Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Palladium-Catalyzed Cyanide Metathesis: Utilization of Benzyl Cyanide as an Operator-Benign Reagent for Aryl Halide Cyanations

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1. General experimental details:

Melting points were recorded on a BÜCHI 535. NMR spectra were obtained on a Bruker AVANCE DMX500 spectrometer operating at 500 MHz or 400 MHz for ^{1}H-NMR, 125 MHz or 100 MHz for ^{13}C-NMR in $CDCl_3$.Chemicals were either purchased or purified by standard techniques without special instructions. 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: s = singlet, d = doublet, t = triplet, m = multiplet. Coupling constants J, were reported in hertz unit(Hz). Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ as an internal standard. ^{13}C NMR spectra were obtained by using the same NMR spectrometers and chemical shifts were reported in ppm referenced to the center line of a triplet at 77.36 ppm of $CDCl_3$.

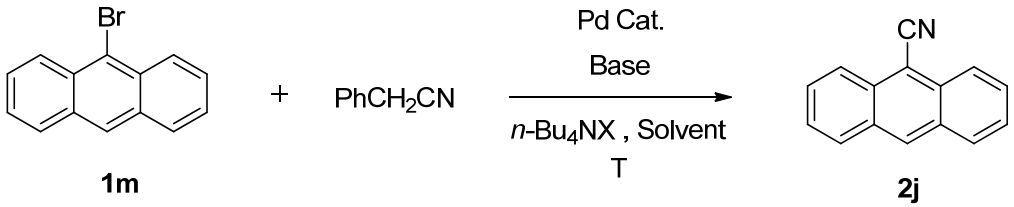
Typical experimental procedures for the reaction of aryl halide and benzyl cyanide: A 25mL round-bottom flask was charged with aryl halide (1 mmol), benzyl cyanide (176 mg, 1.5 mmol), K_2CO_3 (690 mg, 5 mmol), *n*-Bu_4NBr (322 mg, 1 mmol), $Pd(OAc)_2$ (11.2 mg, 0.05 mmol), and DMF (5 mL). The reaction mixture was stirred at 90 °C (oil bath) for 8 h. After cooling to room temperature, the resultant mixture was added to 30mL water, extracted with DCM (3×5 mL), and dried over anhydrous Na_2SO_4. The dichloromethane was evaporated under reduced pressure and the residue was purified by flash column chromatography on a silica gel to give the products.

Procedure for 1c to 2c in 5 mmol scale: 1c (1.17 g, 5 mmol), benzyl cyanide (878 mg, 7.5 mmol), K_2CO_3 (3.45 g, 25 mmol), *n*-Bu_4NBr (1.61 g, 5 mmol), $Pd(OAc)_2$ (56 mg, 0.25 mmol), and DMF (30 mL). The reaction gave **2c** (345 mg) in 52% yield along with 4,4'-dimethoxy-1,1'-biphenyl (226 mg) in 42% yield.

Procedure for the reaction of 1p with benzyl cyanide in 5 mmol scale: 1p (1.23 g, 5 mmol), benzyl cyanide (878 mg, 7.5 mmol), K_2CO_3 (3.45 g, 25 mmol), *n*-Bu_4NBr (1.61 g, 5 mmol), $Pd(OAc)_2$ (56 mg, 0.25 mmol), and DMF (30 mL). The reaction gave a mixture (440 mg) of **2na** and **2nb** in 46% yield.

2. Optimization of reaction conditions for the preparation of 2j

Table S1 Screening of reaction condition of 9-bromoanthracene and benzyl cyanide catalyzed by palladium[a]

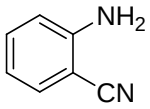


Entry	Pd Cat.	Base (equiv.)	*n*-Bu_4NX (equiv.)	Solvent	Temp (°C)	Yield(%)[b]
1	5%$PdCl_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	86
2	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	88
3	5% $PdCl_2(PPh_3)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	n.d.
4	5% $Pd(OAc)_2$ 10%PPh_3	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	n.d.
5[c]	5%$Pd(PPh_3)_4$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	trace
6[c]	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	15
7	2.5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	trace
8	3% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	trace
9	4% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	78
10	10% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	90	86
11	5% $Pd(OAc)_2$	K_2CO_3 (4)	*n*-Bu_4NBr (1)	DMF	90	83
12	5% $Pd(OAc)_2$	K_2CO_3 (2)	*n*-Bu_4NBr (1)	DMF	90	80
13	5% $Pd(OAc)_2$	K_2CO_3 (1)	*n*-Bu_4NBr (1)	DMF	90	70
14	5% $Pd(OAc)_2$	K_2CO_3 (0)	*n*-Bu_4NBr (1)	DMF	90	40
15	5% $Pd(OAc)_2$	$NaHCO_3$ (5)	*n*-Bu_4NBr (1)	DMF	90	40
16	5% $Pd(OAc)_2$	NaOAc (5)	*n*-Bu_4NBr (1)	DMF	90	trace
17	5% $Pd(OAc)_2$	Et_3N (5)	*n*-Bu_4NBr (1)	DMF	90	trace
18	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (0.5)	DMF	90	66
19	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (2)	DMF	90	77
20	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (0)	DMF	90	59
21	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NCl (1)	DMF	90	77
22	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NI (1)	DMF	90	53
23	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-$Bu_4NF{\cdot}3H_2O$ (1)	DMF	90	n.d
24	5% $Pd(OAc)_2$	K_2CO_3 (0)	*n*-Bu_4NBr (0)	DMF	90	trace
25	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMAc	90	34
26	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	Dioxane	90	54
27	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMSO	90	n.d
28	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	THF	90	trace
29	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	110	85
30	5% $Pd(OAc)_2$	K_2CO_3 (5)	*n*-Bu_4NBr (1)	DMF	70	6

[a] *Reaction conditions*: unless otherwise specified,the reaction was carried out under air, 8 h. [b] Isolated yield. [c] under N_2.

3. Spectral data for the products:

2-aminobenzonitrile (2a)

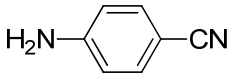


brown solid, m.p. 49-50 ^{o}C (Lit.[1], 48-50 ^{o}C)

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 (d, *J* = 7.8 Hz, 1H), 7.34-7.31 (m, 1H), 6.75-6.72 (m, 2H), 4.43 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) : δ 149.9, 134.3, 132.6, 118.2, 117.9, 115.4, 96.2.

4-aminobenzonitrile (2b)

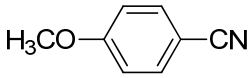


yellow solid, m.p. 85-87 ^{o}C (Lit.[1], 84-86 ^{o}C)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.42 (d, *J* = 8.5 Hz, 2H), 6.65 (d, *J* = 8.5 Hz, 2H), 4.18 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 150.6, 134.1, 120.5, 114.7, 100.4.

4-methoxybenzonitrile (2c)

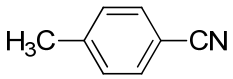


white solid, m.p. 60-61 ^{o}C (Lit.[2], 60-62 ^{o}C)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.59 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 163.1, 134.2, 119.5, 115.0, 104.2, 55.8.

4-methylbenzonitrile (2d)

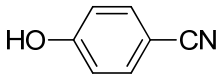


white solid, m.p. 29-30 ^{o}C (Lit.[3], 29-30 ^{o}C)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.53 (d, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 2H), 2.42 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 143.9, 132.2, 130.0, 119.4, 109.4, 22.0.

4-hydroxybenzonitrile (2e)

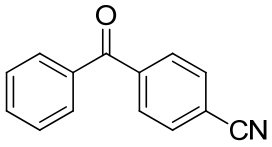


white solid, m.p. 112-113 ^{o}C (Lit.[4], 111-113 ^{o}C)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.57 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.58 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 160.4, 134.6, 119.5, 116.8, 103.5.

4-benzoylbenzonitrile (2f)

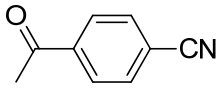


white solid, m.p. 113-114 °C (Lit.[5], 113-114 °C)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.88 (d, J = 8.0 Hz, 2H), 7.81-7.78 (m, 4H), 7.65 (dd, J_1 = J_2 = 7.2 Hz, 1H), 7.52 (dd, J_1 = J_2 = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 195.3, 141.5, 136.5, 133.6, 132.4, 130.5, 130.3, 128.9, 118.3, 115.9.

4-acetylbenzonitrile (2g)

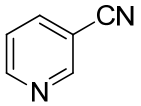


white solid, m.p. 57-58 °C (Lit.[6], 56-58 °C)

^{1}H NMR (500 MHz, $CDCl_3$) : δ 8.05 (d, J = 8.3 Hz, 2H), 7.79 (d, J = 8.3 Hz, 2H), 2.66 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) : δ 196.8, 140.2, 132.8, 129.0, 118.2, 116.7, 27.1.

3-cyanopyridine (2h)

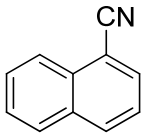


white solid, m.p. 51-52 °C (Lit.[7], 50-51 °C)

^{1}H NMR (500 MHz, $CDCl_3$) : δ 8.92 (s, 1H), 8.85-8.84 (m, 1H), 8.00 (dd, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 1H), 7.49-7.46 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) : δ 153.2, 152.7, 139.5, 123.8, 116.7, 110.3.

1-naphthonitrile (2i)

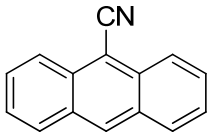


white solid, m.p. 36-37 °C (Lit.[2], 35-36 °C)

^{1}H NMR (500 MHz, $CDCl_3$) : δ 8.21 (d, J = 8.3 Hz, 1H), 8.05 (d, J = 8.3 Hz, 1H), 7.89 (dd, J_1 = 9.0 Hz, J_2 = 7.5 Hz, 2H), 7.67 (dd, J_1 = 7.0 Hz, J_2 = 7.5 Hz, 1H), 7.60 (dd, J_1 = 8.0 Hz, J_2 = 7.0 Hz, 1H), 7.50 (dd, J_1 = 7.5 Hz, J_2 = 8.0 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) : δ 133.5, 133.1, 132.8, 132.6, 128.9, 128.8, 127.8, 125.3, 125.1, 118.1, 110.4.

anthracene-9-carbonitrile (2j)

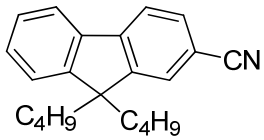


yellow solid, m.p. 175-176 °C (Lit.[8], 173-177 °C)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.60 (s, 1H), 8.37 (d, J = 8.4 Hz, 2H), 8.03 (d, J = 8.4 Hz, 2H), 7.68 (dd, J_1 = J_2 = 7.6 Hz, 2H), 7.55 (dd, J_1 = J_2 = 7.6 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) : δ 133.5, 133.0, 130.8, 129.2, 129.2, 126.6, 125.5, 117.5, 105.5.

9,9-dibutyl-9H-fluorene-2-carbonitrile (2k)



white solid, m.p. 103-104 °C

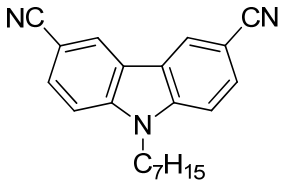
^{1}H NMR (500 MHz, $CDCl_3$) : δ 7.77-7.73 (m, 2H), 7.64-7.61 (m, 2H), 7.39-7.37 (m, 3H), 2.01-1.95 (m, 4H), 1.11-1.03 (m, 4H), 0.67 (t, J = 7.4 Hz, 6H), 0.58-0.48 (m, 4H).

^{13}C NMR (125 MHz, $CDCl_3$) : δ 151.7, 151.6, 146.0, 139.4, 131.5, 129.2, 127.5, 126.7, 123.4, 121.1, 120.5, 120.2, 110.1, 55.7, 40.2, 26.1, 23.2, 14.0.

IR (KBr) : 2951, 2929, 2860, 2220, 1466, 1452, 831, 737, 590 cm^{-1}.

HRMS : cacld. for $C_{22}H_{25}N$ [M^+], 303.1987; found, 303.1985.

9-heptyl-9H-carbazole-3,6-dicarbonitrile (2l)



yellow solid, m.p. 172-173 °C

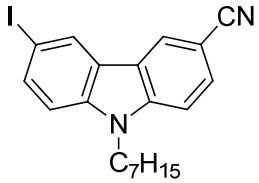
^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.41 (s, 2H), 7.79 (d, J = 8.6 Hz, 2H), 7.53 (d, J = 8.6 Hz, 2H), 4.36 (t, J = 7.2 Hz, 2H), 1.94-1.83 (m, 2H), 1.35-1.25 (m, 8H), 0.86 (t, J = 6.7 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 143.0, 130.6, 126.0, 122.4, 120.1, 110.5, 103.7, 44.1, 31.9, 29.2, 29.1, 27.4, 22.8, 14.3.

IR (KBr) : 2926, 2856, 2220, 1596, 1483, 821, 593 cm^{-1}.

HRMS : cacld. for $C_{21}H_{21}N_3$ [M^+], 315.1735; found, 315.1737.

9-heptyl-6-iodo-9H-carbazole-3-carbonitrile (2m)



brown solid, m.p. 117-118 °C

^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.39 (s, 1H), 8.31 (s, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 4.28 (t, *J* = 7.2 Hz, 2H), 1.89-1.79 (m, 2H), 1.32-1.24 (m, 8H), 0.85 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ 142.2, 140.4, 135.6, 129.9, 129.8, 125.7, 124.6, 121.9, 120.6, 111.6, 109.9, 102.4, 83.1, 43.8, 31.9, 29.3, 29.1, 27.4, 22.8, 14.3.

IR (KBr) : 3474, 3414, 2928, 2853, 2221, 1479, 802 cm^{-1}.

HRMS : cacld. for $C_{20}H_{21}IN_2$ [M^+], 416.0749; found, 416.0747.

4. The detection of CN^- by the picric acid strip

Preparation of the picric acid strip:

Picric acid strip was prepared by wetting filter paper with a solution of 5.0 g of sodium bicarbonate and 0.5 g picric acid in 100 mL water. After drying the paper, it was cut into strips for use.

Strip test of the cyanide anion:

Tartaric acid (0.2 g) and the target solution (1.5 mL) were added into a flask. A sealed plastic vial, with a number of holes and a strip inside, was placed above the reaction mixture. The flask was heated in the water bath under 80 °C for 20 minutes. The strip turned red indicating the existence of CN^-.[10]

Table S2 Detection of CN^- by the picric acid strip [a]

Entry	9-Br anthracene 0.5 mmol	$Pd(OAc)_2$ 0.025 mmol	*n*-Bu_4NBr 0.5 mmol	K_2CO_3 2.5 mmol	Cyanation reagent 0.75 mmol	color
1					$PhCH_2CN$	yellow
2	√	√	√	√	$PhCH_2CN$	pink
3		√	√	√	$PhCH_2CN$	pink
4				√	$PhCH_2CN$	yellow
5			√		$PhCH_2CN$	yellow
6			√	√	$PhCH_2CN$	yellow
7		√			$PhCH_2CN$	yellow
8					$K_3[Fe(CN)_6]$ [b]	pink
9					NaCN [b]	red

[a] *Reaction conditions*: The mixture was heated under 90 °C in 3 mL DMF for 2 h. [b] 0.25 mmol $K_3[Fe(CN)_6]$ or NaCN was tested.

5. References

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6. ^{1}H NMR and ^{13}C NMR of the products

Figure S1 ^{1}H-NMR spectrum of **2a**

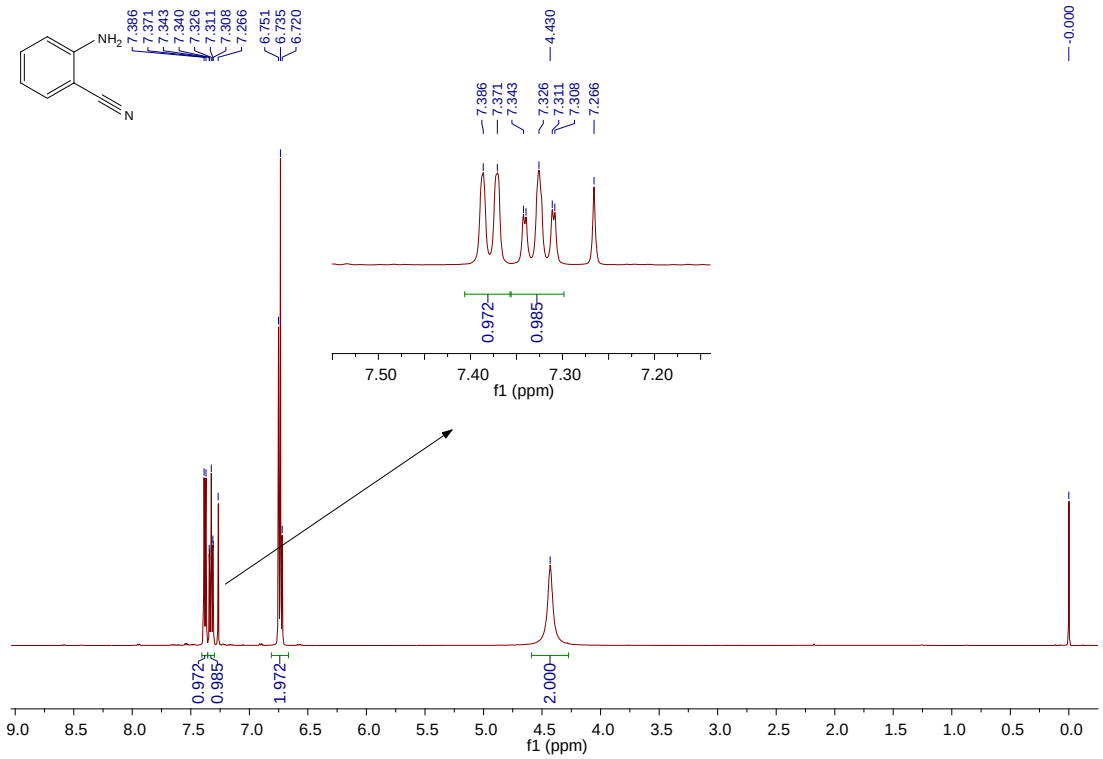


Figure S2 ^{13}C-NMR spectrum of **2a**

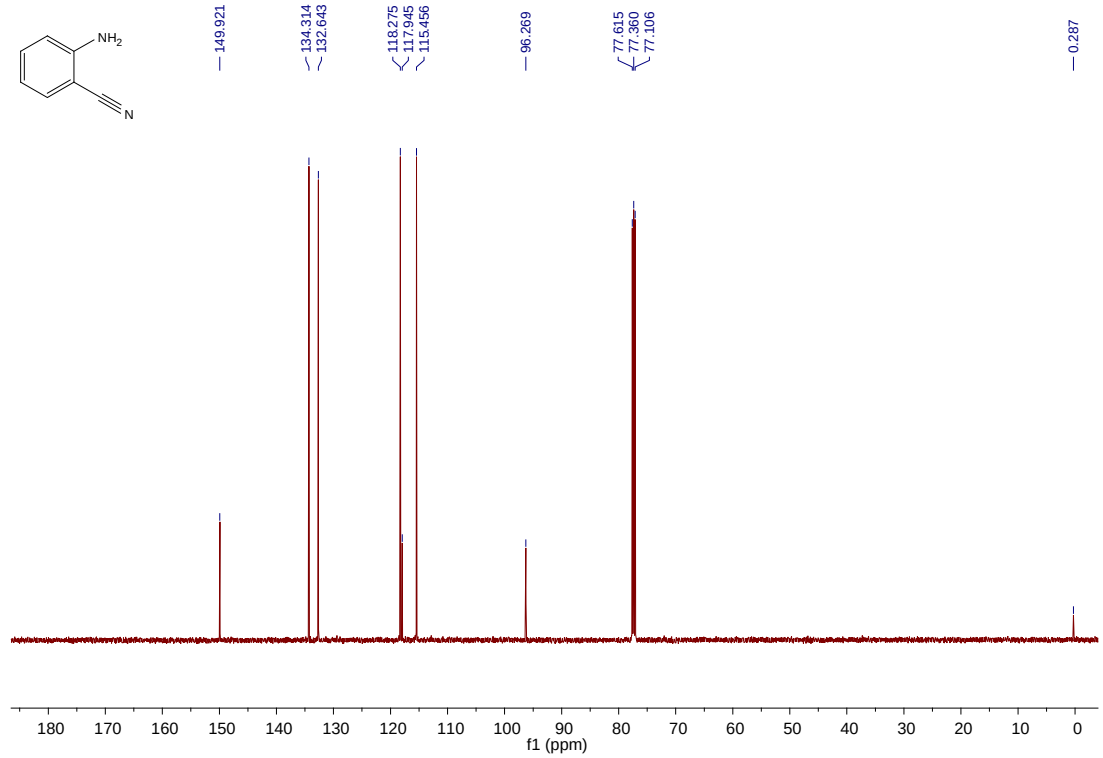


Figure S3 ^{1}H-NMR spectrum of **2b**

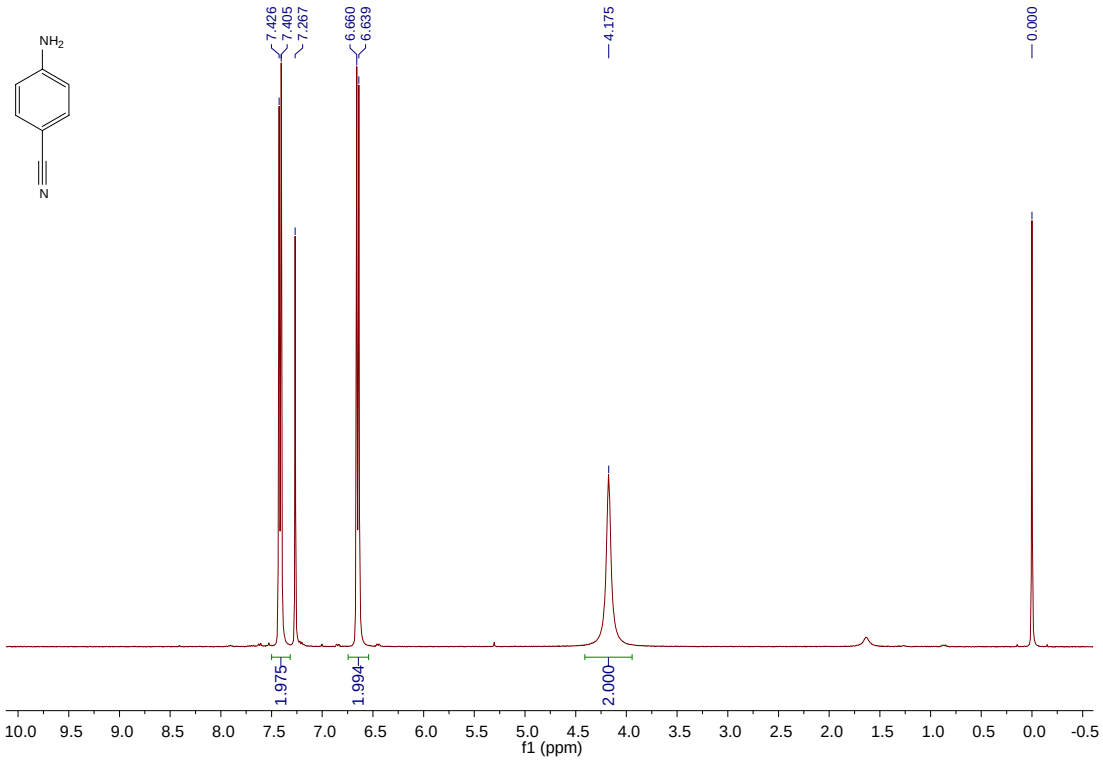


Figure S4 ^{13}C-NMR spectrum of **2b**

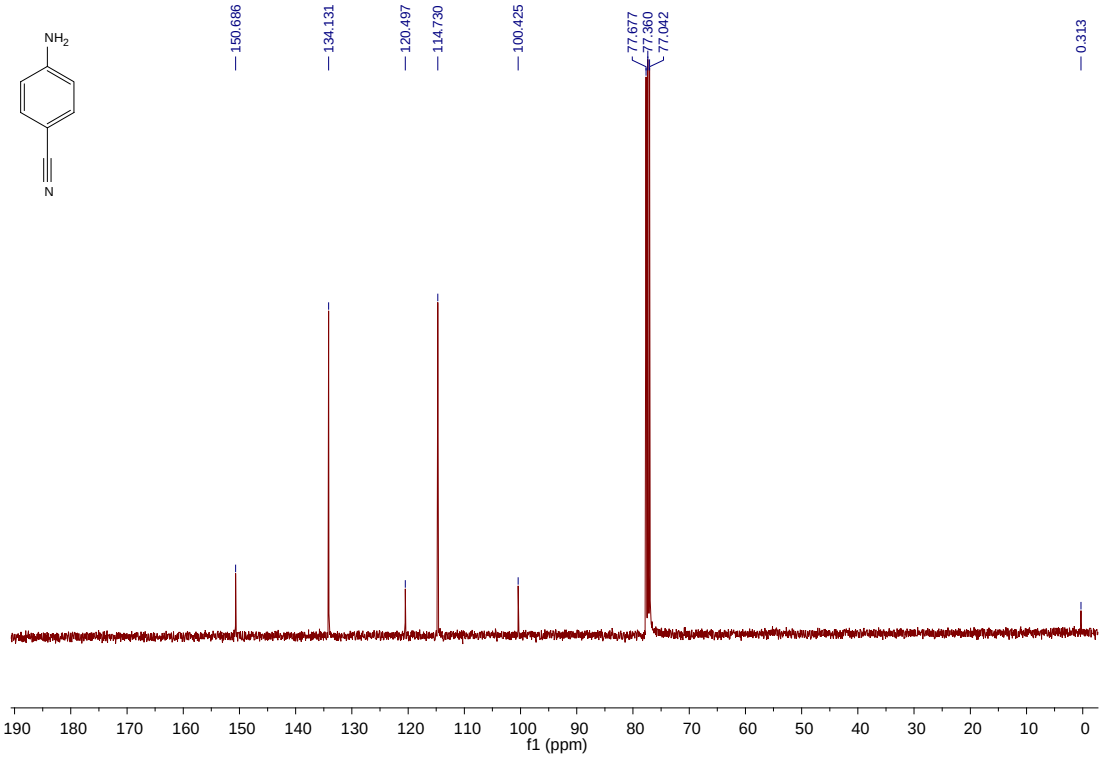


Figure S5 ^{1}H-NMR spectrum of **2c**

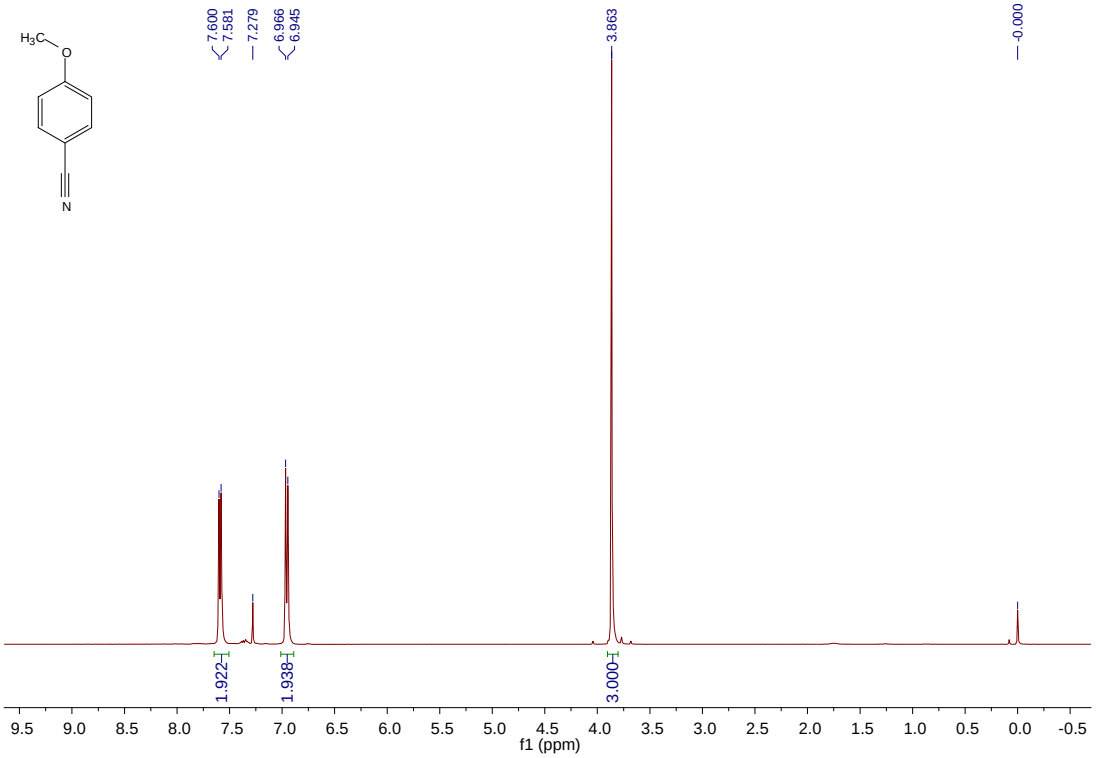


Figure S6 ^{13}C-NMR spectrum of **2c**

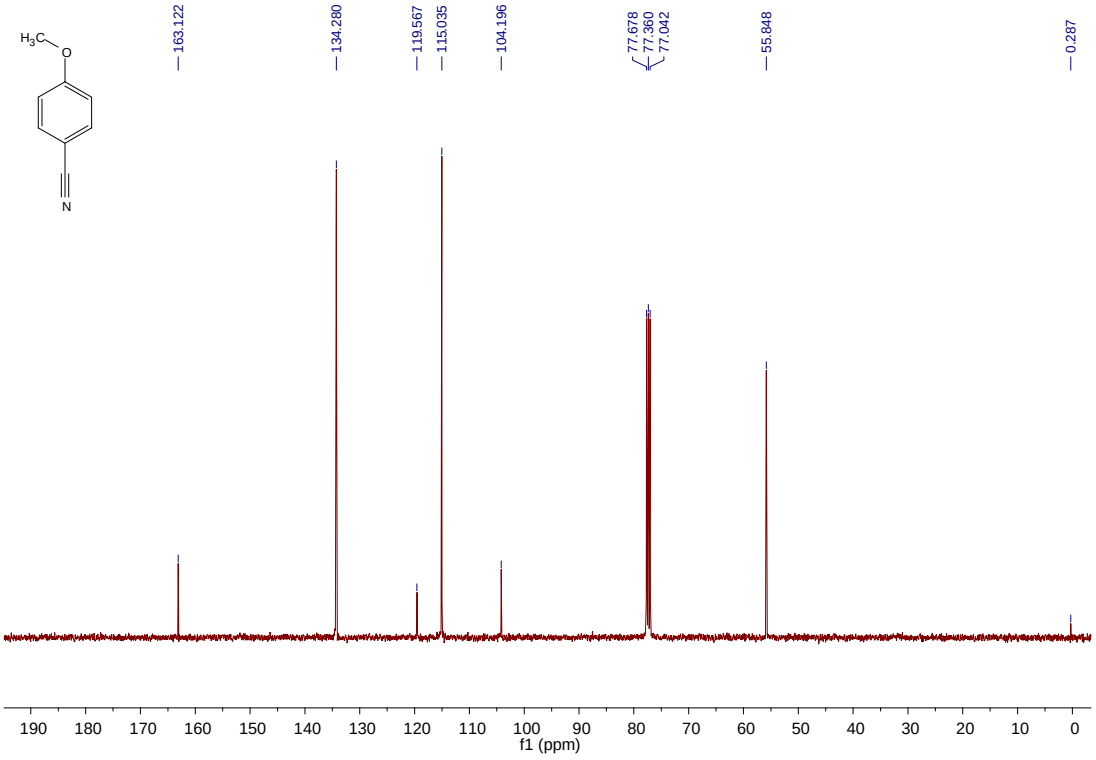


Figure S7 ^{1}H-NMR spectrum of **2d**

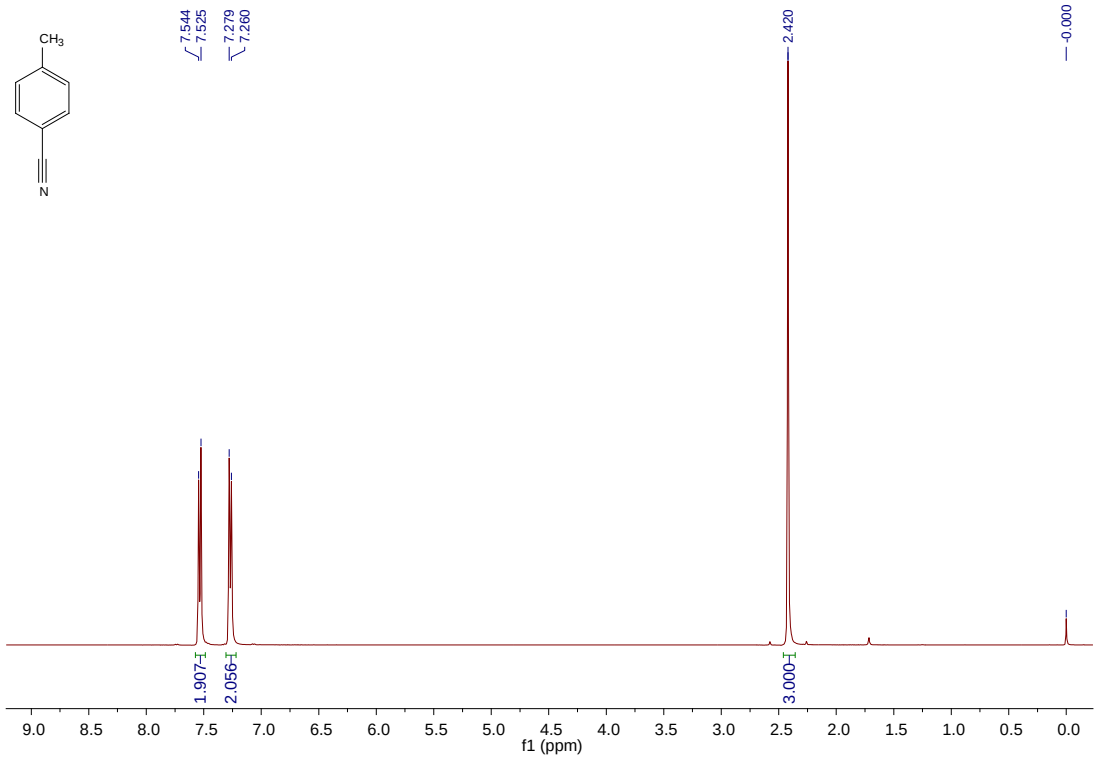


Figure S8 ^{13}C-NMR spectrum of **2d**

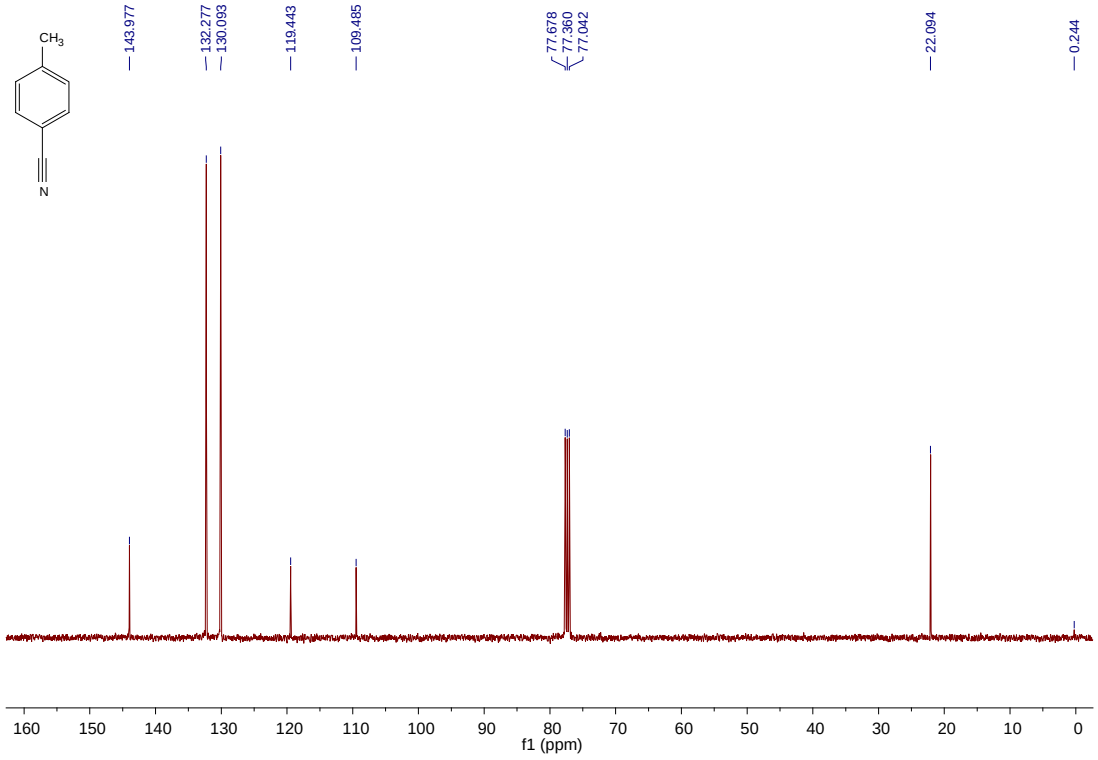


Figure S9 ^{1}H-NMR spectrum of **2e**

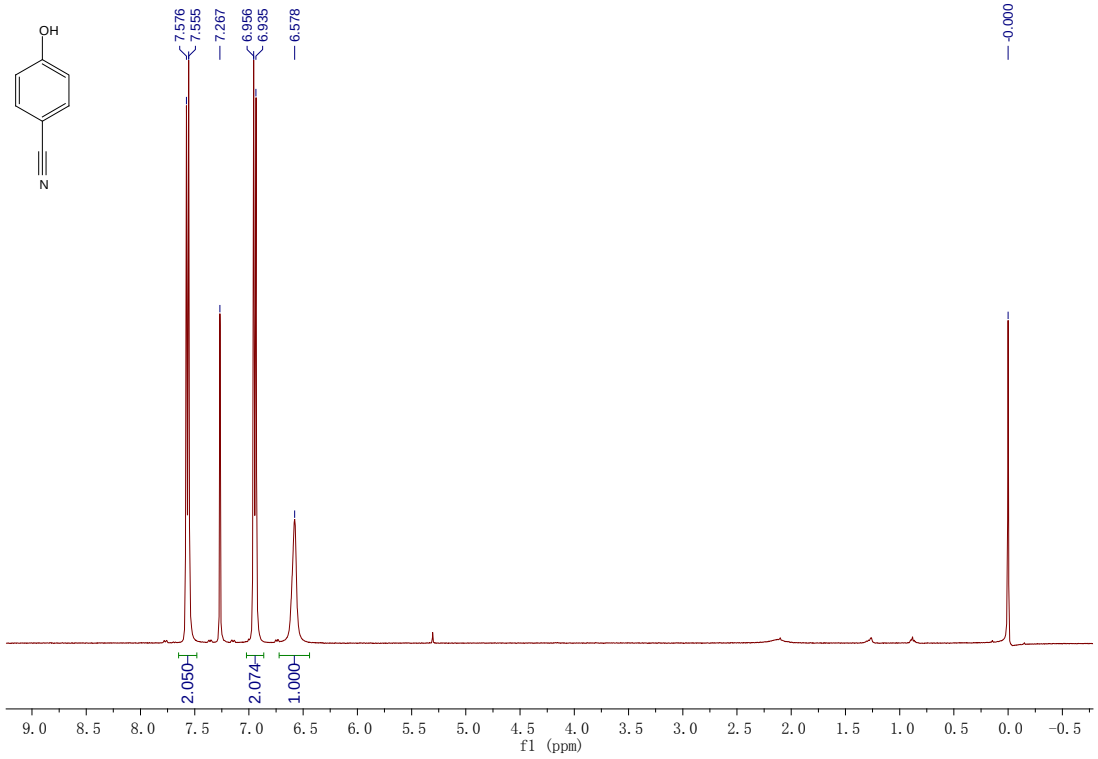


Figure S10 ^{13}C-NMR spectrum of **2e**

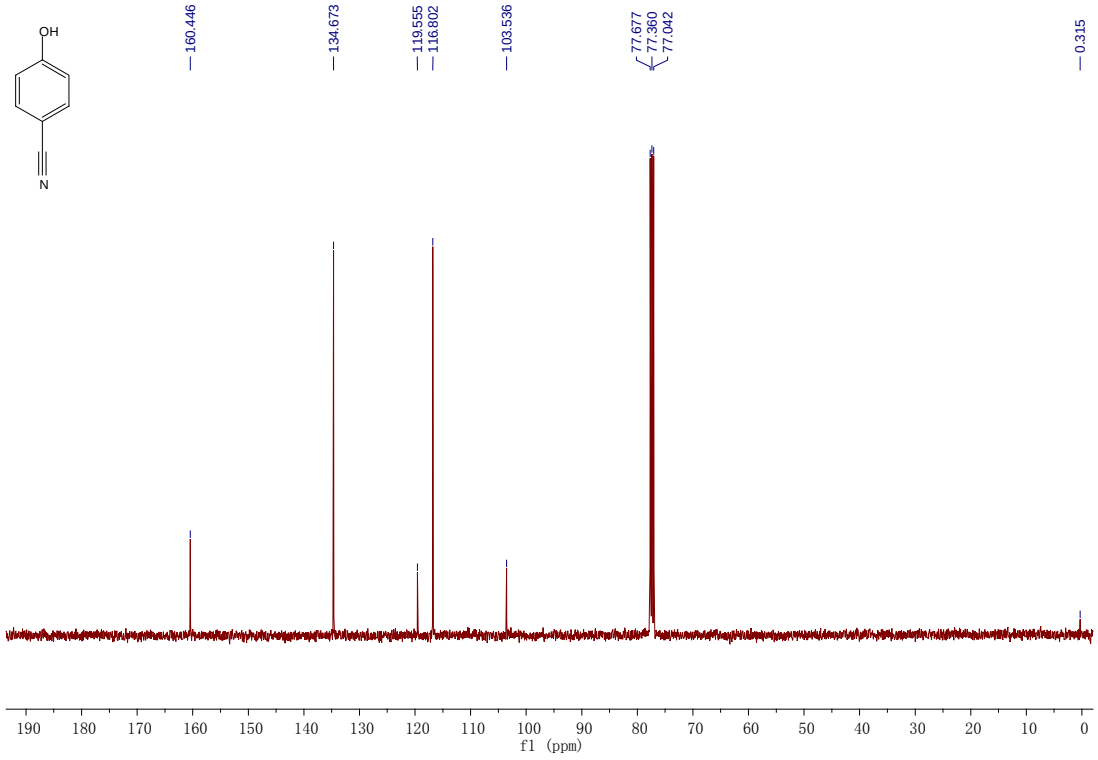


Figure S11 ^{1}H-NMR spectrum of **2f**

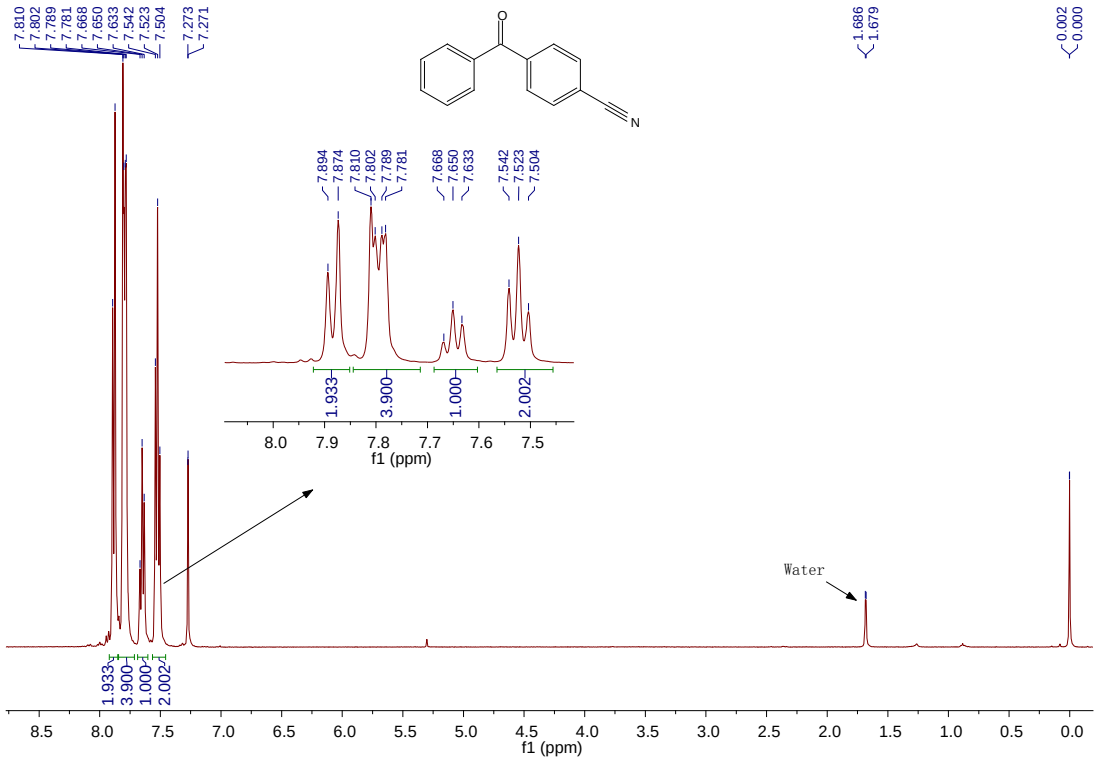


Figure S12 ^{13}C-NMR spectrum of **2f**

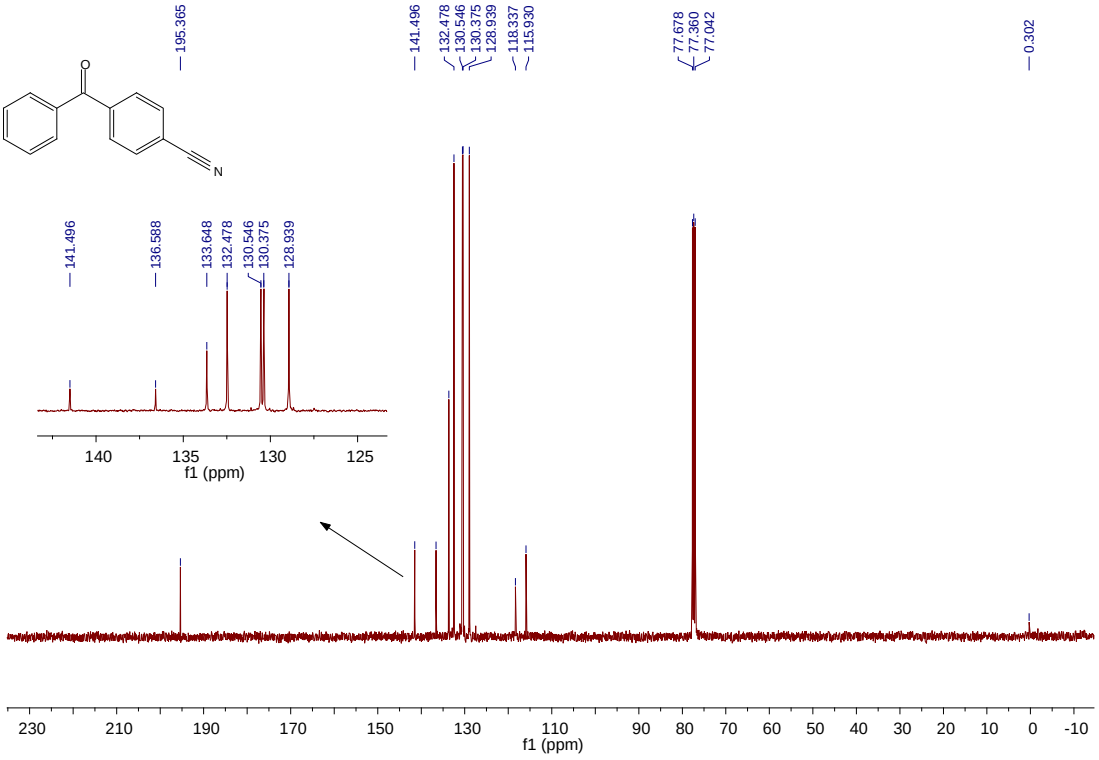


Figure S13 ^{1}H-NMR spectrum of **2g**

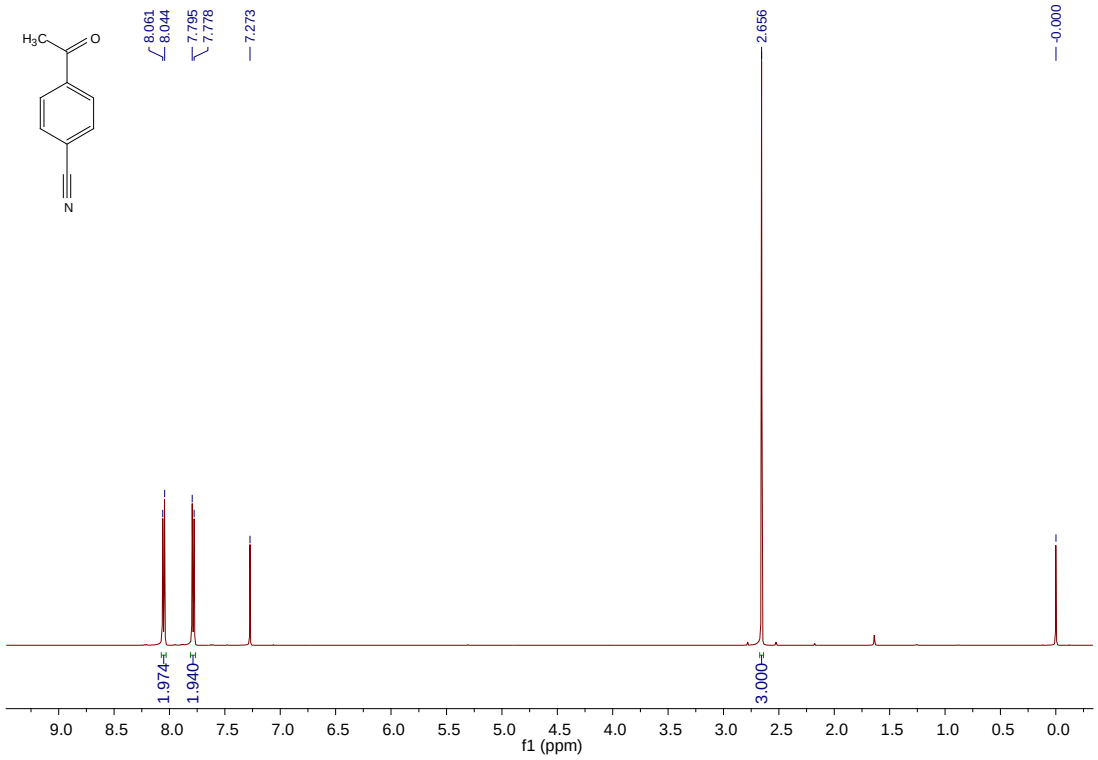


Figure S14 ^{13}C-NMR spectrum of **2g**

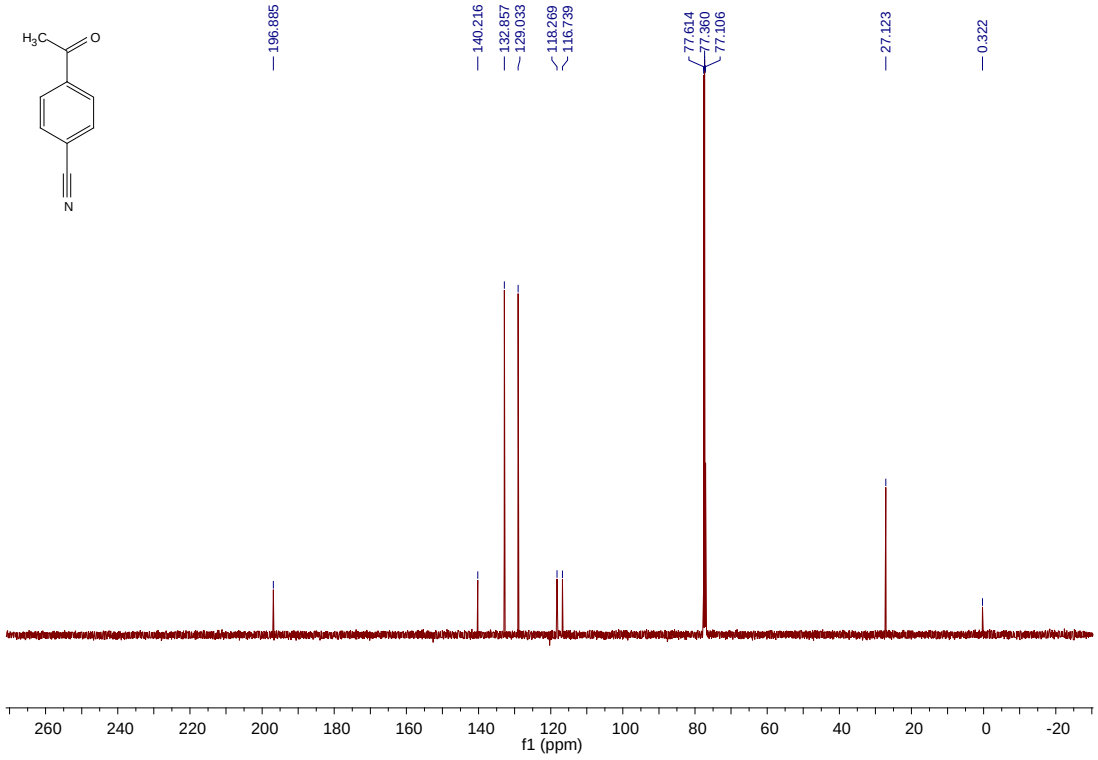


Figure S15 ^{1}H-NMR spectrum of **2h**

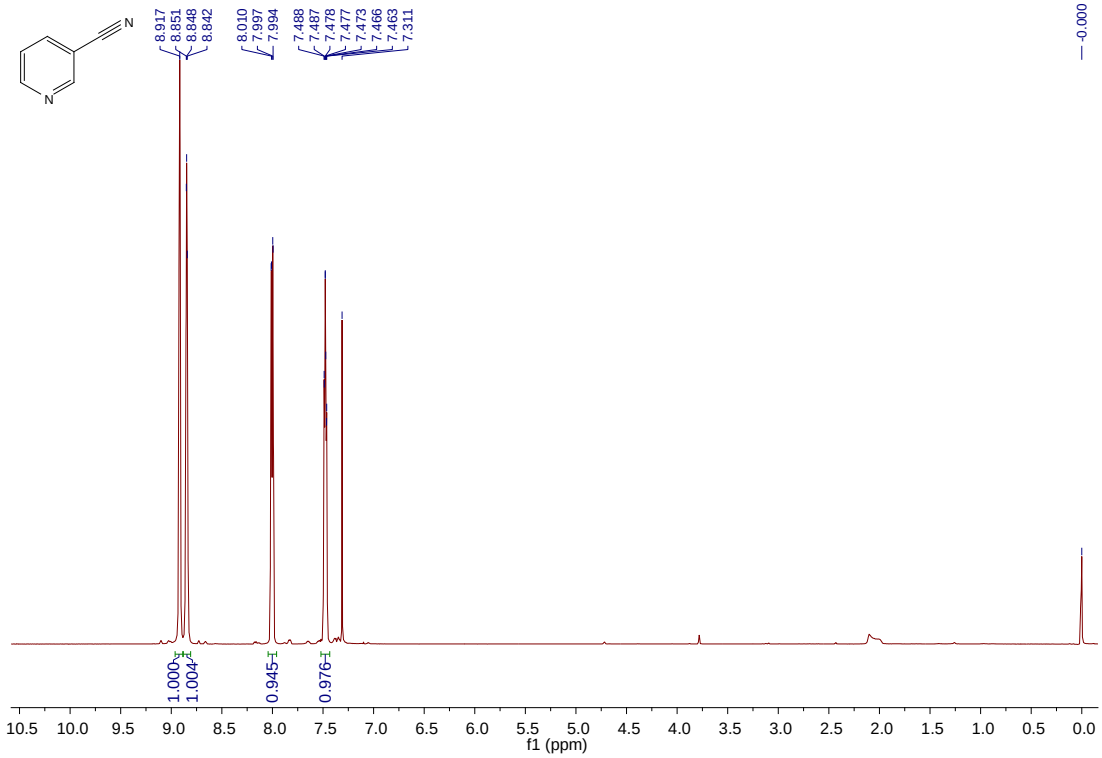


Figure S16 ^{13}C-NMR spectrum of **2h**

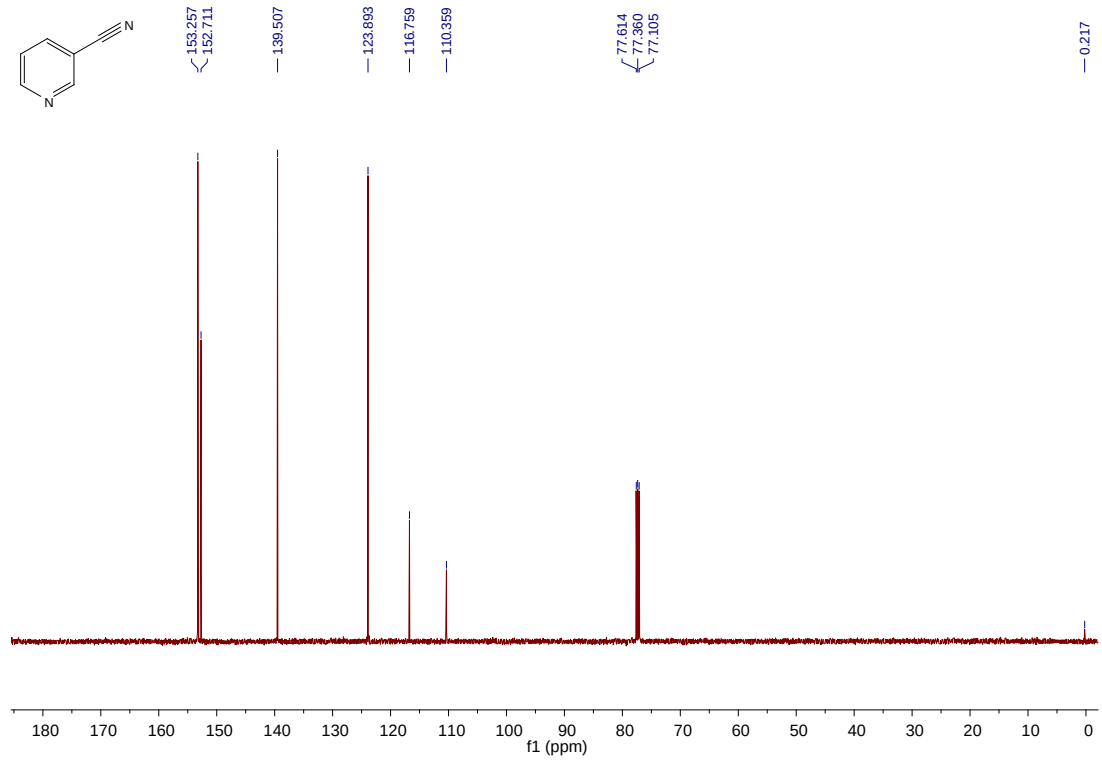


Figure S17 ^{1}H-NMR spectrum of **2i**

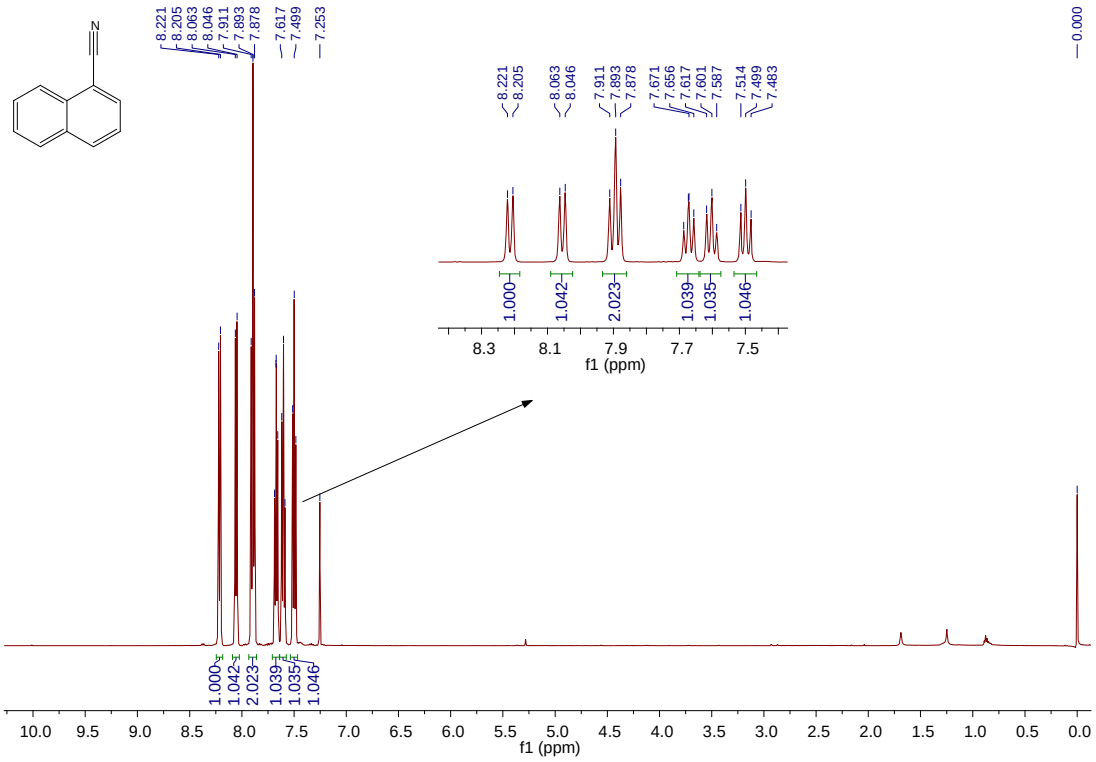


Figure S18 ^{13}C-NMR spectrum of **2i**

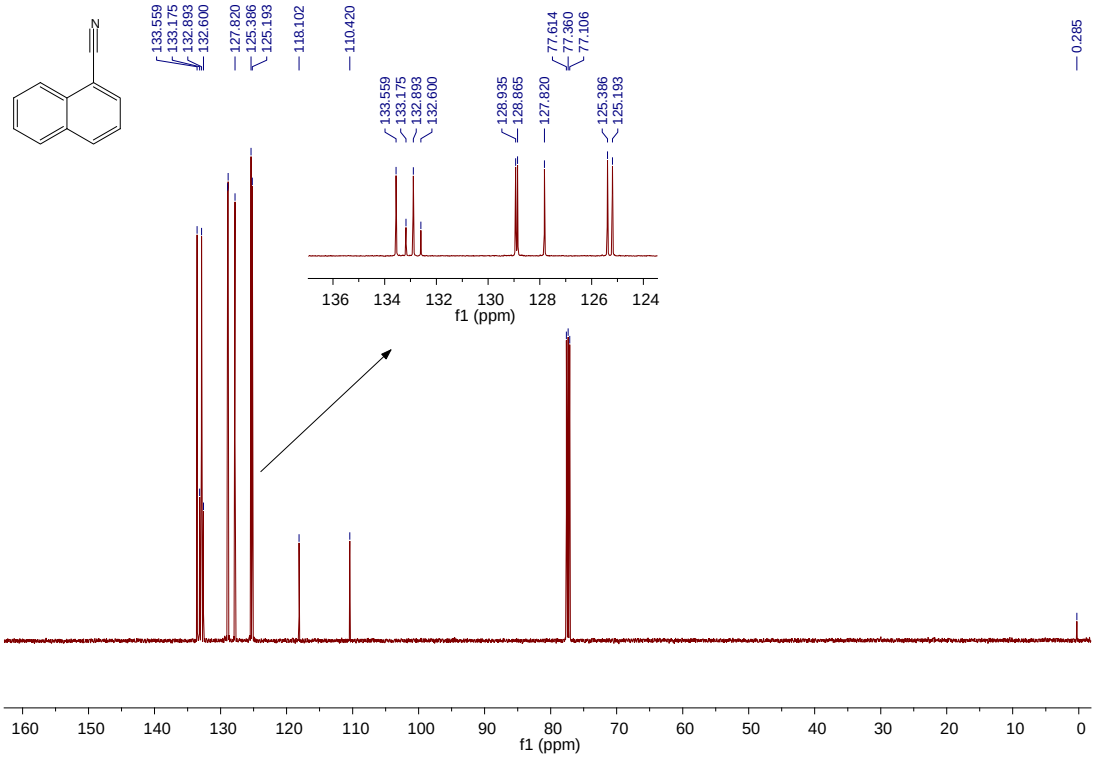


Figure S19 ^{1}H-NMR spectrum of **2j**

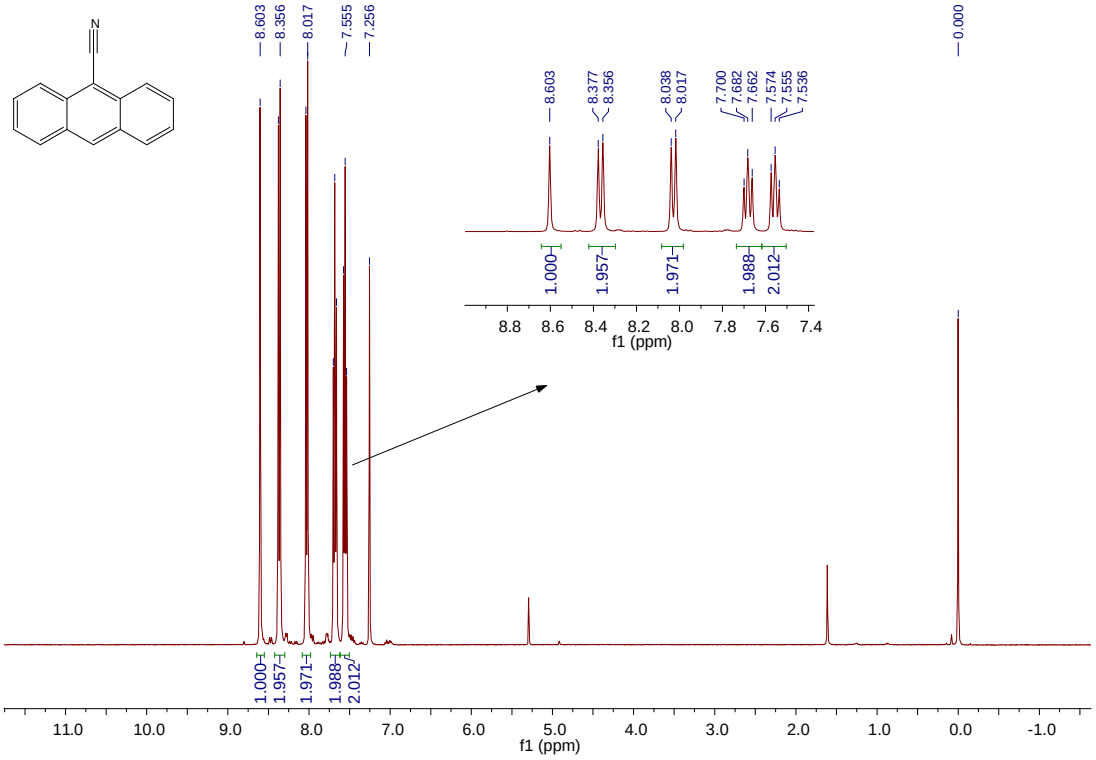


Figure S20 ^{13}C-NMR spectrum of **2j**

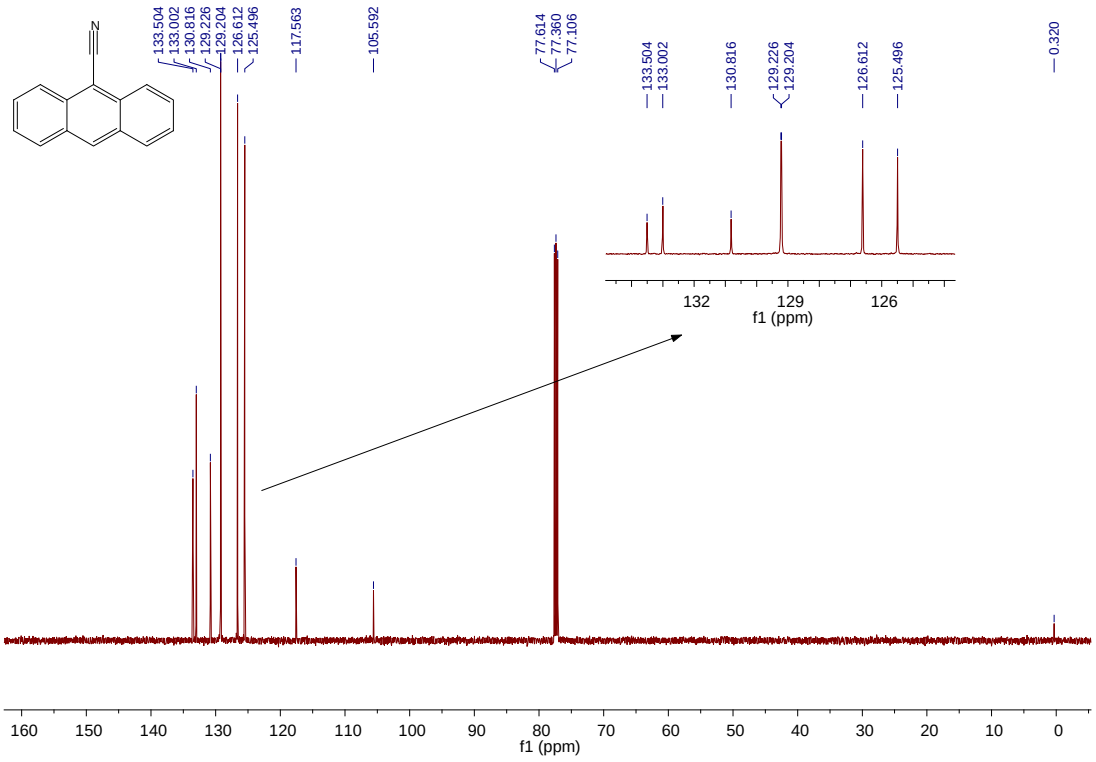


Figure S21 ^{1}H-NMR spectrum of **2k**

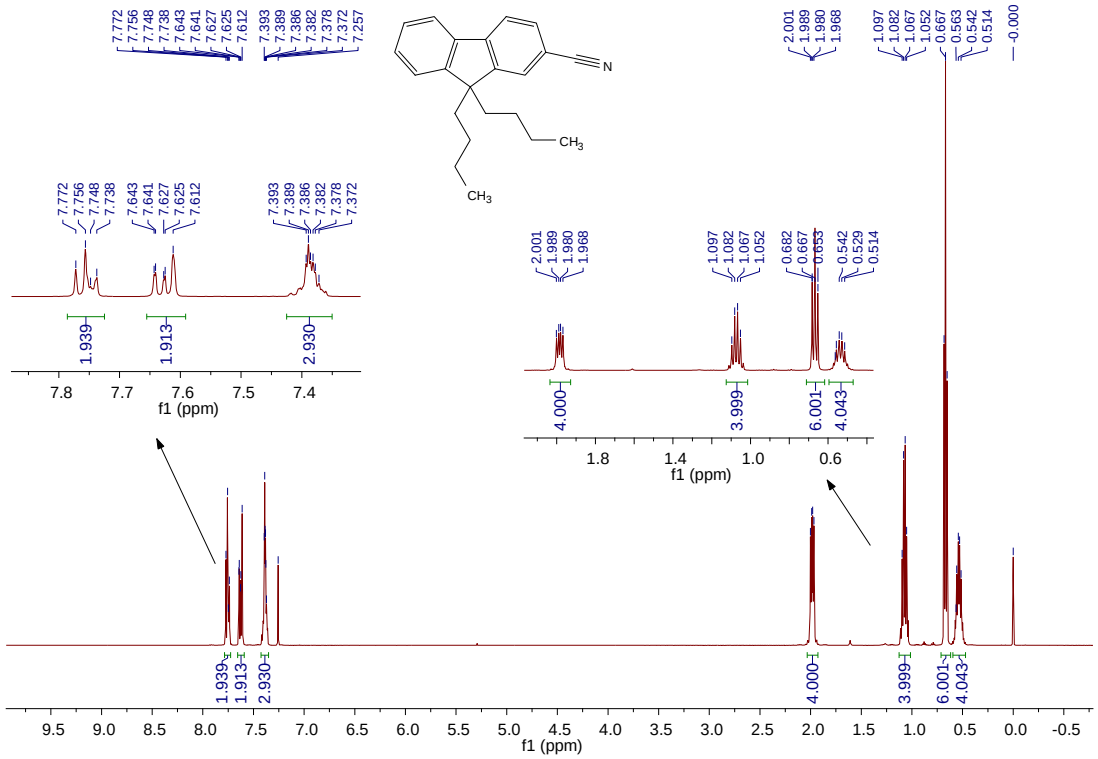


Figure S22 ^{13}C-NMR spectrum of **2k**

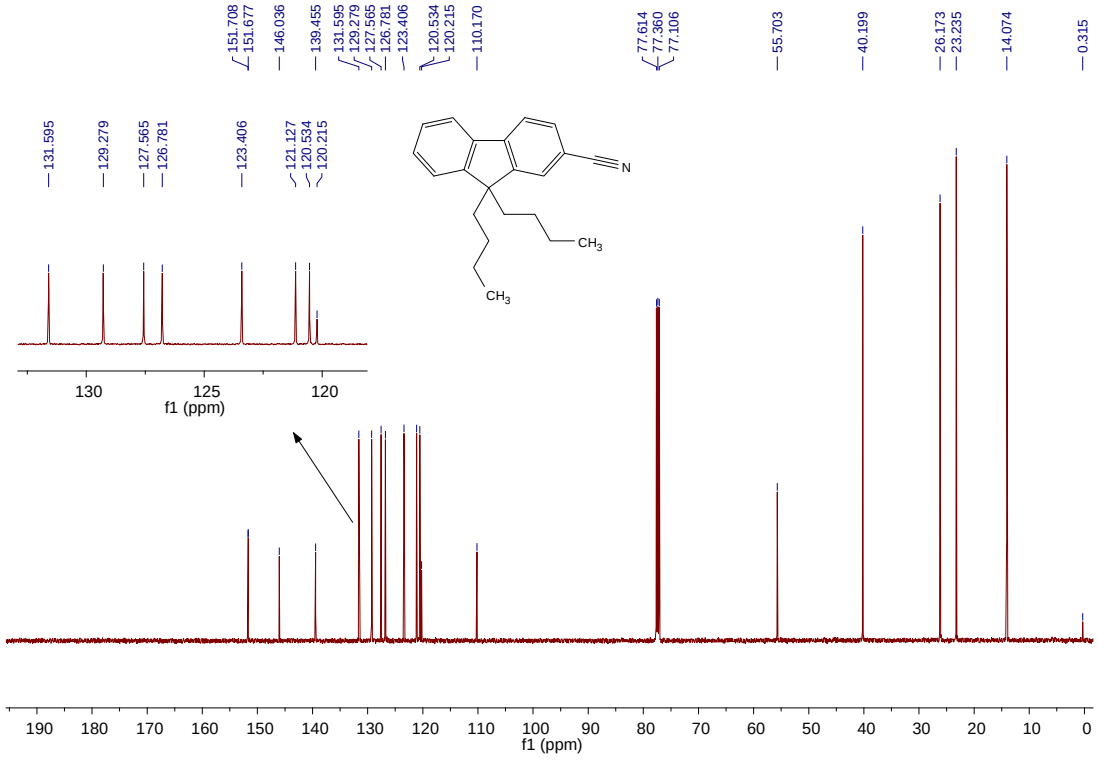


Figure S23 ^{1}H-NMR spectrum of **2l**

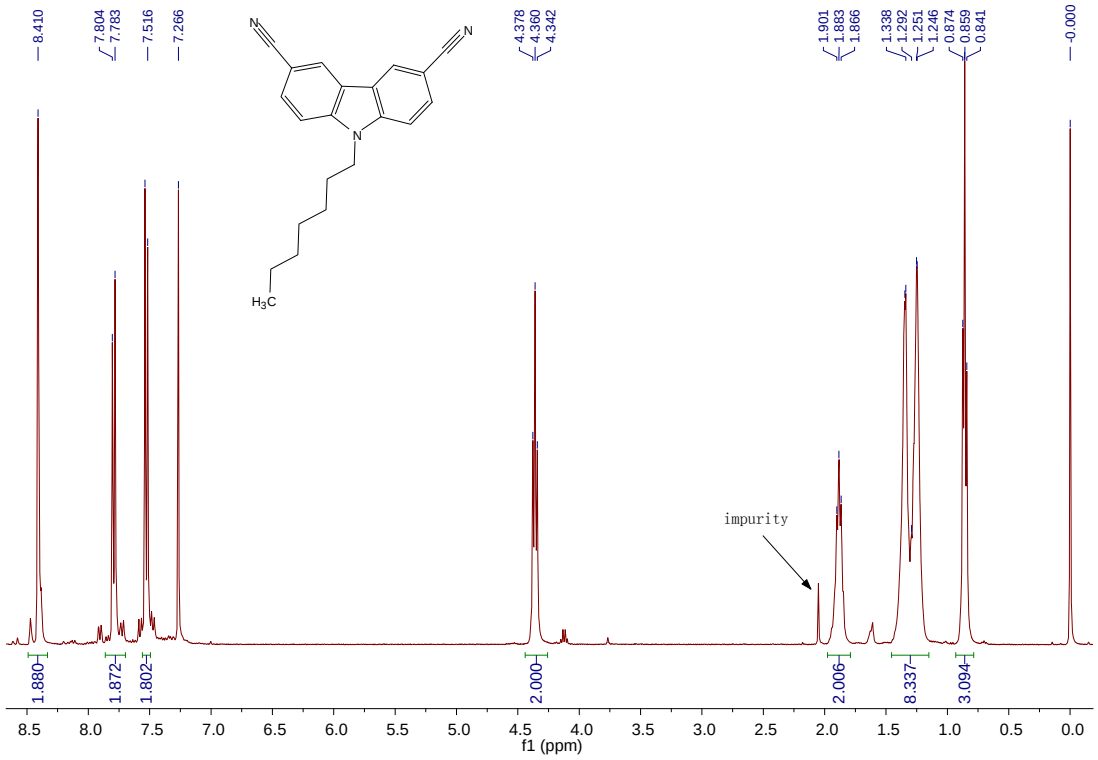


Figure S24 ^{13}C-NMR spectrum of **2l**

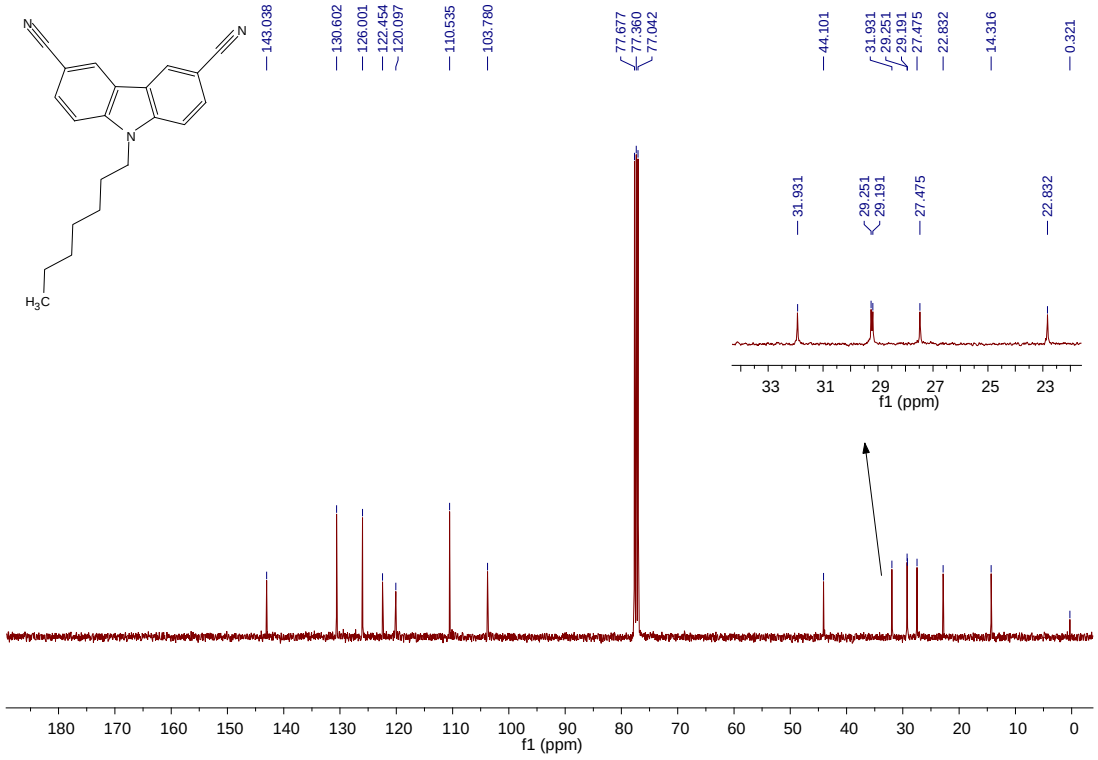


Figure S25 ^{1}H-NMR spectrum of **2m**

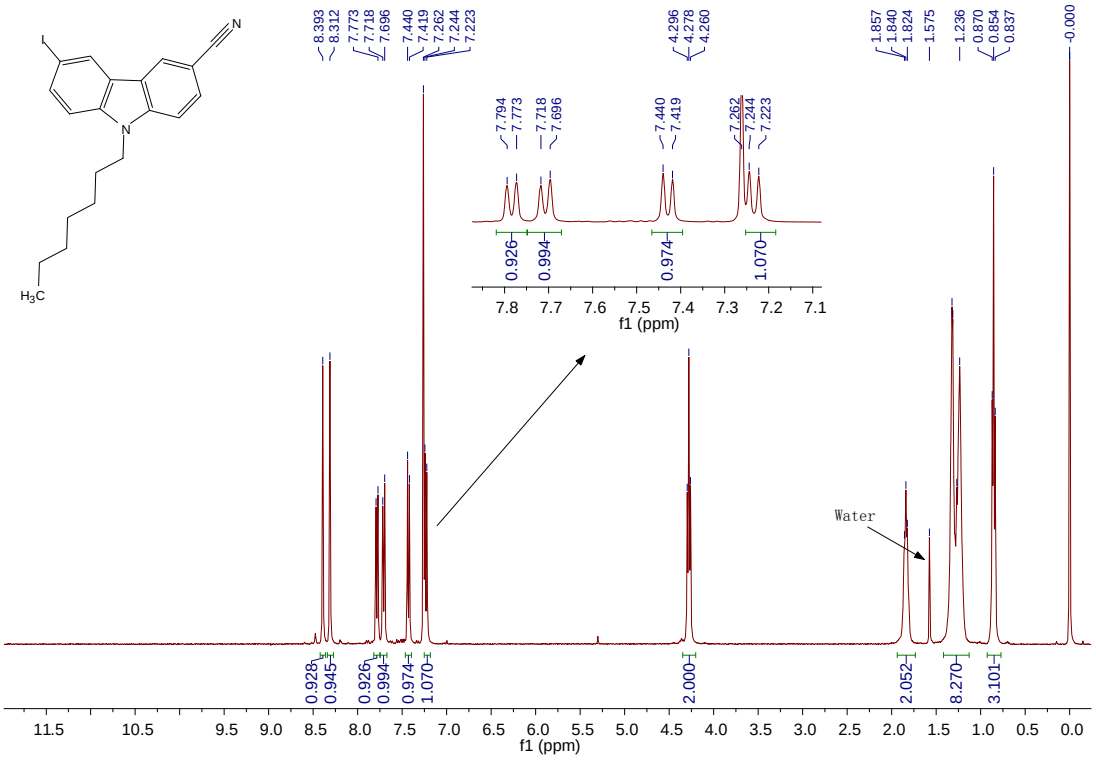
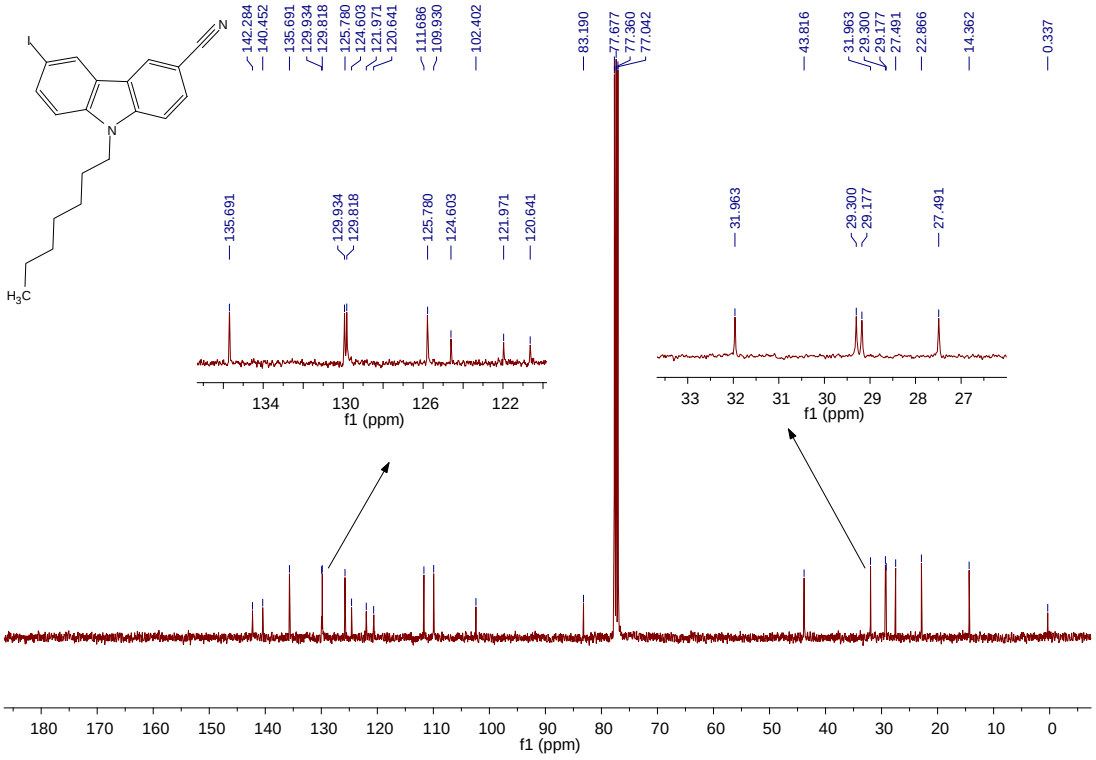


Figure S26 ^{13}C-NMR spectrum of **2m**



7. Other data

Figure S27 ^{1}H-NMR spectrum of 4,4'-dimethyl-1,1'-biphenyl

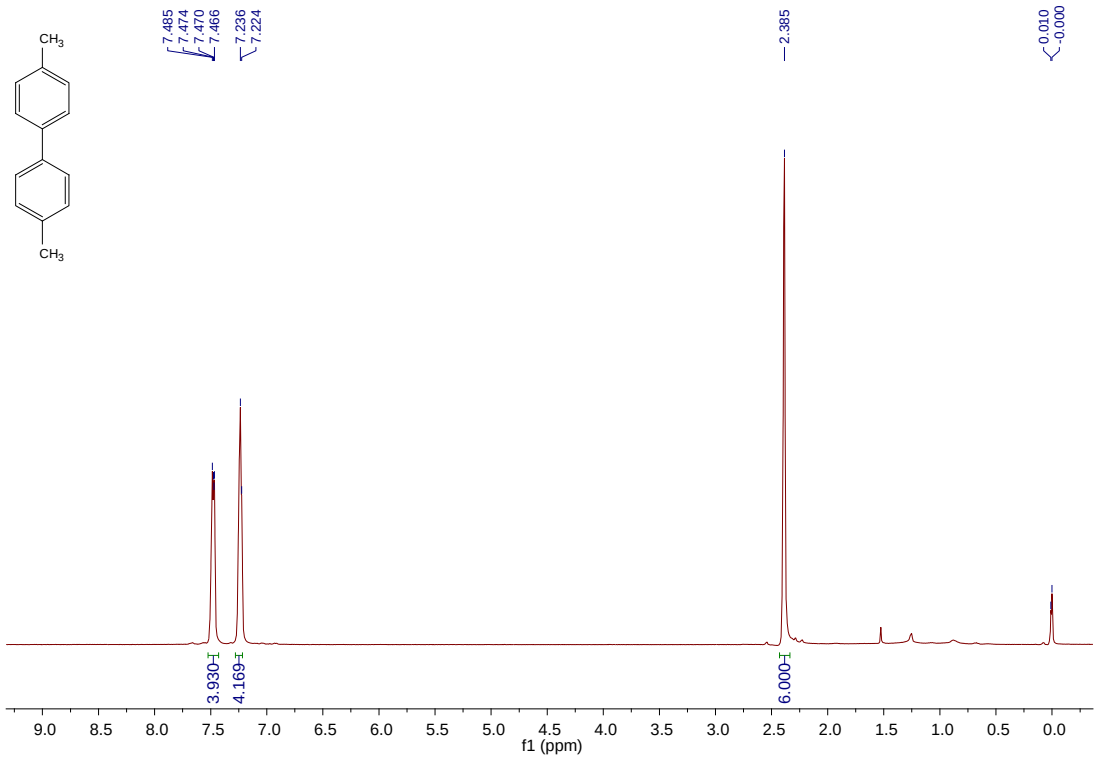


Figure S28 ^{13}C-NMR spectrum of 4,4'-dimethyl-1,1'-biphenyl

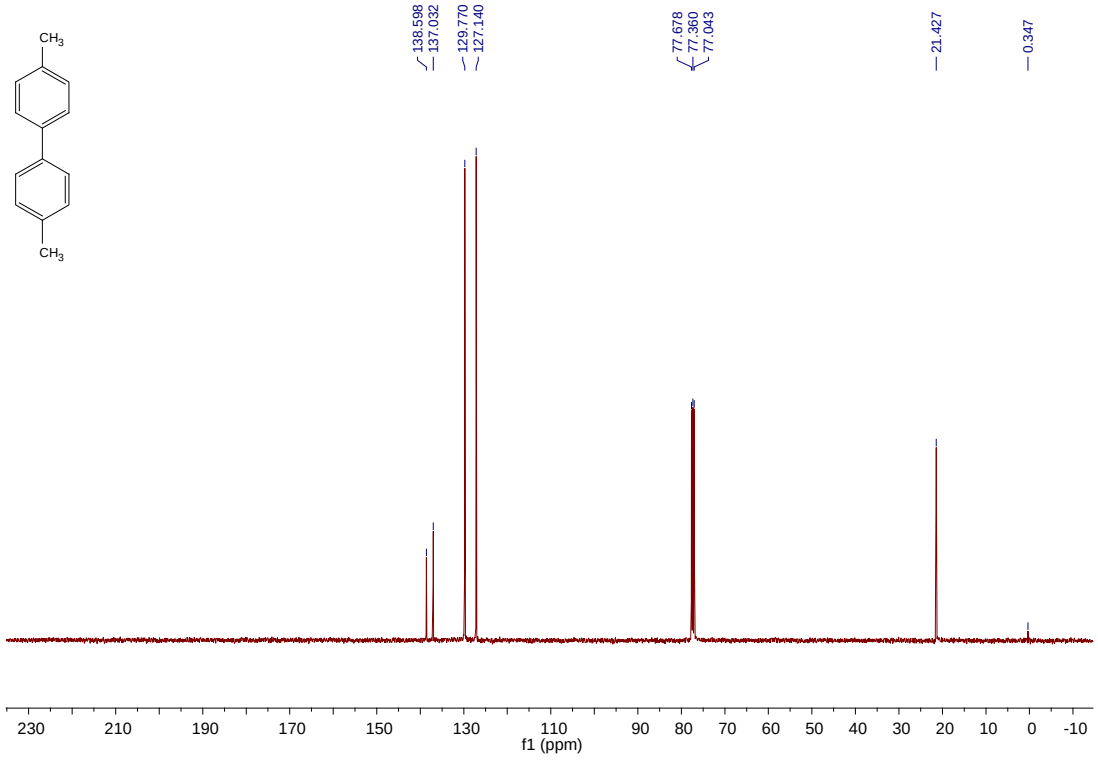


Figure S29 ^{1}H-NMR spectrum of 4,4'-dimethoxy-1,1'-biphenyl

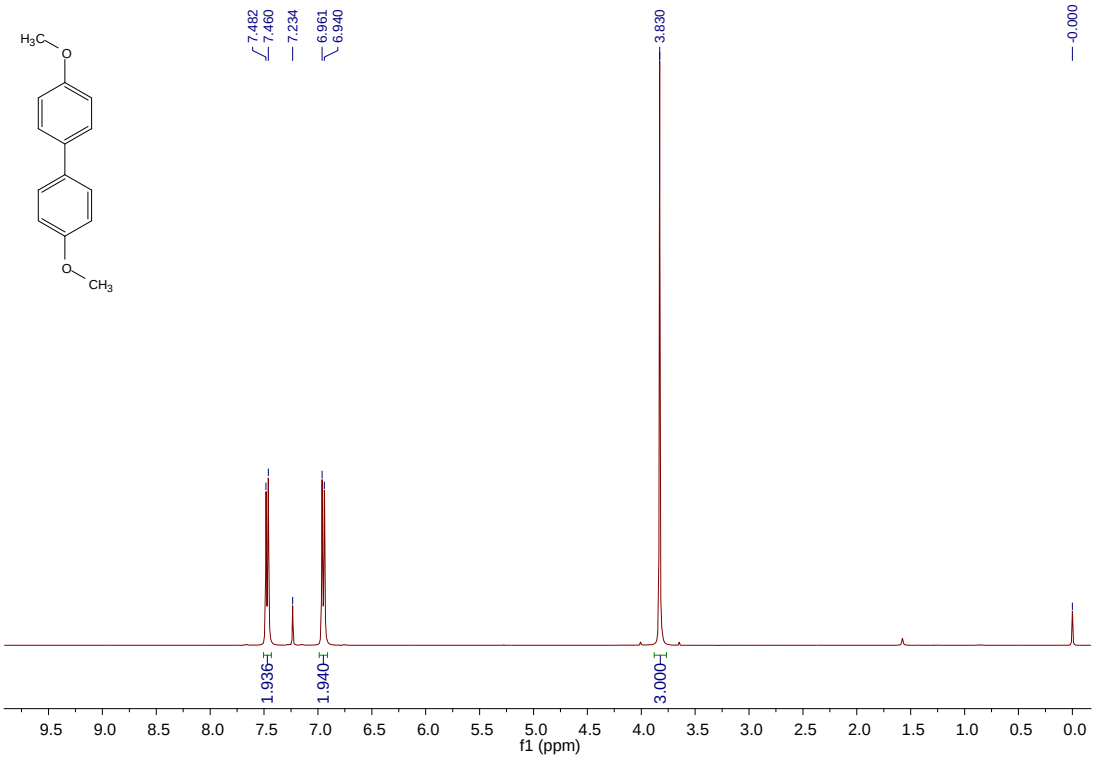


Figure S30 ^{13}C-NMR spectrum of 4,4'-dimethoxy-1,1'-biphenyl

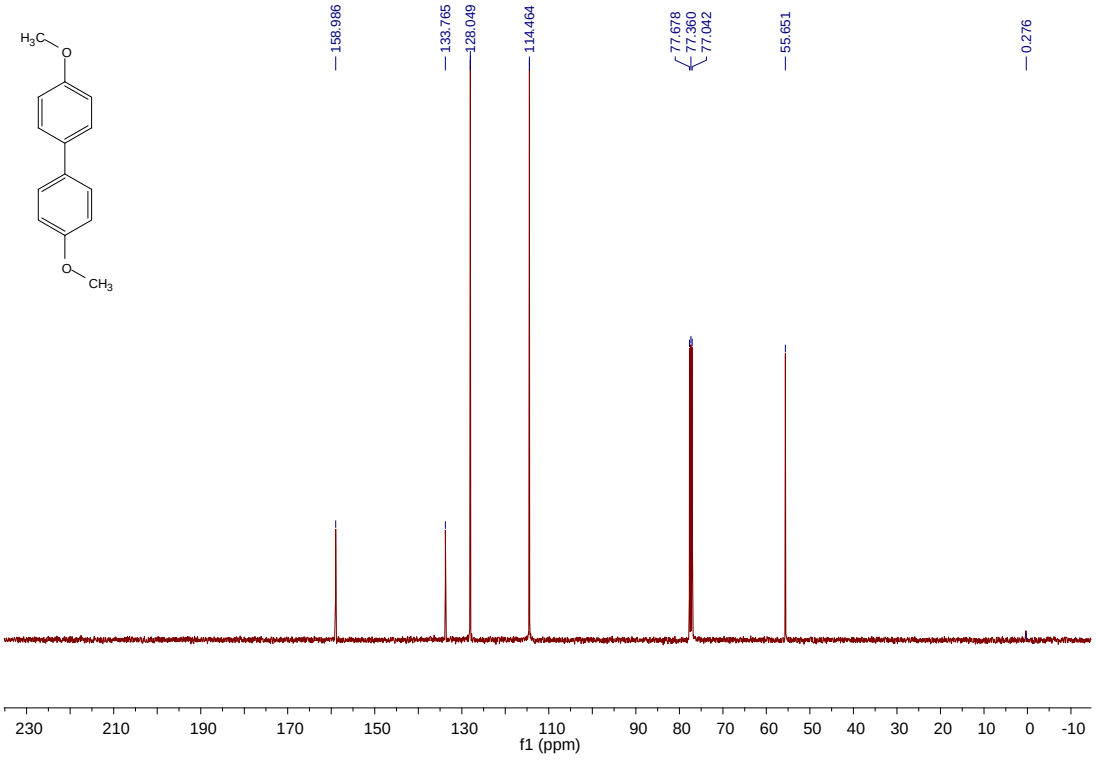


Figure S31 ^{1}H-NMR spectrum of the mixture of **2na** and **2nb**

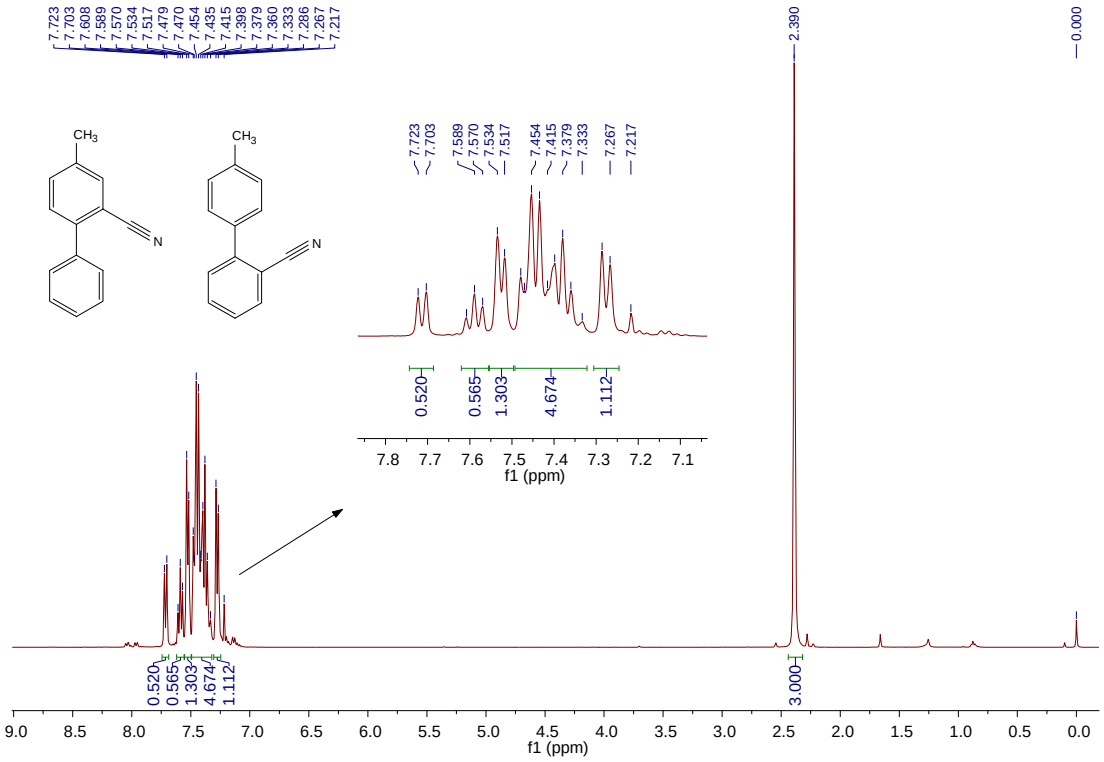
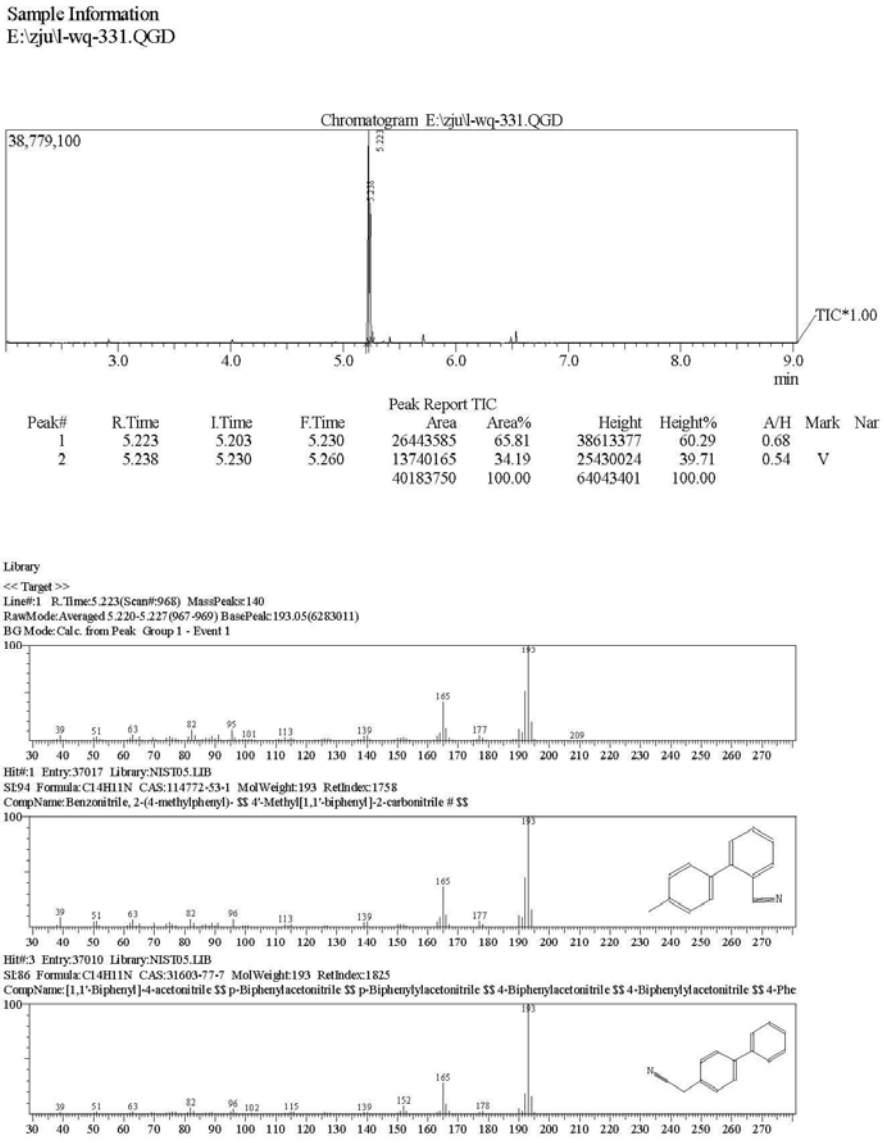
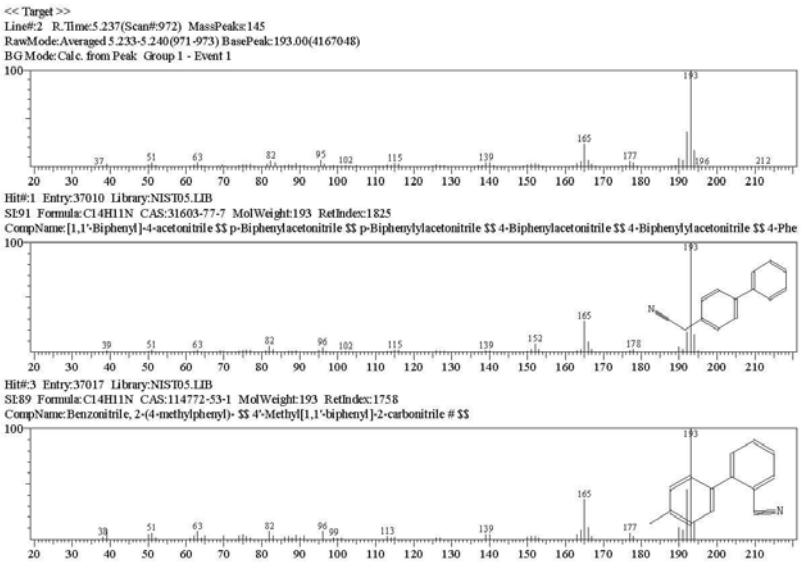


Figure S32 GC-MS result of the mixture of **2na** and **2nb**

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Line#:2 R.Time:5.237(Scan#:972) MassPeaks:145
RawMode:Averaged 5.233-5.240(971-973) BasePeak:193.00(41670-48)
BG Mode:Calc. from Peak Group 1 - Event 1
Hit#:1 Entry:37010 Library:NIST05.LIB
SI:91 Formula:C14H11N CAS:31603-77-7 MolWeight:193 RetIndex:1825
CompName:[1,1'-Biphenyl]-4-acetonitrile $$ p-Biphenylacetonitrile $$ p-Biphenylylacetonitrile $$ 4-Biphenylacetonitrile $$ 4-Biphenylylacetonitrile $$ 4-Phe
Hit#:3 Entry:37017 Library:NIST05.LIB
SI:89 Formula:C14H11N CAS:114772-53-1 MolWeight:193 RetIndex:1758
CompName:Benzonitrile, 2-(4-methylphenyl)- $$ 4'-Methyl[1,1'-biphenyl]-2-carbonitrile # $$