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Electronic Supplementary Information

Cu-mediated Nitrogen-Atom Transfer via C≡N Bond Cleavage

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Content

I. General information

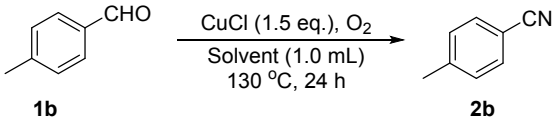
Except where otherwise noted, all reactions were carried out in 25 mL sealed Schlenk tubes under anhydrous conditions and O_2 atmosphere, and monitored by GC and/or GC-MS. All solvents were dried and distilled before use according to the standard methods. Column chromatography was performed using Silica Gel 60 (particle size 300-400 μm). The ^1H and ^{13}C NMR spectra were recorded on a 400 MHz spectrometer (400 MHz for ^1H and 100 MHz for ^{13}C NMR spectroscopy). $CDCl_3$ or DMSO-d_6 was used as the solvent. Chemical shifts for ^1H NMR are referred to internal Me_4Si (0 ppm) and reported as follows: chemical shift (δ ppm), multiplicity, integration and coupling constant (Hz). Data for ^{13}C NMR are reported in ppm relative to the center line of a triplet at 77.0 ppm for chloroform-*d*. GC-MS results were recorded on GC-MS QP2010, and GC analysis was performed on GC 2010 plus. The electron ionization (EI) method was used as the ionization method for the HRMS measurement, and the mass analyzer type is TOF for EI.

II. Typical experimental procedure for the synthesis of aryl nitriles

An oven-dried 25 mL Schlenk tube, which was equipped with a magnetic stir bar and charged with CuCl (29.7 mg, 0.3 mmol), was evacuated and backfilled with oxygen three times. Then, CH_3CN (0.67 mL), DMAc (0.33 mL), and 4-methoxybenzaldehyde **1a** (27.2 mg, 0.2 mmol) were added. The reaction mixture was stirred at 130 °C for 24 h and monitored by GC or GC-MS. After completion of the reaction, the resulting solution was cooled to room temperature, and washed with saturated NH_4Cl solution (10.0 mL). The product was extracted with $CHCl_3$ (5.0 mL × 3), filtered and dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by column chromatography on silica gel with ethyl acetate / petroleum ether (1 / 10) to afford white solid 4-methoxybenzonitrile **2a** in 83% yield (22.1 mg).

III. Optimization of reaction conditions

***Table S1*. Optimization of solvent[a]**



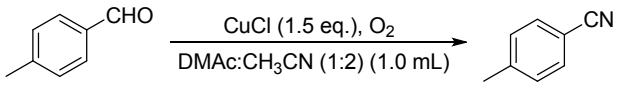
1b **2b**

Entry	Solvent	Yield %[b]
1	CH_3CN	40
2	DMAc	None
3	DMAc:CH_3CN (4:1)	Trace
4	DMAc:CH_3CN (2:1)	29
5	DMAc:CH_3CN (1:1)	86
6	DMAc:CH_3CN (1:2)	90
7	DMAc:CH_3CN (1:3)	80
8	DMAc:CH_3CN (1:9)	56
9	DMSO:CH_3CN (1:2)	14
10	NMP:CH_3CN (1:2)	18
11[c]	DMAc:CH_3CN (1:2)	None
12[d]	DMAc:CH_3CN (1:2)	Trace

[a]Reaction conditions: **1b** (24.0 mg, 0.2 mmol), CuCl (29.7 mg, 0.3 mmol), solvent (1.0 mL), 130 °C, 24 h.

[b]GC yield. [c]under N_2. [d]under air.

Table S2. Optimization of temperature and time[a]

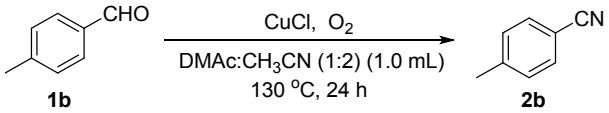


1b **2b**

Entry	T/°C	t/h	Yield %[b]
1	100	24	Trace
2	120	24	40
3	130	24	90
4	140	24	91
5	130	12	32
6	130	16	54
7	130	20	70
8	130	28	92

[a]Reaction conditions: **1b** (24.0 mg, 0.2 mmol), CuCl (29.7 mg, 0.3 mmol), solvent (1.0 mL), 130 °C, 24 h. [b]GC yield.

Table S3. Optimization of copper loading[a]

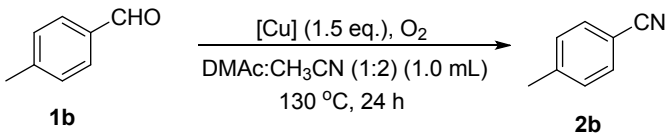


1b **2b**

Entry	CuCl (eq.)	Yield %[b]
1	0.2	Trace
2	1.0	57
3	1.1	68
4	1.2	79
5	1.3	82
6	1.4	87
7	1.5	90
8	2.0	91

[a] Reaction conditions: **1b** (24.0 mg, 0.2 mmol), solvent (1.0 mL), 130 °C, 24 h. [b]GC yield.

Table S4. Optimization of Cu salts[a]



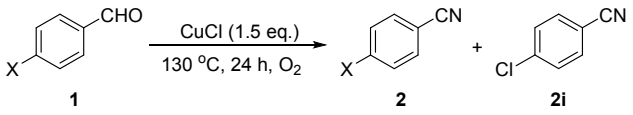
1b **2b**

Entry	[Cu]	Yield %[b]
1	Cu	None
2	CuCl	90

3	CuBr	38
4	CuI	None
5	Cu_2O	None
6	CuSCN	None
7	$[Cu(CH_3CN)]_4PF_6$	None
8	$CuCl_2$	10
9	$CuBr_2$	5.1
10	$Cu(OAc)_2$	15
11	$Cu(NO_3)_2{\cdot}3H_2O$	13
12	$CuSO_4$	None
13	$Cu(OH)_2$	Trace
14	$Cu(OH)_2CO_3$	None
15	CuO	None

[a]Reaction conditions: **1b** (24.0 mg, 0.2 mmol), [Cu] (0.3 mmol), 130 °C, 24 h. [b]GC yield.

IV. Reactions of 4-Bromobenzaldehyde and 4-Iodobenzaldehyde with acetonitrile



1 **2** **2i**

Entry	**X**	Yield %	Yield %
1	-Br	**2s**, 64[a] (85)[b]	**2i**, 17[a] (4)[b]
2	-I	**2t**, 52[a] (80)[b]	**2i**, 23[a] (8)[b]

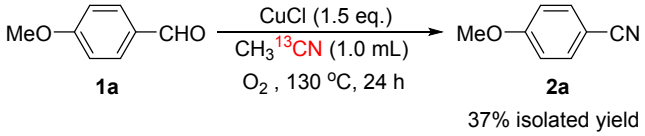
[a]Conditions A: aldehyde **1** (0.2 mmol), CuCl (0.3 mmol), CH_3CN (0.67 mL), DMAc (0.33 mL) in 25 mL tube under O_2, 130 °C, 24 h, GC yields. [b]Conditions B: aldehyde **1** (0.2 mmol), benzeneacetonitrile (0.3 mmol), CH_3CN (1.0 mL), GC yields.

V. Investigation on the reaction mechanism

1. ^{13}C Labeled CH_3CN and 4-methoxybenzaldehyde Test

Acetonitrile-1-^{13}C (99 atom%, ^{13}C, cat. No. 485160) were purchased from Aldrich, Anisaldehyde-[7-^{13}C] (98% atom%, ^{13}C, cat. No. A673202) were purchased from TRG, the isotope reagents were used without further purification.

(1)



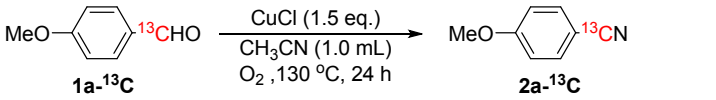
1a **2a**

37% isolated yield

An oven-dried 25 mL Schlenk tube, which was equipped with a magnetic stir bar and charged with CuCl (29.7 mg, 0.3 mmol), was evacuated and backfilled with oxygen three times. Then, $CH_3{}^{13}CN$ (1.0 mL) and 4-methoxybenzaldehyde **1a** (27.2 mg, 0.2 mmol) were added. The reaction mixture was stirred at 130 °C

for 24 h and monitored by GC or GC-MS. After completion of the reaction, the resulting solution was cooled to room temperature, and washed with saturated NH_4Cl solution (10.0 mL). The product was extracted with $CHCl_3$ (5.0 mL × 3), filtered and dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1 / 10) to afford white solid 4-methoxybenzonitrile **2a** in 37% yield (9.8 mg).

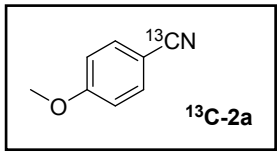
(2)



1a-^{13}C **2a-^{13}C**

39% isolated yield (98.5% ^{13}C)

An oven-dried 25 mL Schlenk tube, which was equipped with a magnetic stir bar and charged with CuCl (29.7 mg, 0.3 mmol), was evacuated and backfilled with oxygen three times. Then, CH_3CN (1.0 mL) and Anisaldehyde-[7-^{13}C] (27.4 mg, 0.2 mmol) were added. The reaction mixture was stirred at 130 °C for 24 h and monitored by GC or GC-MS. After completion of the reaction, the resulting solution was cooled to room temperature, and washed with saturated NH_4Cl solution (10.0 mL). The product was extracted with $CHCl_3$ (5.0 mL × 3), filtered and dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by column chromatography on silica gel with ethyl acetate / petroleum ether (1 / 10) to afford white solid 4-methoxybenzonitrile **2a-^{13}C** in 39% yield (10.5 mg).

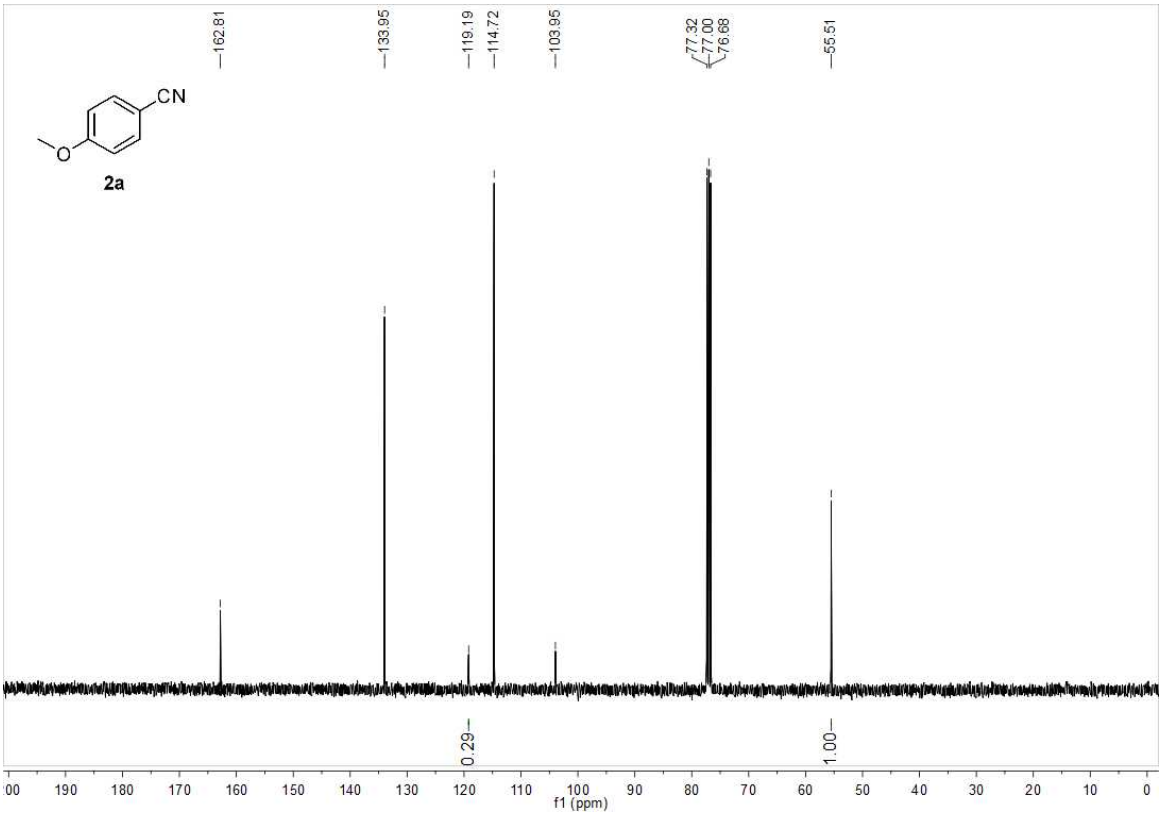


4-Methoxybenzonitrile-^{13}C (**^{13}C-2a**): 98.5% of ^{13}C incorporation; **HRMS** (ESI+) exact mass calc'd for $(C_7{}^{13}CH_7NO)^+$ $(M+H)^+$ requires m/z: 134.0571, found m/z: 134.0559.

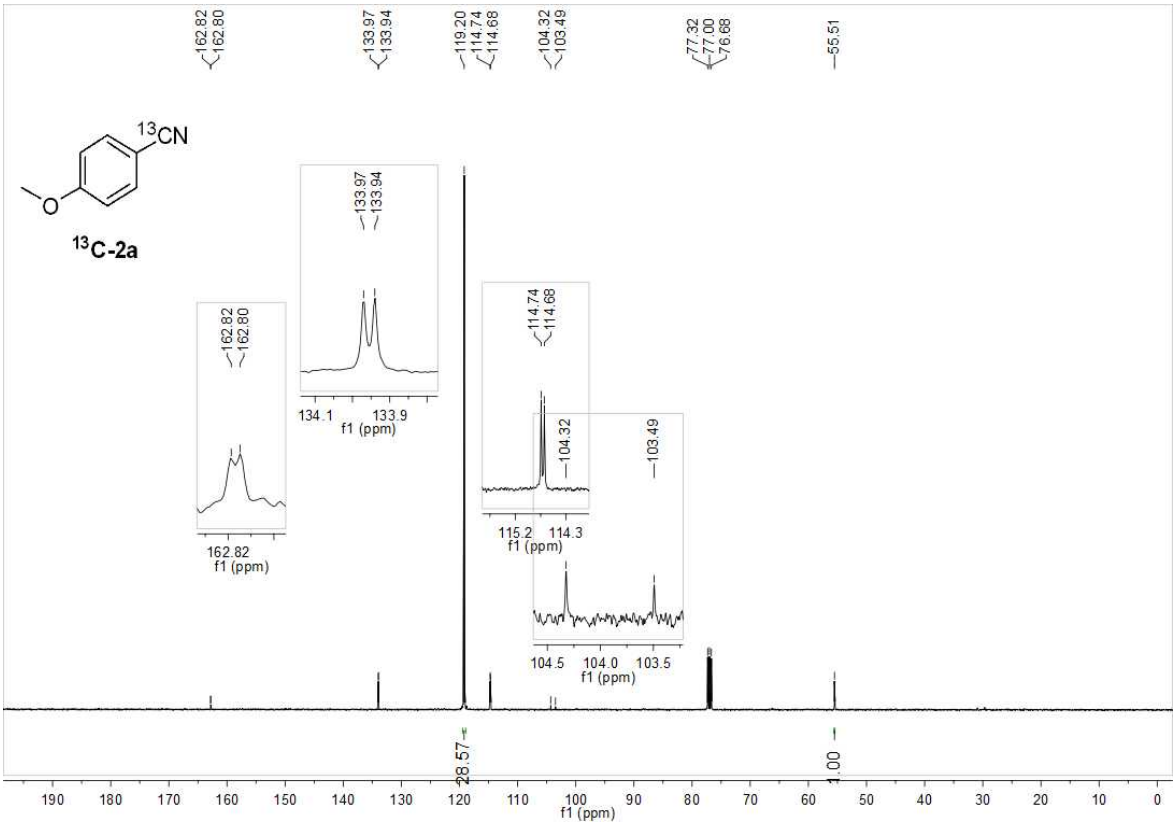
4-Methoxybenzonitrile (2a): Inverse gated decoupling ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5 (int. = 1.00), 119.1 (-C≡N, int. = 0.29)

4-Methoxybenzonitrile-^{13}C (2a-^{13}C): Inverse gated decoupling ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5 (int. = 1.00), 119.2 (-C≡N, int. = 28.57). (^{13}C incorporation: 28.57 / 0.29 = 98.5%).[1]

Copies of ^{13}C NMR charts of 2a

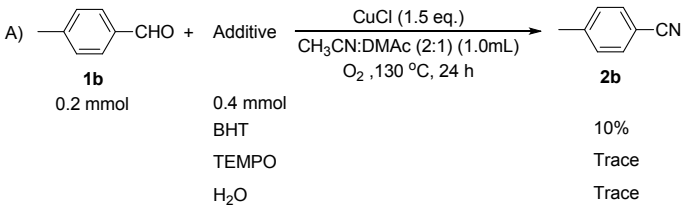


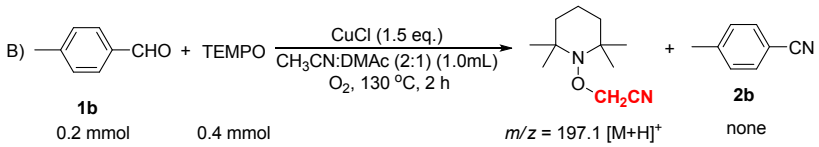
Copies of ^{13}C NMR charts of ^{13}C-2a



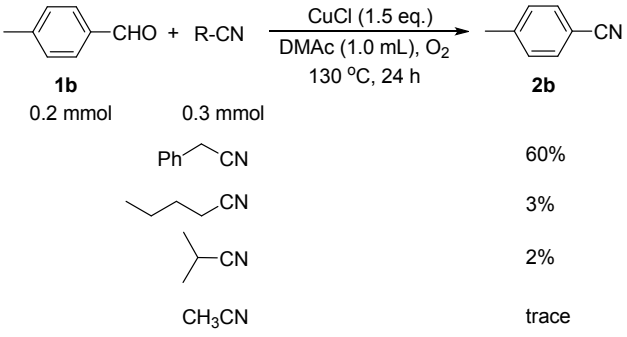
2. Control experiments

(1) The free-radical experiments

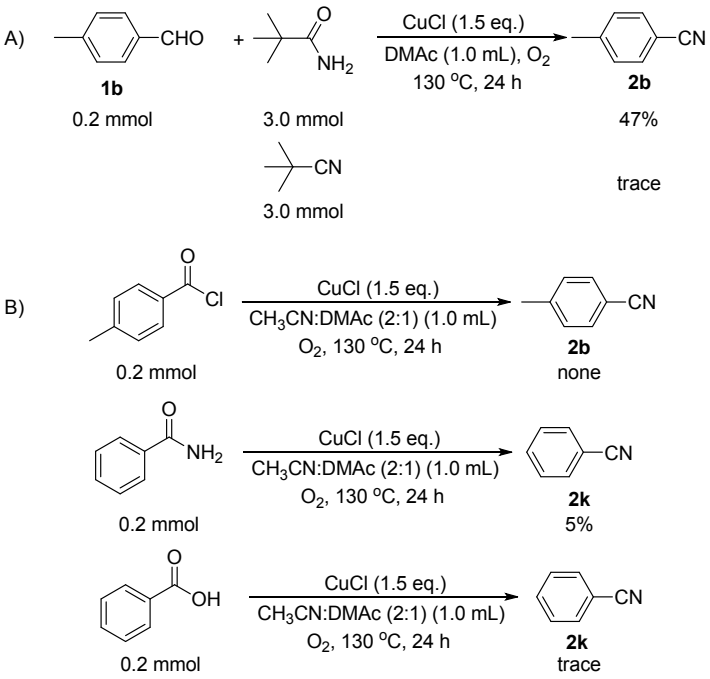




(2) Reactivities of nitriles

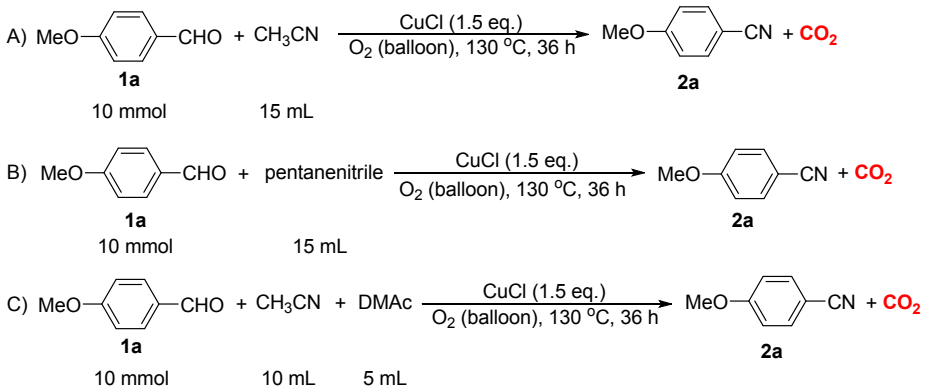


(3) Reactivities of other substrates



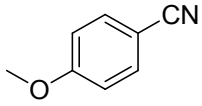
3. The capture of CO_2

The reactions were carried out under standard conditions with a large scale. After completion of the reactions, the reaction systems were contacted with lime-water, they became muddy immediately.



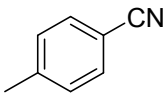
VI. ^{1}H and ^{13}C NMR spectra data of the products

4-Methoxybenzonitrile (2a)[2]



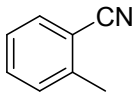
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, J = 9.0 Hz, 2H), 6.95 (d, J = 8.9 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.8, 133.9, 119.1, 114.7, 103.9, 55.5.

4-Methylbenzonitrile (2b)[2]



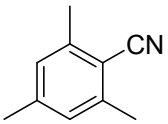
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, J = 8.1 Hz, 2H), 7.27 (d, J = 6.8 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.6, 132.0, 129.7, 119.1, 109.2, 21.8.

2-Methylbenzonitrile (2c)[2]



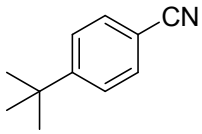
White liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 7.8 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.33–7.27 (m, 2H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.9, 132.6, 132.4, 130.1, 126.1, 118.1, 112.7, 20.4.

2,4,6-Trimethylbenzonitrile (2d)[2]



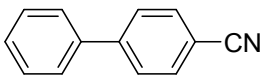
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.93 (s, 2H), 2.48 (s, 6H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.7, 141.9, 128.1, 117.6, 110.2, 21.5, 20.6.

4-(*t*ert-Butyl)benzonitrile (2e)[2]



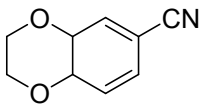
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.5, 131.9, 126.1, 119.1, 109.2, 35.2, 30.9.

4-Phenylbenzonitrile (2f)[3]



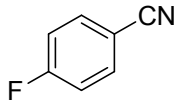
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.4 Hz, 2H), 7.68 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 7.2 Hz, 2H), 7.50-7.41 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.5, 139.0, 132.5, 129.0, 128.5, 127.6, 127.1, 118.8, 110.8.

2,3-Dihydro-1,4-benzodioxine-6-carbonitrile (2g)[4]



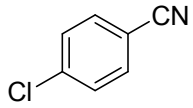
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15–7.12 (m, 2H), 6.91 (d, J = 8.4 Hz, 1H), 4.32-4.27 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.6, 143.7, 125.9, 121.2, 118.8, 118.2, 104.4, 64.5, 64.0.

4-Fluorobenzonitrile (2h)[2]



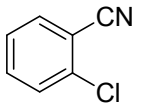
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70-7.65 (m, 2H), 7.20-7.14 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0 (d, $J_{C\text{-}F}$ = 256.7 Hz), 134.6 (d, $J_{C\text{-}F}$ = 9.3 Hz), 118.0, 116.8 (d, $J_{C\text{-}F}$ = 22.7 Hz), 108.5 (d, $J_{C\text{-}F}$ = 3.7 Hz).

4-Chlorobenzonitrile (2i)[2]



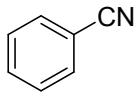
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, J = 8.5 Hz, 2H), 7.46 (d, J = 8.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.5, 133.3, 129.6, 117.9, 110.7.

2-Chlorobenzonitrile (2j)[5]



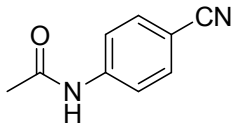
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (dd, J = 7.8, 1.3 Hz, 1H), 7.57–7.50 (m, 2H), 7.39–7.35 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.8, 133.9, 133.8, 130.0, 127.1, 115.9, 113.3.

Benzonitrile (2k)[2]



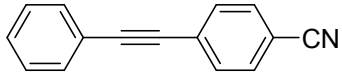
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65–7.58 (m, 3H), 7.47 (t, J = 7.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.7, 132.0, 129.0, 118.7, 112.3.

***N*-(4-cyanophenyl)acetamide (2l)**[1b]



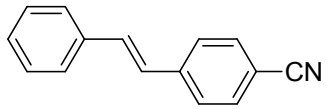
White solid. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.38 (s, 1H), 7.74 (s, 4H), 2.08 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 169.1, 143.4, 133.2, 119.1, 118.9, 104.6, 24.2.

4-(Phenylethynyl)benzonitrile (2m)[6]



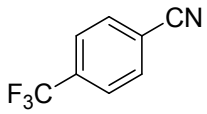
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 8.3 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.55-7.53 (m, 2H), 7.39–7.36 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.0, 132.0, 131.7, 129.1, 128.4, 128.2, 122.1, 118.5, 111.4, 93.7, 87.6.

(*E*)-4-styrylbenzonitrile (2n)[7]



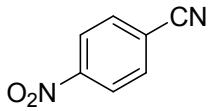
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 7.4 Hz, 2H), 7.39 (t, J = 7.5 Hz, 2H), 7.32 (t, J = 7.3 Hz, 1H), 7.22 (d, J = 16.3 Hz, 1H), 7.09 (d, J = 16.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.8, 136.2, 132.4, 132.3, 128.8, 128.6, 126.8, 126.8, 126.6, 119.0, 110.5.

4-(Trifluoromethyl)benzonitrile (2o)[5]



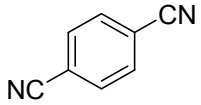
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 8.3 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.5 (d, $J_{C\text{-}F}$ = 33.3 Hz), 132.6, 126.1 (q, $J_{C\text{-}F}$ = 3.7 Hz), 123.0 (d, $J_{C\text{-}F}$ = 272.9 Hz), 117.4, 116.0.

4-Nitrobenzonitrile (2p)[2]



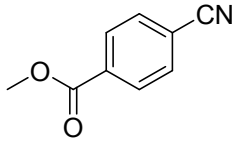
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.8 Hz, 2H), 7.89 (d, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.4, 130.4, 124.2, 118.3, 116.7.

Terephthalonitrile (2q)[2]



White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.7, 116.9, 116.7.

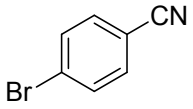
Methyl 4-cyanobenzoate (2r)[3]



White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, J = 8.1 Hz, 2H), 7.74 (d, J = 8.2 Hz, 2H), 3.95 (s, 3H).

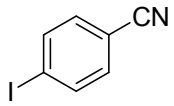
^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 133.8, 132.1, 129.9, 117.8, 116.2, 52.6.

4-bromobenzonitrile (2s)[2]



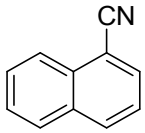
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.3, 132.6, 128.0, 118.0, 111.2.

4-Iodobenzonitrile (2t)[2]



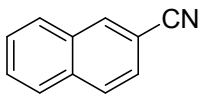
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.4, 133.1, 118.2, 111.7, 100.3.

1-Naphthonitrile (2u)[3]



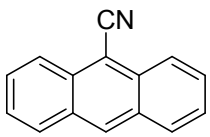
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, J = 8.3 Hz, 1H), 8.08 (d, J = 8.3 Hz, 1H), 7.92 (dd, J = 7.4, 5.2 Hz, 2H), 7.70 (t, J = 7.2 Hz, 1H), 7.62 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 7.8Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.2, 132.8, 132.6, 132.3, 128.6, 128.5, 127.5, 125.1, 124.8, 117.8, 110.1.

2-Naphthonitrile (2v)[3]



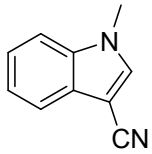
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 1H), 7.89 (t, J = 8.4 Hz, 3H), 7.66-7.58 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.5, 134.0, 132.1, 129.1, 128.9, 128.3, 127.9, 127.5, 126.2, 119.1, 109.2.

Anthracene-9-carbonitrile (2w)[3]



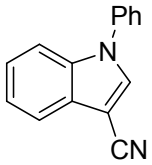
Yellow-green solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (s, 1H), 8.42 (d, J = 8.7 Hz, 2H), 8.07 (d, J = 8.5 Hz, 2H), 7.73–7.69 (m, 2H), 7.60–7.56 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.3, 132.7, 130.6, 128.9, 126.3, 125.2, 117.2, 105.4.

1-Methyl-1*H*-indole-3-carbonitrile (2x)[8]



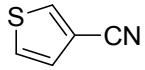
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, J = 7.9 Hz, 1H), 7.53 (s, 1H), 7.39–7.27 (m, 3H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.9, 135.5, 127.6, 123.7, 122.0, 119.7, 115.9, 110.2, 85.2, 33.5.

1-Phenyl-1*H*-indole-3-carbonitrile (2y)[8]



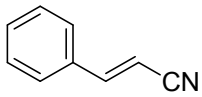
White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84–7.82 (m, 1H), 7.81 (s, 1H), 7.60–7.56 (m, 2H), 7.53–7.47 (m, 4H), 7.37–7.32 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.7, 135.5, 134.6, 130.0, 128.3, 127.9, 124.8, 124.5, 122.7, 120.0, 115.5, 111.5, 88.0.

Thiophene-3-carbonitrile (2z)[9]



Pale yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (dd, J = 3.0, 1.0 Hz, 1H), 7.43 (dd, J = 5.1, 3.0 Hz, 1H), 7.30 (dd, J = 5.1, 1.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.3, 128.6, 127.2, 115.0, 110.6.

Cinnamonitrile (2za)[2]



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.38 (m, 6H), 5.89 (d, J = 16.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 133.4, 131.1, 129.0, 127.2, 118.1, 96.2.

VII. References

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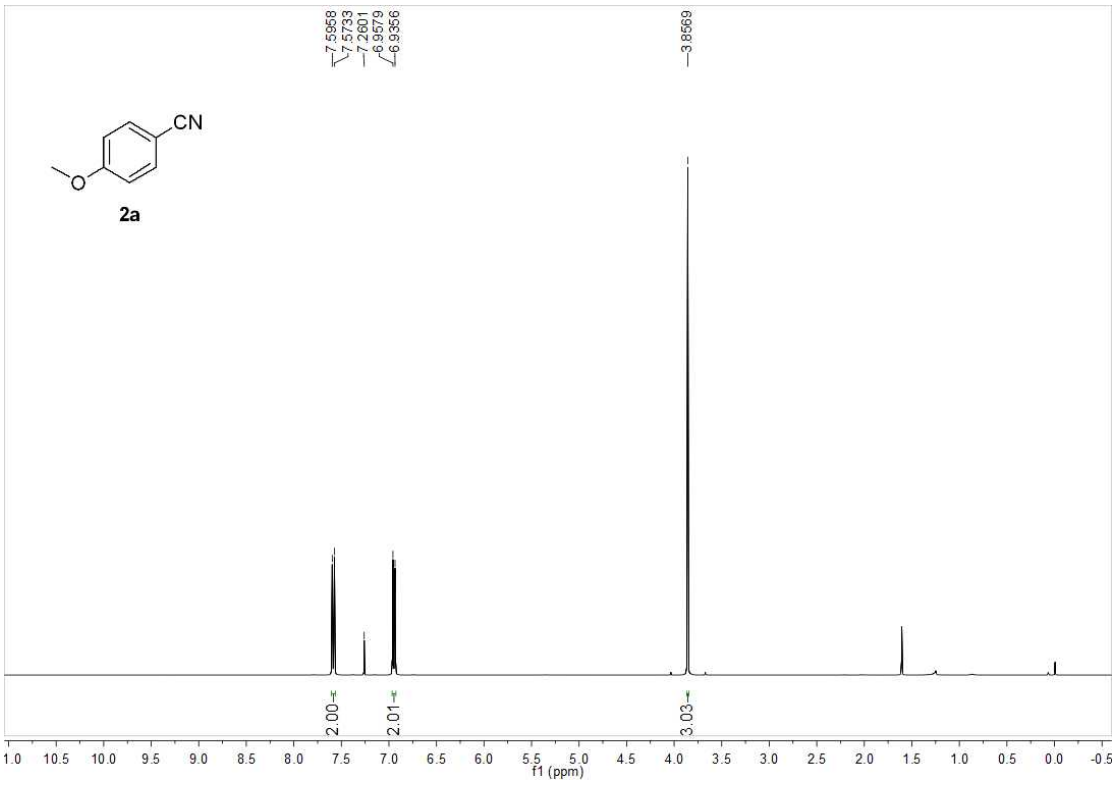
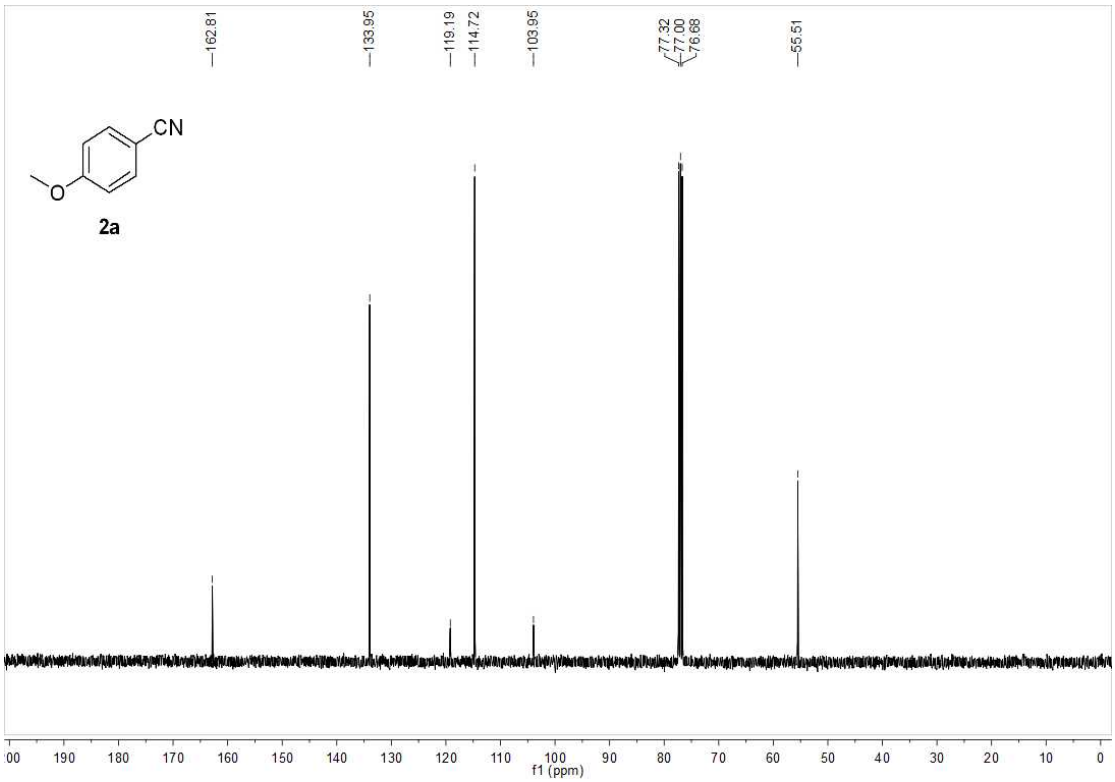
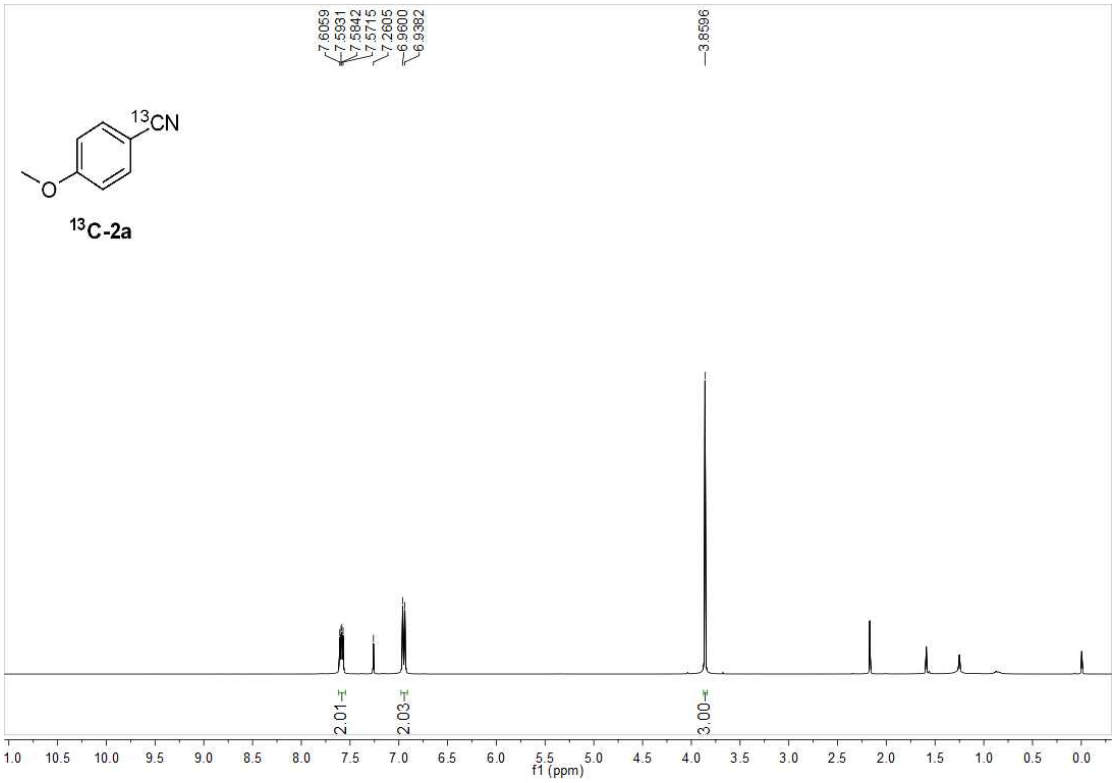
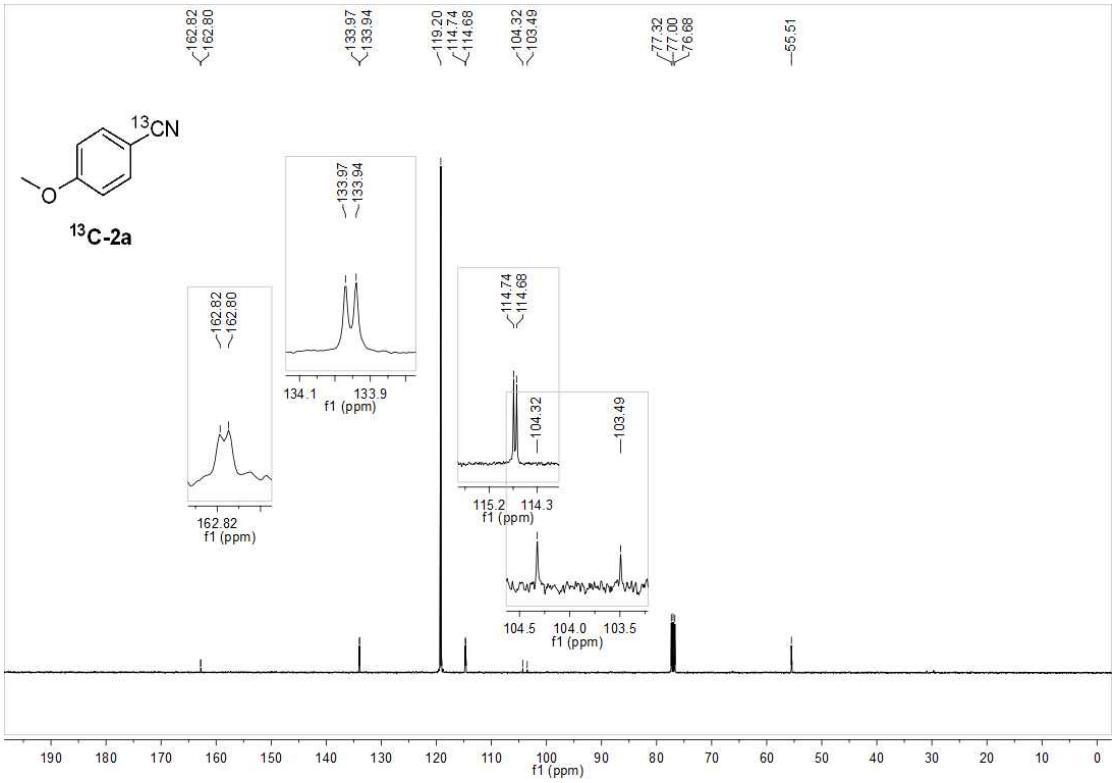
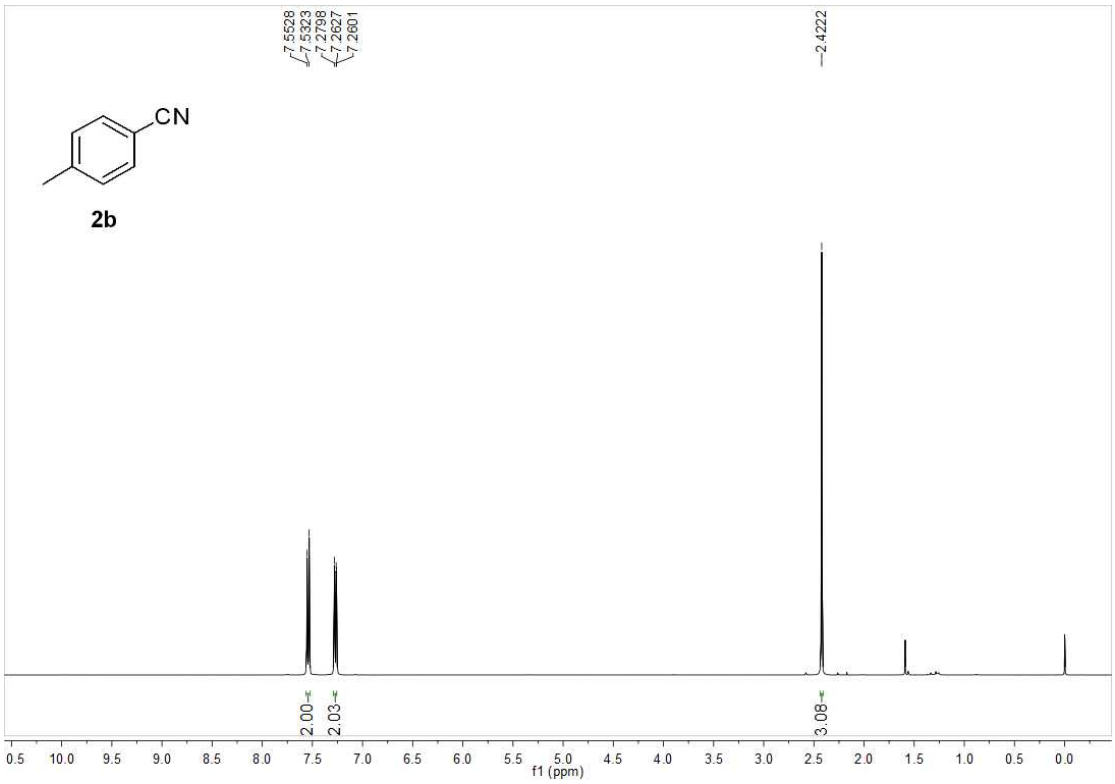
VIII. Copies of ^{1}H and ^{13}C NMR charts of the products

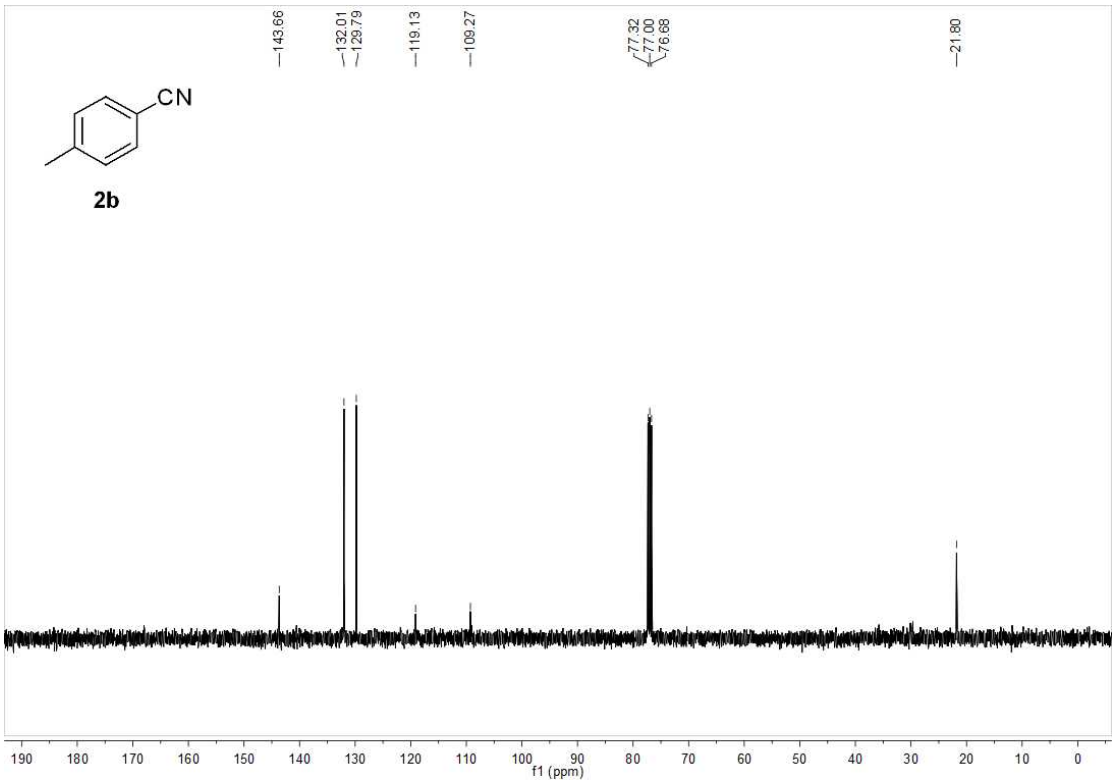


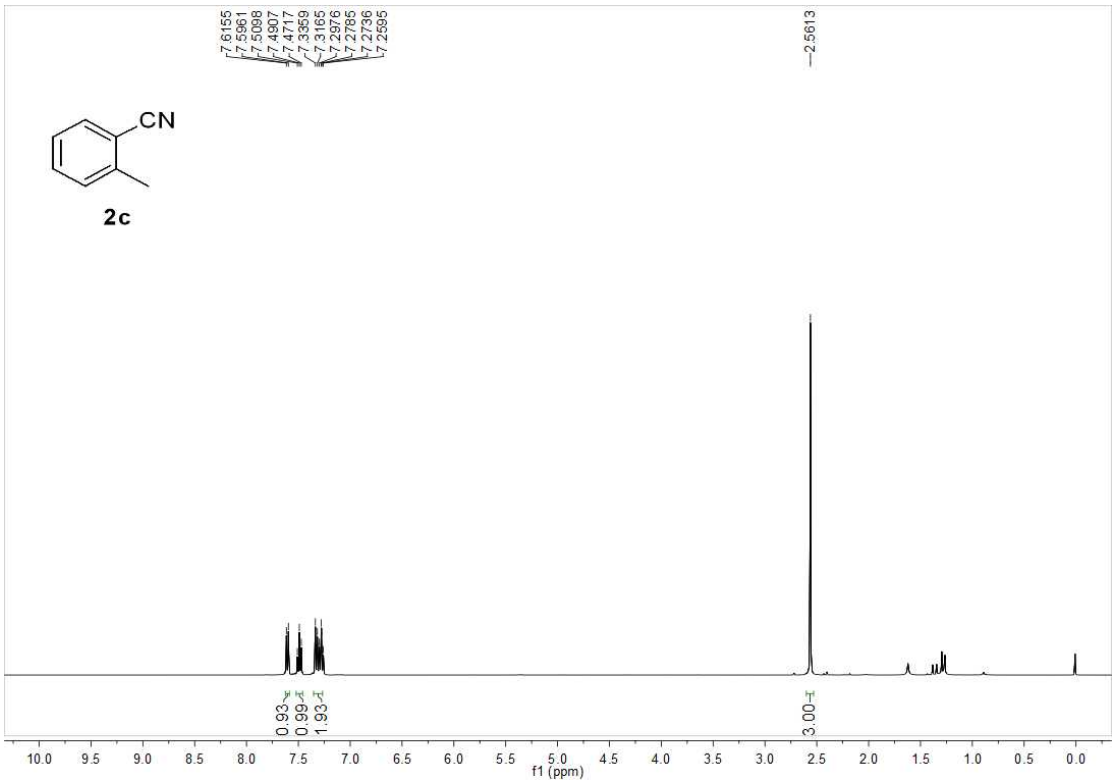


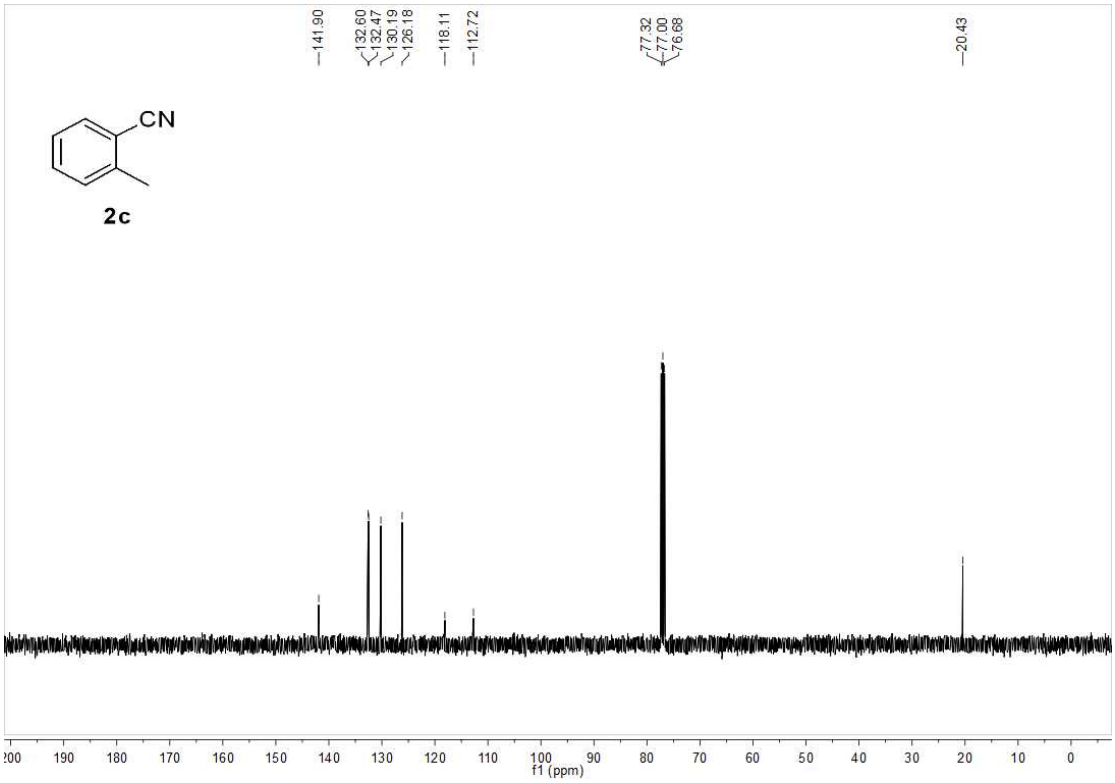

7.6059
7.5931
7.5842
7.5715
7.2605
6.9600
6.9382
3.8596
13CN
O
13C-2a
2.01
2.03
3.00
f1 (ppm)

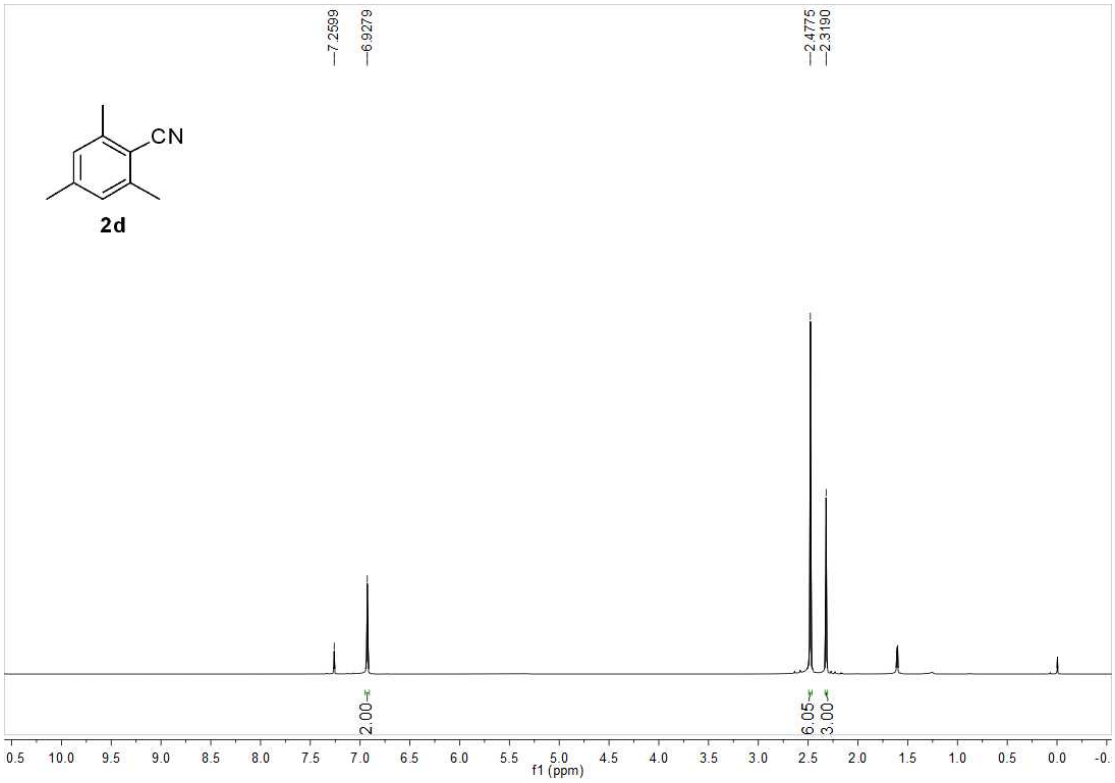

162.82
162.80
133.97
133.94
119.20
114.74
114.68
104.32
103.49
77.32
77.00
76.68
55.51
13CN
O
13C-2a
f1 (ppm)

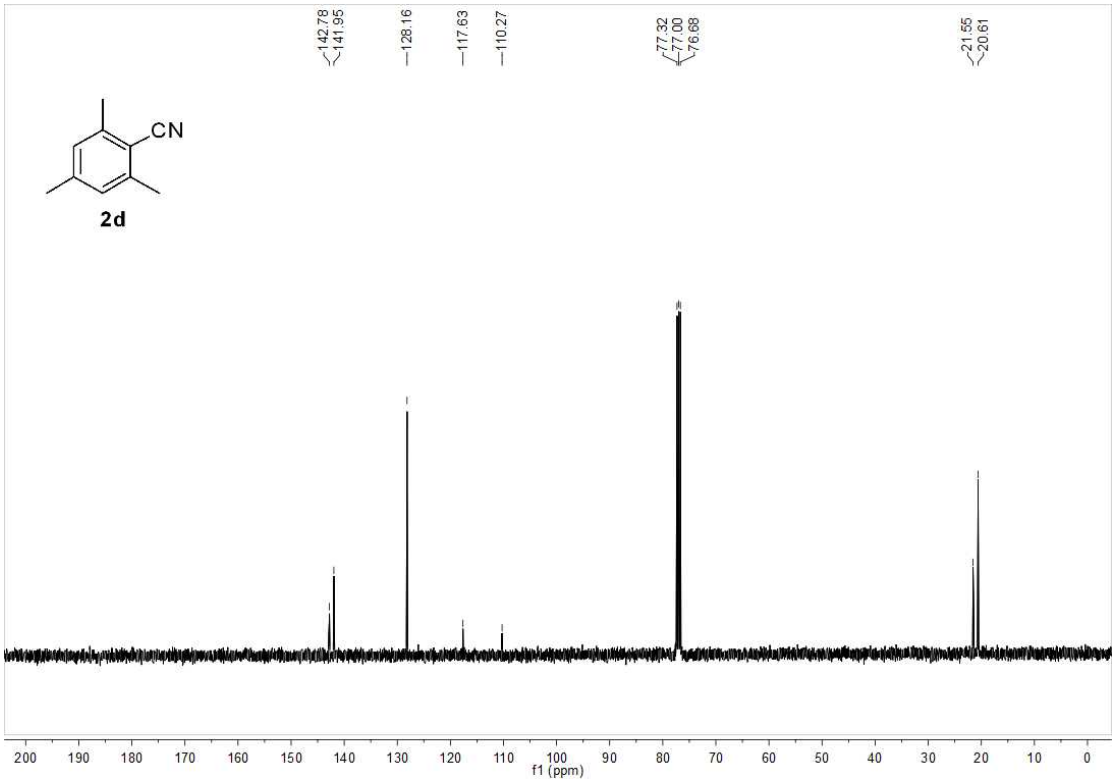

7.5528
7.5323
7.2798
7.2627
7.2601
2.4222
CN
2b
2.00
2.03
3.08
f1 (ppm)

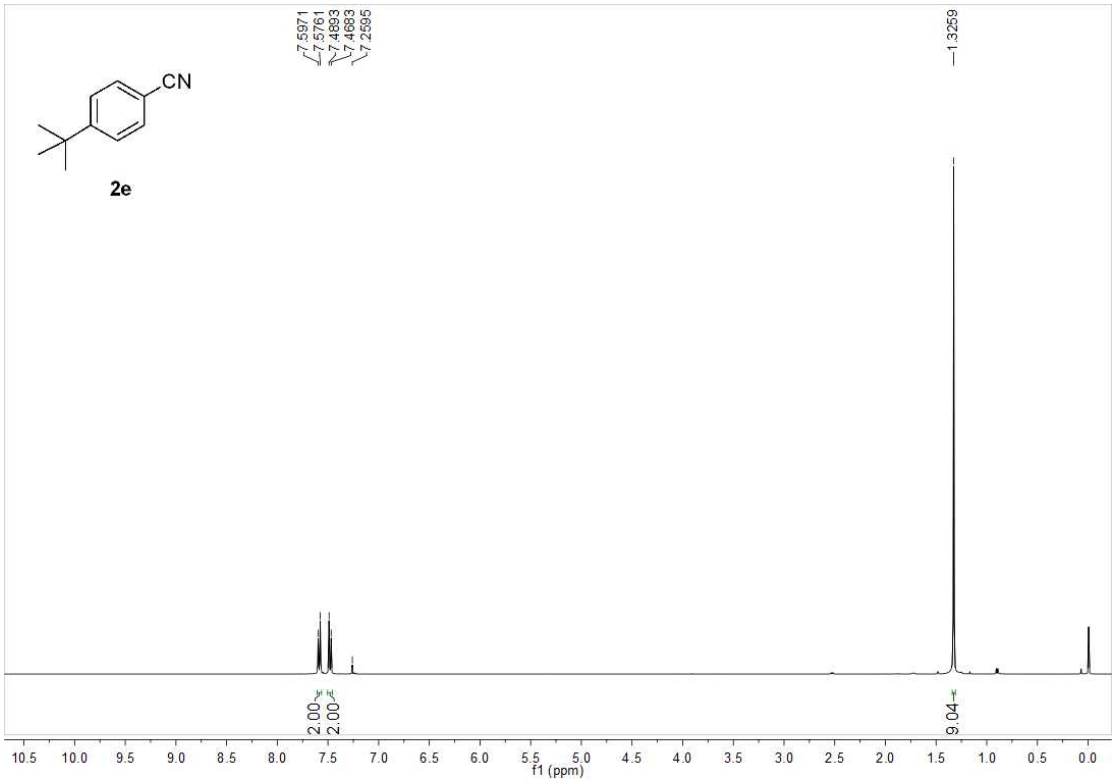

143.66
132.01
129.79
119.13
109.27
77.32
77.00
76.68
21.80
CN
2b
f1 (ppm)

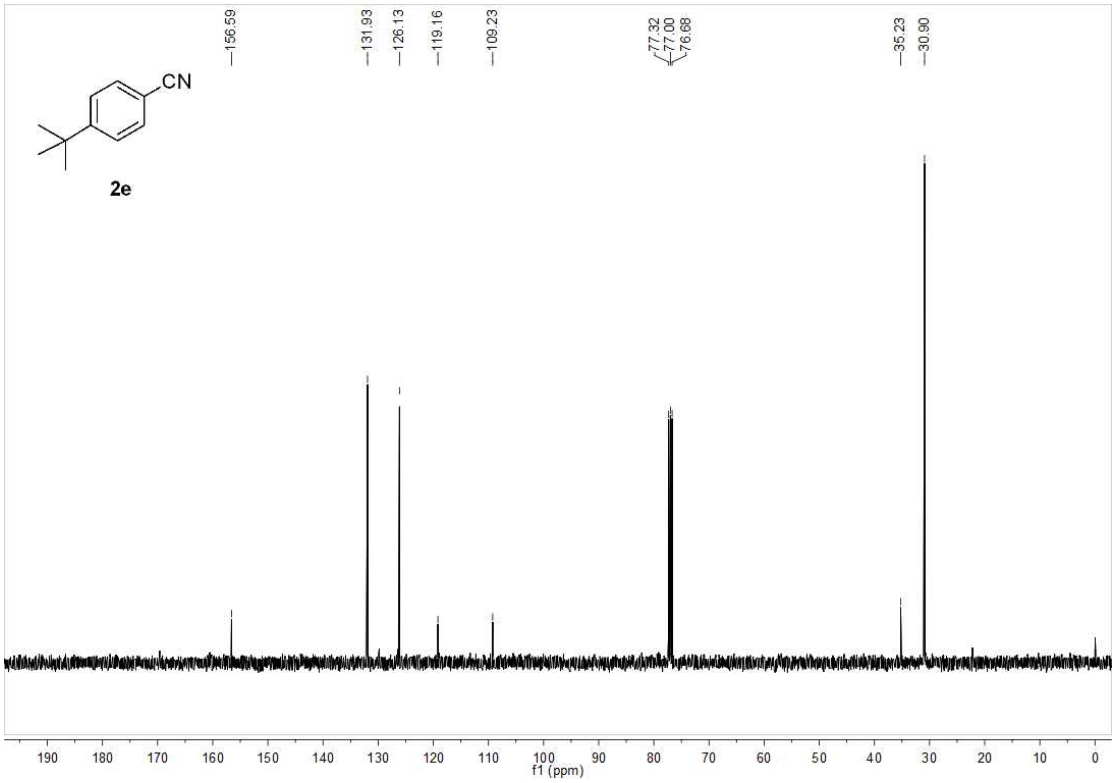

7.6155
7.5961
7.5098
7.4907
7.4717
7.3359
7.3165
7.2976
7.2785
7.2736
7.2595
2.5613
CN
2c
0.93
0.99
1.93
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

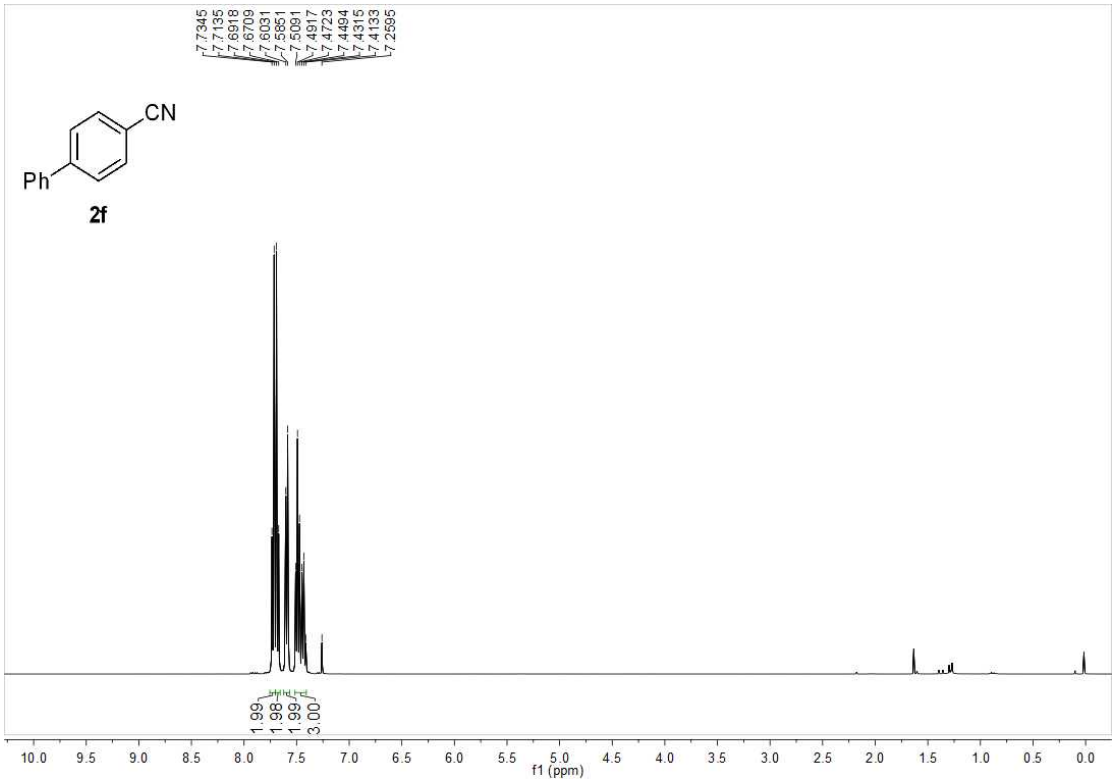

141.90
132.60
132.47
130.19
126.18
118.11
112.72
77.32
77.00
76.68
20.43
CN
2c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

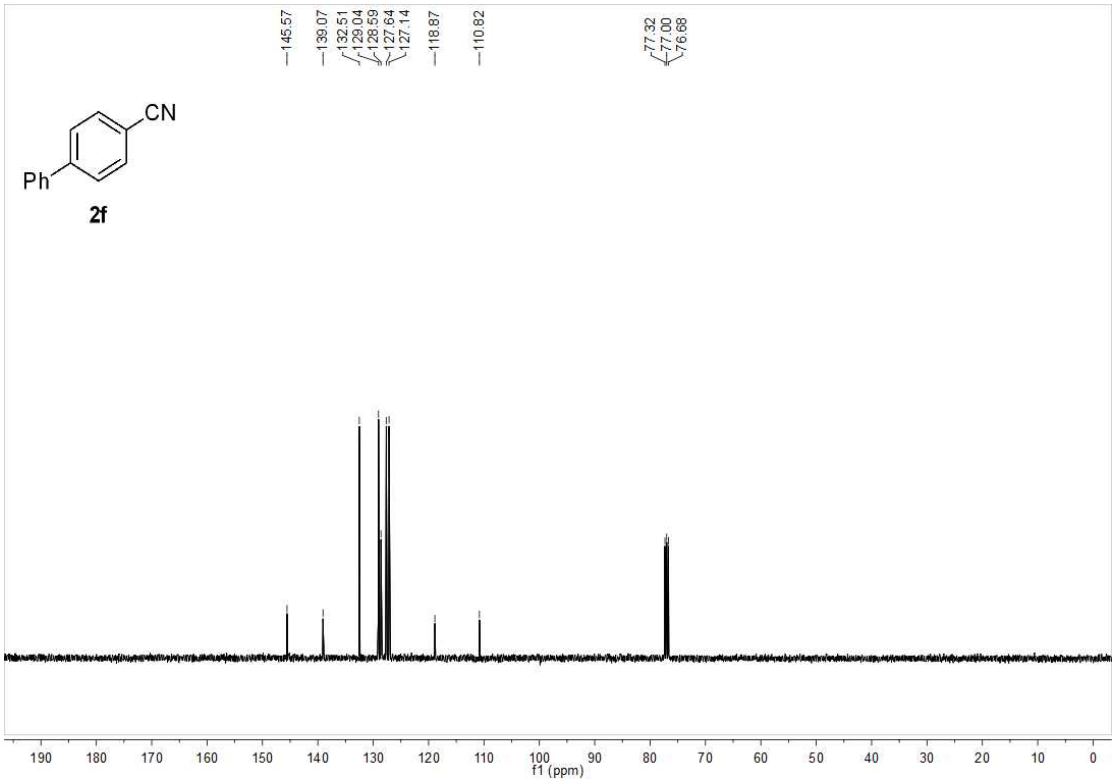

7.2599
6.9279
2.4775
2.3190
CN
2d
2.00
6.05
3.00
f1 (ppm)

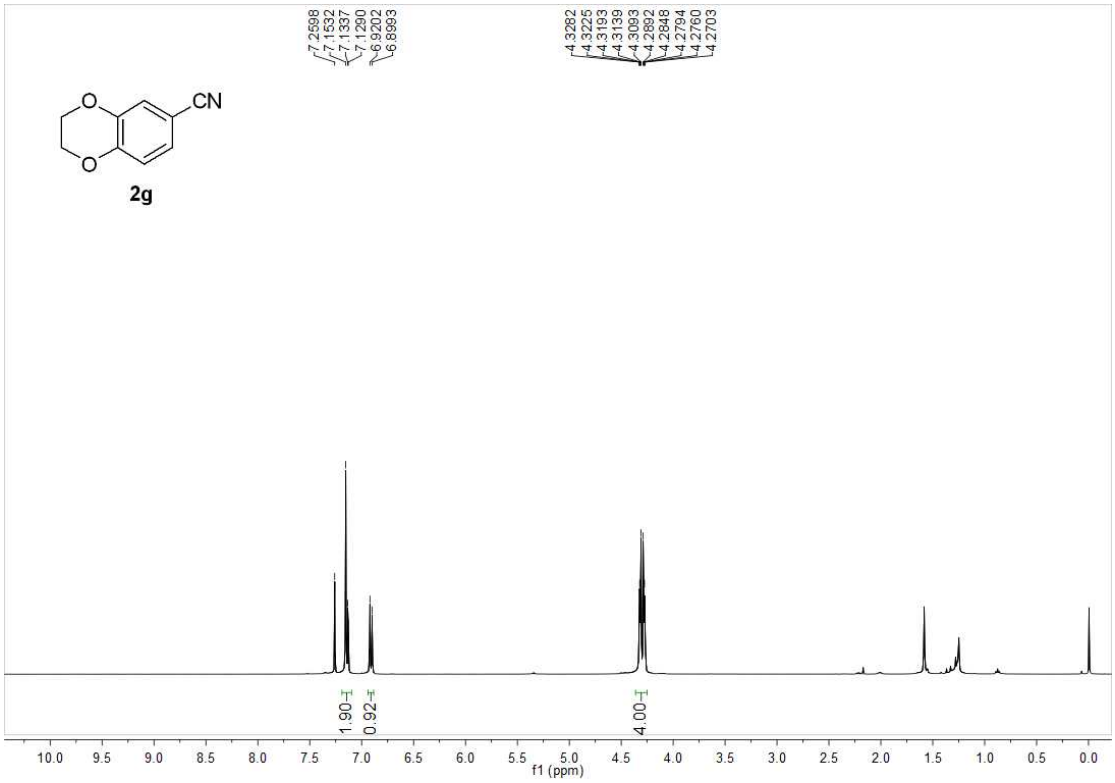

142.78
141.95
128.16
117.63
110.27
77.32
77.00
76.68
21.55
20.61
CN
2d
f1 (ppm)

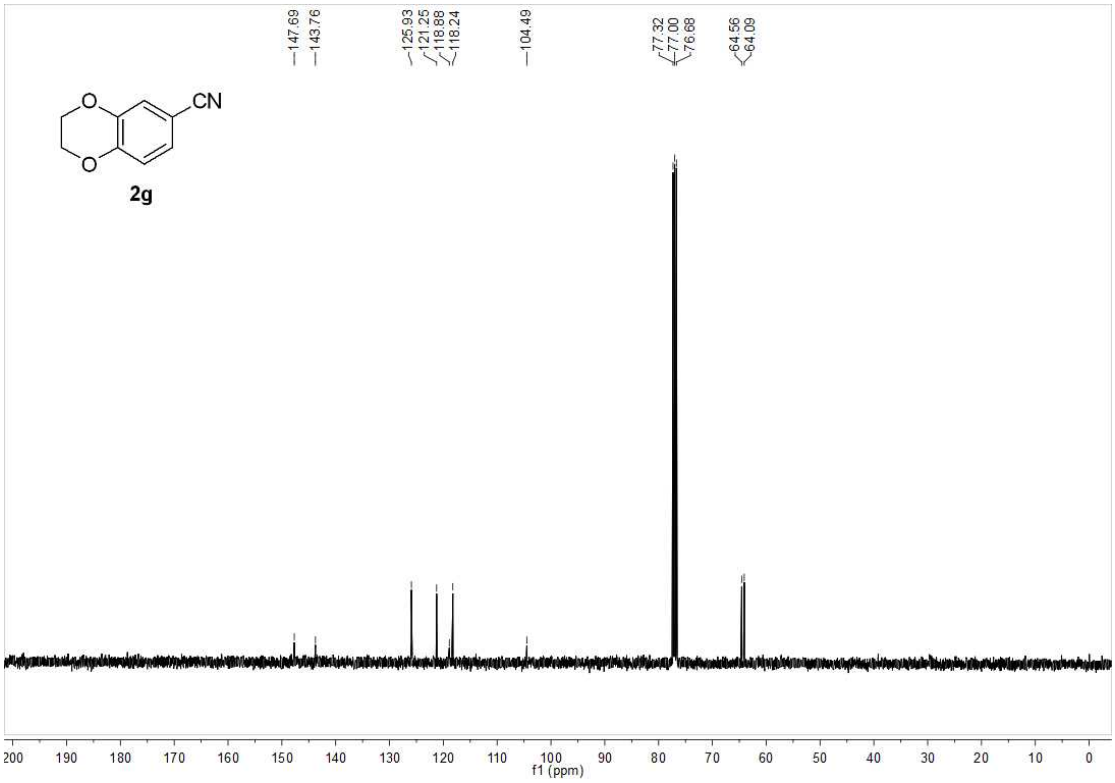

7.5971
7.5761
7.4893
7.4683
7.2595
1.3259
CN
2e
2.00
2.00
9.04
f1 (ppm)

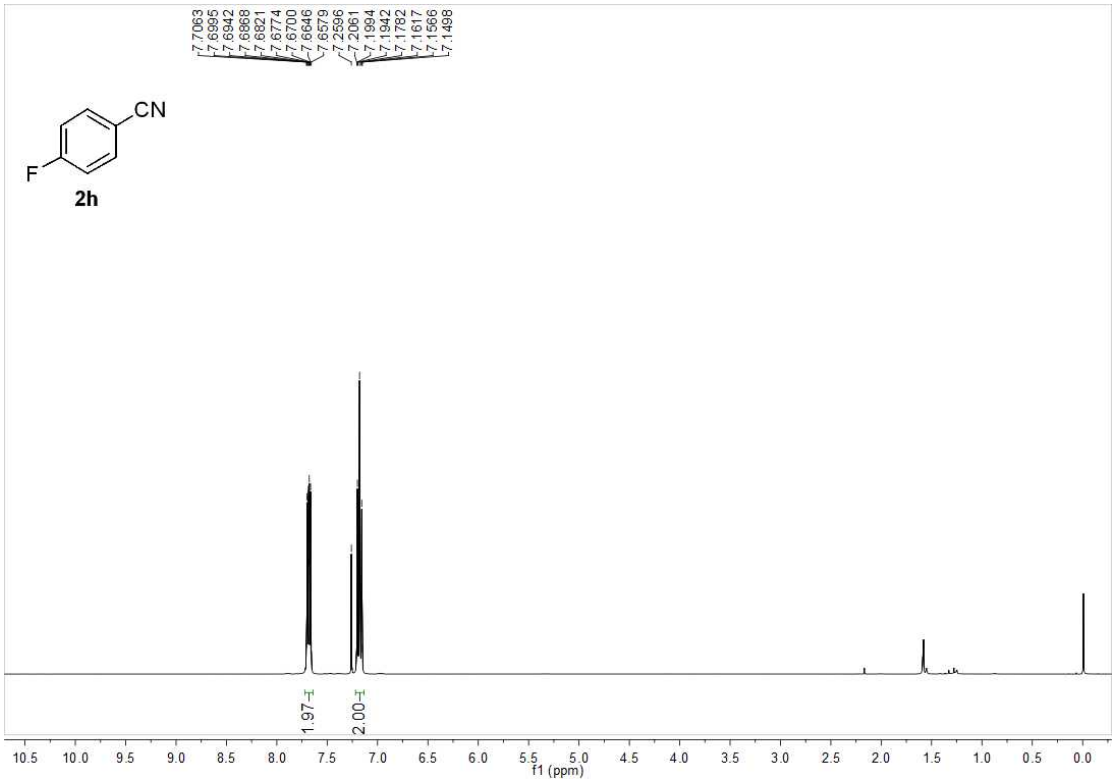

156.59
131.93
126.13
119.16
109.23
77.32
77.00
76.68
35.23
30.90
CN
2e
f1 (ppm)


7.7345
7.7135
7.6818
7.6709
7.6031
7.5851
7.5091
7.4917
7.4723
7.4494
7.4315
7.4133
7.2595
CN
Ph
2f
1.99
1.98
1.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


145.57
139.07
132.51
129.04
128.59
127.64
127.14
118.87
110.82
77.32
77.00
76.68
CN
Ph
2f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.2598
7.1532
7.1337
7.1290
6.9202
6.8993
4.3282
4.3225
4.3193
4.3139
4.3093
4.2892
4.2848
4.2794
4.2760
4.2703
CN
O
O
2g
1.90
0.92
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.69
143.76
125.93
121.25
118.88
118.24
104.49
77.32
77.00
76.68
64.56
64.09
CN
O
O
2g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.6942
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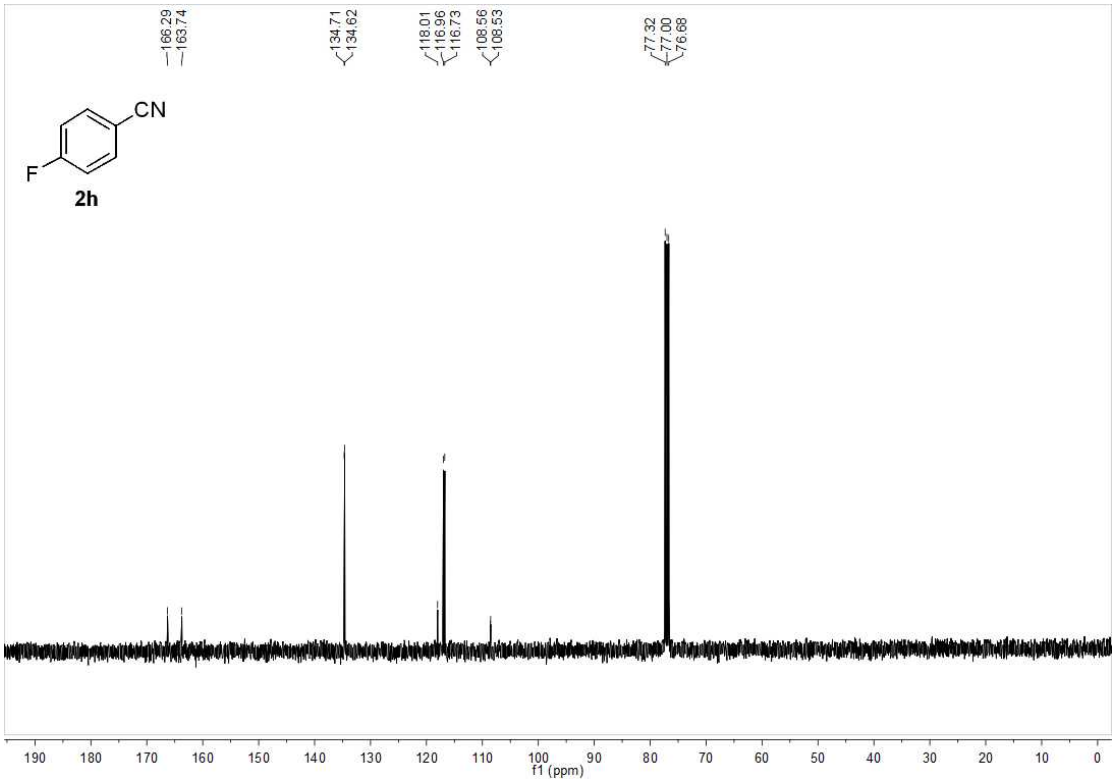
7.6821
7.6774
7.6700
7.6646
7.6579
7.2596
7.2061
7.1994
7.1942
7.1782
7.1617
7.1566
7.1498
CN
F
2h
1.97
2.00
f1 (ppm)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163.74
134.71
134.62
118.01
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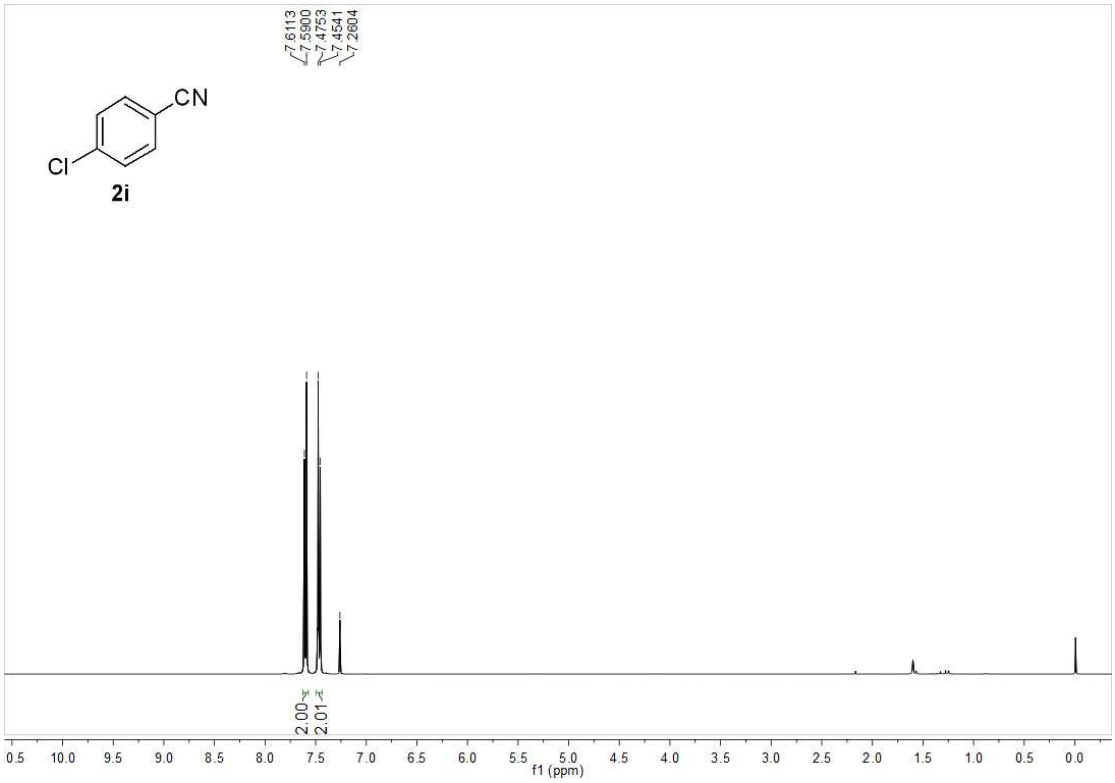
116.73
108.56
108.53
77.32
77.00
76.68
CN
F
2h
f1 (ppm)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7.4753
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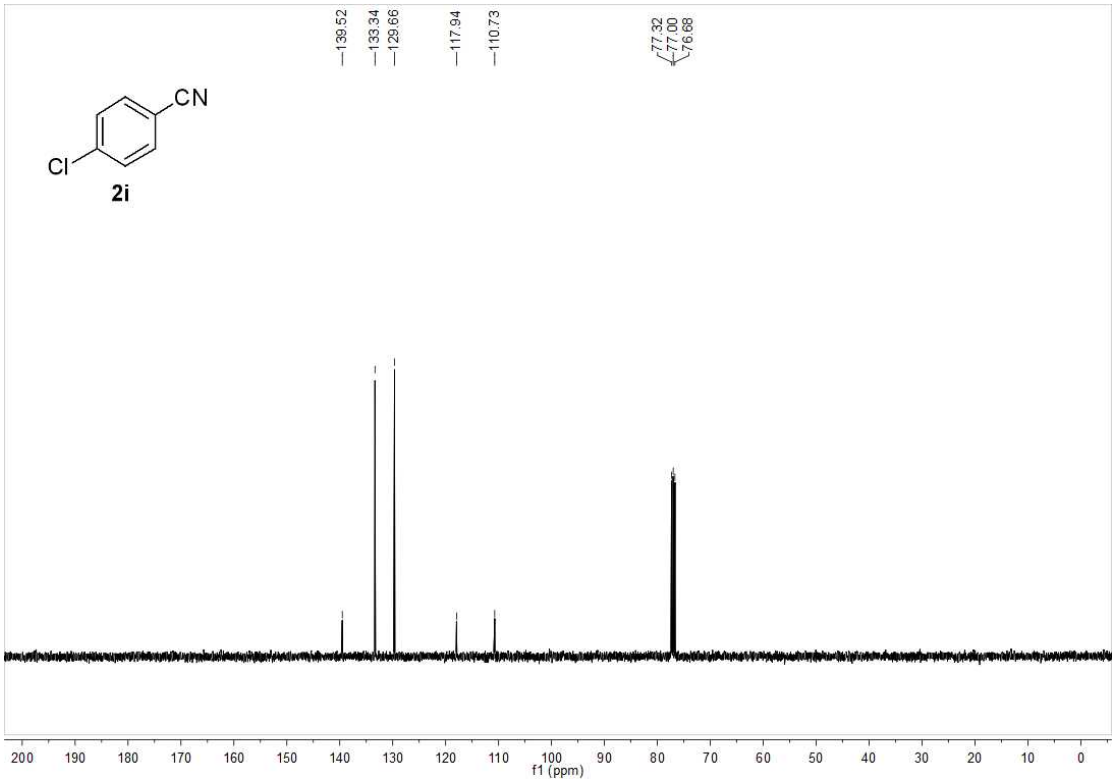
7.2604
CN
Cl
2i
2.00
2.01
f1 (ppm)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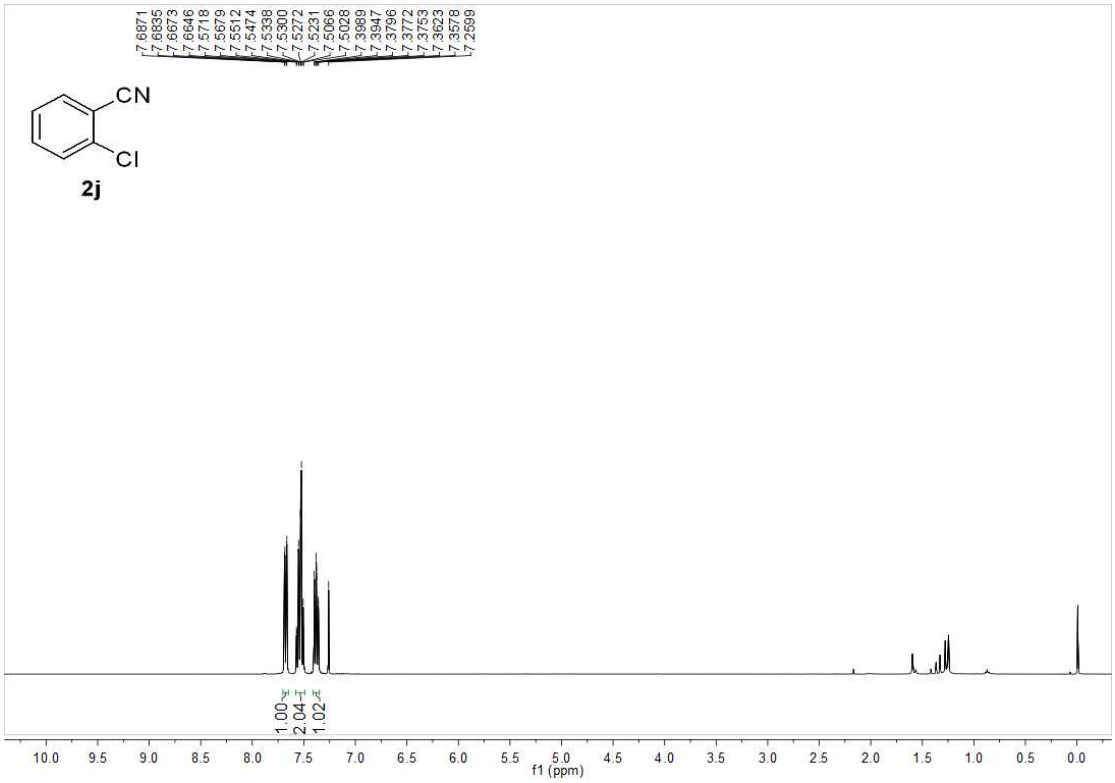
77.32
77.00
76.68
CN
Cl
2i
f1 (ppm)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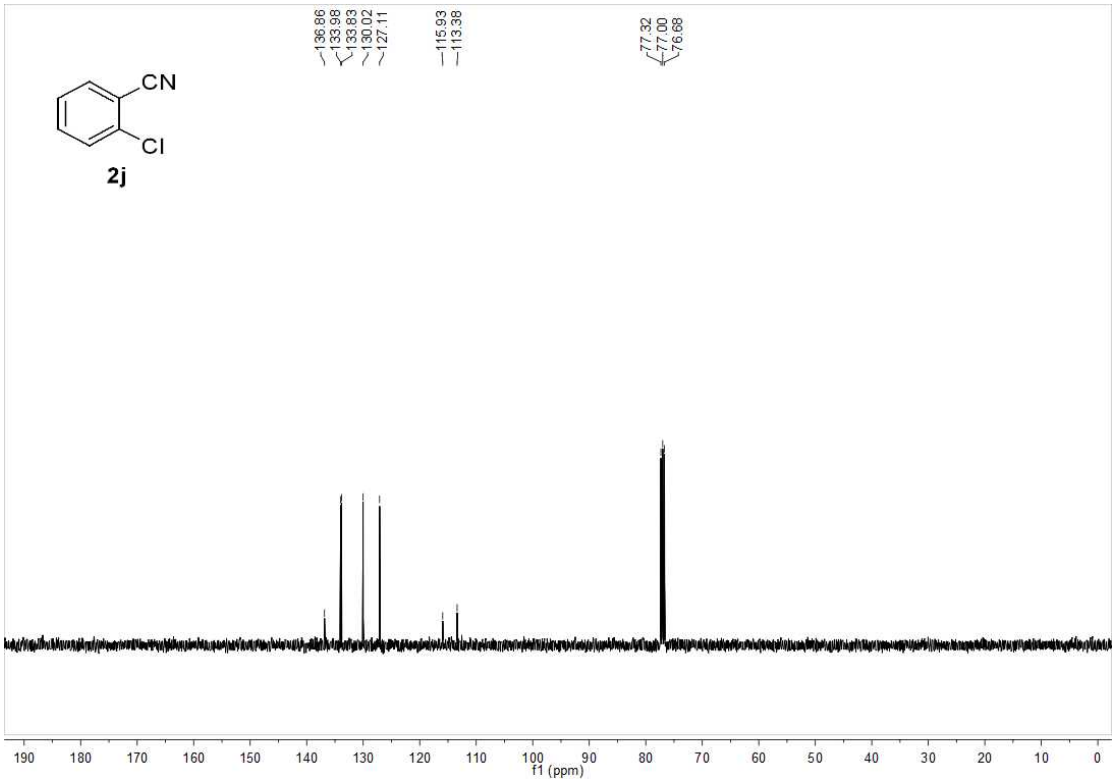
7.5338
7.5300
7.5272
7.5231
7.5066
7.5028
7.3989
7.3947
7.3796
7.3772
7.3753
7.3623
7.3578
7.2599
CN
Cl
2j
1.00
2.04
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


136.86
133.98
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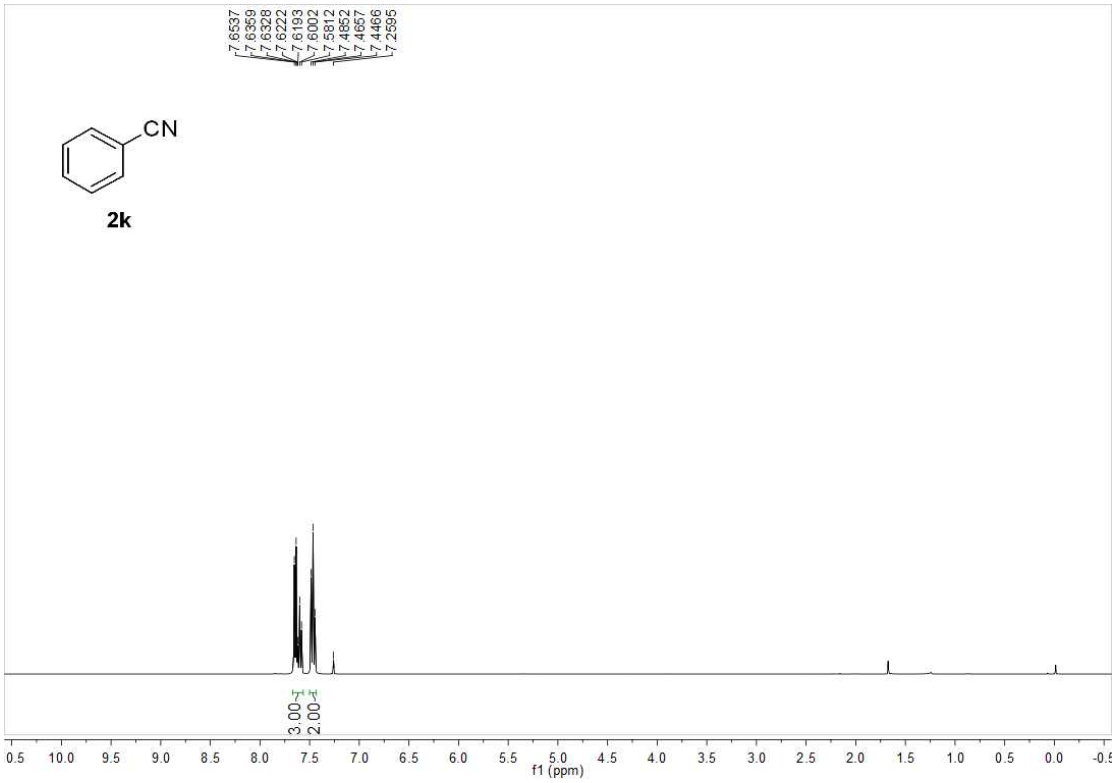
130.02
127.11
115.93
113.38
77.32
77.00
76.68
CN
Cl
2j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.6359
7.6328
7.6222
7.6193
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7.4657
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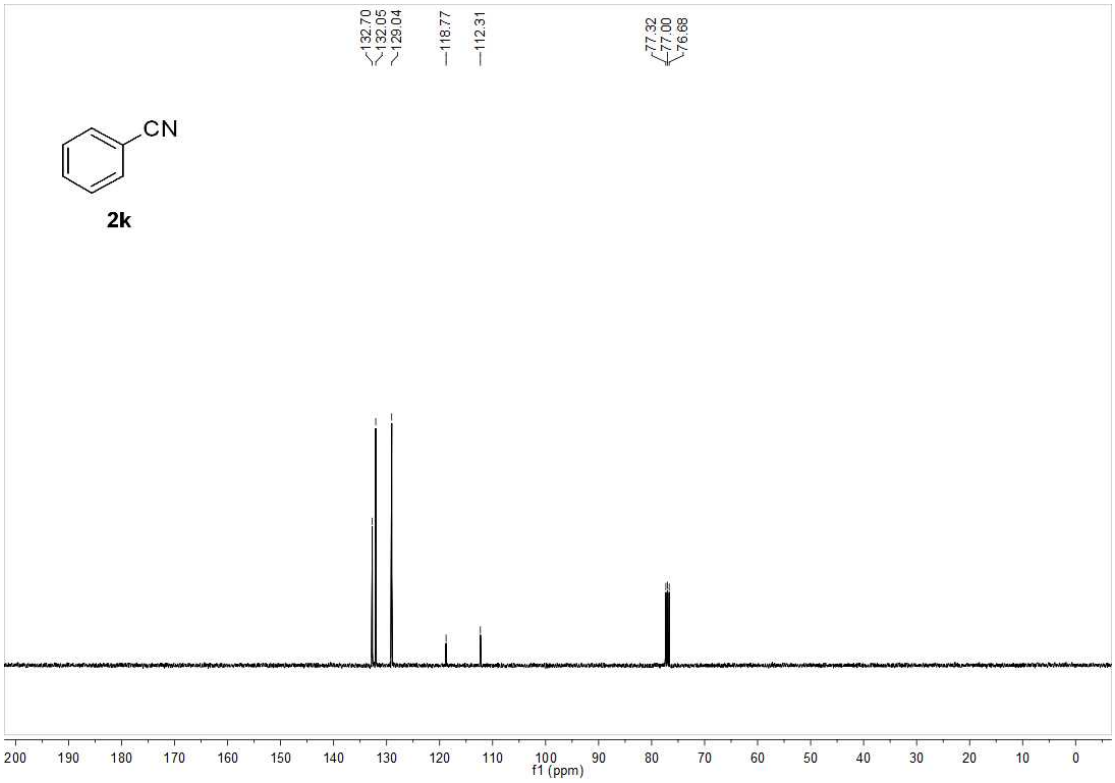
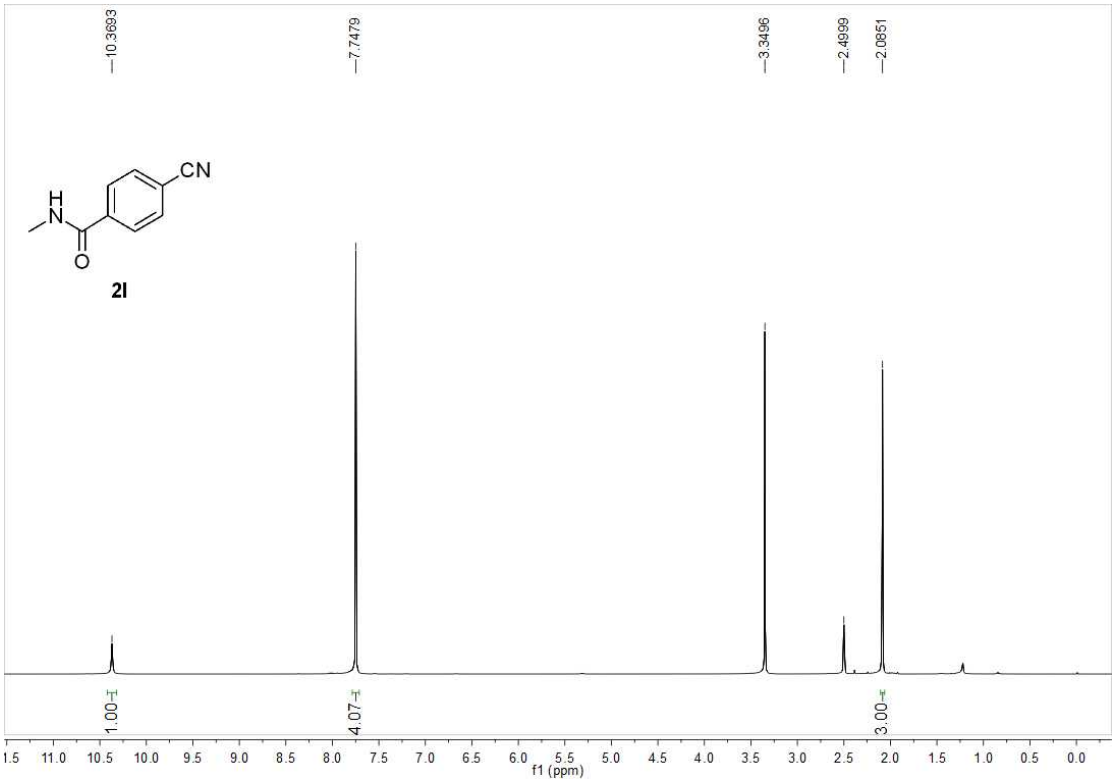
7.2595
CN
2k
3.00
2.00
f1 (ppm)


132.70
132.05
129.04
118.77
112.31
77.32
77.00
76.68
CN
2k
f1 (ppm)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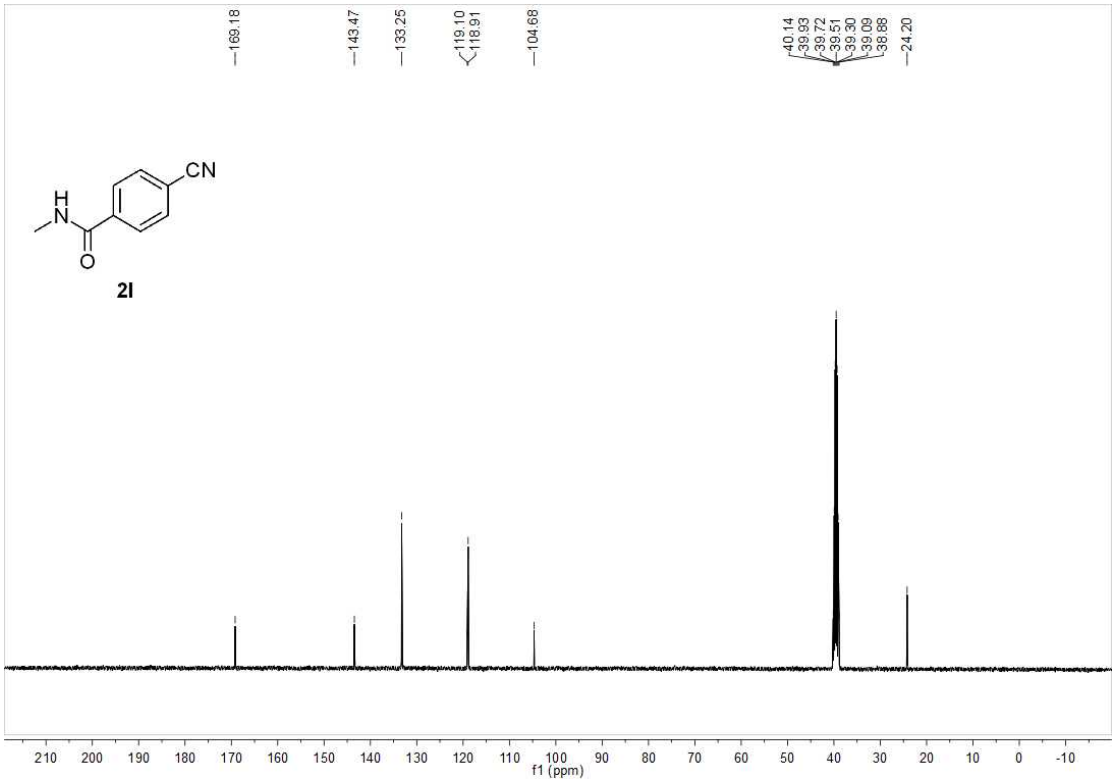
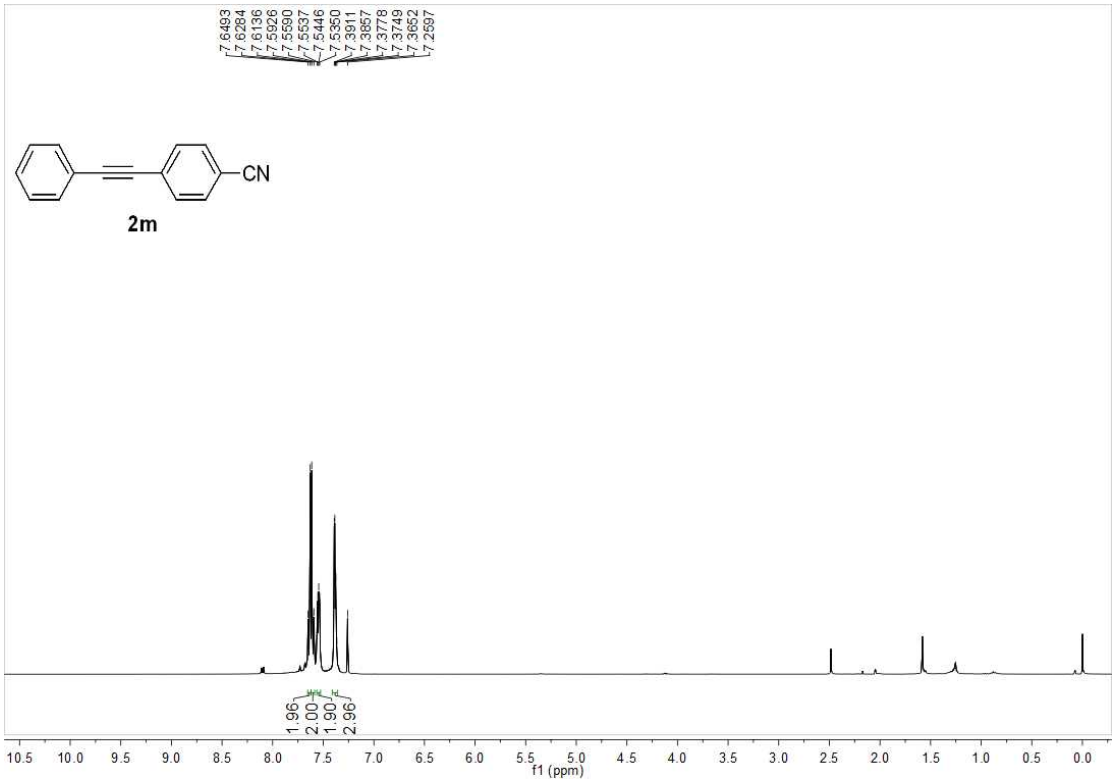
3.3496
2.4999
2.0851
CN
H
N
O
2l
1.00
4.07
3.00
f1 (ppm)


169.18
143.47
133.25
119.10
118.91
104.68
40.14
39.93
39.72
39.51
39.30
39.09
38.88
24.20
CN
H
N
O
2l
f1 (ppm)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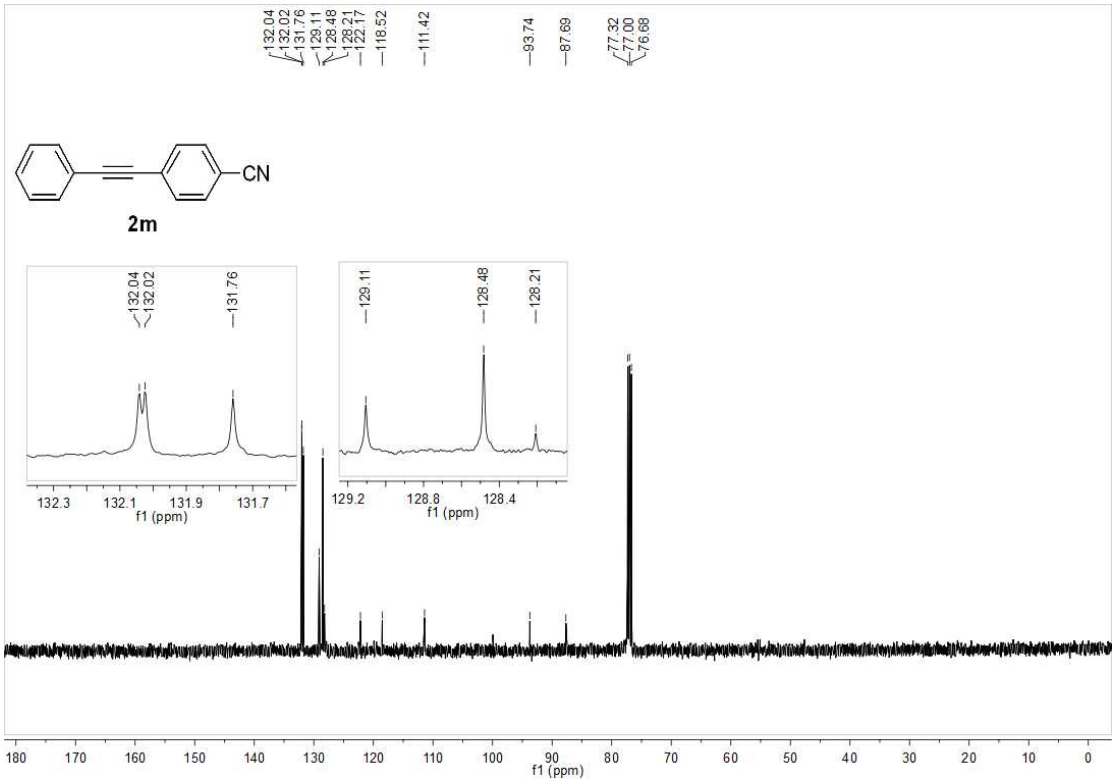
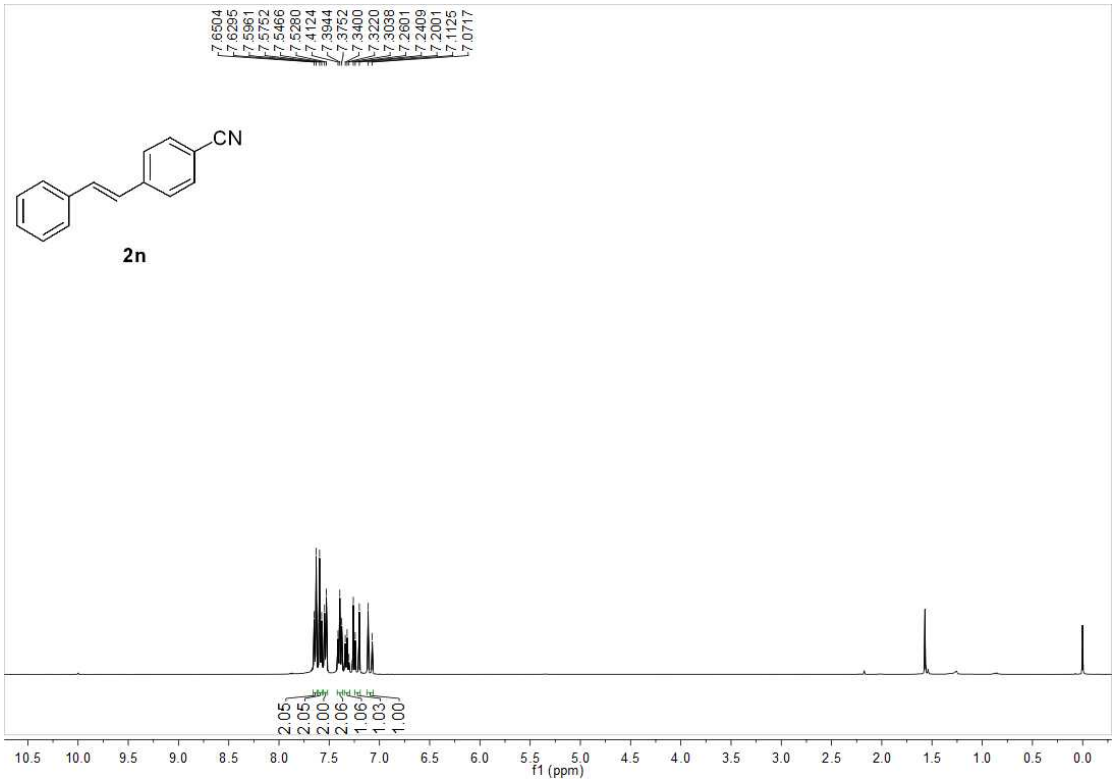
7.6284
7.6136
7.5926
7.5590
7.5537
7.5446
7.5350
7.3911
7.3857
7.3778
7.3749
7.3652
7.2697
CN
2m
1.96
2.00
1.90
2.96
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


132.04
132.02
131.76
129.11
128.48
128.21
122.17
118.52
111.42
93.74
87.69
77.32
77.00
76.68
CN
2m
132.3 132.1 131.9 131.7
f1 (ppm)
129.2 128.8 128.4
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.6295
7.5961
7.5752
7.5466
7.5280
7.4124
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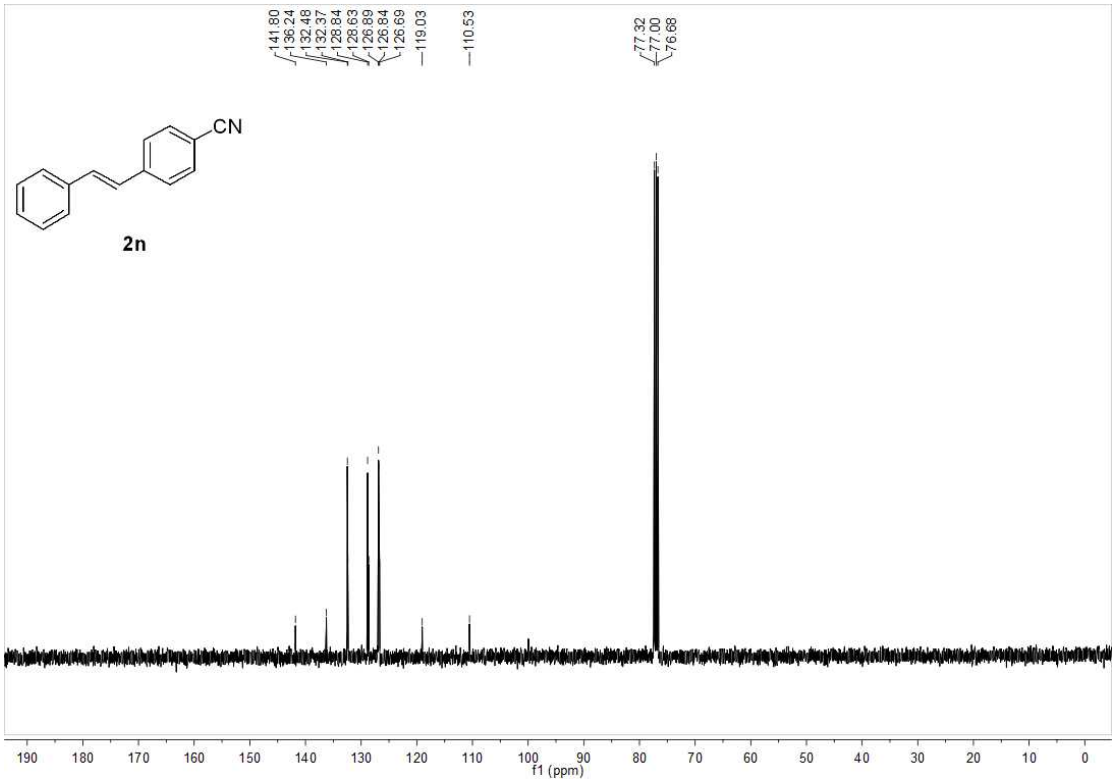
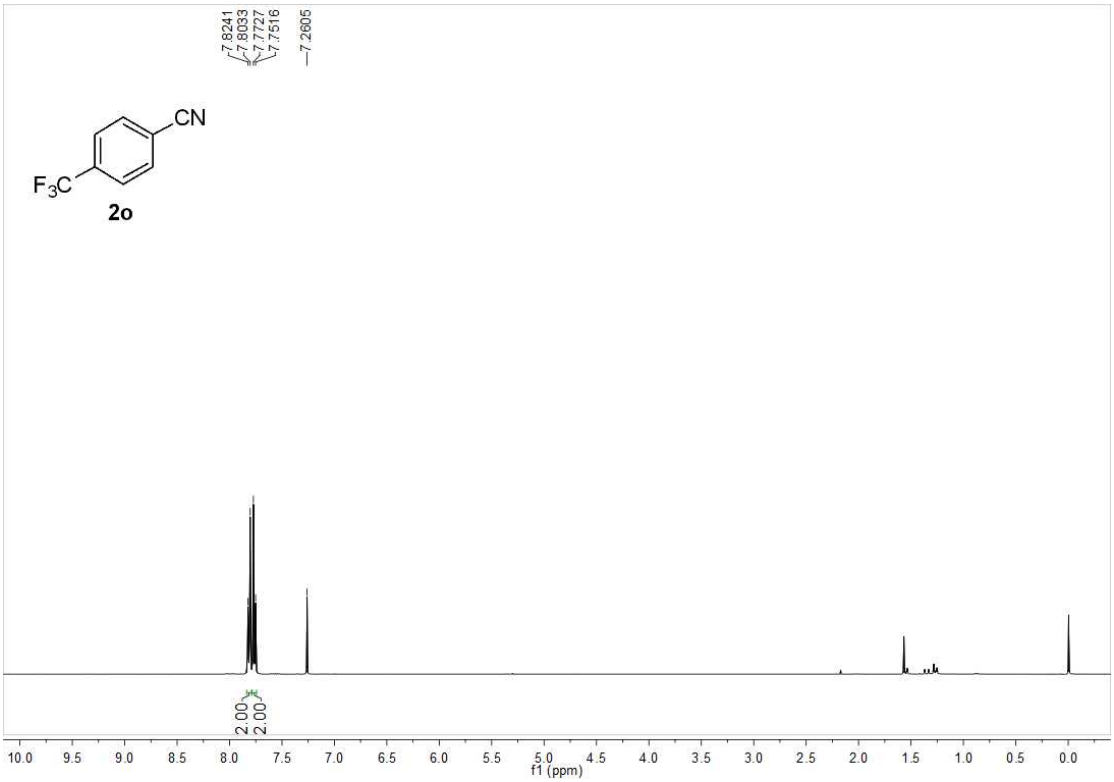
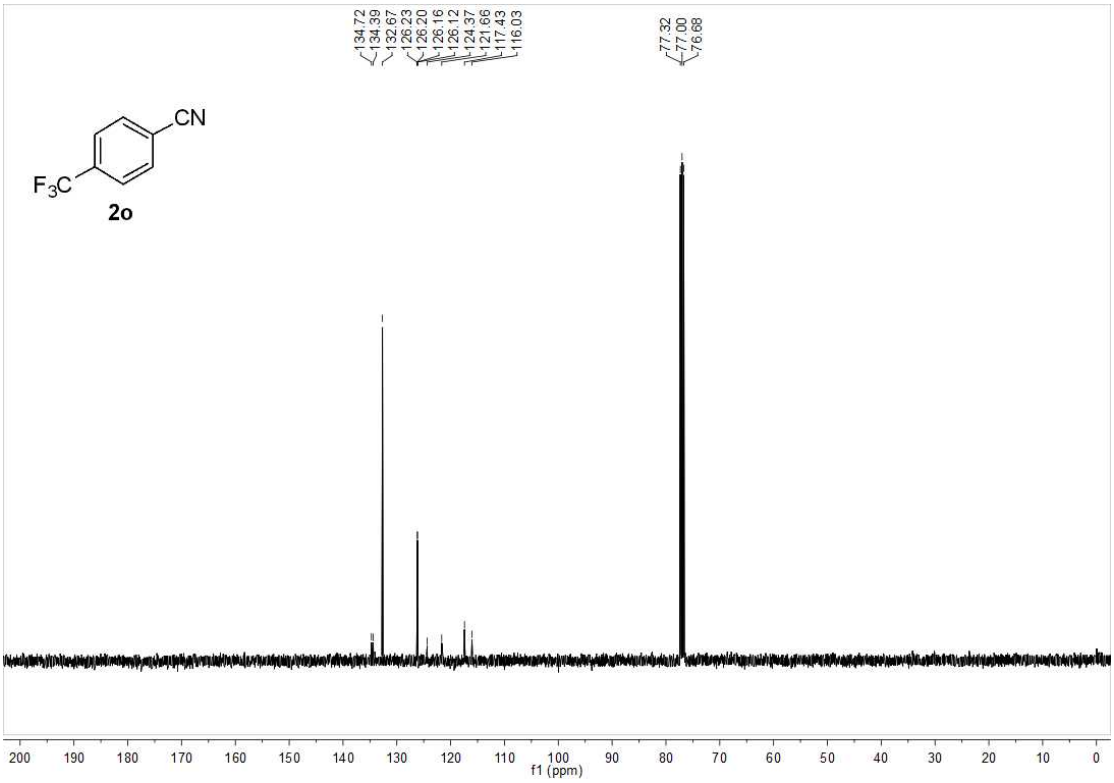
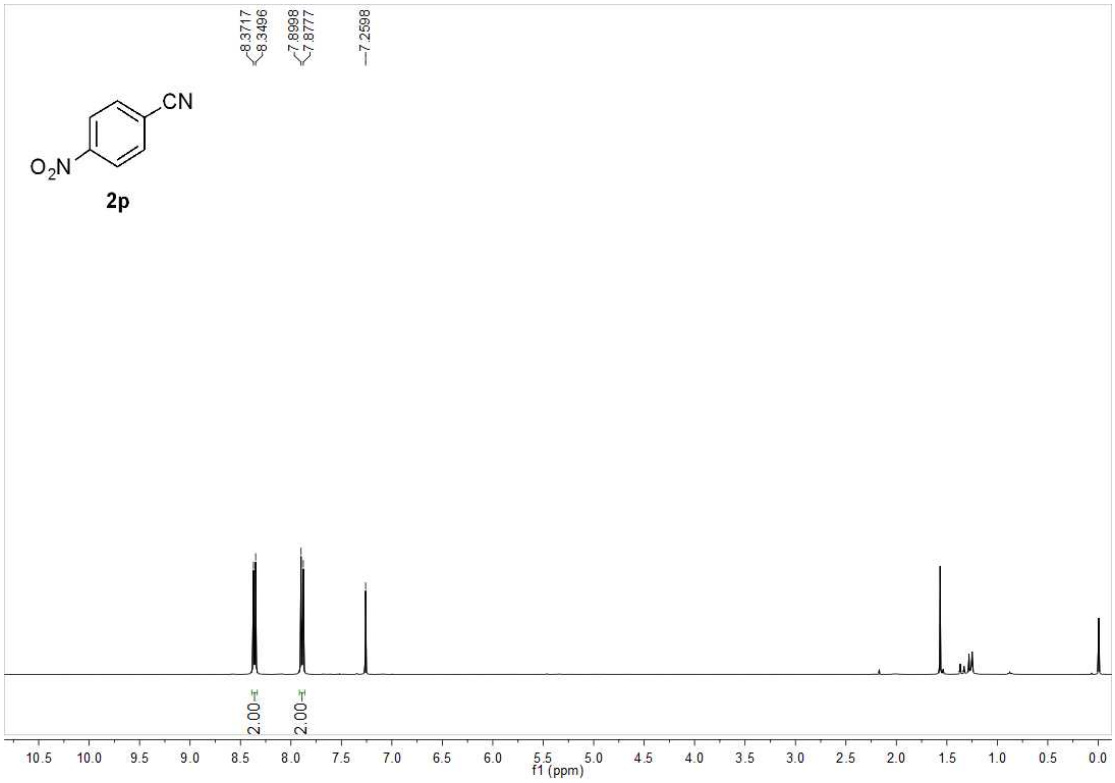
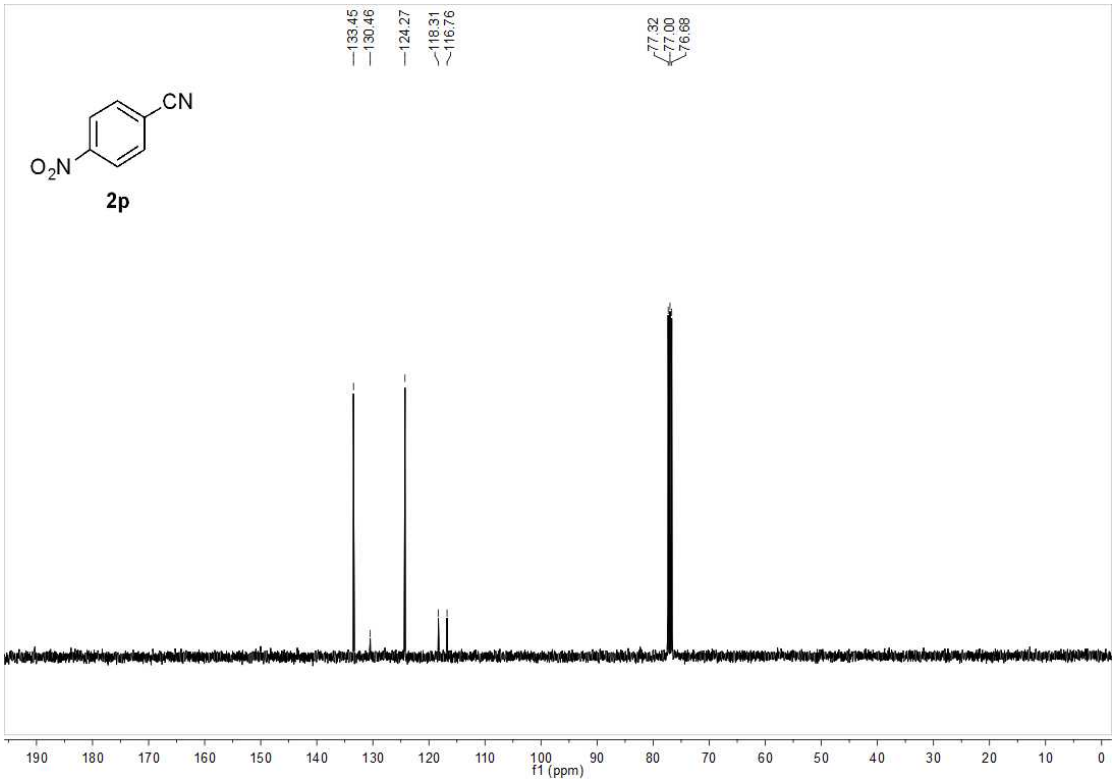
7.3752
7.3400
7.3220
7.3038
7.2601
7.2409
7.2001
7.1125
7.0717
CN
2n
2.05
2.05
2.00
2.06
1.06
1.03
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

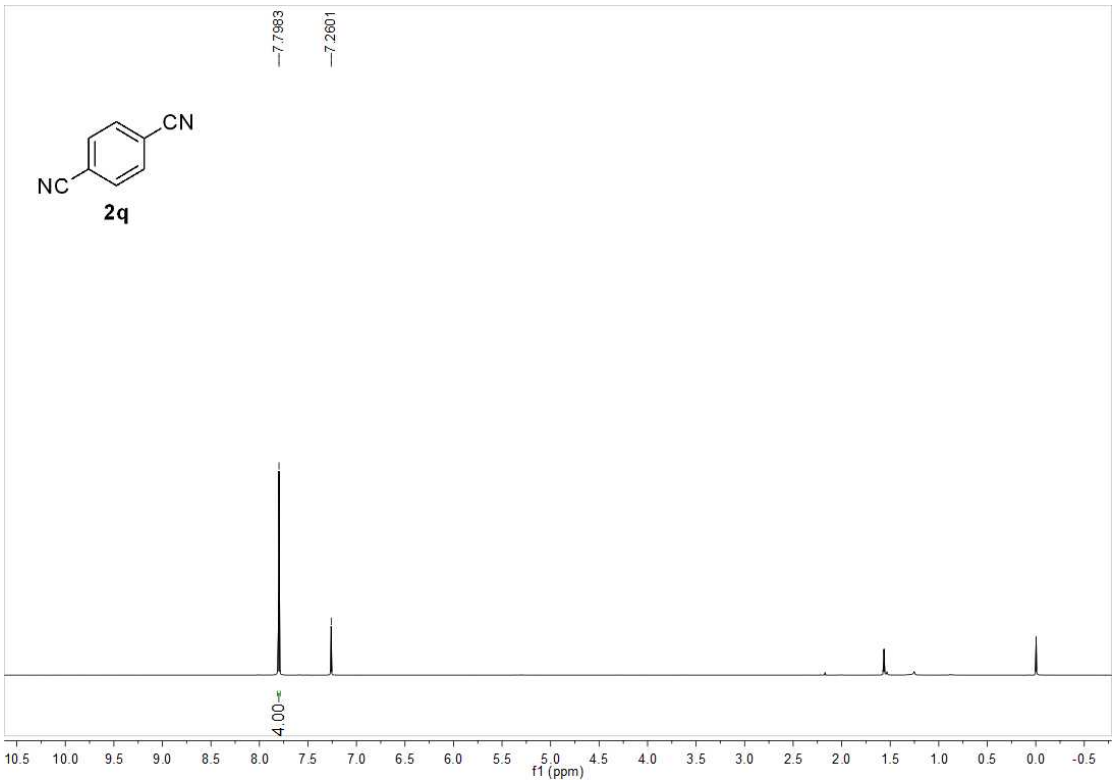

141.80
136.24
132.48
132.37
128.84
128.63
128.89
126.84
126.69
119.03
110.53
77.32
77.00
76.68
CN
2n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.8241
7.8033
7.7727
7.7516
7.2605
CN
F3C
2o
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


134.72
134.39
132.67
126.23
126.20
126.16
126.12
124.37
121.66
117.43
116.03
77.32
77.00
76.68
CN
F3C
2o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.3717
8.3496
7.8998
7.8777
7.2598
CN
O_2N
2p
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


133.45
130.46
124.27
118.31
116.76
77.32
77.00
76.68
CN
O_2N
2p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.7983
7.2601
CN
NC
2q
4.00
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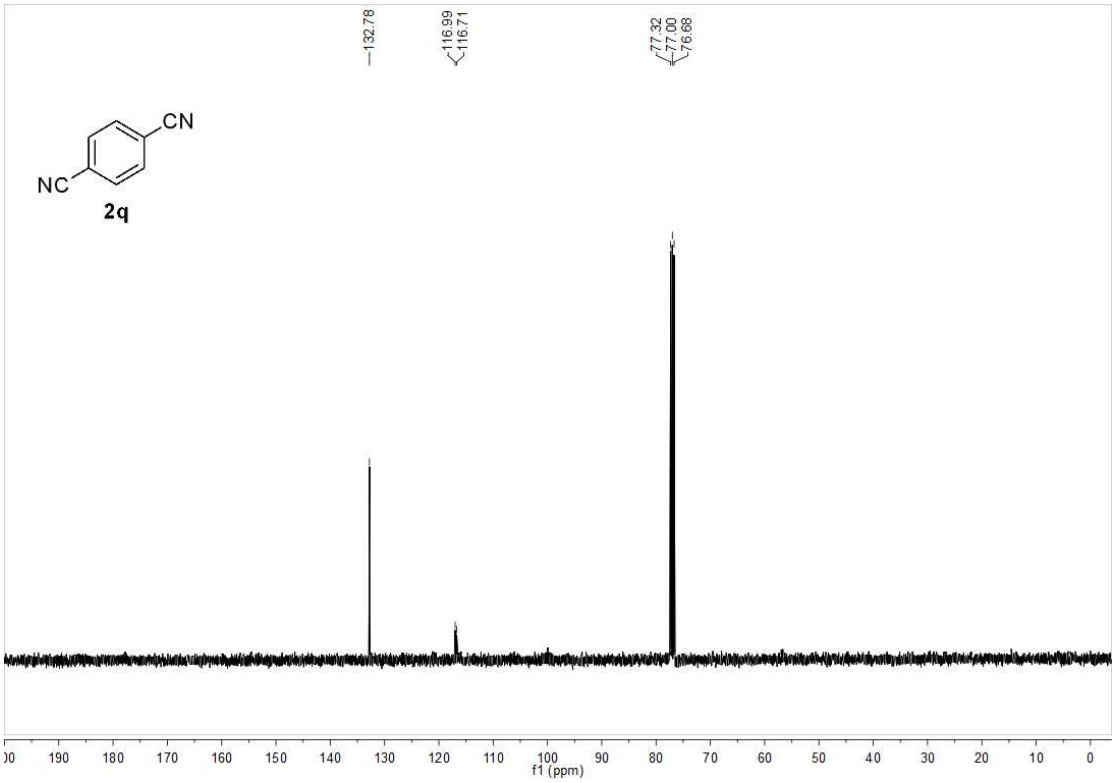
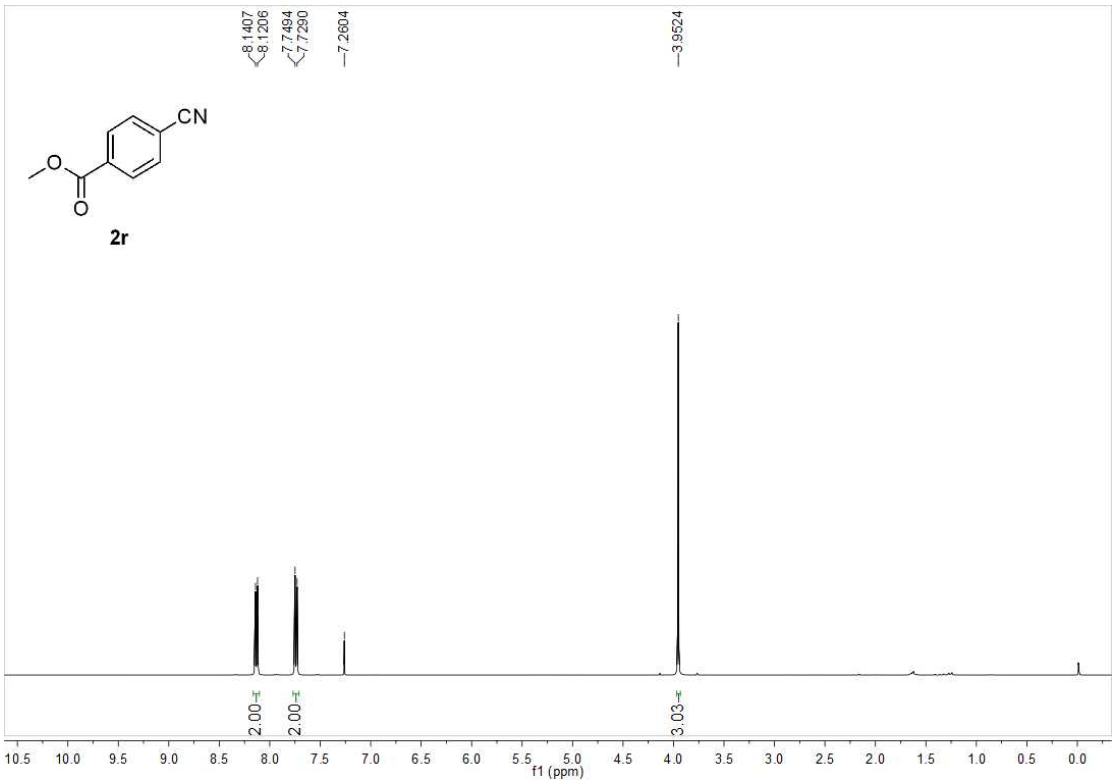
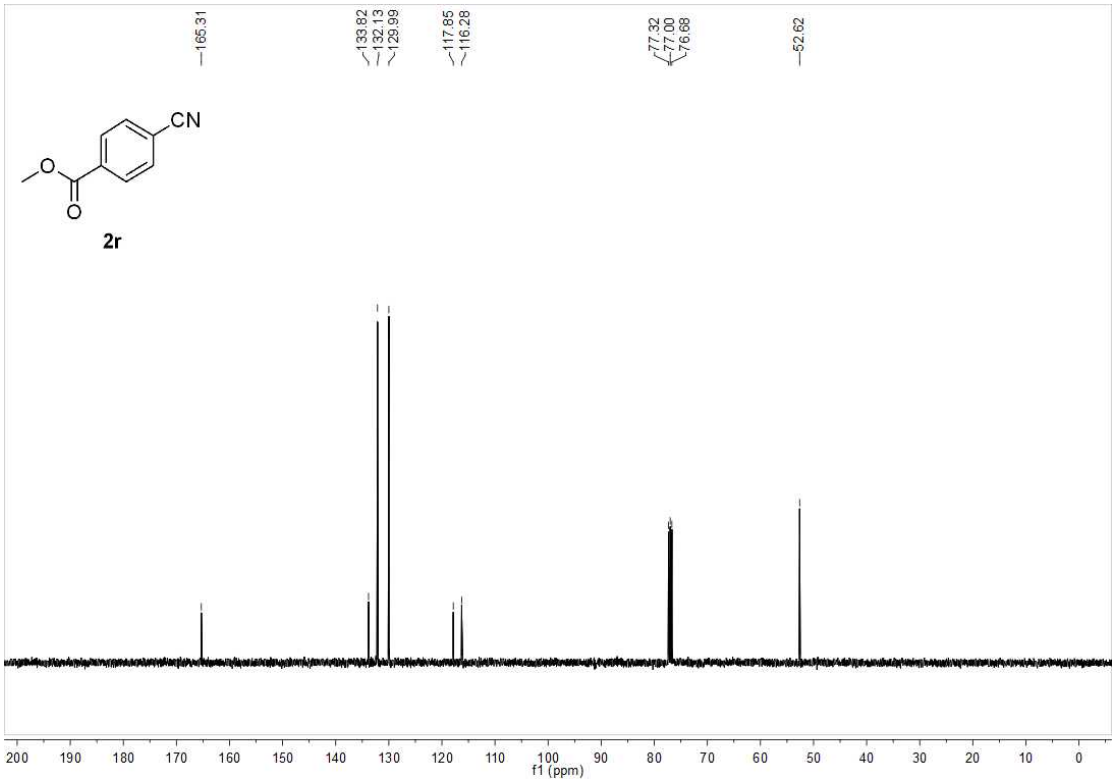
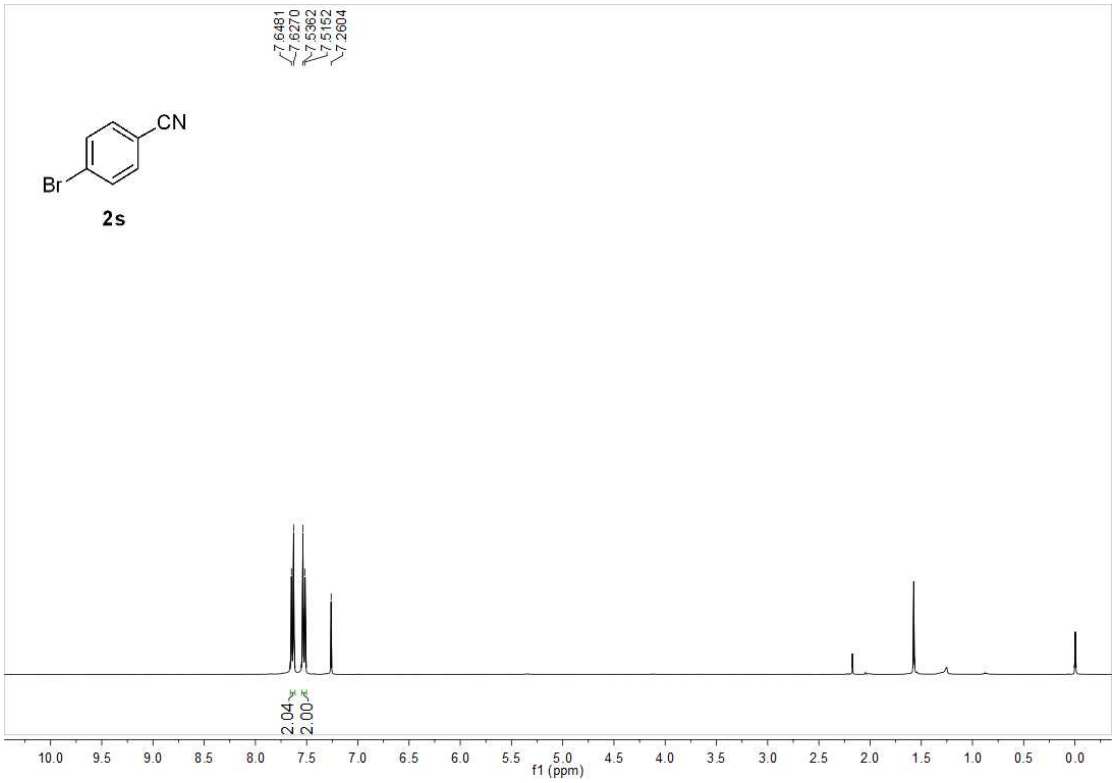
f1 (ppm)


132.78
116.99
116.71
77.32
77.00
76.68
CN
NC
2q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.1407
8.1206
7.7494
7.7290
7.2604
3.9524
CN
O
O
2r
2.00
2.00
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.31
133.82
132.13
129.99
117.85
116.28
77.32
77.00
76.68
52.62
CN
O
O
2r
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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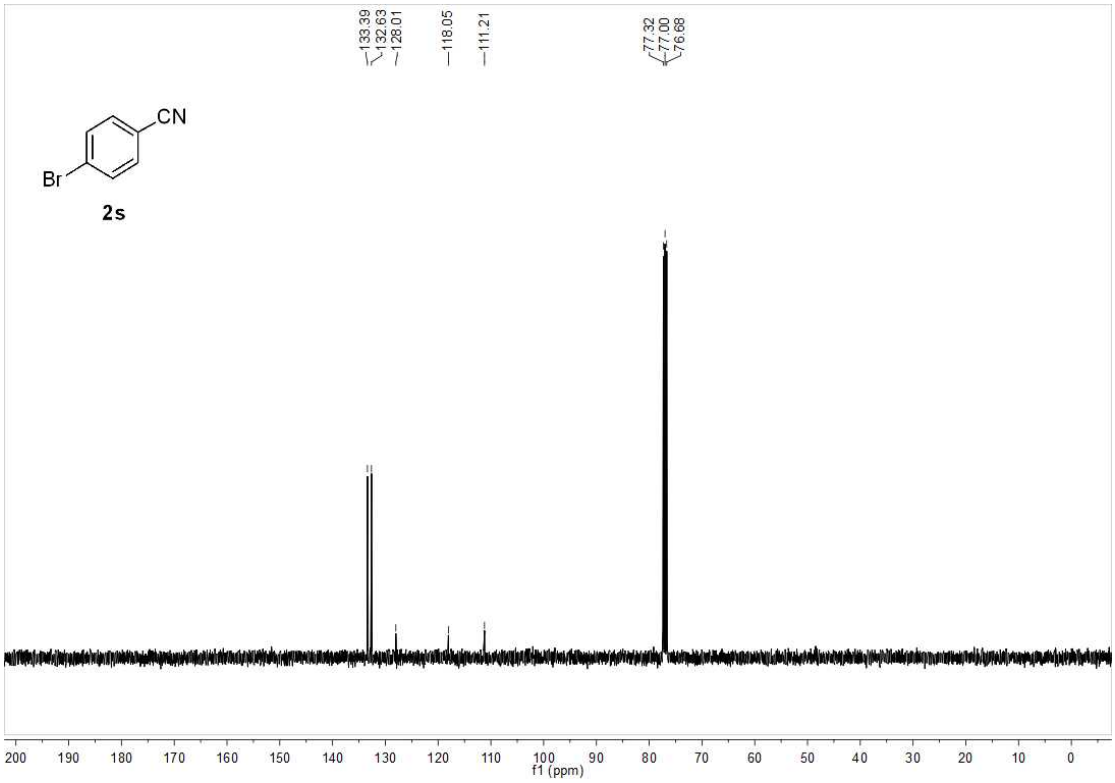
7.5362
7.5152
7.2604
CN
Br
2s
2.04
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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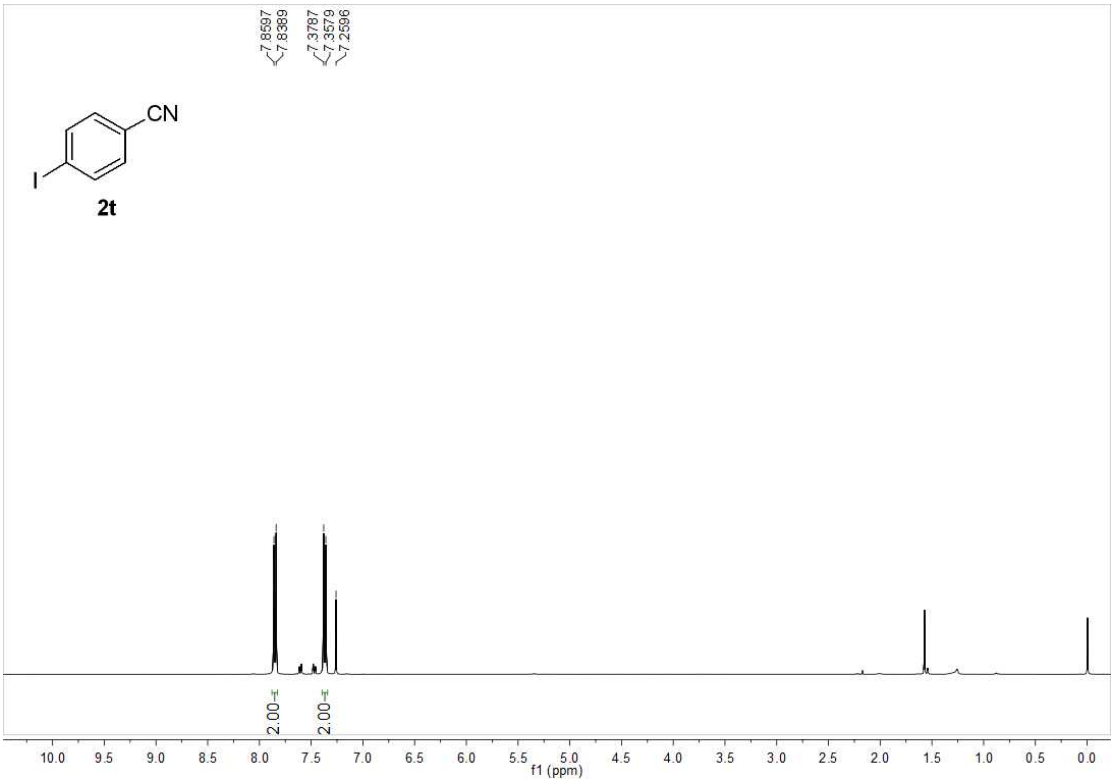
132.63
128.01
118.05
111.21
77.32
77.00
76.68
CN
Br
2s
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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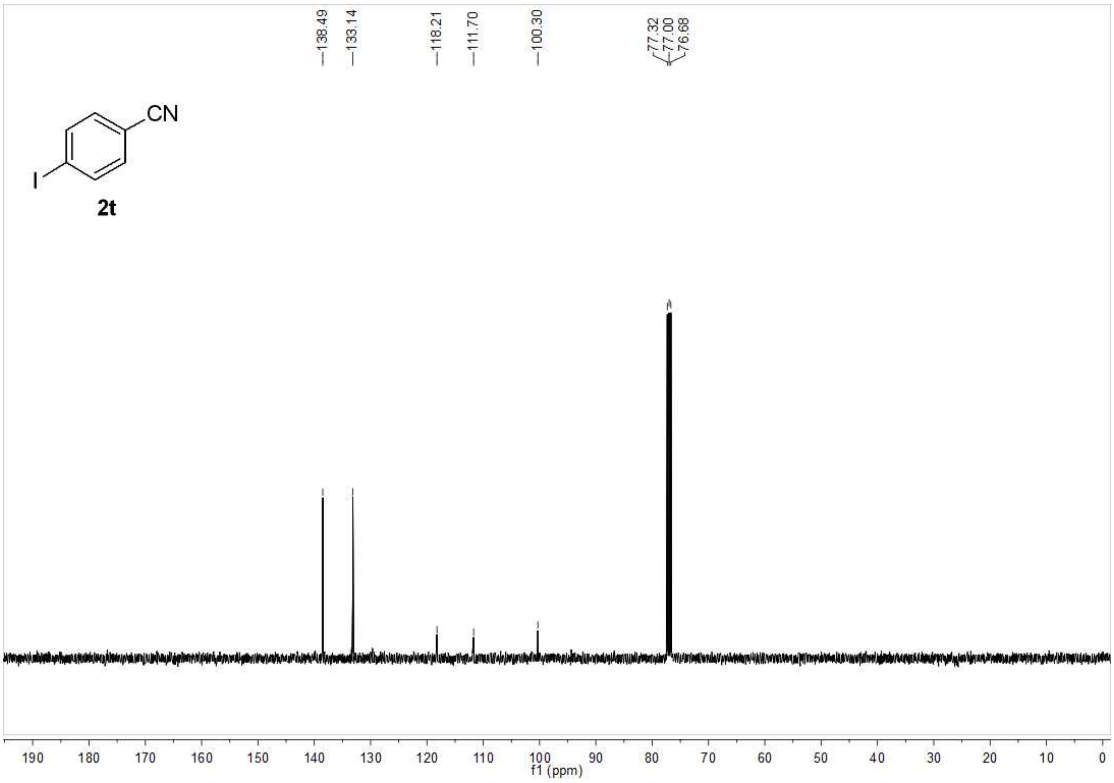
7.8389
7.3787
7.3579
7.2596
CN
I
2t
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.14
118.21
111.70
100.30
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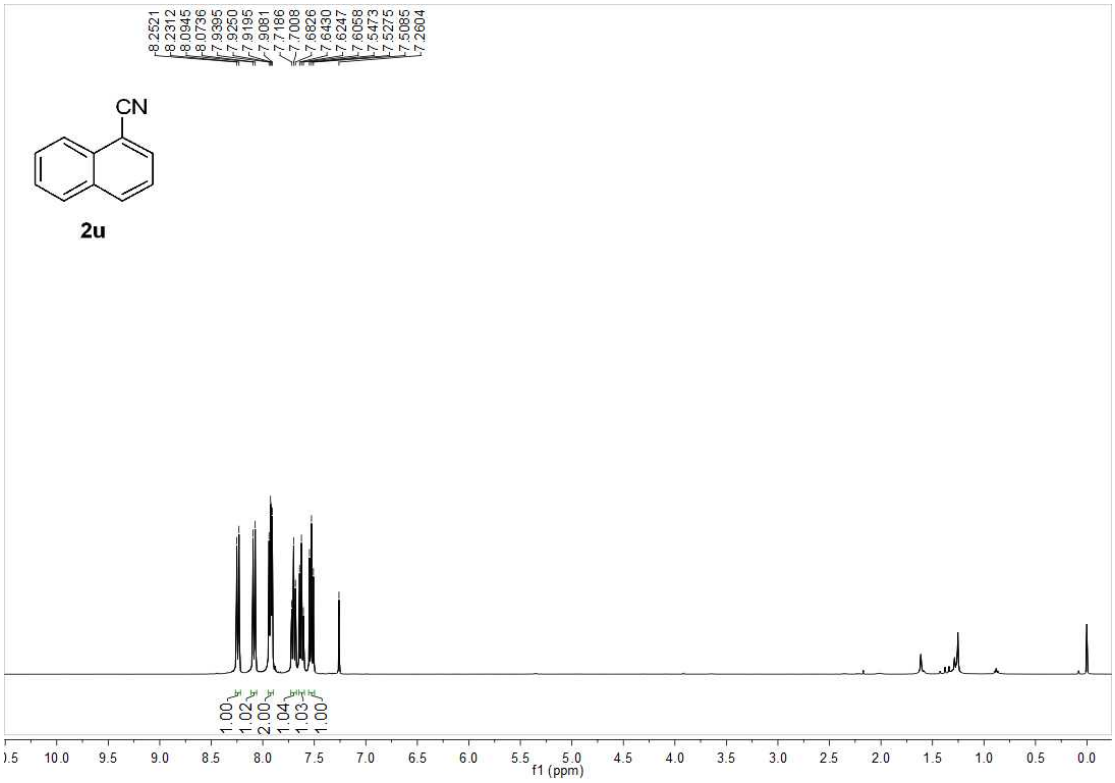
77.00
76.68
CN
I
2t
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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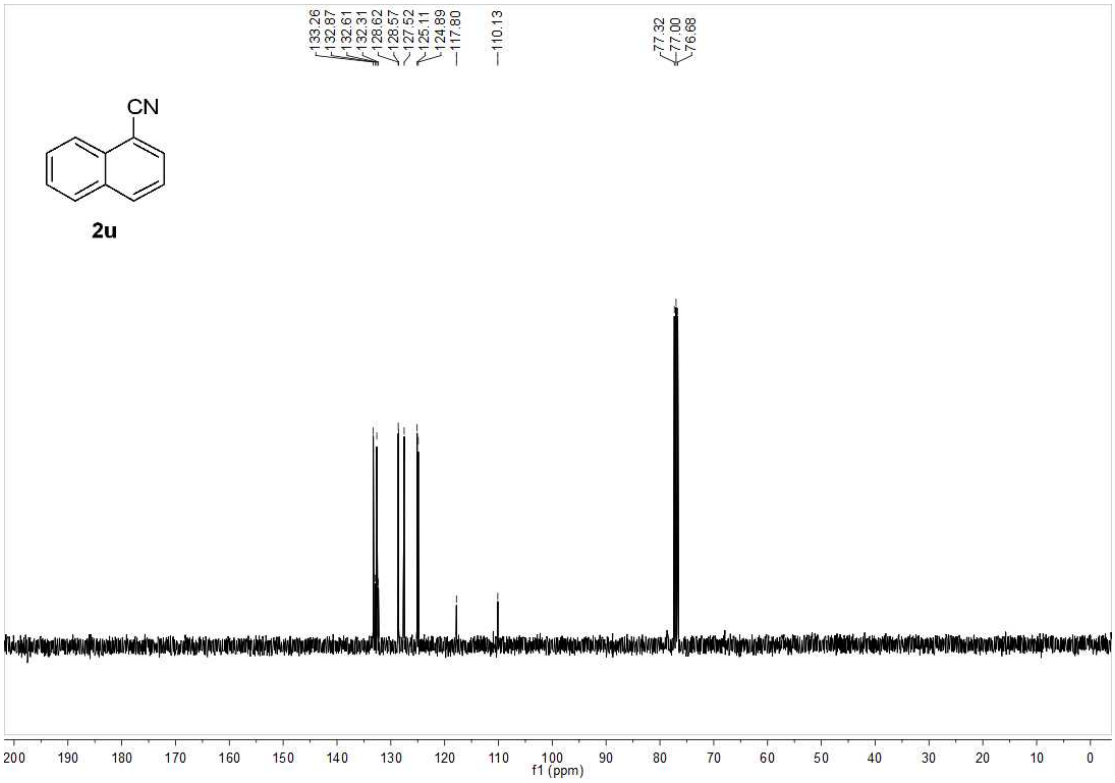
8.0945
8.0736
7.9395
7.9250
7.9195
7.9081
7.7186
7.7008
7.6826
7.6430
7.6247
7.6058
7.5473
7.5275
7.5085
7.2604
CN
2u
1.00
1.02
2.00
1.04
1.03
1.00
f1 (ppm)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132.87
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125.11
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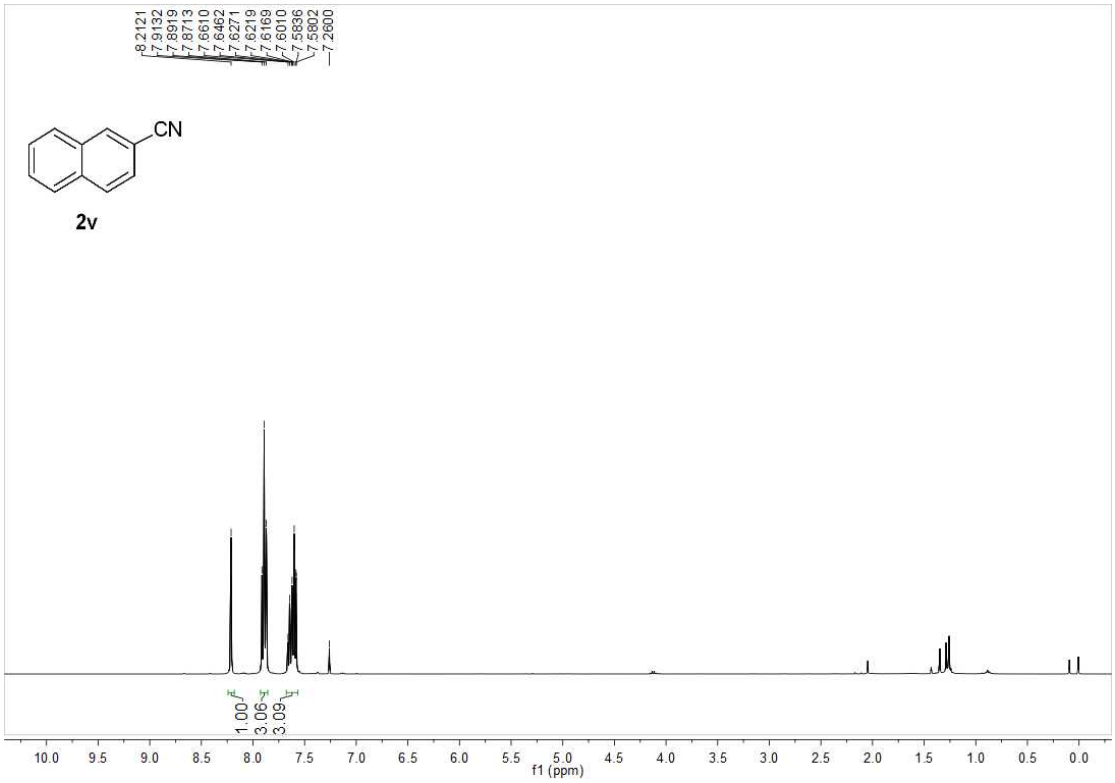
110.13
77.32
77.00
76.68
CN
2u
f1 (ppm)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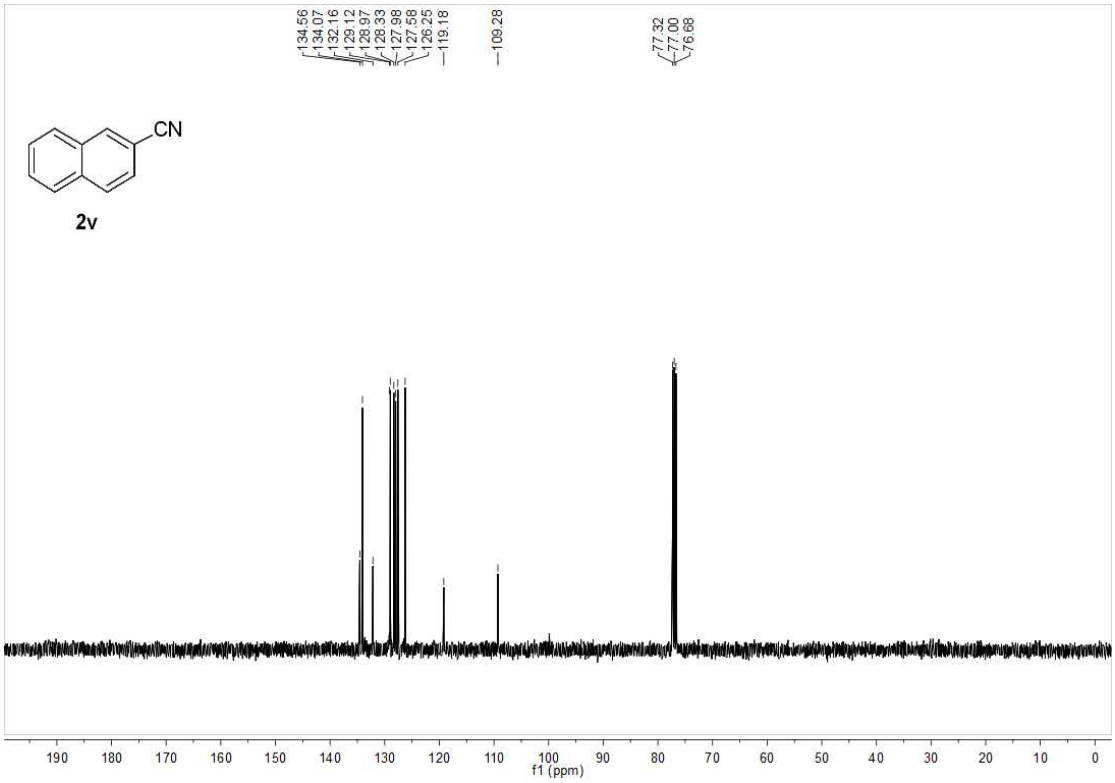
7.6610
7.6462
7.6271
7.6219
7.6169
7.6010
7.5836
7.5802
7.2600
CN
2v
1.00
3.06
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


134.56
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132.16
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128.97
128.33
127.98
127.58
126.25
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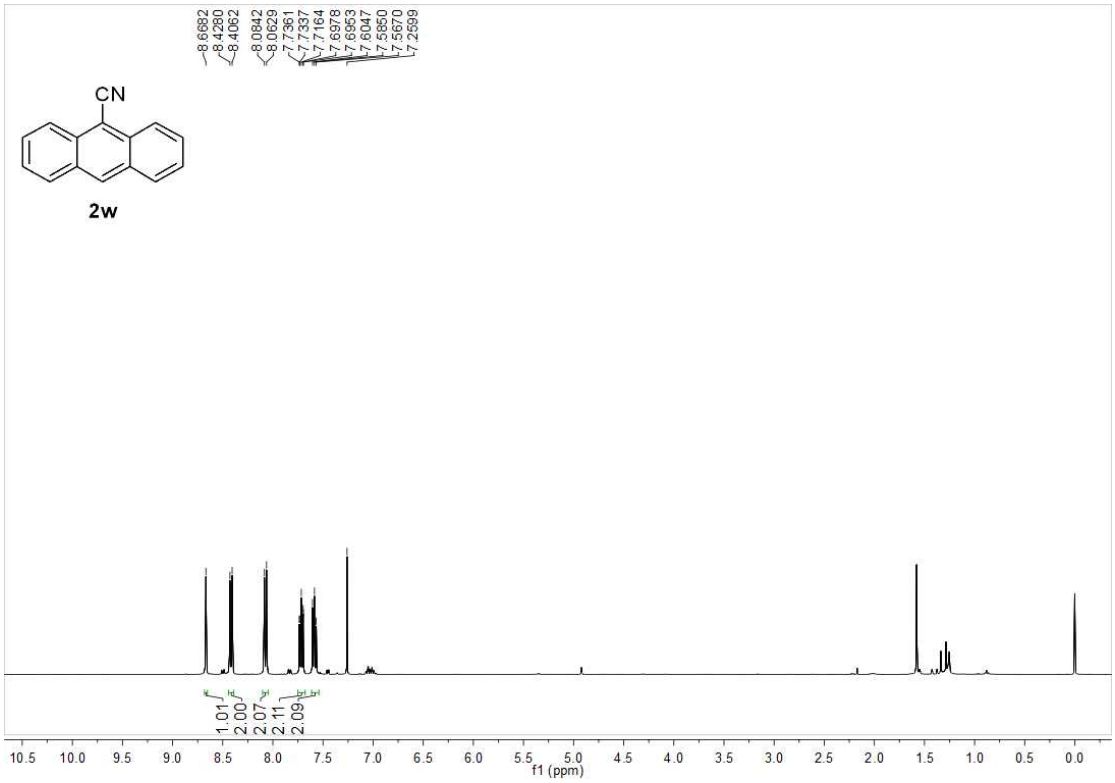
109.28
77.32
77.00
76.68
CN
2v
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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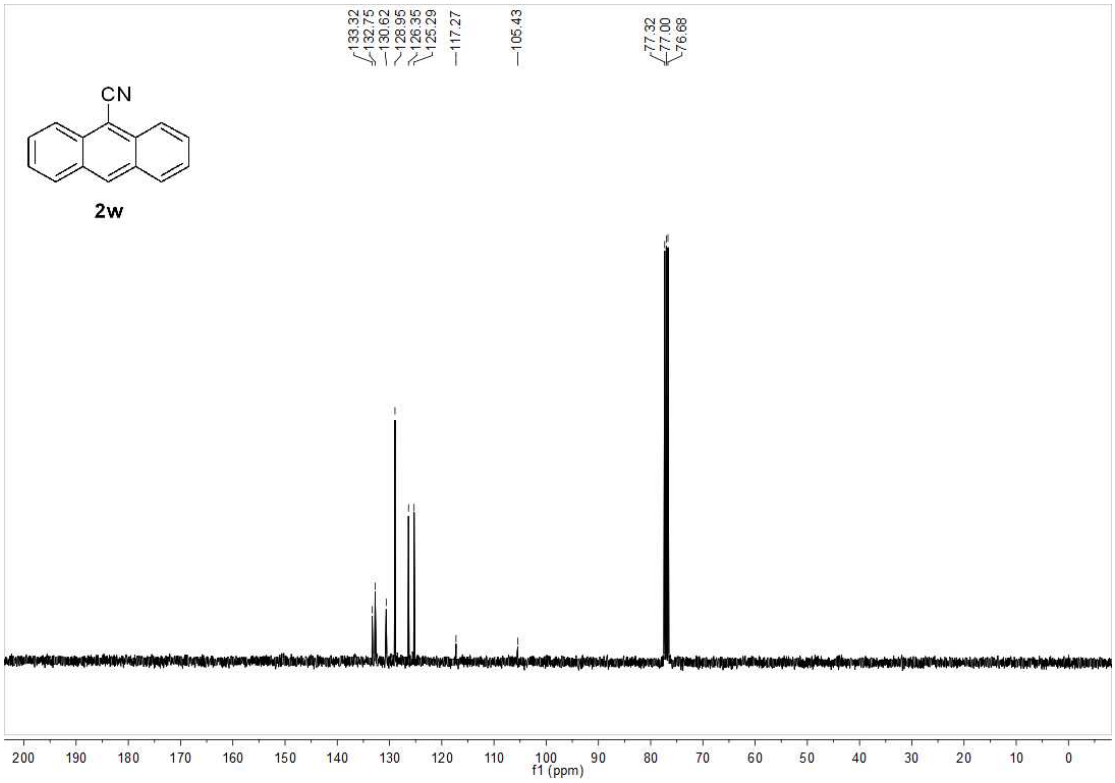
7.7164
7.6978
7.6953
7.6047
7.5850
7.5670
7.2599
CN
2w
1.01
2.00
2.07
2.11
2.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.95
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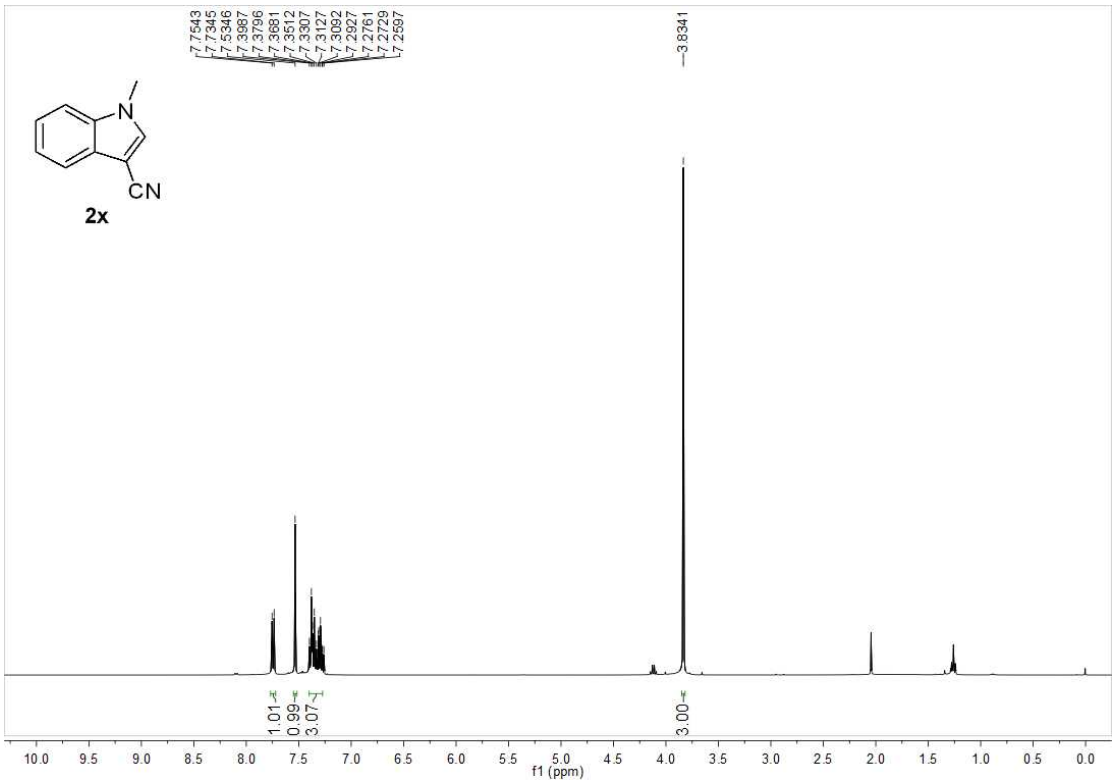
125.29
117.27
105.43
77.32
77.00
76.68
CN
2w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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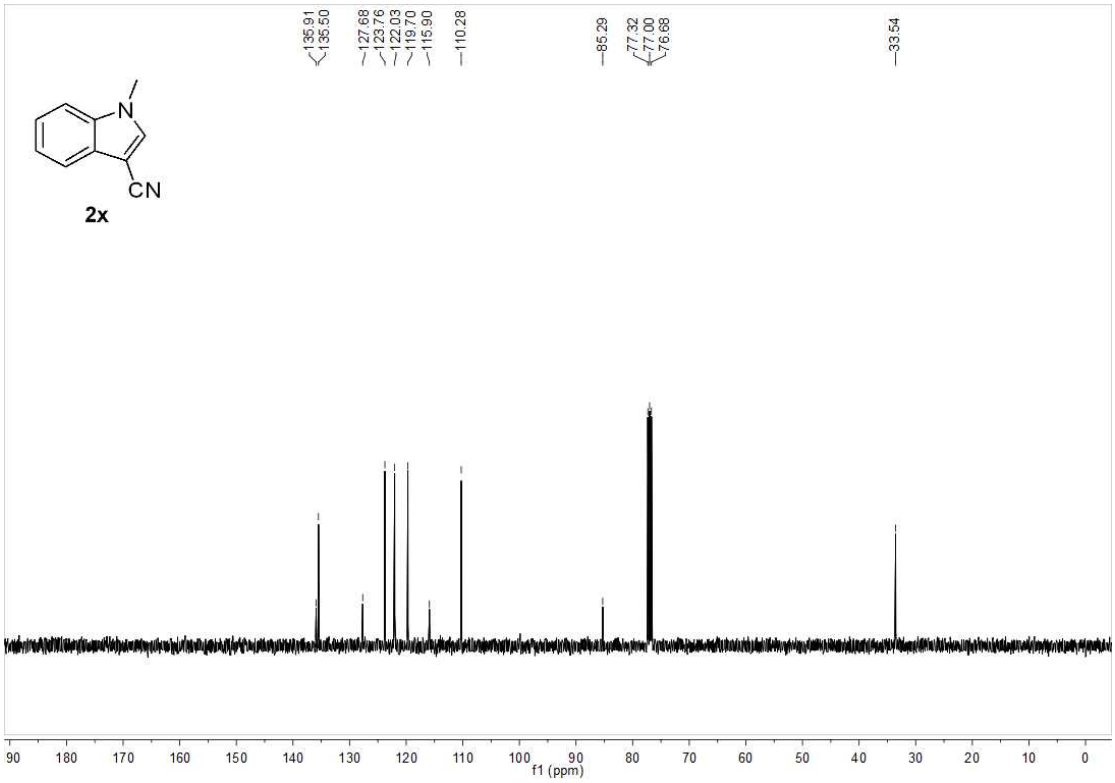
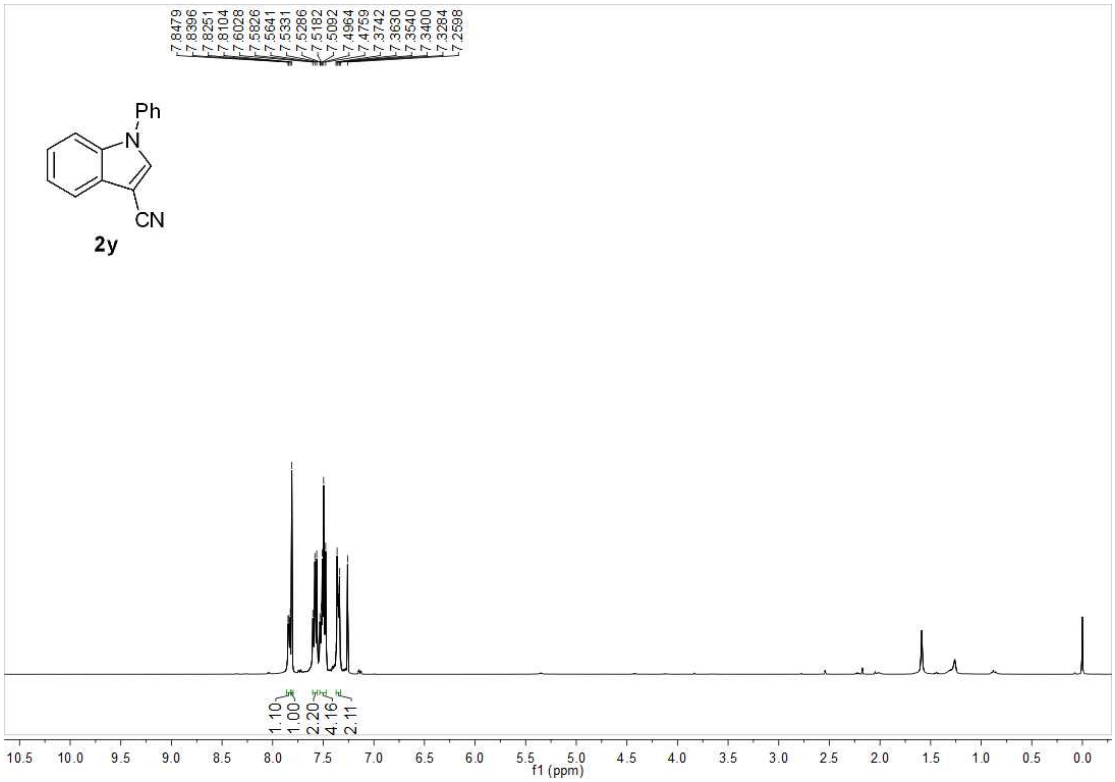
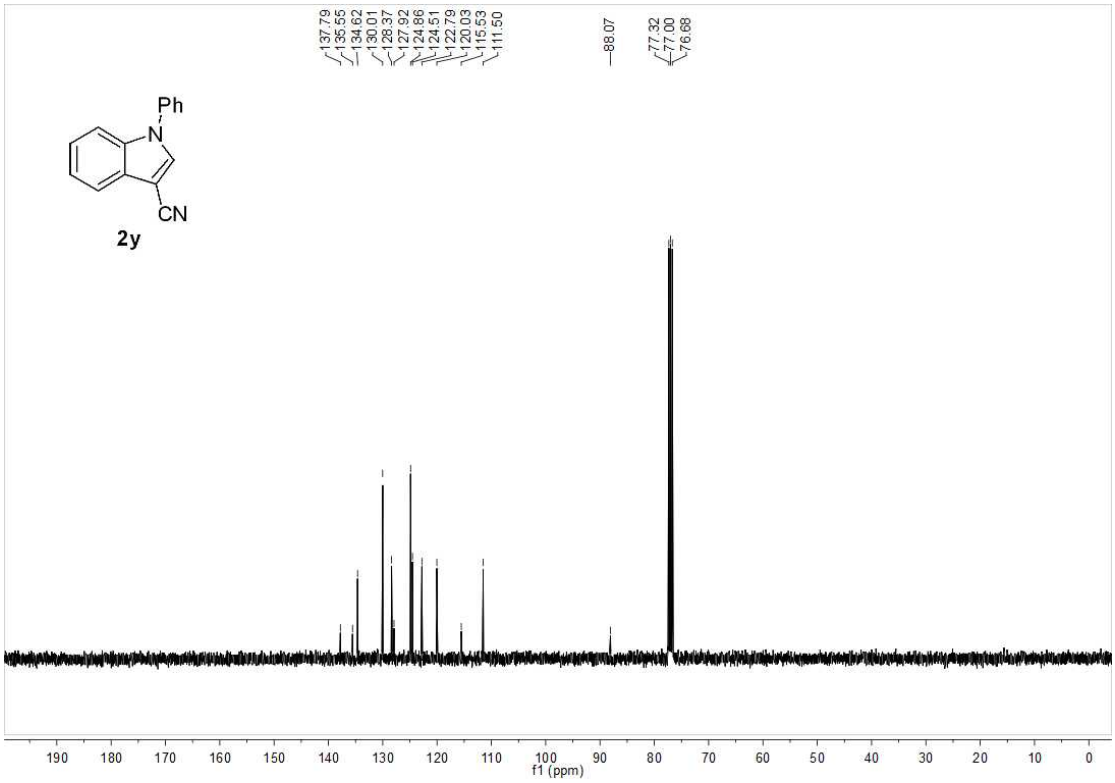
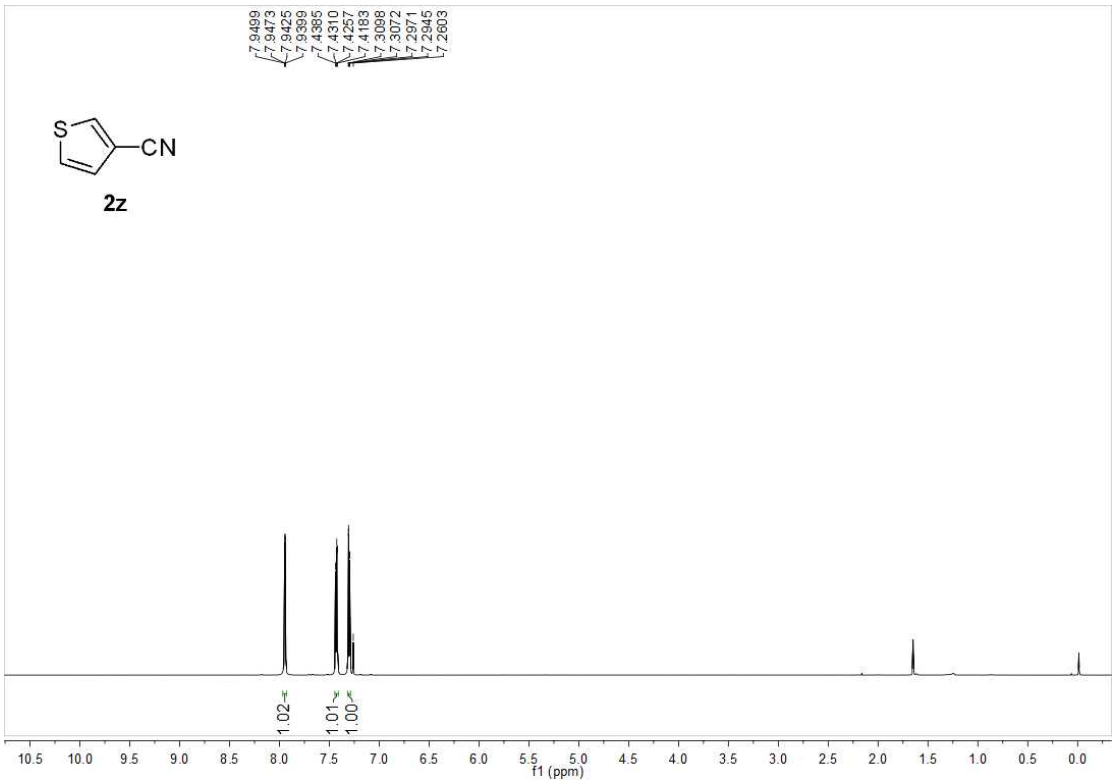
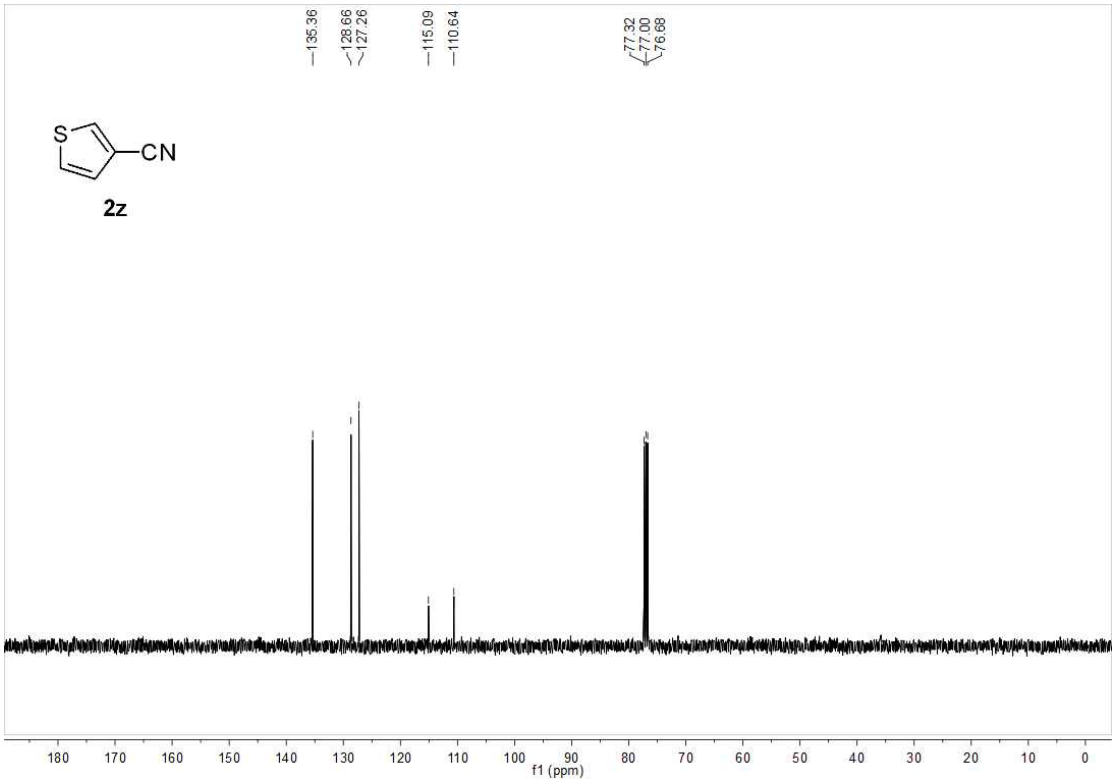
7.3681
7.3512
7.3307
7.3127
7.3092
7.2927
7.2761
7.2729
7.2597
3.8341
N
CN
2x
1.01
0.99
3.07
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

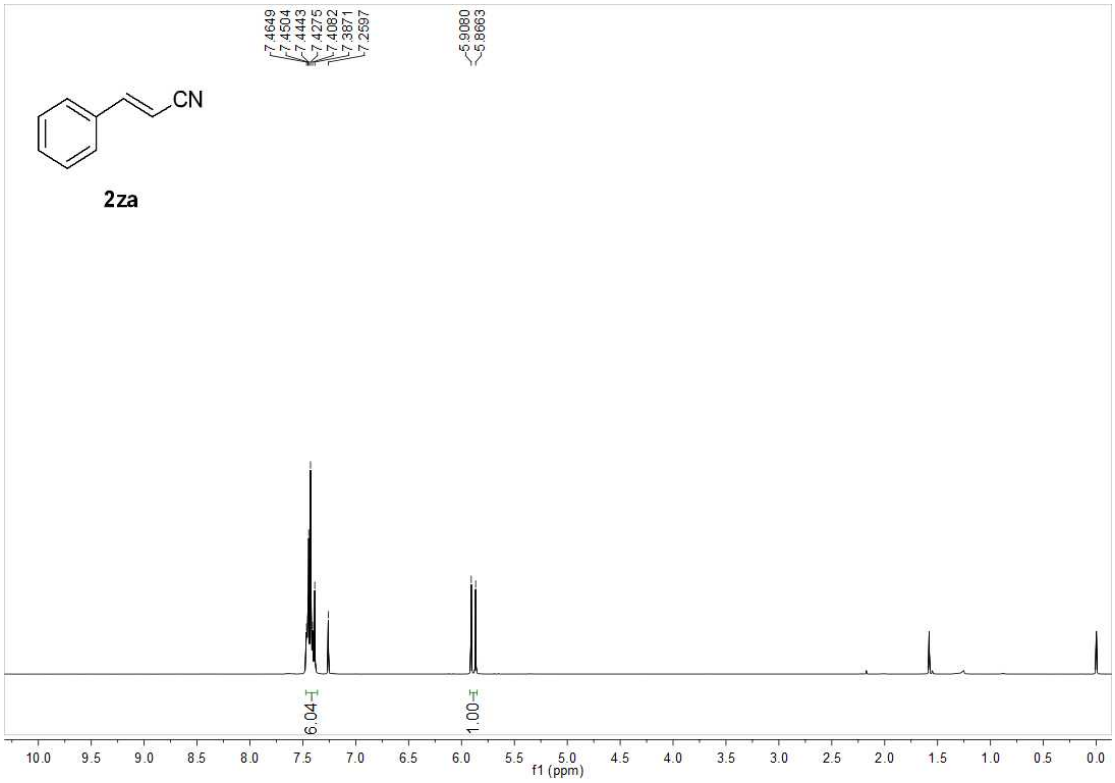

135.91
135.50
127.68
123.76
122.03
119.70
115.90
110.28
85.29
77.32
77.00
76.68
33.54
N
CN
2x
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

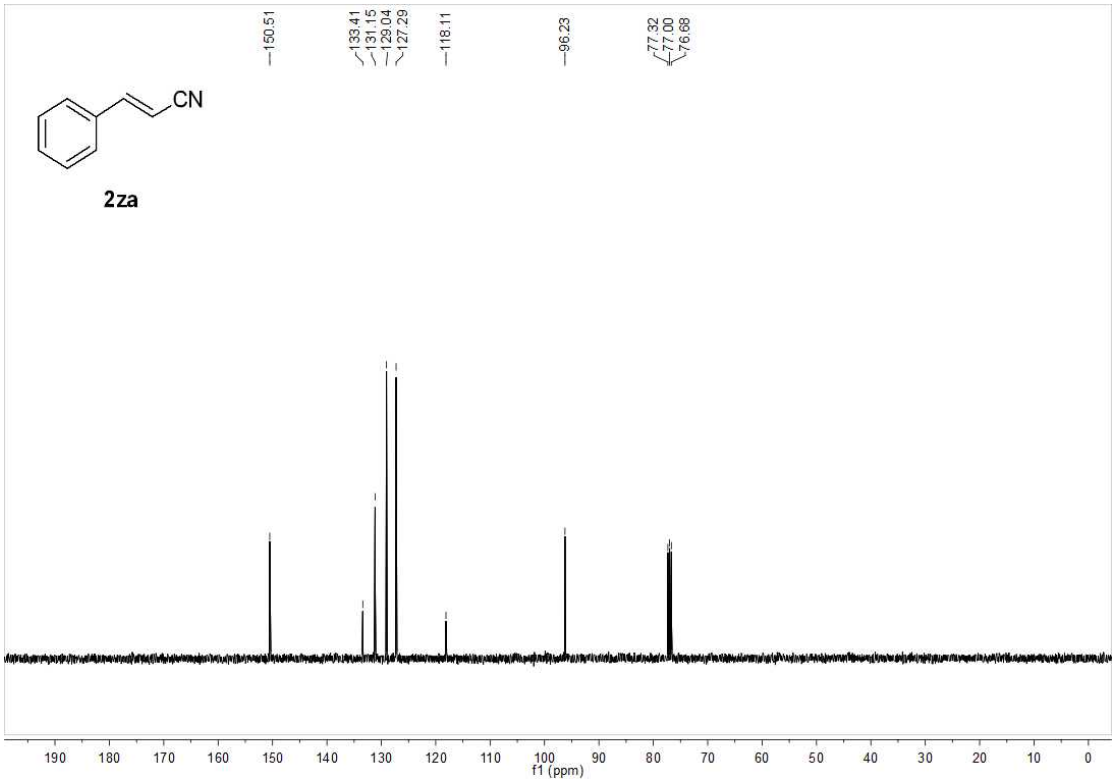

7.8479
7.8396
7.8251
7.8104
7.6028
7.5826
7.5641
7.5331
7.5286
7.5182
7.5092
7.4964
7.4759
7.3742
7.3630
7.3540
7.3400
7.3284
7.2598
Ph
N
CN
2y
1.10
1.00
2.20
4.16
2.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.79
135.55
134.62
130.01
128.37
127.92
124.86
124.51
122.79
120.03
115.53
111.50
88.07
77.32
77.00
76.68
Ph
N
CN
2y
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.9499
7.9473
7.9425
7.9399
7.4385
7.4310
7.4257
7.4183
7.3098
7.3072
7.2971
7.2945
7.2603
S
CN
2z
1.02
1.01
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


135.36
128.66
127.26
115.09
110.64
77.32
77.00
76.68
S
CN
2z
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.4649
7.4504
7.4443
7.4275
7.4082
7.3871
7.2597
5.9080
5.8863
CN
2za
6.04
1.00
f1 (ppm)


150.51
133.41
131.15
129.04
127.29
118.11
96.23
77.32
77.00
76.68
CN
2za
f1 (ppm)