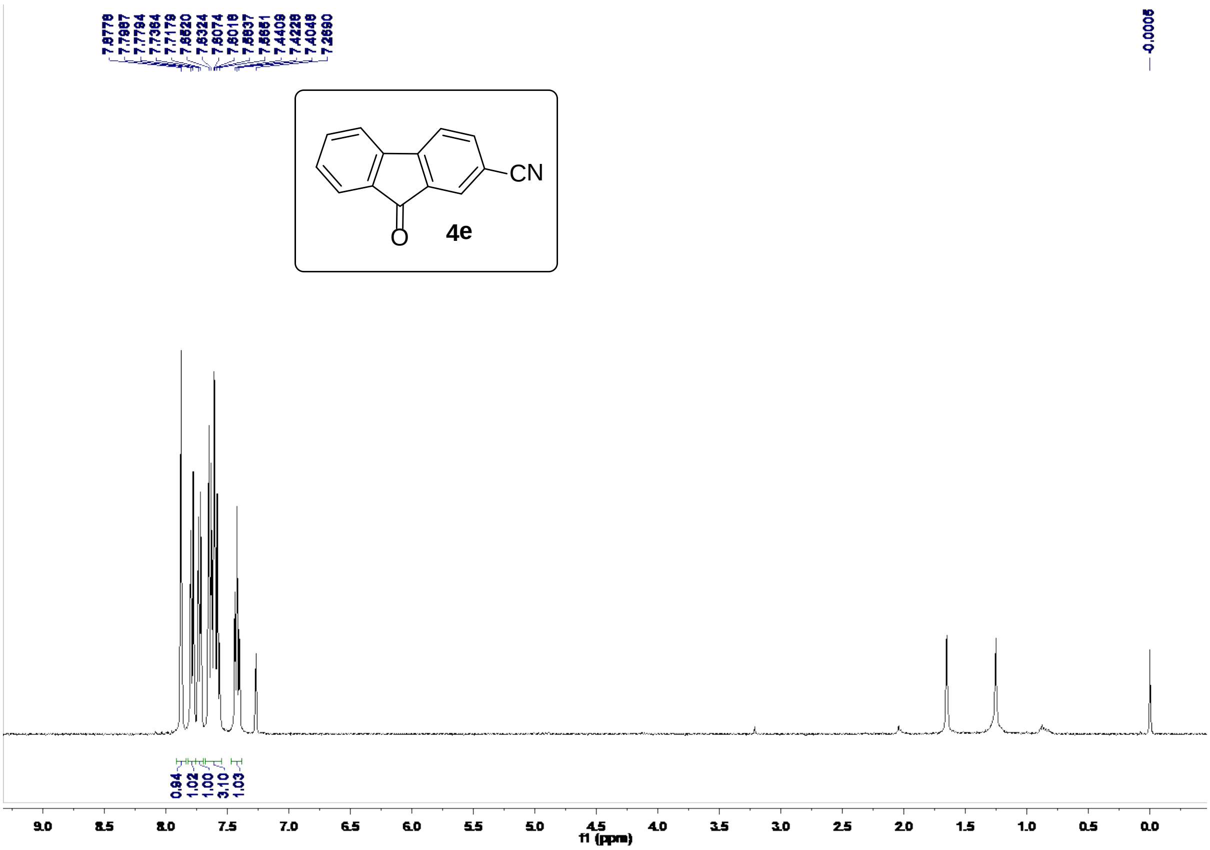


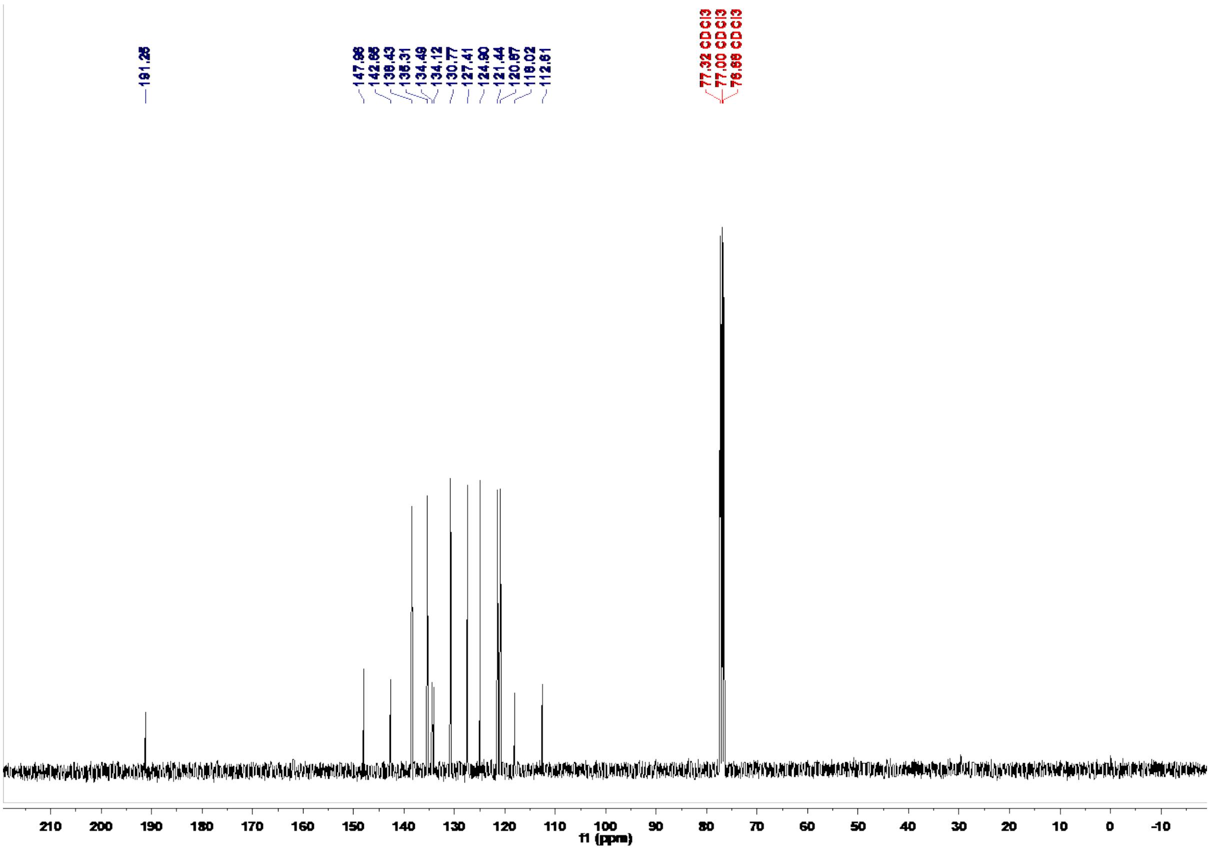
Phenanthrene-9-carbonitrile (4d)



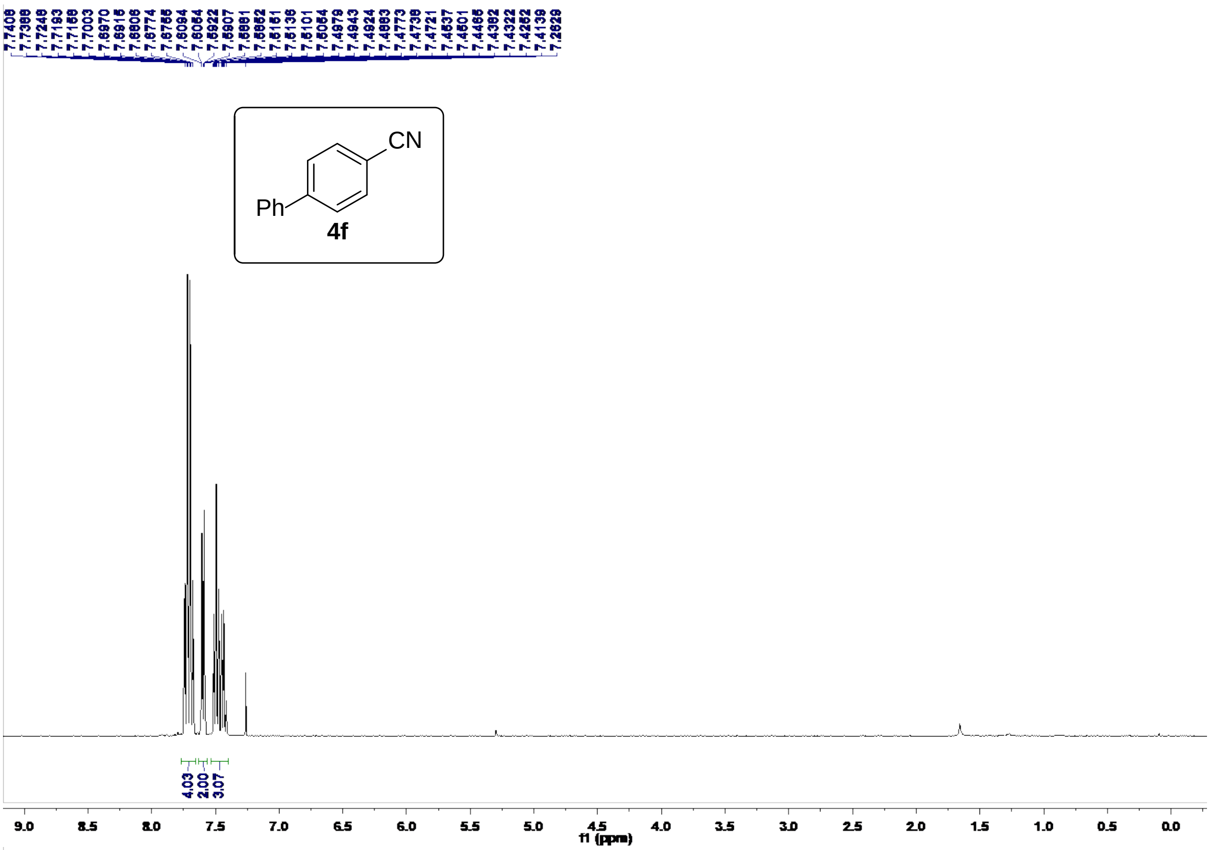


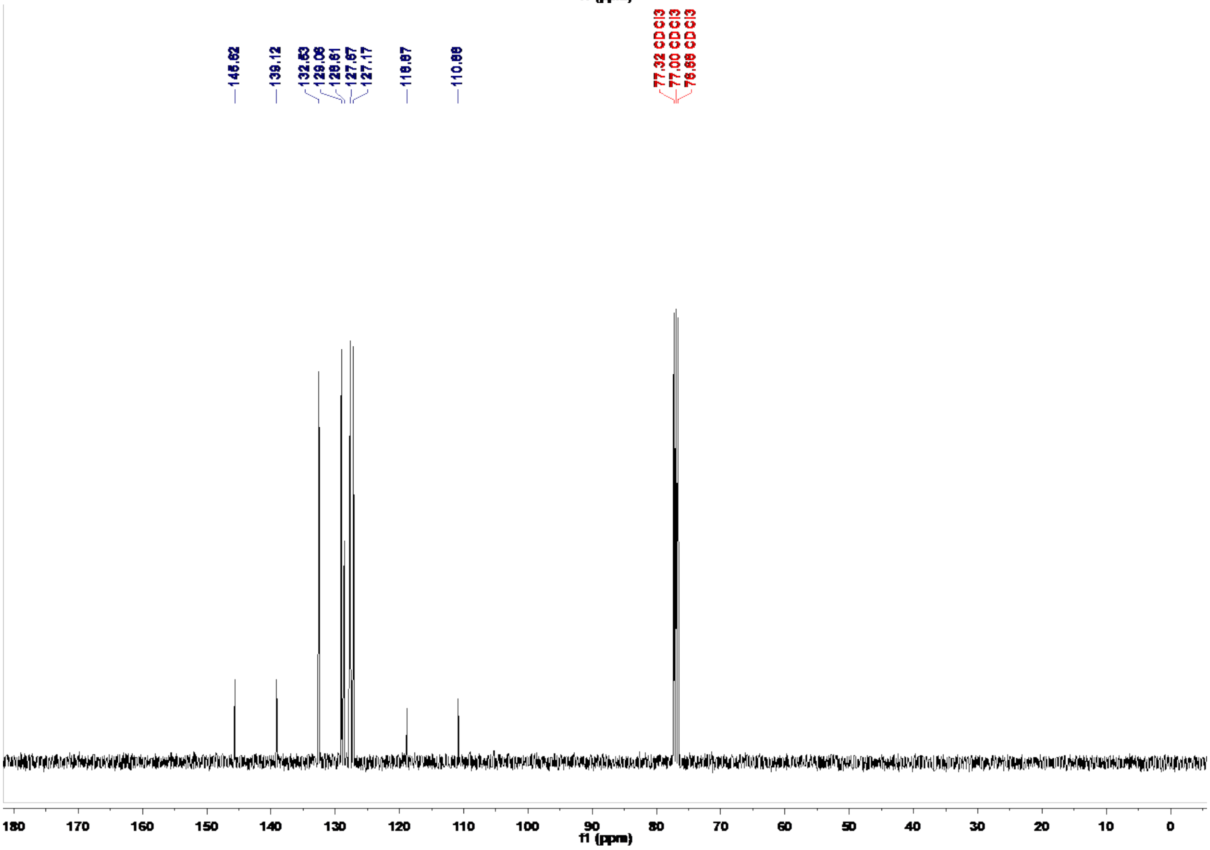
2-Cyano-9*H*-fluoren-9-one (4e)



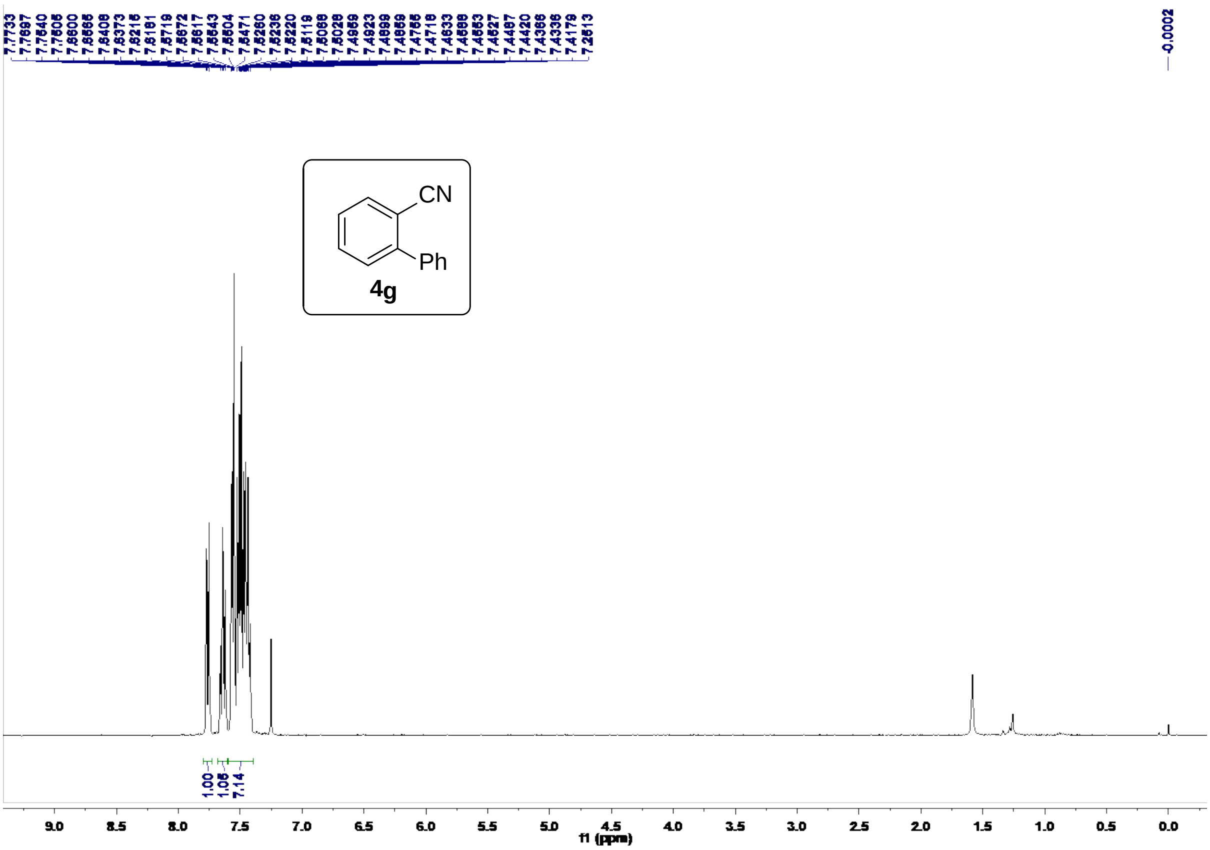


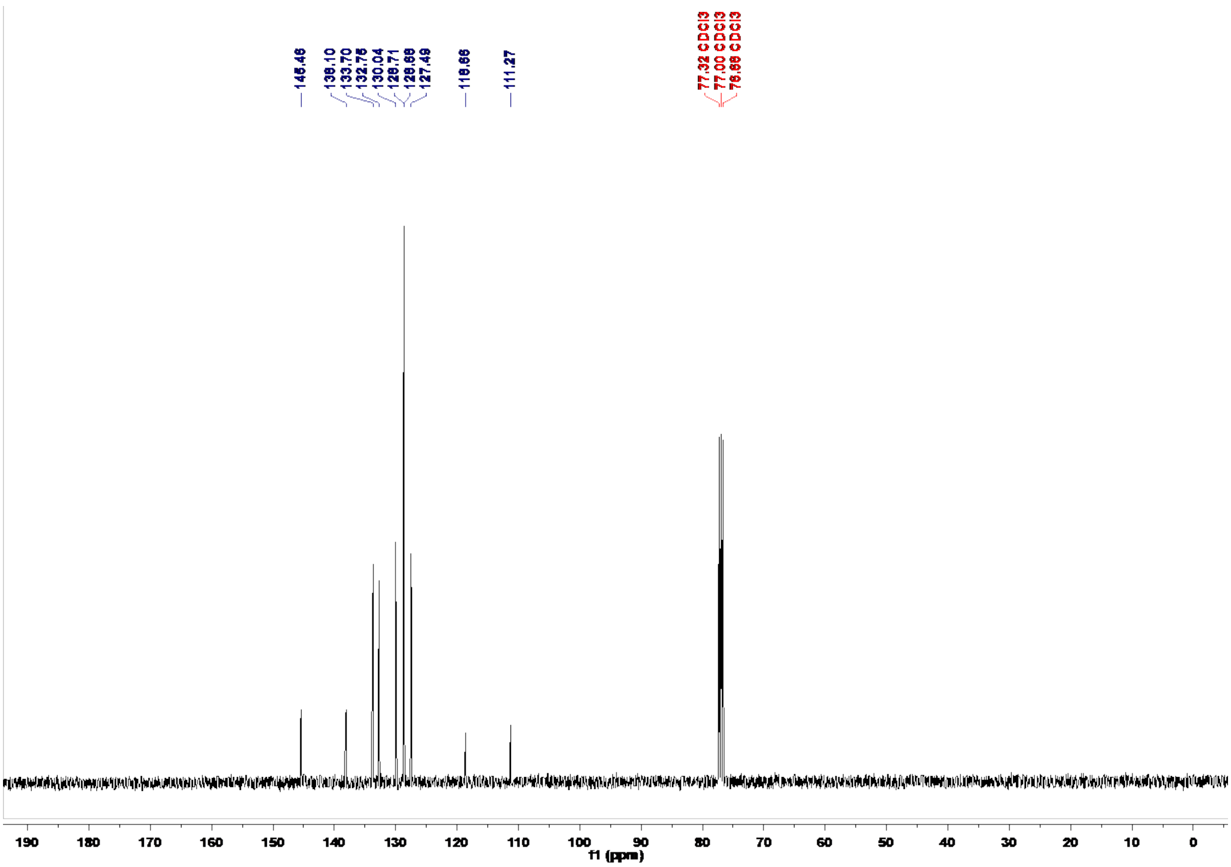
4-Phenylbenzonitrile (4f)



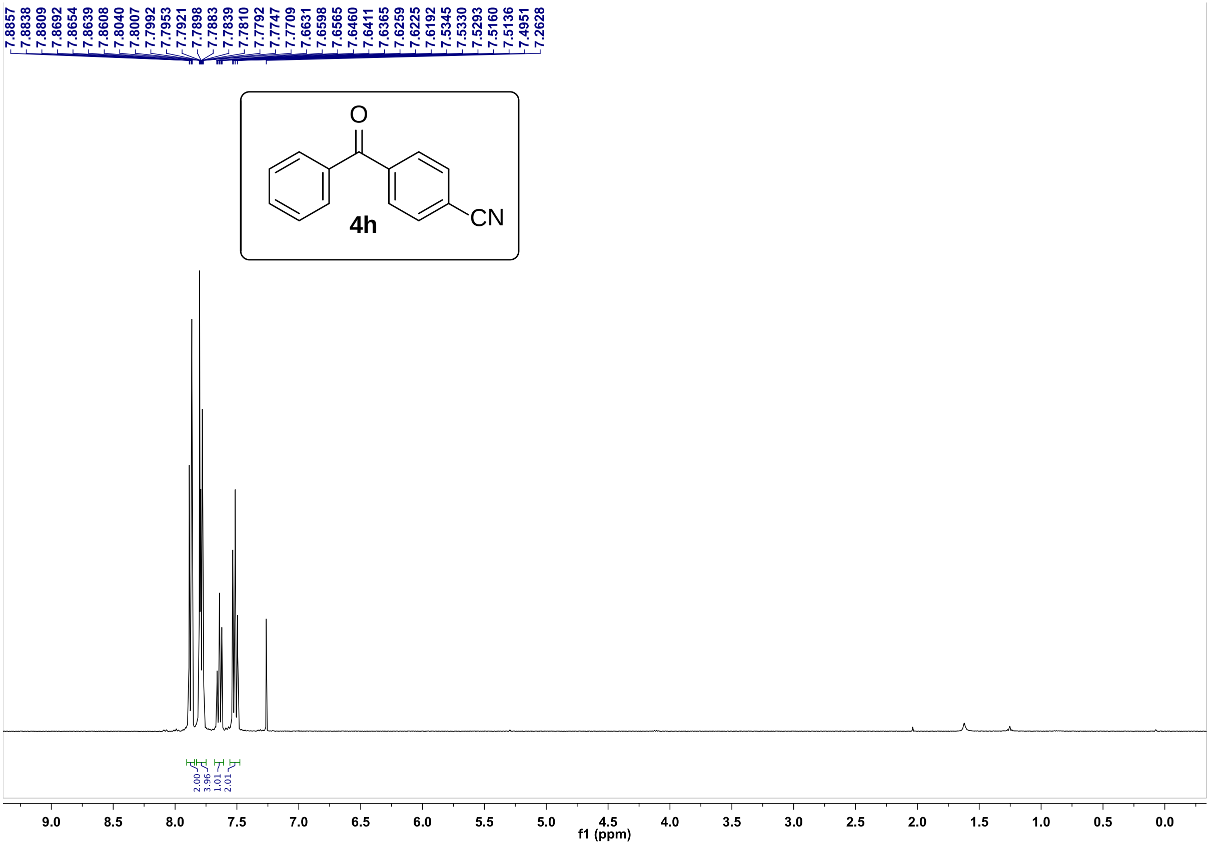


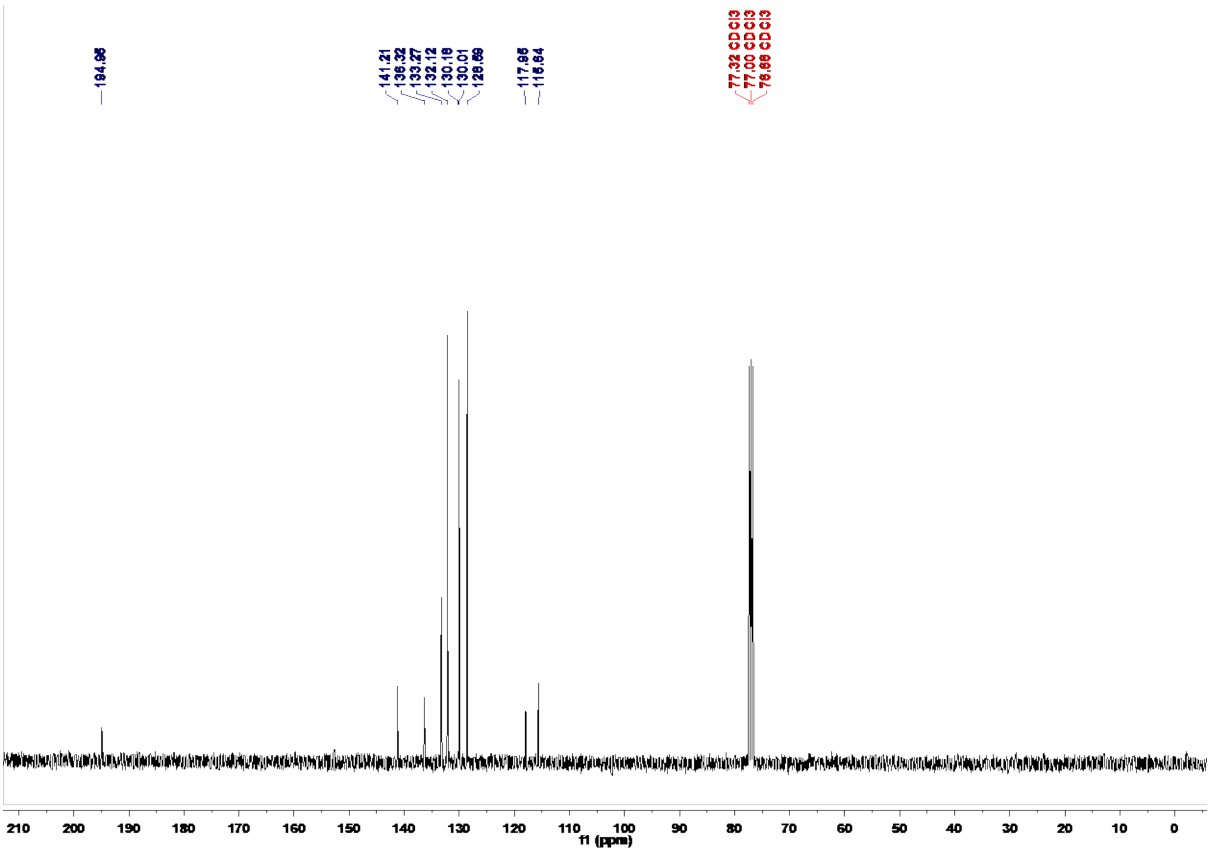
2-Phenylbenzonitrile (4g)



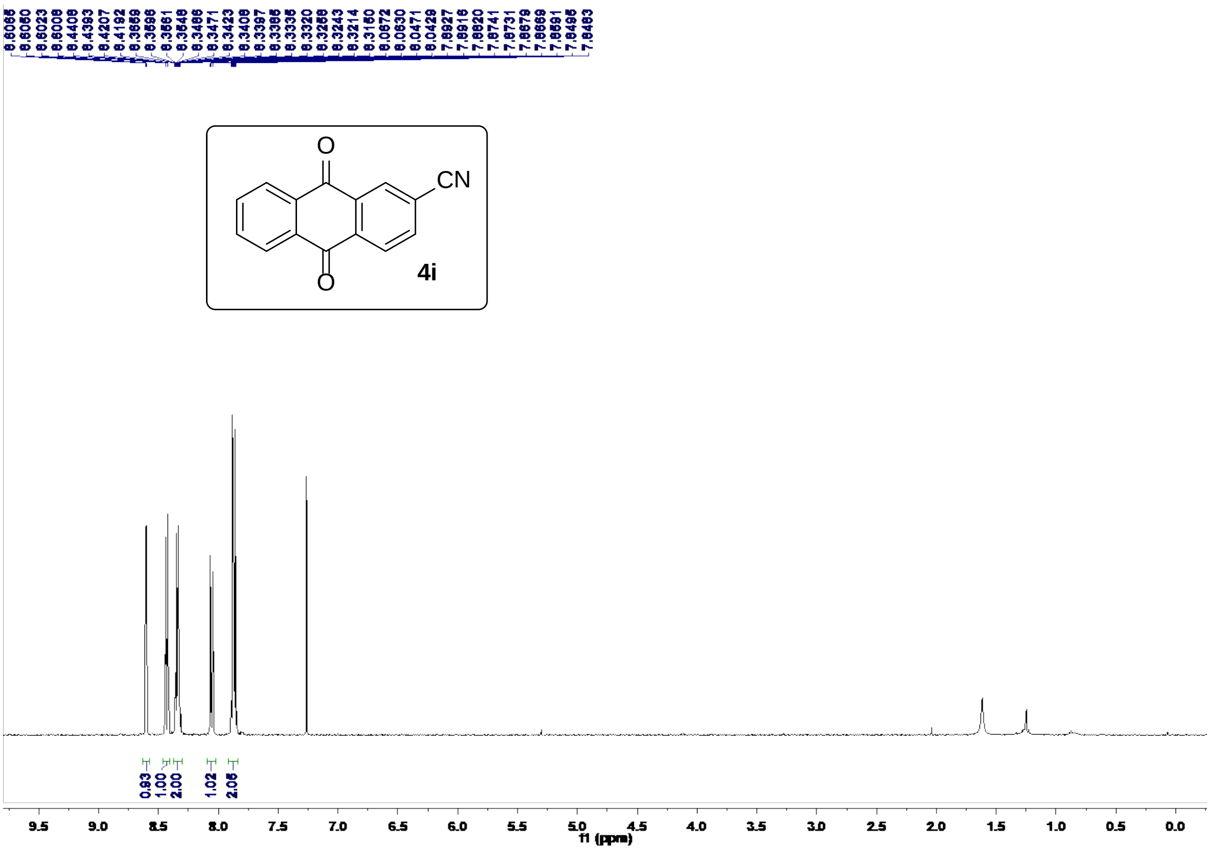


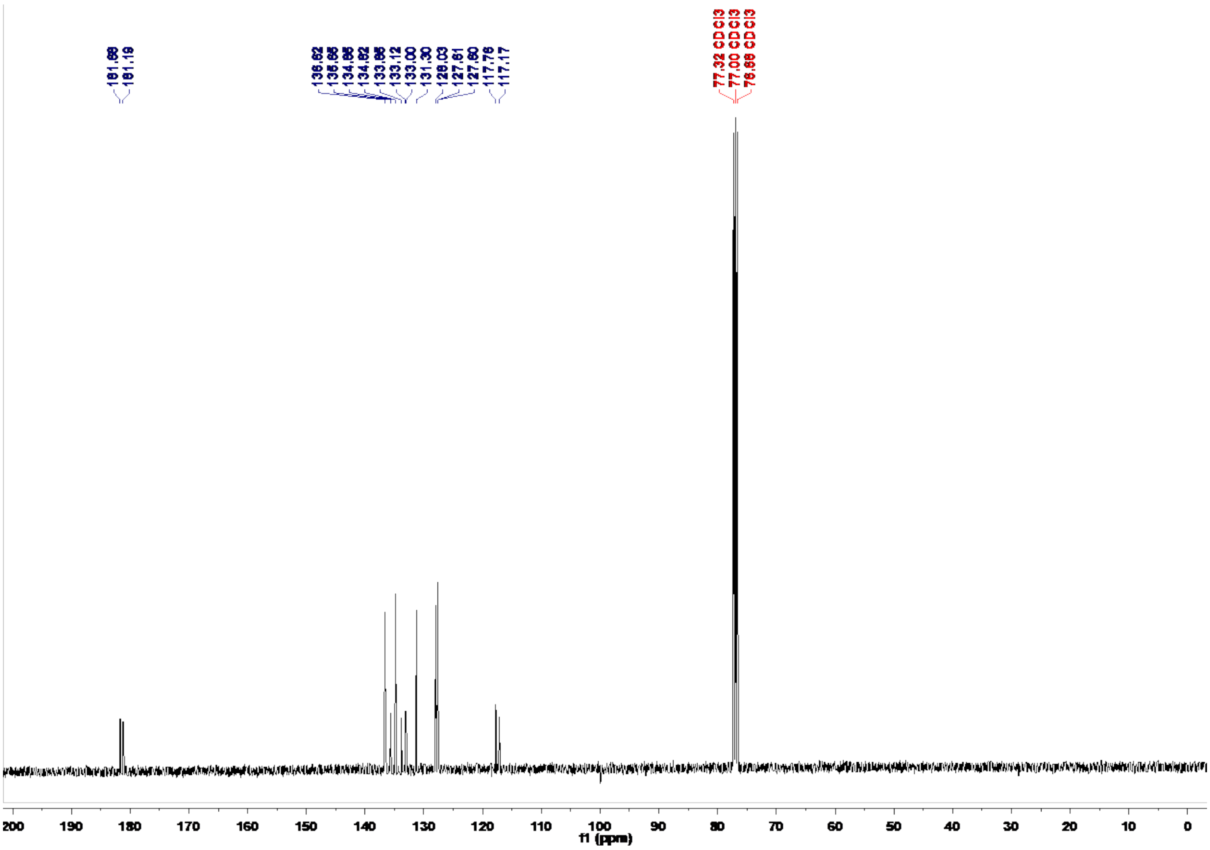
4-Cyanobenzophenone (4h)



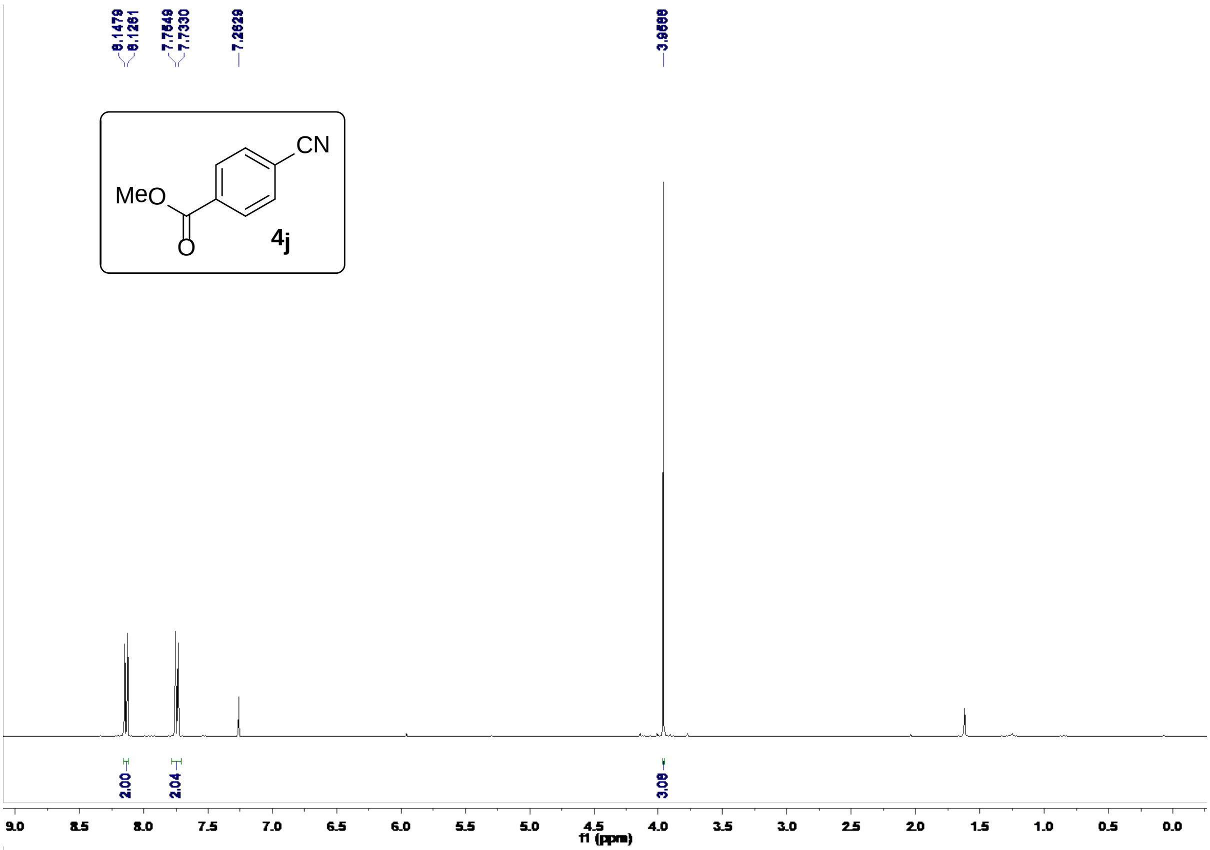


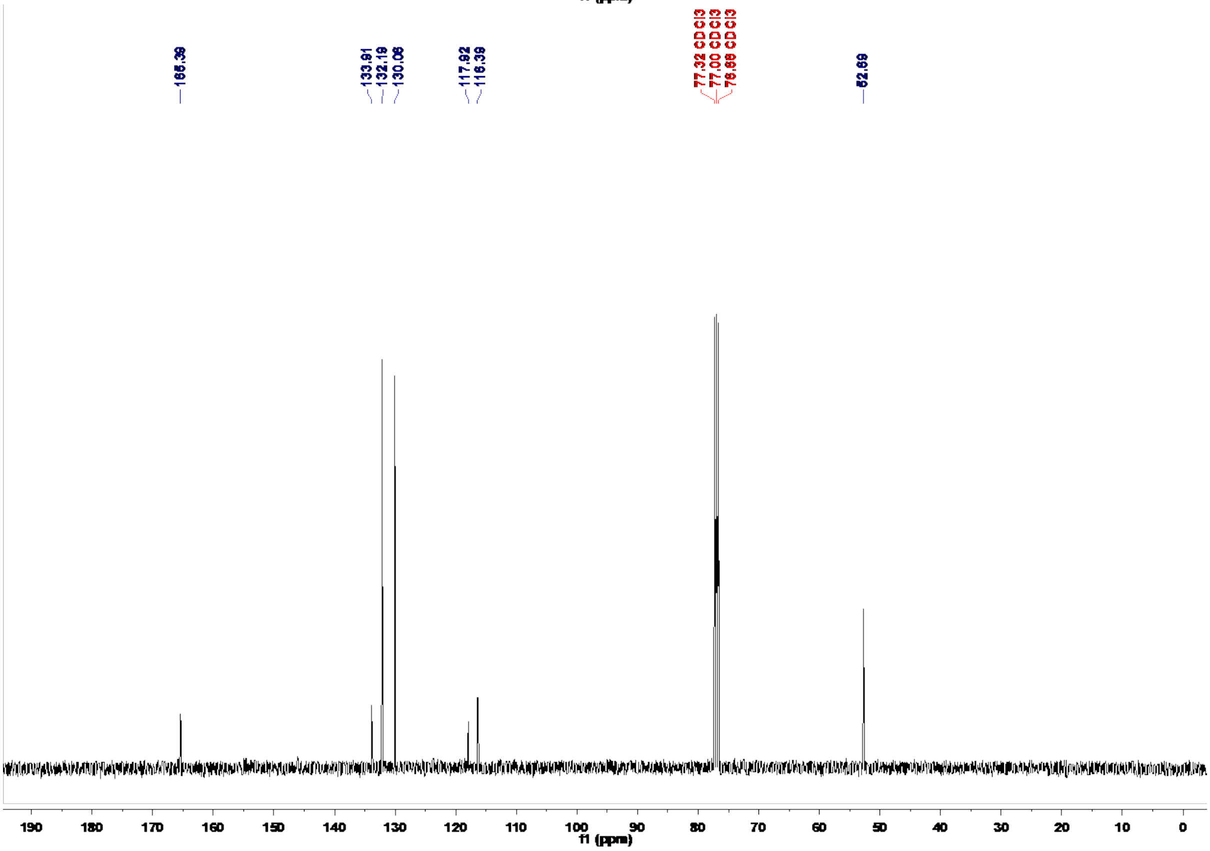
9,10-Dioxo-9,10-dihydroanthracene-2-carbonitrile (4i)



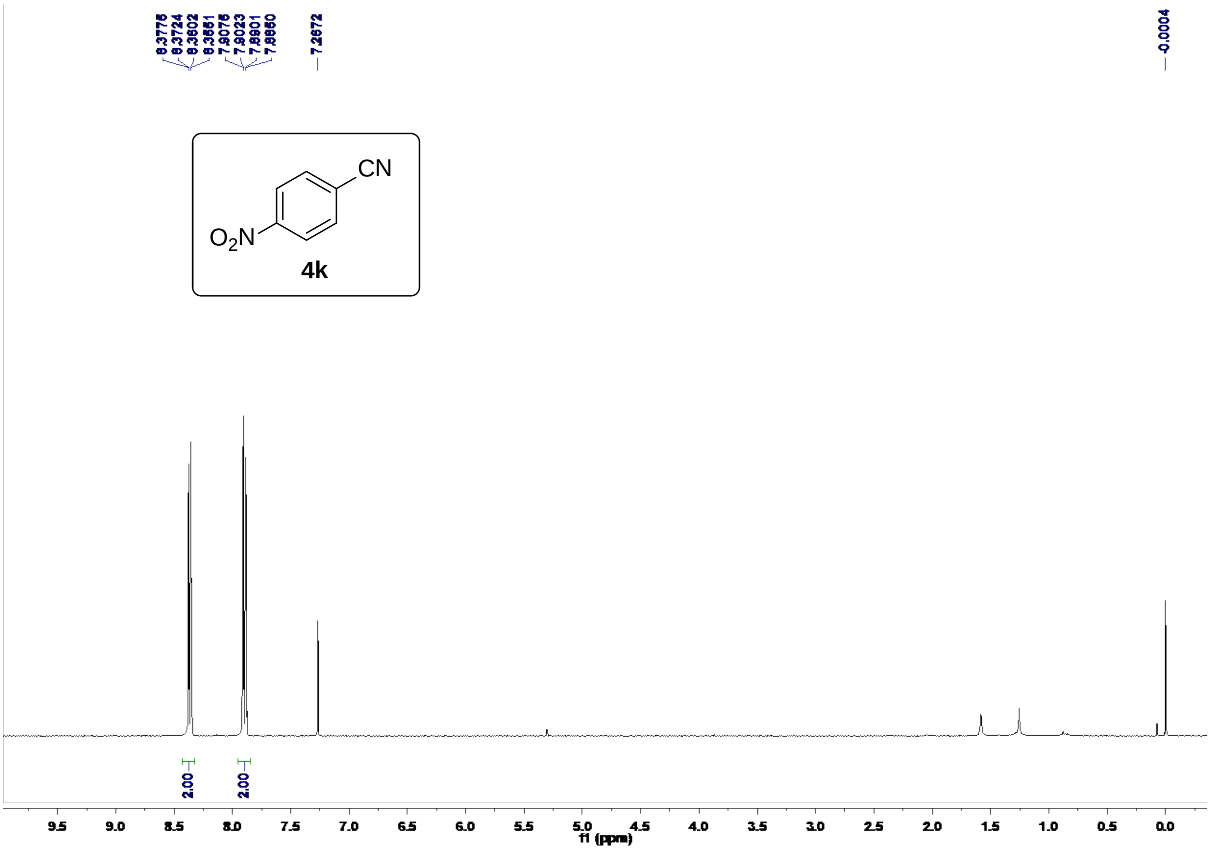


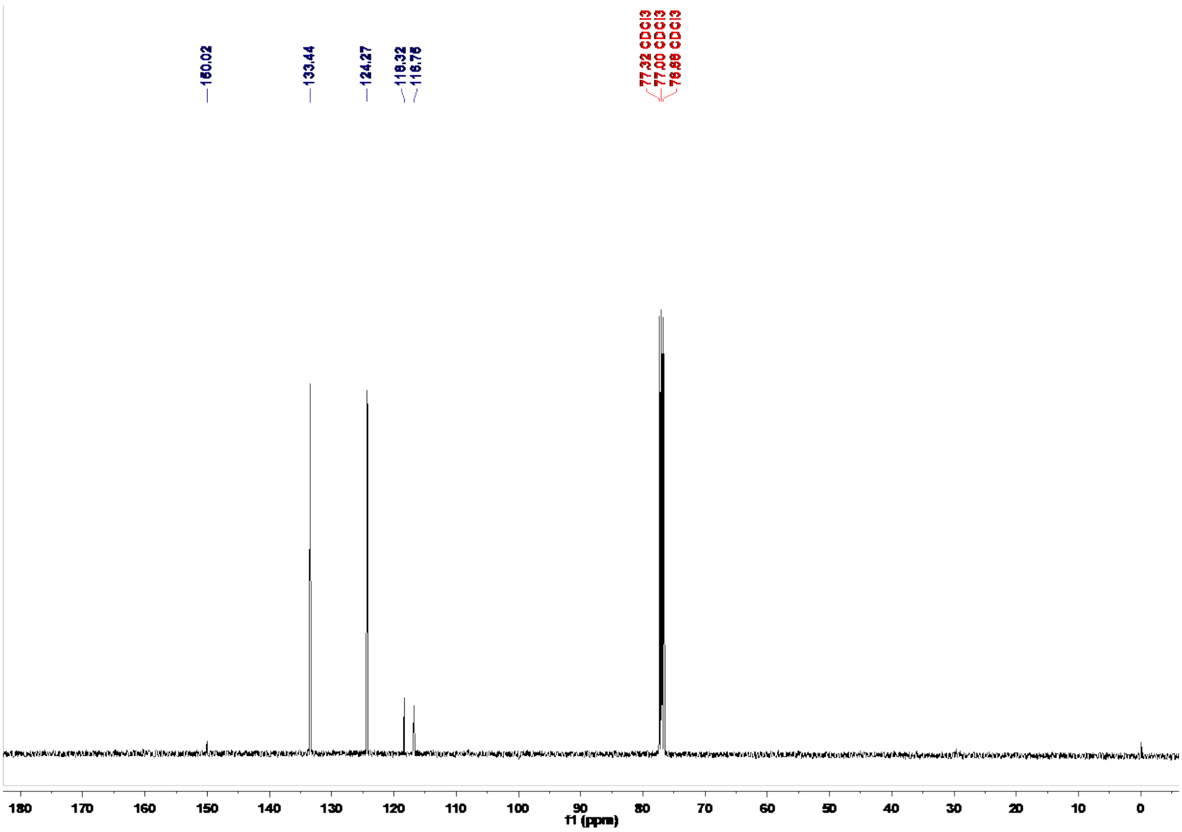
Methyl 4-cyanobenzoate (4j)



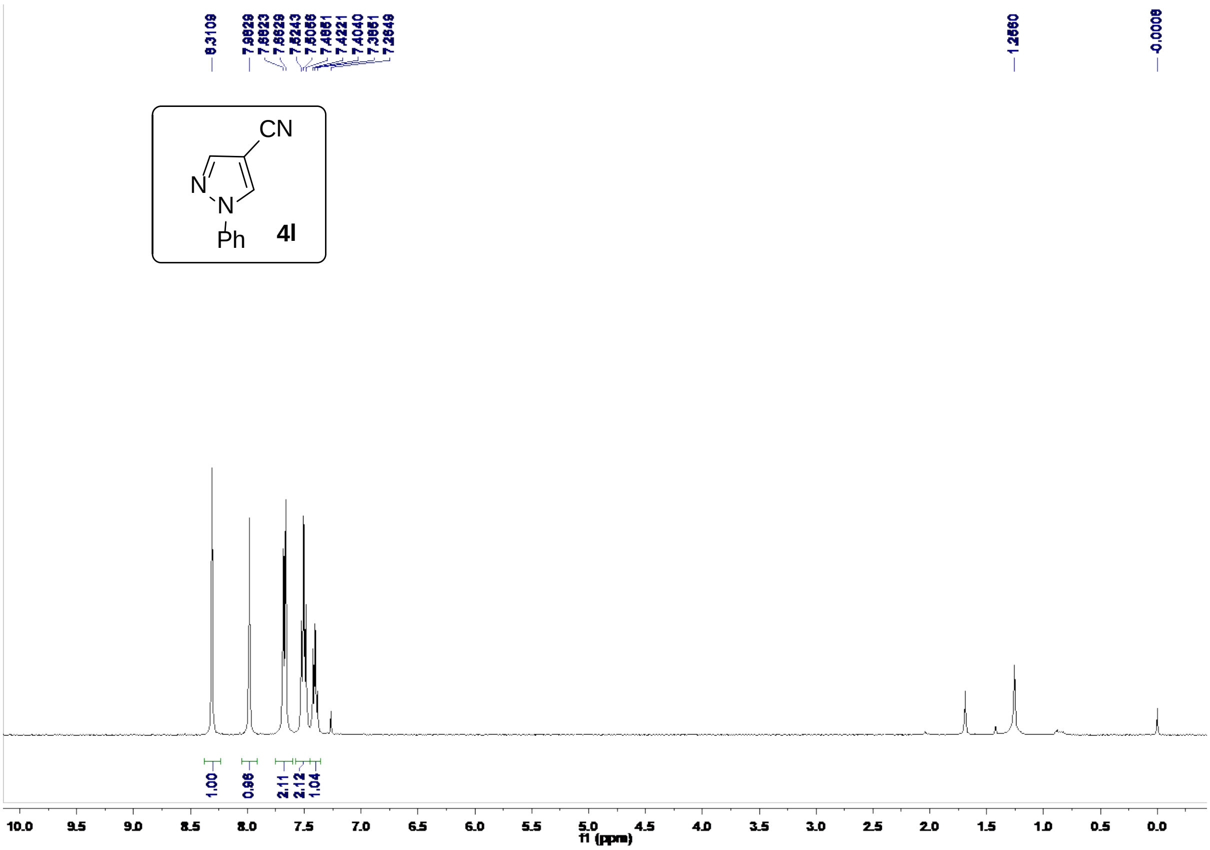


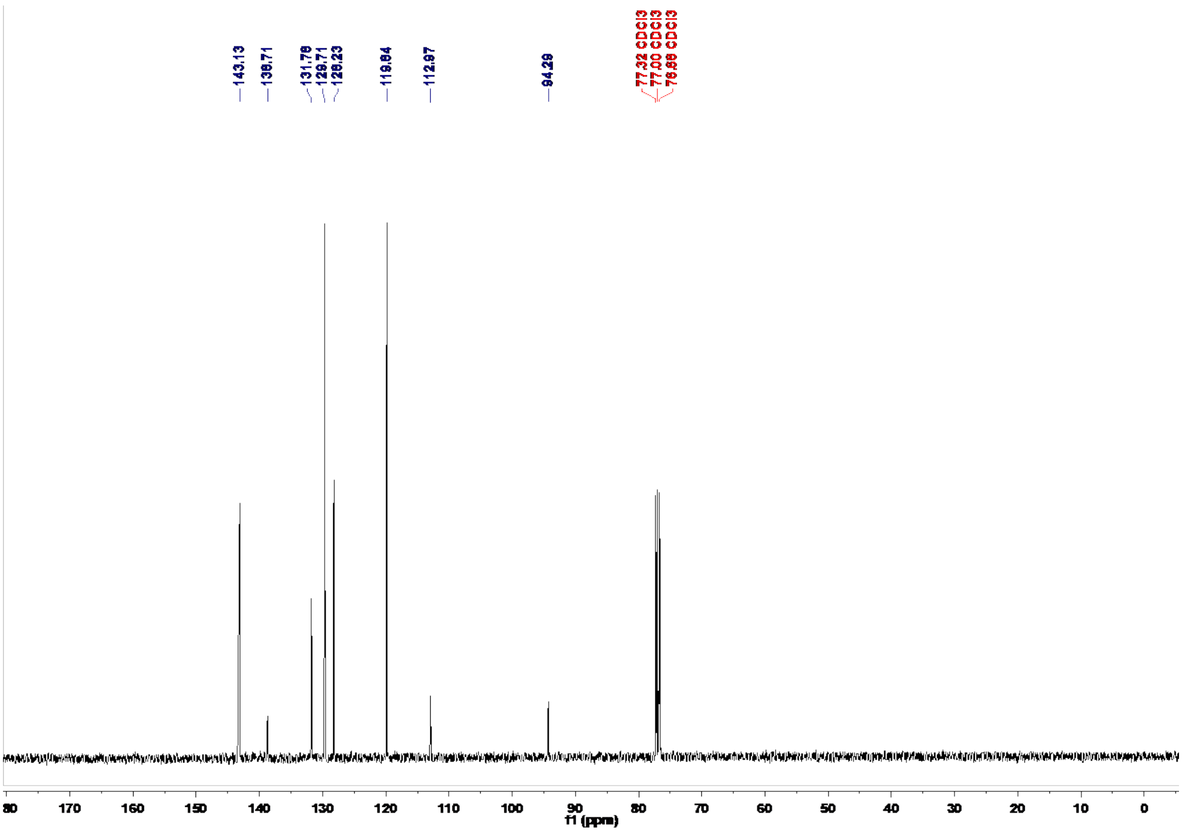
4-Nitrobenzonitrile (4k)



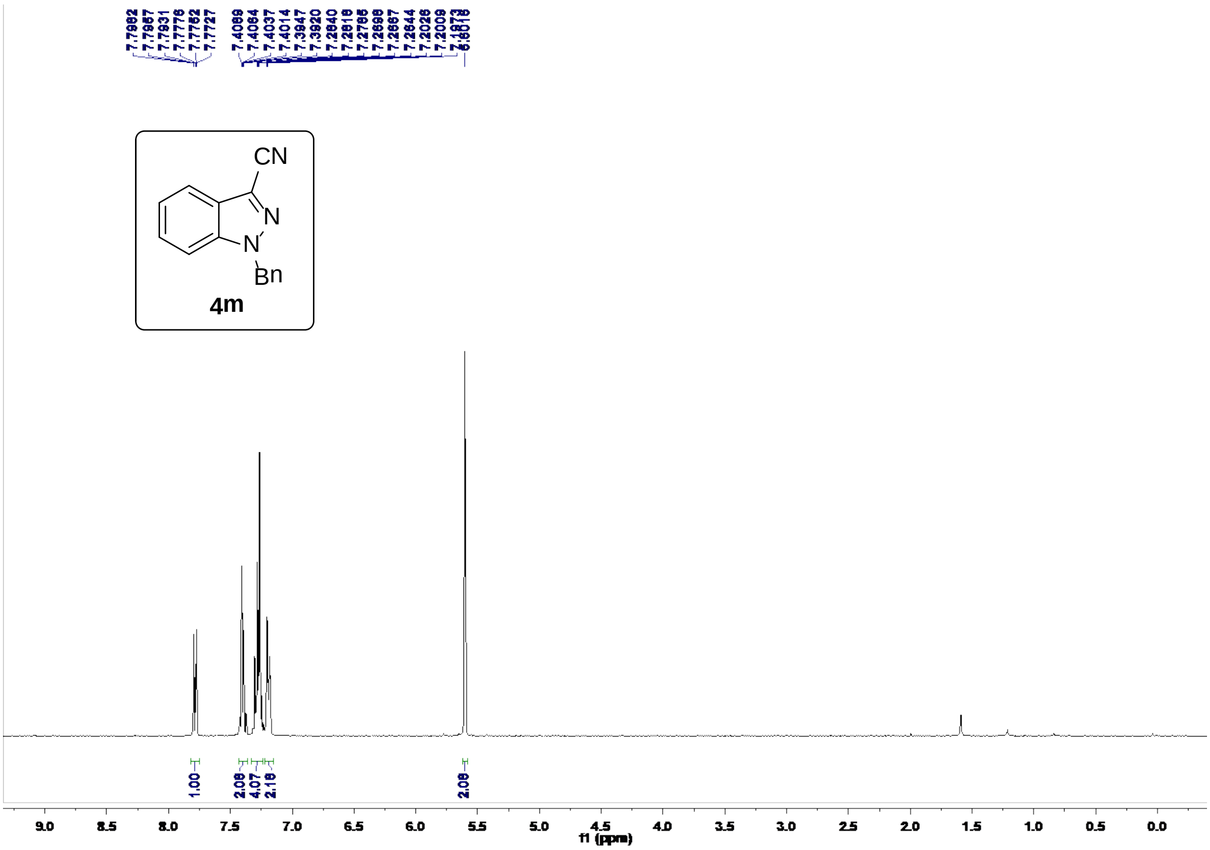


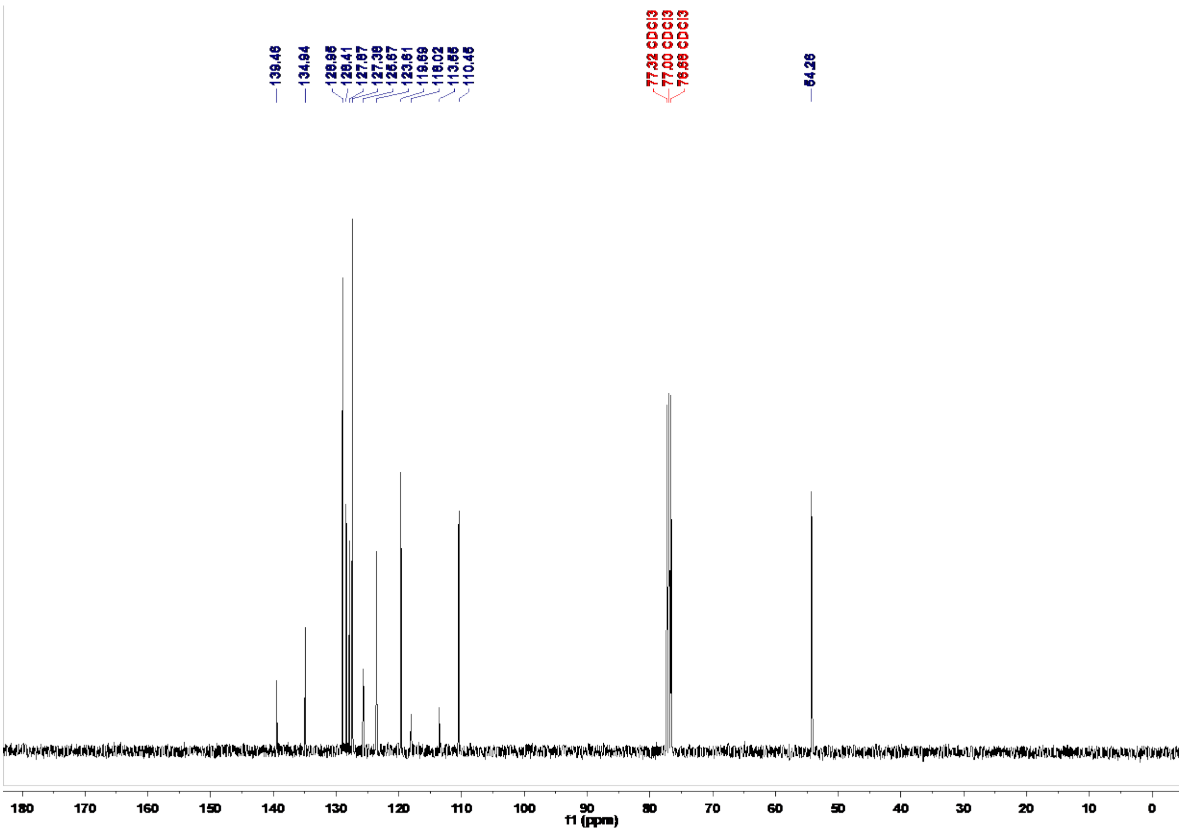
1-Phenyl-1*H*-pyrazole-4-carbonitrile (4l)





1-Benzyl-1*H*-indazole-3-carbonitrile (4m)





2-Cyano-9*H*-xanthen-9-one (4n)