Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Electromagnetic Mill Promoted Mechanochemical Palladium-catalyzed Solid State Cyanidation of Aryl Bromides Using Non-toxic $K_4[Fe(CN)_6]$

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Table of contents

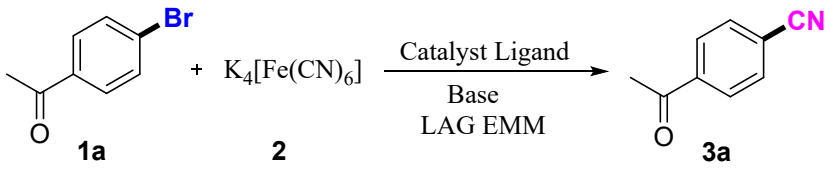
1. General Information

The starting materials were obtained from commercial suppliers and used as received. The ferromagnetic rod used is SUS304 stainless steel, which is purchased from Donghuan Feiada Metal Co., Ltd. and then processed by ourselves. Solvents were purchased from commercial suppliers. Purifications of reactions products were carried out by flash chromatography using Merck silica gel (40-63 μm). All mechanochemical reactions were carried out using grinding vesseis in a Megnetic grinding machine. The reaction bottles used were commercially available 10 ml flat bottom flask. The grinding medium is customized ferromagnetic rods. 1H NMR (400 MHz), 13C NMR (100 MHz) were measured on a Brucker Avance 400 MHz spectrometer. Chemical shifts are reported in parts per million (ppm, δ) downfield from residual solvents peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are designated as singlet (s), doublet (d), triplet (t), …. Splitting patterns that could not be interpreted or easily visualized are designated as multiplet (m). Electrospray mass spectra were obtained using an ESI/TOF Mariner Mass Spectrometer. Unless otherwise noted, all other commercially available reagents and solvents were used without further purification.

About the magnetic grinding used: The magnetic grinding machine (Figure S1) is self-developed and has not yet been put into commercial use, The magnetic field strength is about 0.2T.

Figure S1. Magnetic Grinding equipment

2. Optimization of the reaction conditions

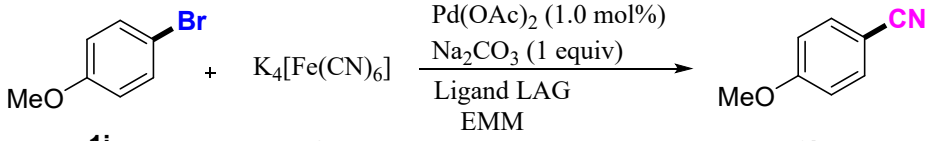


1a 2 3a

entry	catalyst	ligand	base	LAG	yield(%)[a]
1	$Pd(OAc)_2$	DPPF	Na_2CO_3	---	39
2	$Pd_2(dba)_3$	DPPF	Na_2CO_3	---	trace
3	$Pd(PPh_3)_4$	DPPF	Na_2CO_3	---	27
4	$PdCl_2(pcy_3)_2$	DPPF	Na_2CO_3	---	trace
5	$Pd(dba)_2$	DPPF	Na_2CO_3	---	trace
6	$PdCl_2$(dppf)	DPPF	Na_2CO_3	---	trace
7	$Pd(OAc)_2$	DPPE	Na_2CO_3	---	trace
8	$Pd(OAc)_2$	Xantphos	Na_2CO_3	---	50
9	$Pd(OAc)_2$	DPCP	Na_2CO_3	---	---
10	$Pd(OAc)_2$	Bis(2-diphenylphosphinophenyl)ether	Na_2CO_3	---	trace
11	$Pd(OAc)_2$	TXP-2,4	Na_2CO_3	---	trace
12	$Pd(OAc)_2$	DPPP	Na_2CO_3	---	trace
13	$Pd(OAc)_2$	PhDavePhos	Na_2CO_3	---	17
14	$Pd(OAc)_2$	DPPM	Na_2CO_3	---	trace
15	$Pd(OAc)_2$	DCyPFc	Na_2CO_3	---	12
16	$Pd(OAc)_2$	Xphos	Na_2CO_3	---	34
17	$Pd(OAc)_2$	Xantphos	Na_2CO_3	DMF	37
18	$Pd(OAc)_2$	Xantphos	Na_2CO_3	MeCN	45
19	$Pd(OAc)_2$	Xantphos	Na_2CO_3	1,4-dioxane	58
20	$Pd(OAc)_2$	Xantphos	Na_2CO_3	DMSO	34
21	$Pd(OAc)_2$	Xantphos	Na_2CO_3	Toluene	45
22	$Pd(OAc)_2$	Xantphos	Na_2CO_3	Methanol	45
23	$Pd(OAc)_2$	Xantphos	Na_2CO_3	Acetone	51
24	$Pd(OAc)_2$	Xantphos	Na_2CO_3	NMP	20
25	$Pd(OAc)_2$	Xantphos	Cs_2CO_3	1,4-dioxane	trace
26	$Pd(OAc)_2$	Xantphos	Et_3N	1,4-dioxane	trace
27	$Pd(OAc)_2$	Xantphos	KOH	1,4-dioxane	---
28	$Pd(OAc)_2$	Xantphos	CsF	1,4-dioxane	trace
29[b]	$Pd(OAc)_2$	Xantphos	Na_2CO_3	1,4-dioxane	45
30[c]	$Pd(OAc)_2$	Xantphos	Na_2CO_3	1,4-dioxane	68
31[d]	$Pd(OAc)_2$	Xantphos	Na_2CO_3	1,4-dioxane	54
32[e]	**$Pd(OAc)_2$**	**Xantphos**	**Na_2CO_3**	**1,4-dioxane**	**84**
33[f]	$Pd(OAc)_2$	Xantphos	Na_2CO_3	1,4-dioxane	35

Reaction conditions: 1a (1 mmol), 2 (0.3 mmol), catalyst (0.015 mmol), ligand (0.0225 mmol), base (1 mmol), LAG (0.2 mL), in a flat bottom flask (10 mL) with ferromagnetic rods (0.3 mm×15 mm,4 g), EMM, 50 Hz, 3 h. TXP-2,4 = Tris(2,4-dimethylphenyl)phosphine, DCyPFc = 1,1'-Bis(dicyclohexylphosphino)-ferrocene.

DPCP=cyclohexyldiphenylphosphine
[a] Isolated yields. [b] ferromagnetic rods (0.5 mm×10 mm). [c] ferromagnetic rods (0.3 mm×15 mm). [d] ferromagnetic rods (1.0 mm×5 mm). [e] $Pd(OAc)_2$ (1.0 mol%). [f] $Pd(OAc)_2$ (0.5 mol%).



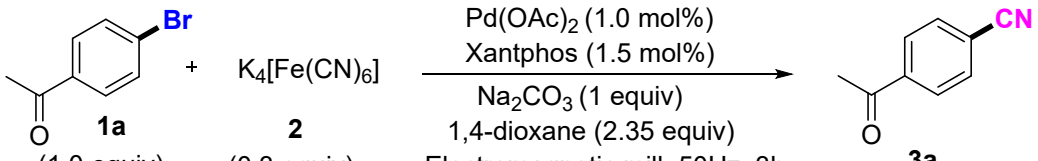
1j **2** **3j**

entry	catalyst	ligand	base	LAG	yield(%)[a]
1	$Pd(OAc)_2$	Xantphos	Na_2CO_3	1,4-dioxane	---
2	$Pd(OAc)_2$	DPPF	Na_2CO_3	1,4-dioxane	45
3	$Pd(OAc)_2$	DPPM	Na_2CO_3	1,4-dioxane	45
4	$Pd(OAc)_2$	DTBPF	Na_2CO_3	1,4-dioxane	61
5	$Pd(OAc)_2$	DCyPFc	Na_2CO_3	1,4-dioxane	---
6	$Pd(OAc)_2$	DTBPF	Na_2CO_3	DMA	59
7	$Pd(OAc)_2$	DTBPF	Na_2CO_3	DMF	---
8	**$Pd(OAc)_2$**	**DTBPF**	**Na_2CO_3**	**Methanol**	**87**
9	$Pd(OAc)_2$	DTBPF	Na_2CO_3	MeCN	68
10	$Pd(OAc)_2$	DTBPF	Na_2CO_3	Acetone	---
11	$Pd(OAc)_2$	DTBPF	Na_2CO_3	Toluene	54
12	$Pd(OAc)_2$	DTBPF	Na_2CO_3	DMSO	---

Reaction conditions: 1j (1 mmol), 2 (0.3 mmol), $Pd(OAc)_2$ (0.01 mmol), ligand (0.015 mmol), Na_2CO_3 (1 mmol), LAG (0.2 mL), in a flat bottom flask (10 mL) with ferromagnetic rods (0.3 mm×15 mm, 4 g), EMM, 50 Hz, 3 h. [a] Isolated yields. DCyPFc=1,1'-Bis(dicyclohexylphosphino)ferrocene DTBPF=1,1'-bis(di-tert-butylphosphino)ferrocene.

3. General procedure for Palladium-catalyzed Cyanidation of Aryl Bromides

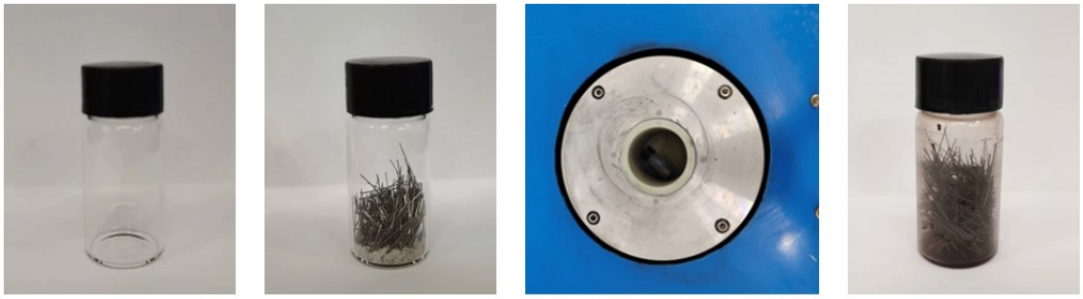
1) Procedure I: Pd-catalyzed cyanidation reaction of 4-bromoacetophenone under EMM.



1a (1.0 equiv) **2** (0.3 equiv) **3a**

Aryl halide **1a** (199.04 mg, 1 mmol 1.0 equiv), $K_4[Fe(CN)_6]$ **2** (110.5 mg , 0.3 mmol, 0.3 equiv), $Pd(OAc)_2$ (2.2 mg. 0.01 mmol) and Xantphos (8.68 mg, 0.015mmol), Na_2CO_3 (106.0 mg, 1mmol 1.0 equiv), 1,4-dioxane (0.2 mL, 2.35 equiv), ferromagnetic rods 4 g (a diameter of 0.3 mm and a length of 15 mm) were placed in a flat bottom

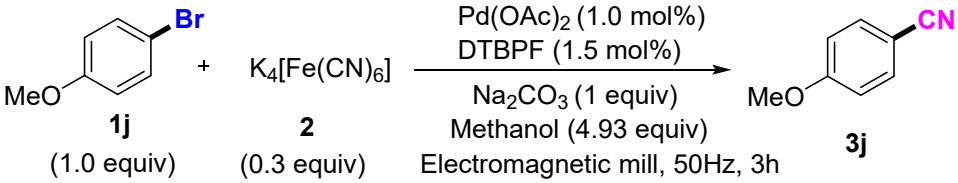
flask. Put it in magnetic grinder. After 3 h, the mixture was dissolved in EA. Then filter out the inorganic salt from the mixture with sand core funnel. The organic phase was spun dry, evaporated and recrystallization to give compound **3a** (121.9 mg, 84% yield). If the reaction is good and the product is solid, we directly perform recrystallization to obtain the purified product. If recrystallization is not possible, flash chromatography is used to obtain the purified product.



1. Reaction bottle | 2. Chemicals and ferromagnetic rods were added | 3. Bottle was placed in reaction unit | 4. Reaction end state in reaction flask

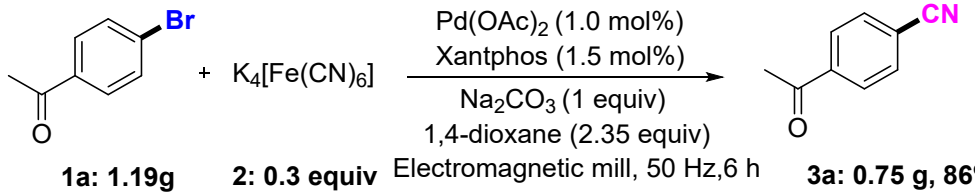
Figure S2. Set-up procedure for the cyanidation reaction of 4-bromoacetophenone.

2) Procedure II: Pd-catalyzed cyanidation reaction of 4-bromoanisole under EMM.



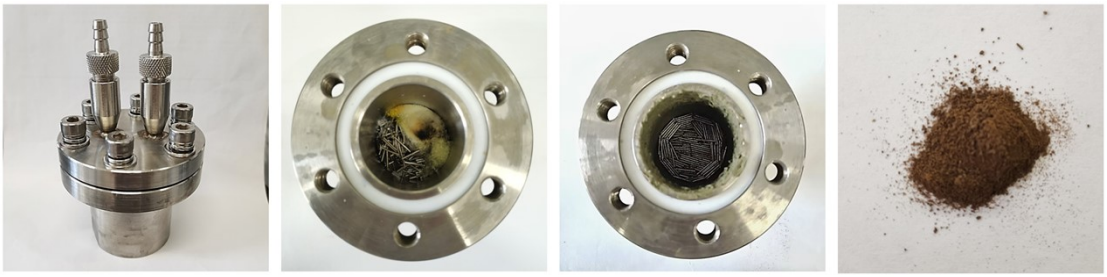
Aryl halide **1j** (93.52 mg, 0.5 mmol 1.0 equiv), $K_4[Fe(CN)_6]$ **2** (55.25 mg , 0.15 mmol, 0.3 equiv), $Pd(OAc)_2$ (1.1 mg. 0.005mmol) and DTBPF (1,1'-bis(di-tert-butylphosphino)ferrocene) (3.56mg, 0.0075mmol), Na_2CO_3 (53.0mg, 0.5 mmol 1.0 equiv), Methanol (0.1 mL, 4.93 equiv), ferromagnetic rods 4 g (a diameter of 0.3 mm and a length of 15 mm) were placed in a flat bottom flask. Put it in magnetic grinder. After 3 h, the mixture was dissolved in EA. Then filter out the inorganic salt from the mixture with sand core funnel. The organic phase was spun dry, evaporated and recrystallization to give compound **3j** (57.9 mg, 87% yield). If the reaction is good and the product is solid, we directly perform recrystallization to obtain the purified product. If recrystallization is not possible, flash chromatography is used to obtain the purified product.

3) Procedure III: Cyanidation reaction of 4-bromoacetophenone at gram-scale reaction



1a: 1.19g **2: 0.3 equiv** **3a: 0.75 g, 86%**

Aryl halide **1a** (1.19 g, 6.0 mmol 1.0 equiv), $K_4[Fe(CN)_6]$ **2** (0.66 g , 1.8 mmol, 0.3 equiv), $Pd(OAc)_2$ (0.0135 g, 0.06mmol) and Xantphos (0.054 g, 0.09mmol), Na_2CO_3 (0.636 g, 6.0 mmol 1.0 equiv), 1,4-dioxane (1.2 mL, 2.35 equiv), ferromagnetic rods 20 g (a diameter of 1.0 mm and a length of 10 mm) were placed in a stainless-steel milling jar. Put it in magnetic grinder. After 6 h, the mixture was dissolved in EA. Then filter out the inorganic salt from the mixture with sand core funnel. The organic phase was spun dry, evaporated and recrystallization to give compound **3a** (0.75g, 86% yield).



a. Reactor **b. Before** **c. Finished** **d. Crude product after separation**

Figure S3. Crude product after separating the ferromagnetic rods.

4. Ferromagnetic rods of different specifications

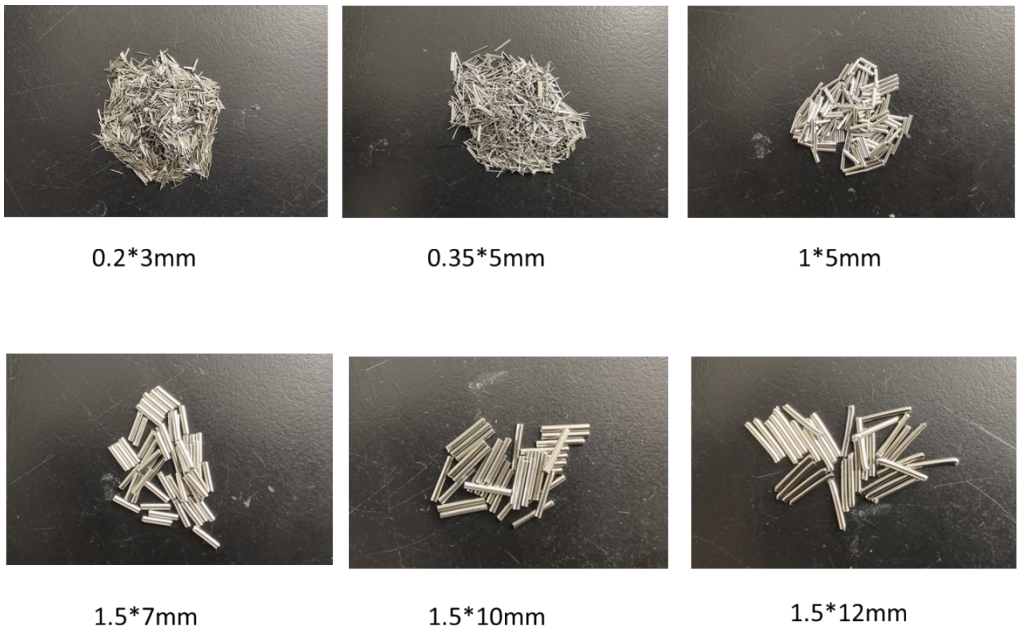


Figure S4. Ferromagnetic rods of different sizes used in experiments

5. SEM-EDS data analysis of ferromagnetic rod (0.35*0.5mm)

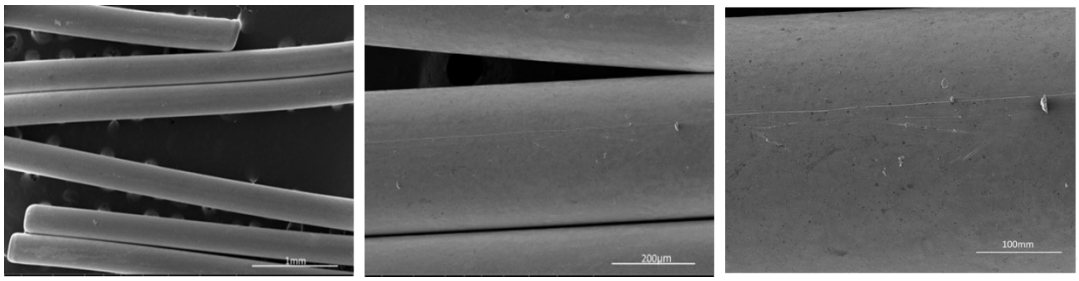
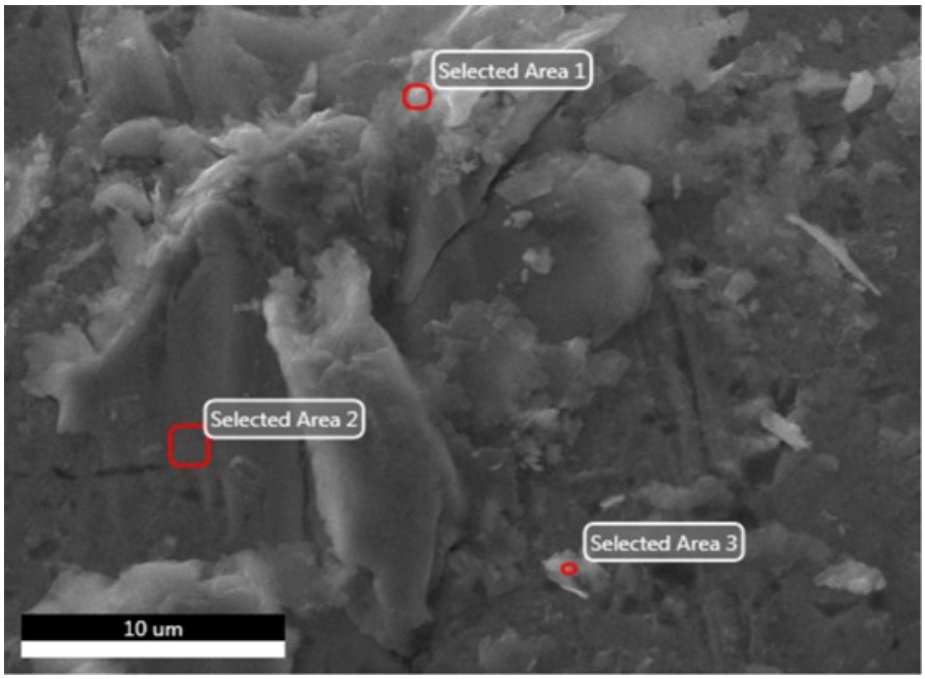
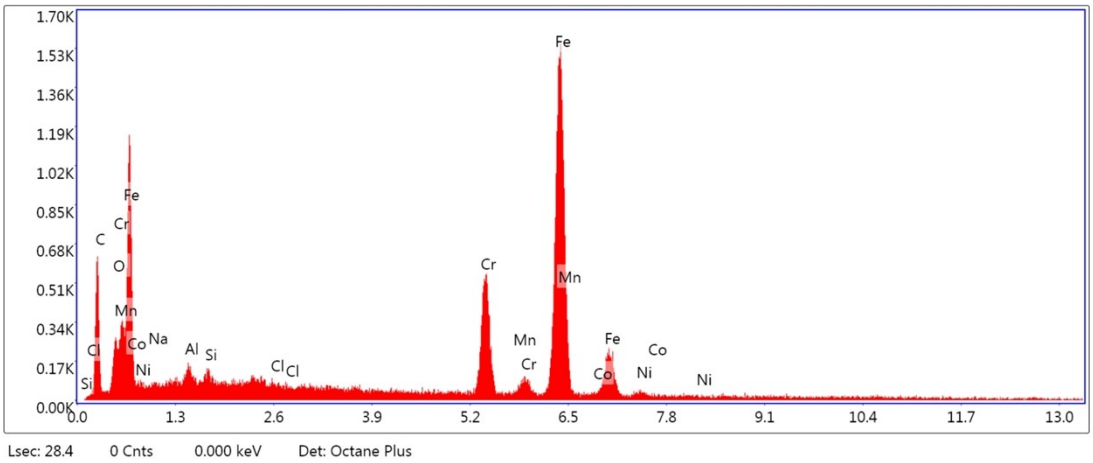


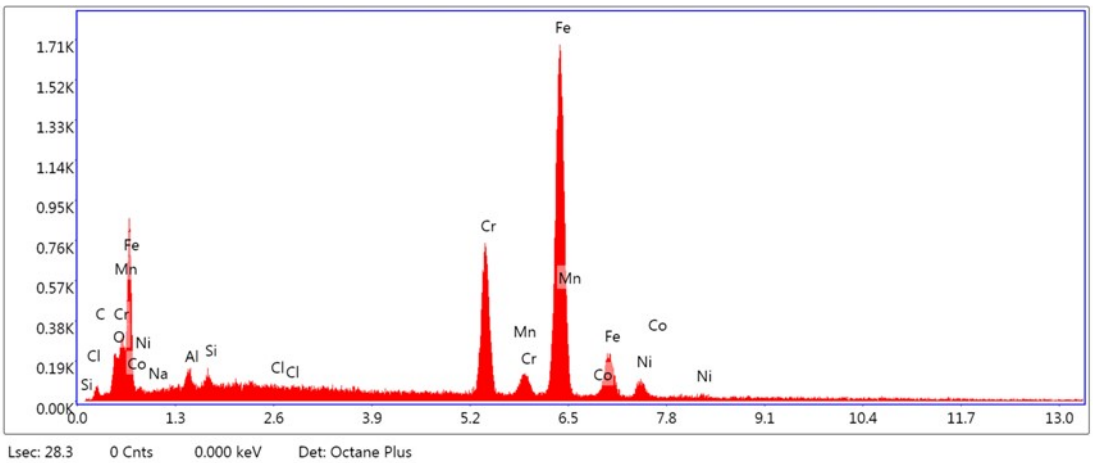
Figure S5. Morphology of ferromagnetic rod under scanning electron microscope



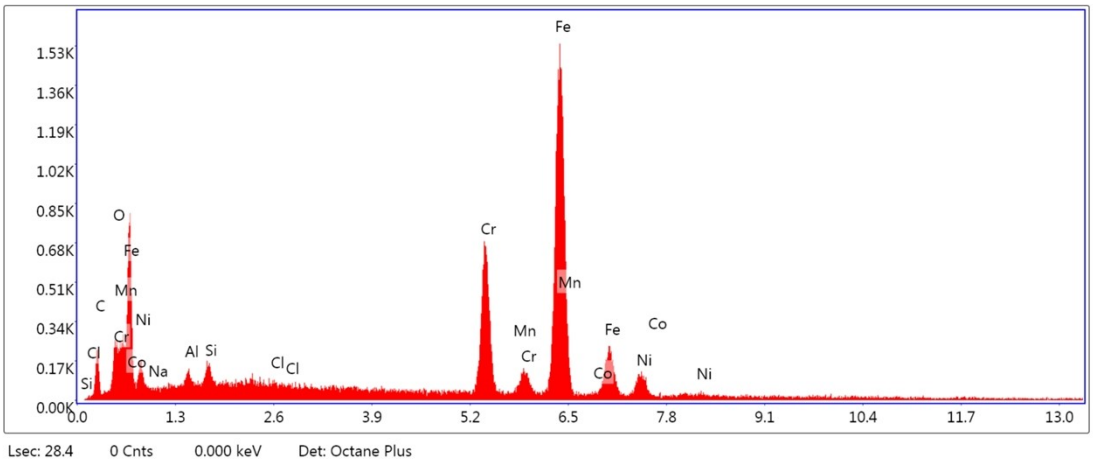
Selected Area 1



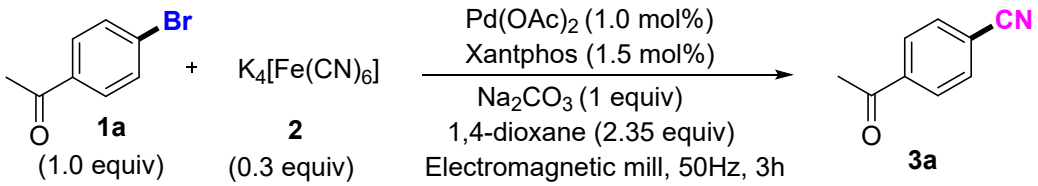
Selected Area 2



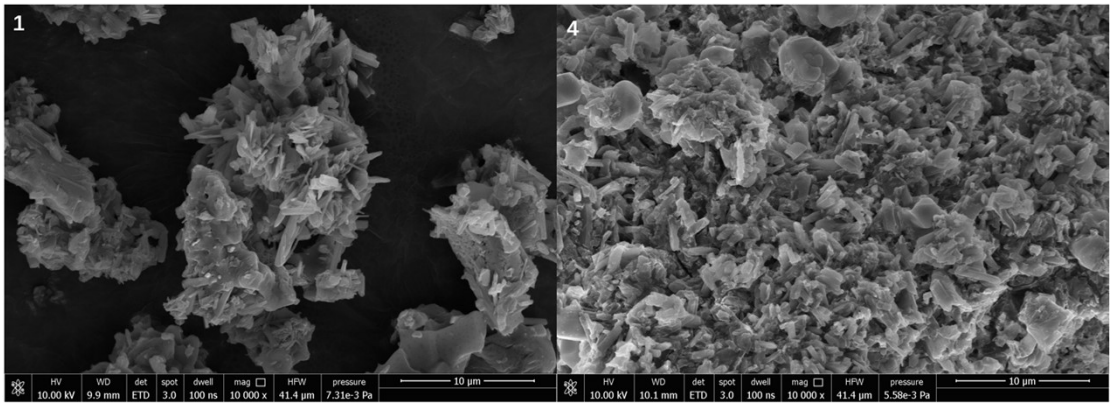
Selected Area 3



6. SEM analysis for crude product and Mapping images of palladium.



Aryl halide **1a** (199.04 mg, 1 mmol 1.0 equiv), $K_4[Fe(CN)_6]$ **2** (110.5 mg , 0.3 mmol, 0.3 equiv), $Pd(OAc)_2$ (2.2 mg. 0.01 mmol) and Xantphos (8.68 mg, 0.015mmol), Na_2CO_3 (106.0 mg, 1mmol 1.0 equiv), 1,4-dioxane (0.2 mL, 2.35 equiv), ferromagnetic rods 4 g (a diameter of 0.3 mm and a length of 15 mm) were placed in a flat bottom flask. Put it in magnetic grinder. Set up a set of control experiment (before the reaction) and one put in the grinder for 3 h (after the reaction). The ferromagnetic rods were separated, and the crude product was ground into powder for SEM analysis and the results as follows:



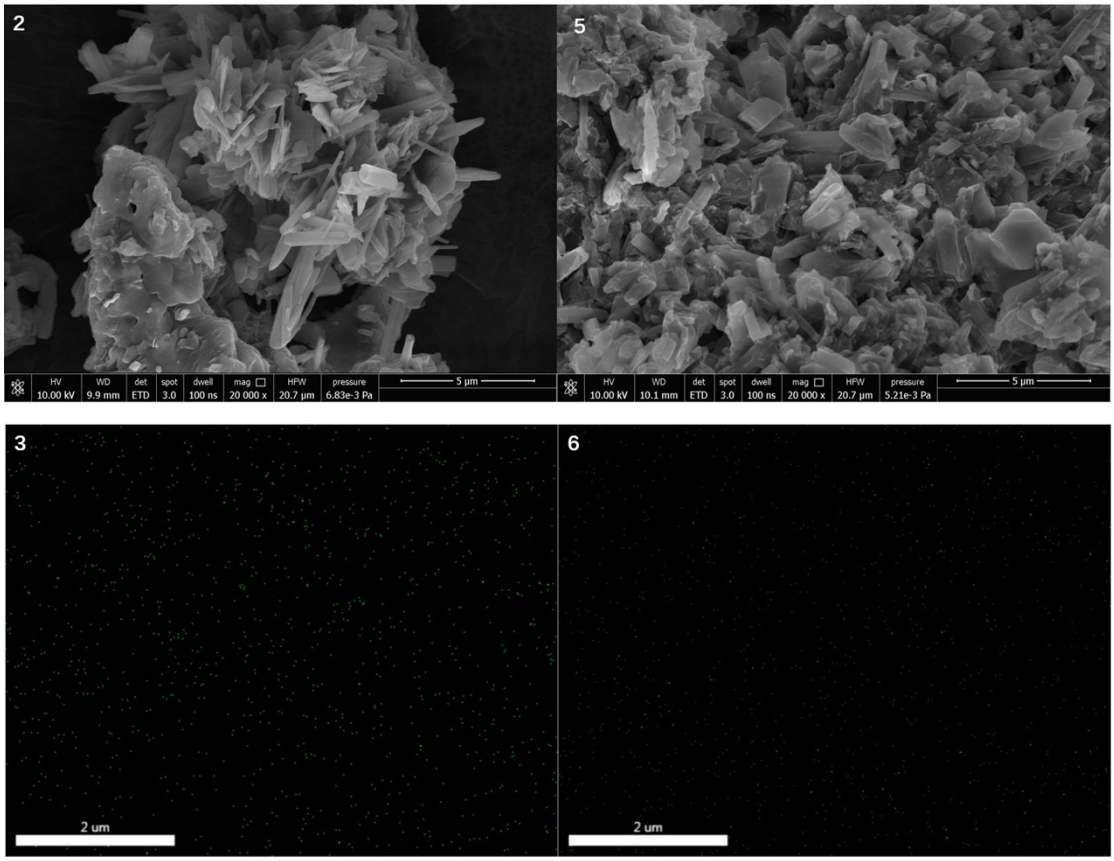
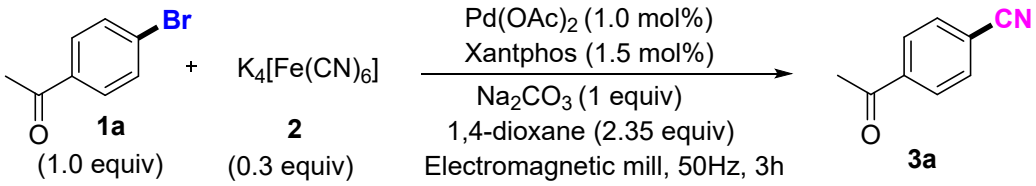


Figure S6. 1 and 2: SEM images of the crude reaction mixtures before the reaction. 3: Mapping images of palladium before the reaction. 4 and 5: SEM images of the crude mixture after three hours of reaction. 6: Mapping image of palladium after the reaction was completed.

7. Temperature for different reaction times

The temperature of the reaction flask was measured at different times using an electronic thermometer gun. The data obtained show that the temperature rises to about 80°C within one hour, and the highest temperature can reach 96°C during the reaction.



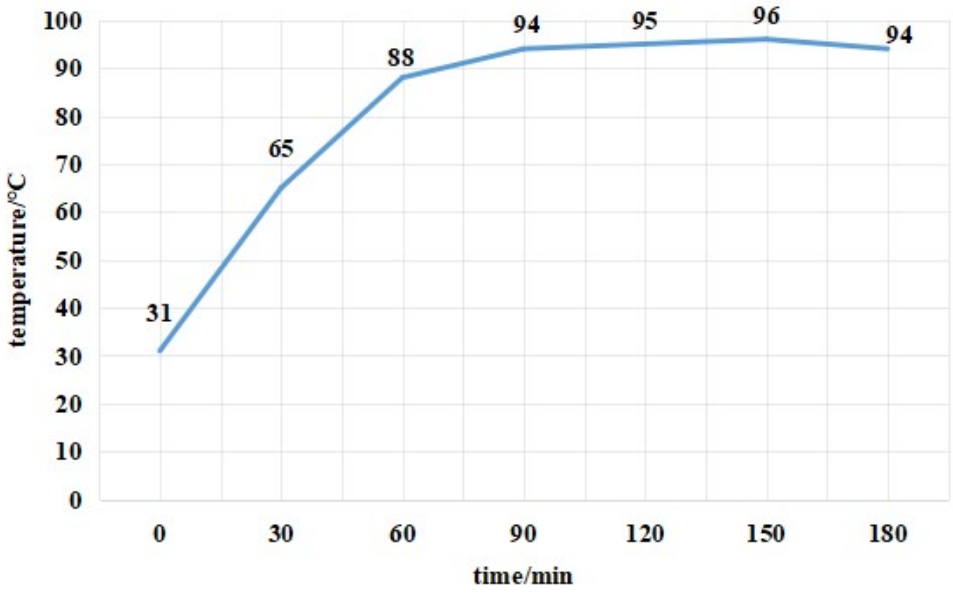
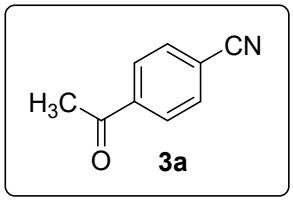


Figure S7. Temperature curve with time. Reaction conditions: 1a (0.5 mmol), 2 (0.15 mmol), $Pd(OAc)_2$ (0.005 mmol), Xantphos (0.0075 mmol), Na_2CO_3 (1 mmol), 1,4-dioxane (0.1 mL), in a flat bottom flask (10 mL) with ferromagnetic rods (0.3 mm×15 mm,4 g), EMM, 50 Hz, 3 h.

8. Characterization of Obtained Products.



4-acetylbenzonitrile

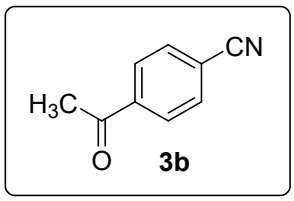
^{1}H and ^{13}C NMR were in agreement with the literature[1].

C_9H_7NO

MW: 145.16 g·mol^{-1} **Light yellow Solid Isolated amounts**: 121.9 mg **Yield**: 84%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.96 (d, J = 7.6 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 2.56 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 196.35, 139.55, 132.19, 128.40, 117.65, 115.92, 26.49.



4-acetylbenzonitrile

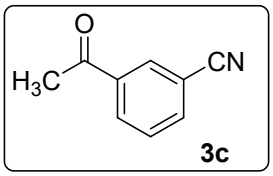
^{1}H and ^{13}C NMR were in agreement with the literature[1].

C_9H_7NO

MW: 145.16 g·mol^{-1} **Light yellow Solid Isolated amounts**: 72.58 mg **Yield**: 50%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.96 (d, J = 7.6 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 2.56 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 196.35, 139.55, 132.19, 128.40, 117.65, 115.92, 26.49.



3-acetylbenzonitrile

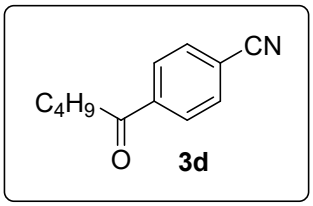
^{1}H and ^{13}C NMR were in agreement with the literature[1].

C_9H_7NO

MW: 145.16 g·mol^{-1} **White Solid** **Isolated amounts**: 117.58 mg **Yield**: 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.25 (s, 1H), 8.19 (d, J = 7.6 Hz, 1H), 7.86 (d, J = 7.2 Hz, 1H), 7.63 (t, J = 7.8 Hz, 1H), 2.65 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$, δ ppm): 195.79, 137.64, 135.94, 132.16, 131.95, 129.63, 117.85, 113.08, 26.53.



4-pentanoylbenzonitrile

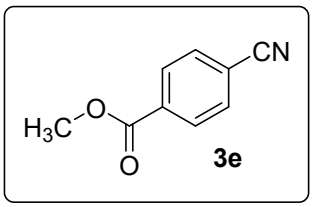
^{1}H and ^{13}C NMR were in agreement with the literature[2]

$C_{12}H_{13}NO$

MW: 187.24 g·mol^{-1} **White Solid** **Isolated amounts**: 159.15 mg **Yield**: 85%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.06 (d, J = 7.6 Hz, 2H), 7.78 (d, J = 7.6 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 1.77-1.69 (m, 2H), 1.47-1.37 (m, 2H), 0.96 (t, J= 7.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 198.91, 139.81, 132.35, 128.31, 117.86, 115.97, 38.46, 25.93, 22.20, 13.77.



methyl 4-cyanobenzoate

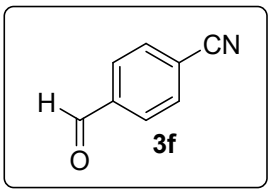
^{1}H and ^{13}C NMR were in agreement with the literature[3]

$C_9H_7NO_2$

MW: 161.16g·mol^{-1} **White Solid** **Isolated amounts**:128.93 mg **Yield**: 80%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.05 (d, J = 8.0 Hz, 2H), 7.67 (d, J = 7.6 Hz, 2H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.24, 133.73, 132.07, 129.92, 117.81, 116.19, 52.58.



3f

4-formylbenzonitrile

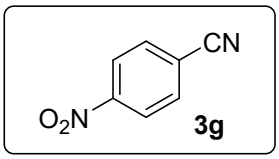
^{1}H and ^{13}C NMR were in agreement with the literature[3]

C_8H_5NO

MW: 131.13 g·mol^{-1} **White Solid Isolated amounts**: 89.17 mg **Yield**: 68%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 10.03 (s, 1H), 7.93 (d, J = 7.2 Hz, 2H), 7.78 (d, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 190.62, 138.45, 132.66, 129.65, 117.53, 117.19.



3g

4-nitrobenzonitrile

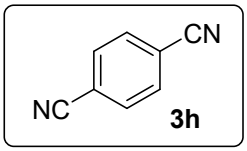
^{1}H and ^{13}C NMR were in agreement with the literature[4].

$C_7H_4N_2O_2$

MW: 148.12 g·mol^{-1} **White Solid Isolated amounts**: 108.13 mg **Yield**: 73%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.38 (d, J = 8.4 Hz, 2H), 7.92 (d, J = 8.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.95, 133.44, 124.24, 118.26, 116.76.



3h

terephthalonitrile

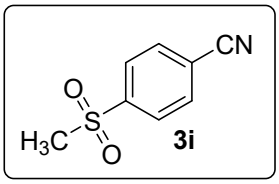
^{1}H and ^{13}C NMR were in agreement with the literature[3]

$C_8H_4N_2$

MW: 128.13 g·mol^{-1} **White Solid Isolated amounts**: 92.25 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.74 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 132.75, 116.97, 116.64.



3i

4-(methylsulfonyl)benzonitrile

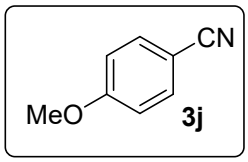
^{1}H and ^{13}C NMR were in agreement with the literature[5]

$C_8H_7N_2OS$

MW: 181.21 g·mol^{-1} **White Solid** **Isolated amounts**: 168.53 mg **Yield**: 93%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.02 (d, J = 7.6 Hz, 2H), 7.84 (d, J = 7.6 Hz, 2H), 3.04 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 144.26, 133.10, 128.06, 117.38, 116.98, 44.06.



4-methoxybenzonitrile

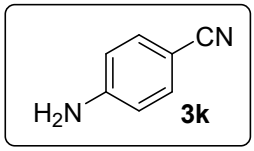
^{1}H and ^{13}C NMR were in agreement with the literature[3]

C_8H_7NO

MW: 133.15 g·mol^{-1} **White Solid** **Isolated amounts**: 115.84 mg **Yield**: 87%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.59 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.4 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 162.78, 133.93, 119.20, 114.69, 103.88, 55.50.



4-aminobenzonitrile

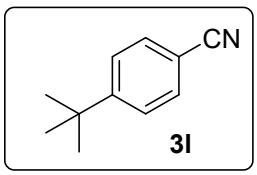
^{1}H and ^{13}C NMR were in agreement with the literature[6]

$C_7H_6N_2$

MW: 118.14 g·mol^{-1} **White Solid** **Isolated amounts**: 81.52 mg **Yield**: 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.41 (d, J = 8.0 Hz, 2H), 6.65 (d, J = 8.0 Hz, 2H), 4.22 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 150.47, 133.68, 120.17, 114.32, 99.77.



4-(tert-butyl)benzonitrile

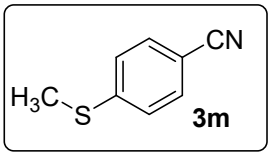
^{1}H and ^{13}C NMR were in agreement with the literature[7]

$C_{11}H_{13}N$

MW: 159.23g·mol^{-1} **White Solid** **Isolated amounts**: 149.68 mg **Yield**: 94%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.59 (d, J = 7.6 Hz, 2H), 7.48 (d, J = 7.2 Hz, 2H), 1.33 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 156.61, 131.95, 126.14, 119.17, 109.26, 35.26, 30.93.



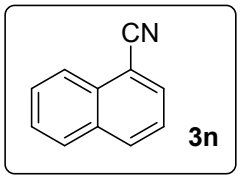
4-(methylthio)benzonitrile
^{1}H and ^{13}C NMR were in agreement with the literature[8]

C_8H_7NS

MW: 149.21 g·mol^{-1} **White Solid Isolated amounts**: 94.00 mg **Yield**: 63%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.45 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 2.43 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 146.02, 132.03, 125.33, 118.89, 107.45, 14.56.



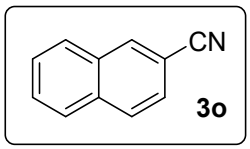
naphthonitrile
^{1}H and ^{13}C NMR were in agreement with the literature[1]

$C_{11}H_7N$

MW: 153.18 g·mol^{-1} **White Solid Isolated amounts**: 110.29 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.11 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.79 (t, J = 7.6 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.4 Hz, 1H), 7.40 (t, J = 7.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 133.18, 132.77, 132.51, 132.20, 128.55, 128.48, 127.43, 124.98, 124.81, 117.73, 110.00.



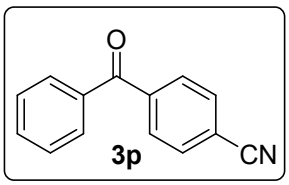
2-naphthonitrile
^{1}H and ^{13}C NMR were in agreement with the literature[3]

$C_{11}H_7N$

MW: 153.18 g·mol^{-1} **White Solid Isolated amounts**: 93.44 mg **Yield**: 61%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.10 (s, 1H), 7.78 (t, J = 8.0 Hz, 3H), 7.52 (dt, J = 17.2, 7.5 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 134.51, 134.03, 132.10, 129.08, 128.95, 128.30, 127.94, 127.55, 126.20, 119.17, 109.22.



4-benzoylbenzonitrile

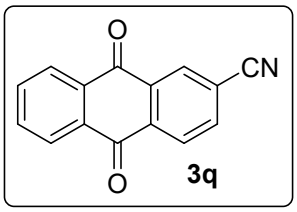
^{1}H and ^{13}C NMR were in agreement with the literature[9]

$C_{14}H_9NO$

MW: 207.23 g·mol^{-1} **White Solid** **Isolated amounts**: 186.51 mg **Yield**: 90%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.88 (d, J = 8.0 Hz, 2H), 7.80 (d, J = 9.2 Hz, 4H), 7.65 (t, J = 13.4 Hz, 1H), 7.52 (t, J = 7.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 195.01, 141.16, 136.25, 133.29, 132.13, 130.20, 130.02, 128.59, 117.98, 115.60.



9,10-dioxo-9,10-dihydroanthracene-2-carbonitrile

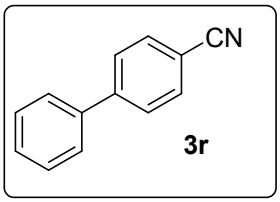
^{1}H and ^{13}C NMR were in agreement with the literature[10]

$C_{15}H_7NO_2$

MW: 233.23 g·mol^{-1} **White Solid** **Isolated amounts**: 205.24 mg **Yield**: 88%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.60 (s, 1H), 8.43 (d, J = 8.0 Hz, 1H), 8.33 (d, J = 2.8 Hz,2H), 8.06 (d, J = 8.0 Hz, 1H), 7.88 (t, J = 2.8 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 181.63, 181.15, 136.61, 135.57, 134.81, 133.76, 133.03, 132.91, 131.25, 128.00, 127.57, 117.68, 117.16.



[1,1'-biphenyl]-4-carbonitrile

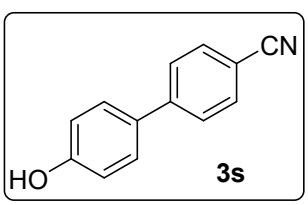
^{1}H and ^{13}C NMR were in agreement with the literature[3]

$C_{13}H_9N$

MW: 179.22 g·mol^{-1} **White Solid** **Isolated amounts**: 163.09 mg **Yield**: 91%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (q, J = 8.0 Hz, 4H), 7.57 (d, J = 7.2 Hz, 2H), 7.47 (t, J = 7.2 Hz, 2H), 7.41 (t, J = 7.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 145.46, 138.97, 132.44, 128.98, 128.54, 127.56, 127.07, 118.82, 110.72.



4'-hydroxy-[1,1'-biphenyl]-4-carbonitrile

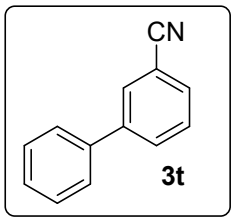
^{1}H and ^{13}C NMR were in agreement with the literature[11]

$C_{13}H_9NO$

MW: 195.22 g·mol^{-1} **White Solid Isolated amounts**: 144.46 mg **Yield**: 74%

^{1}H NMR (400 MHz, DMSO-d6, δ ppm): 9.86 (s, 1H), 7.81 (d, *J* =8.0 Hz, 2H), 7.75 (d, *J* =8.0 Hz, 2H), 7.58 (d, *J* =12.0 Hz, 2H), 6.90 (d, *J* =8.0 Hz, 2H).

^{13}C NMR (100 MHz, DMSO-d6, δ ppm): 158.42, 144.66, 132.74, 128.83, 128.37, 126.57, 119.15, 116.06, 108.78.



[1,1'-biphenyl]-3-carbonitrile

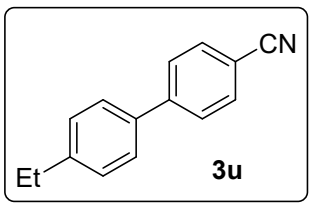
^{1}H and ^{13}C NMR were in agreement with the literature[12]

$C_{13}H_9N$

MW: 179.22 g·mol^{-1} **White Solid Isolated amounts**: 170.26 mg **Yield**: 95%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.83 (s, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.53 (t, J = 8.4 Hz, 3H), 7.47 (t, J = 7.2 Hz, 2H), 7.40 (t, J = 7.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.26, 138.70, 131.37, 130.57, 130.55, 129.50, 129.01, 128.28, 126.95, 118.76, 112.78.



4'-ethyl-[1,1'-biphenyl]-4-carbonitrile

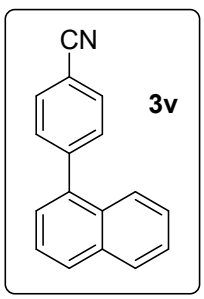
^{1}H and ^{13}C NMR were in agreement with the literature[13]

$C_{15}H_{13}N$

MW: 207.28 g·mol^{-1} **White Solid Isolated amounts**: 128.51 mg **Yield**: 62%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.61 (q, J = 7.6 Hz, 4H), 7.44 (d, J = 7.6 Hz, 2H), 7.24 (d, J = 7.2 Hz, 2H), 2.63 (q, J = 7.6 Hz, 2H), 1.21 (t, J = 7.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 145.57, 145.03, 136.44, 132.52, 128.61, 127.44, 127.11, 119.03, 110.46, 28.53, 15.49.



4-(naphthalen-1-yl)benzonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[14]

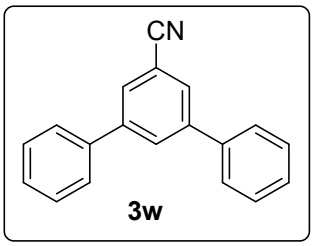
$C_{17}H_{11}N$

MW: 229.28 g·mol^{-1} **White Solid**

Isolated amounts: 96.30mg **Yield**: 42%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.89 (t, J = 7.7 Hz, 2H), 7.72 (dd, J = 16.9, 8.4 Hz, 3H), 7.54 – 7.47 (m, 4H), 7.43 (td, J = 7.6, 6.8, 1.2 Hz, 1H), 7.34 (d, J = 7.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 145.38, 137.96, 131.93, 130.71, 130.59, 128.61, 128.39, 126.88, 126.49, 126.02, 125.19, 124.99, 118.78, 110.90.



[1,1':3',1''-terphenyl]-5'-carbonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[15]

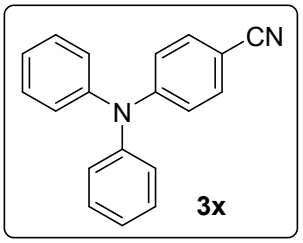
$C_{19}H_{13}N$

MW: 255.32g·mol^{-1} **White Solid**

Isolated amounts: 229.79 mg **Yield**: 90%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.98 (s, 1H), 7.82 (d, J = 4.0 Hz, 2H), 7.60 (d, J = 8.0 Hz, 4H), 7.49 (t, J = 8.0 Hz, 4H), 7.43 (t, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.94, 138.87, 130.32, 129.26, 129.12, 128.45, 127.13, 118.83, 113.34.



4-(diphenylamino)benzonitrile

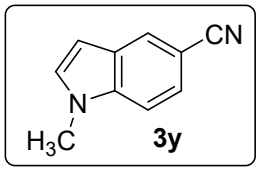
^{1}H and ^{13}C NMR were in agreement with the literature[16]

$C_{19}H_{14}N_2$

MW: 270.34 g·mol^{-1} **White Solid** **Isolated amounts**:135.17 mg **Yield**: 50%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.24 (d, J = 8.0 Hz, 2H), 7.18 (t, J = 8.0 Hz, 4H), 7.01 (t, J = 8.0 Hz, 6H), 6.81 (d, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 151.27, 145.64, 132.91, 129.57, 125.89, 124.93, 119.39, 102.16.



methyl-1H-indole-5-carbonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[17]

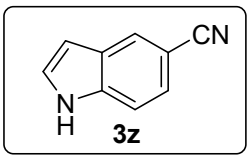
$C_{10}H_8N_2$

MW: 156.19 g·mol^{-1} **White Solid**

Isolated amounts: 87.47 mg **Yield**: 56%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.92 (s, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.33 (d, J = 8.4 Hz, 1H), 7.16 (s, 1H), 6.54 (s, 1H), 3.81 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 137.98, 131.07, 127.98, 126.27, 124.21, 120.81, 109.97, 102.06, 101.95, 32.94.



3z

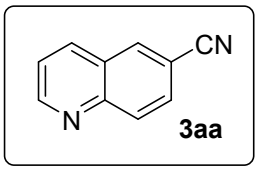
1H-indole-5-carbonitrile
^{1}H and ^{13}C NMR were in agreement with the literature[18]
$C_9H_6N_2$

MW: 142.16 g·mol^{-1} **White Solid**

Isolated amounts: 102.2 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.95 (s, 1H), 7.98 (s, 1H), 7.48 (d, J = 8.4 Hz, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.34 (s, 1H), 6.61 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 137.50, 127.54, 126.61, 126.25, 124.57, 121.00, 112.06, 103.10, 102.20.



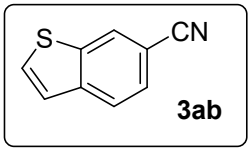
3aa

quinoline-6-carbonitrile
^{1}H and ^{13}C NMR were in agreement with the literature[3]
$C_{10}H_6N_2$

MW: 154.17 g·mol^{-1} **White Solid** **Isolated amounts**: 146.46 mg **Yield**: 95%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.96 (s, 1H), 8.13 (s, 2H), 8.09 (d, J = 8.8 Hz, 1H), 7.75 (d, J = 8.8 Hz, 1H), 7.46 (t, J = 3.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 153.08, 148.86, 136.21, 133.95, 130.82, 129.90, 127.32, 122.56, 118.32, 110.13.



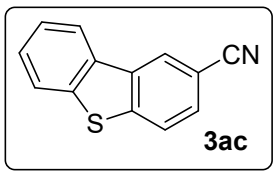
3ab

benzo[b]thiophene-6-carbonitrile
^{1}H and ^{13}C NMR were in agreement with the literature[19]
C_9H_5NS **Melting Point** :41.5 °C -42.0 °C

MW: 159.21 g·mol^{-1} **Transparent liquid** **Isolated amounts**: 105.08 mg **Yield**: 66%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm)： 7.98 (s, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 4.0 Hz, 1H), 7.40 (dd, J = 8.3, 1.4 Hz, 1H), 7.27 – 7.23 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.08, 139.19, 131.06, 126.87, 126.41, 123.99, 123.68, 119.06, 107.06.



dibenzo[b,d]thiophene-2-carbonitrile

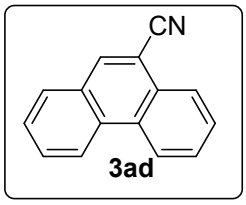
^{1}H and ^{13}C NMR were in agreement with the literature[20]

$C_{13}H_7NS$

MW: 209.27 g·mol^{-1} **White Solid** **Isolated amounts**:110.91 mg **Yield**: 53%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.28 (s, 1H), 8.06 (d, J = 4.0 Hz, 1H), 7.83 (t, J = 8.0 Hz, 2H), 7.62 – 7.57 (m, 1H), 7.53 – 7.45 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.94, 139.45, 135.58, 133.78, 128.67, 127.91, 125.36, 125.06, 123.41, 122.77, 121.75, 119.18, 107.74.



phenanthrene-9-carbonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[4]

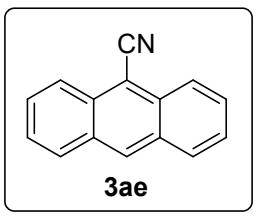
$C_{15}H_9N$

MW: 203.24 g·mol^{-1} **Yellow Solid**

Isolated amounts: 160.56 mg **Yield**: 79%

^{1}H NMR (400 MHz$CDCl_3$, δ ppm): 8.70 (t, J = 8.0 Hz, 2H), 8.35 – 8.21 (m, 2H), 7.93 (d, J = 8.0 Hz, 1H), 7.86 – 7.64 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 135.64, 131.74, 129.98, 129.81, 129.74, 129.48, 128.82, 128.19, 128.09, 127.61, 126.07, 123.06, 122.84, 117.92, 109.35.



anthracene-9-carbonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[12]

$C_{15}H_9N$

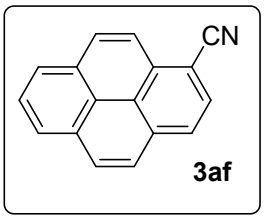
MW: 203.24 g·mol^{-1} **Green Solid**

Isolated amounts: 178.85 mg **Yield**: 88%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.62 (s, 1H), 8.38 (d, J = 8.4 Hz, 2H), 8.04 (d, J = 8.4 Hz, 2H), 7.69 (t, J = 7.6 Hz, 2H), 7.56 (t, J = 7.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 133.22, 132.69, 130.53, 128.90, 128.89, 126.30,

125.21, 117.23, 105.33.



pyrene-1-carbonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[21]

$C_{17}H_9N$

MW: 227.27 g·mol^{-1} **White Solid** **Isolated amounts**: 211.36 mg **Yield**: 93%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.00 (t, J = 8.6 Hz, 3H), 7.90 – 7.85 (m, 4H), 7.76 (d, J = 7.6 Hz, 1H), 7.70 (d, J = 8.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 133.67, 132.40, 130.40, 130.08, 129.99, 129.07, 126.74, 126.68, 126.64, 126.45, 123.97, 123.38, 123.33, 122.93, 118.64, 105.09.

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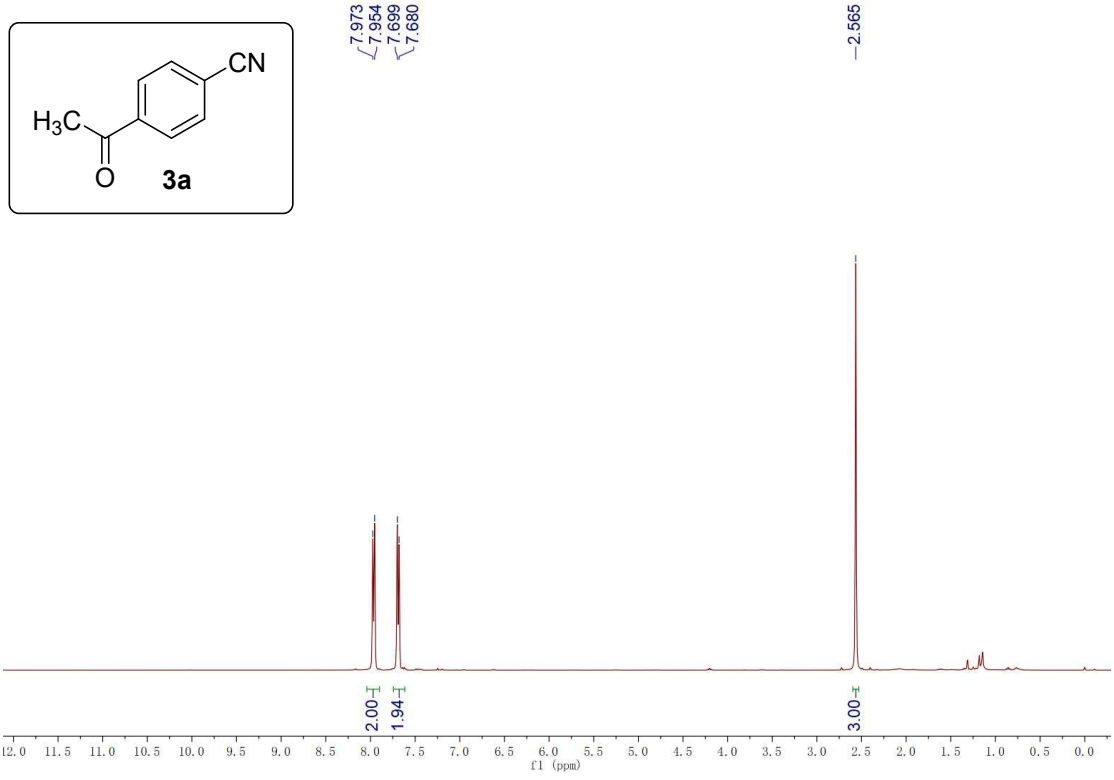
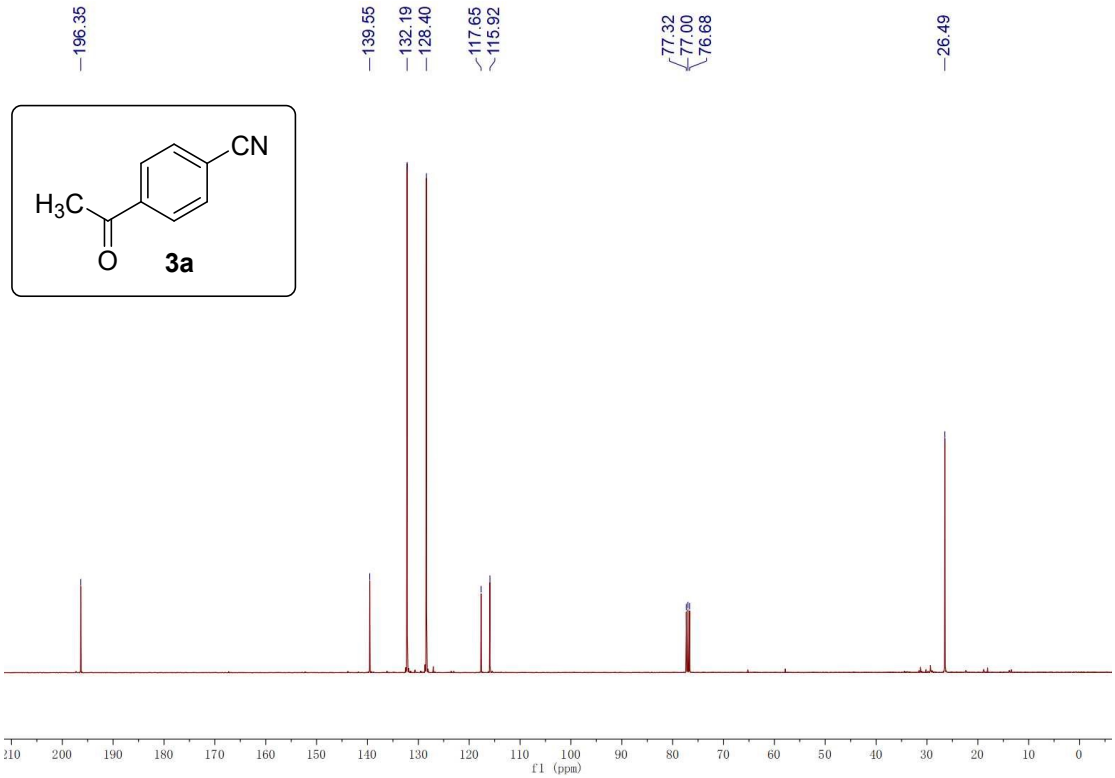
10. Copies of the ^{1}H NMR, ^{13}C NMR

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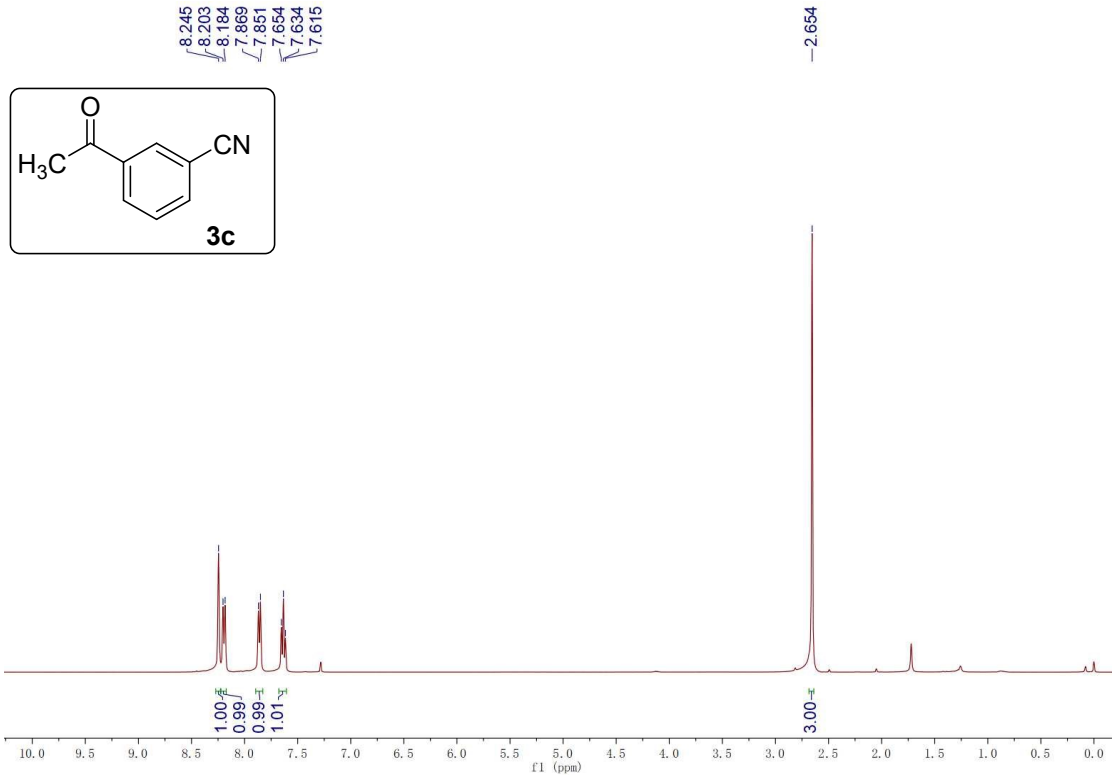
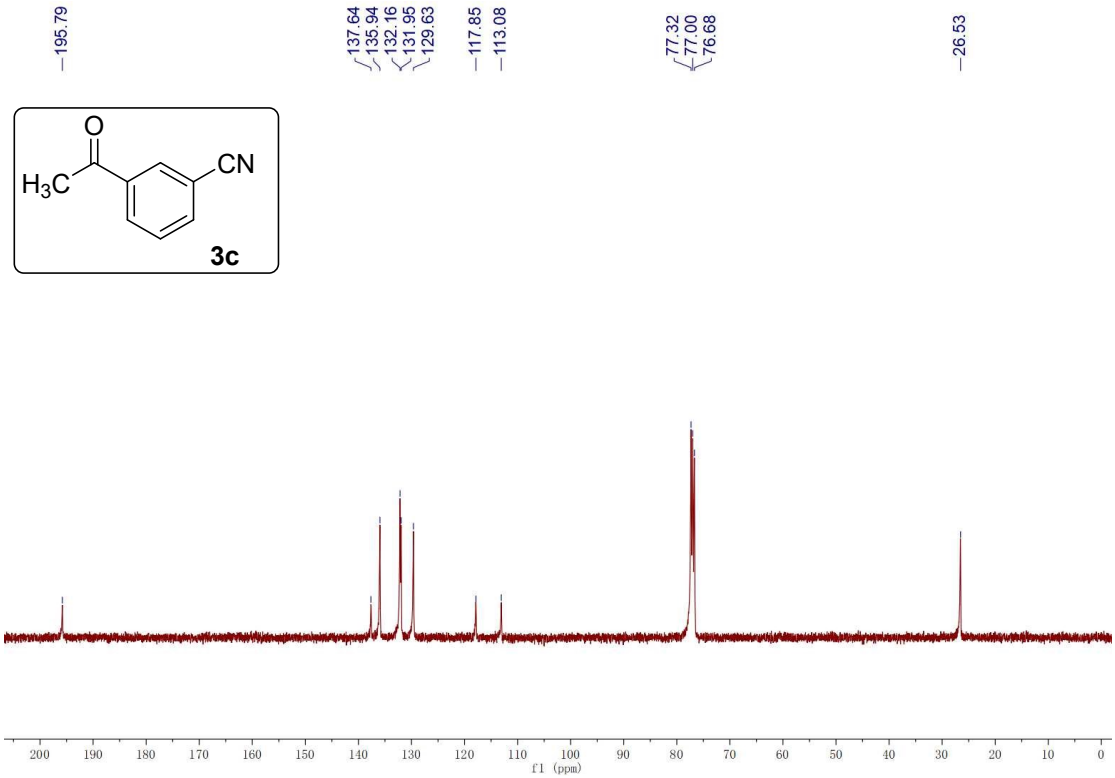
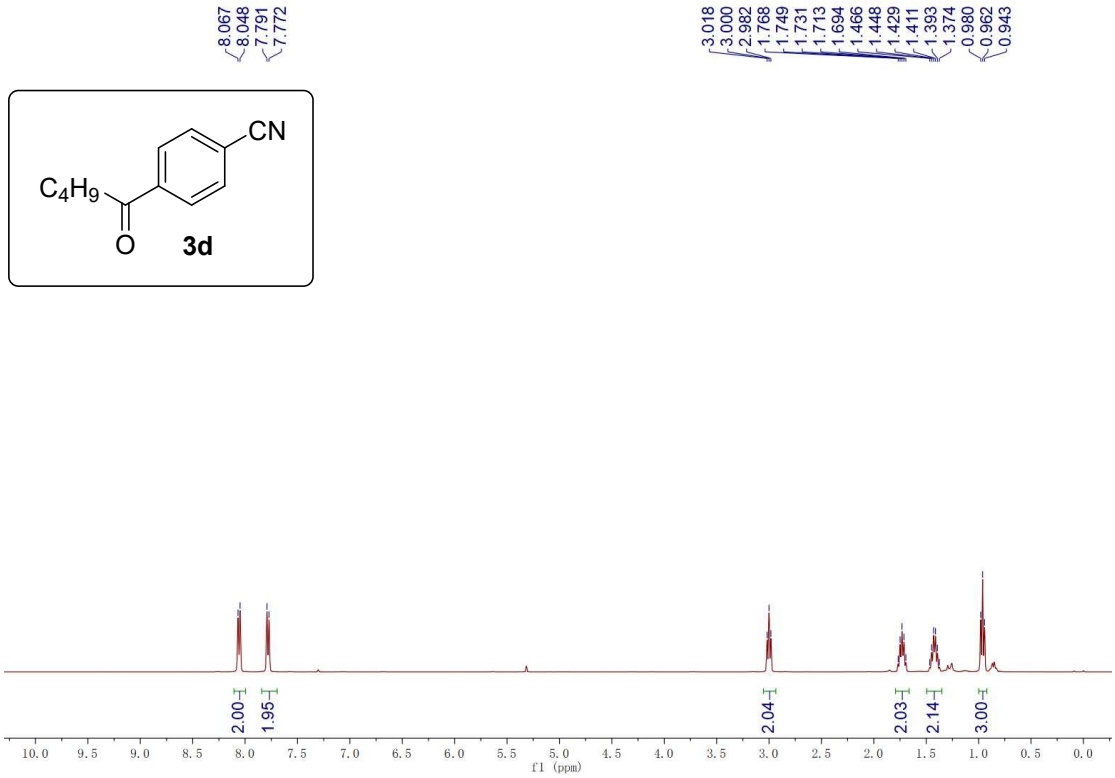
139.55
132.19
128.40
117.65
115.92
77.32
77.00
76.68
26.49
CN
H3C
O
3a
f1 (ppm)


8.245
8.203
8.184
7.869
7.851
7.654
7.634
7.615
2.654
O
H3C
CN
3c
1.00
0.99
0.99
1.01
3.00
f1 (ppm)


195.79
137.64
135.94
132.16
131.95
129.63
117.85
113.08
77.32
77.00
76.68
26.53
O
H3C
CN
3c
f1 (ppm)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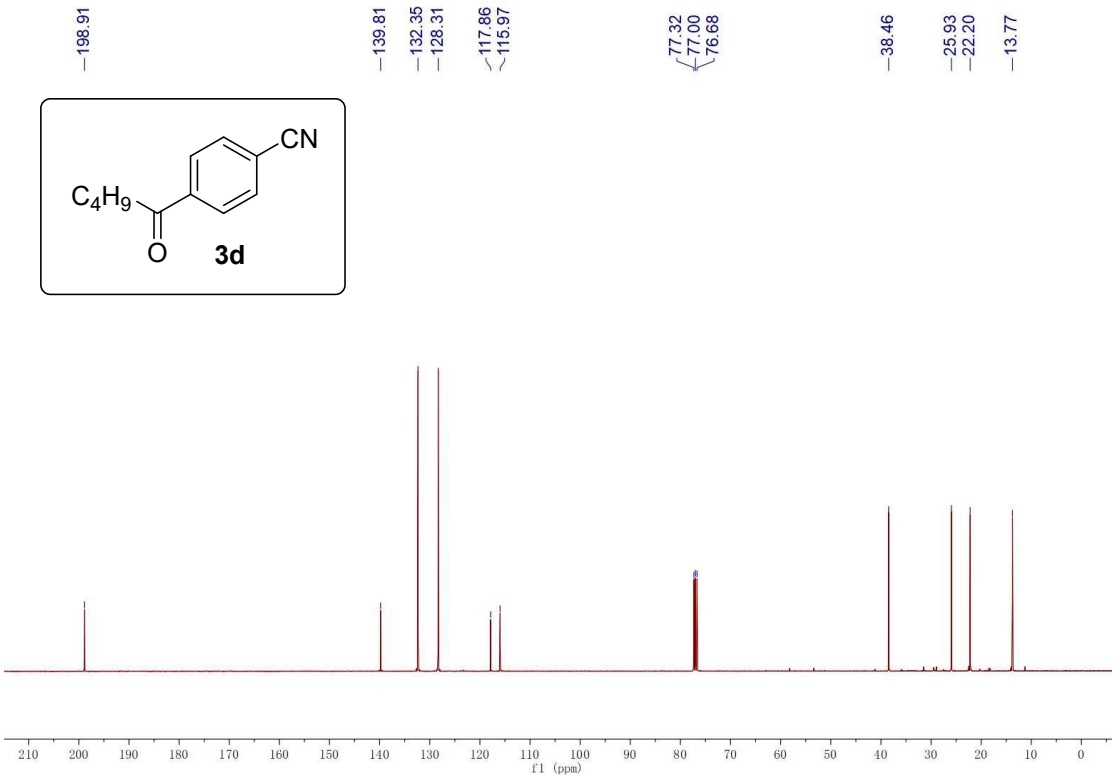
8.048
7.791
7.772
3.018
3.000
2.982
1.768
1.749
1.731
1.713
1.694
1.466
1.448
1.429
1.411
1.393
1.374
0.980
0.962
0.943
CN
C4H9
O
3d
2.00
1.95
2.04
2.03
2.14
3.00
f1 (ppm)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139.81
132.35
128.31
117.86
115.97
77.32
77.00
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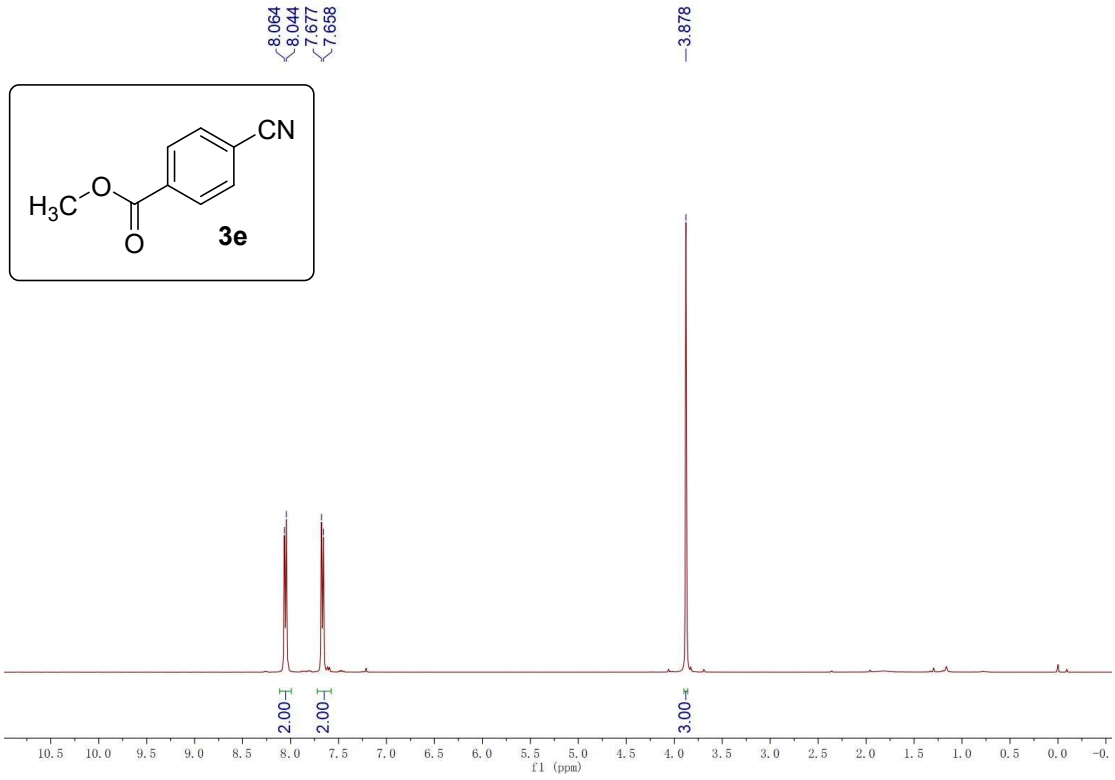
38.46
25.93
22.20
13.77
CN
C4H9
O
3d
f1 (ppm)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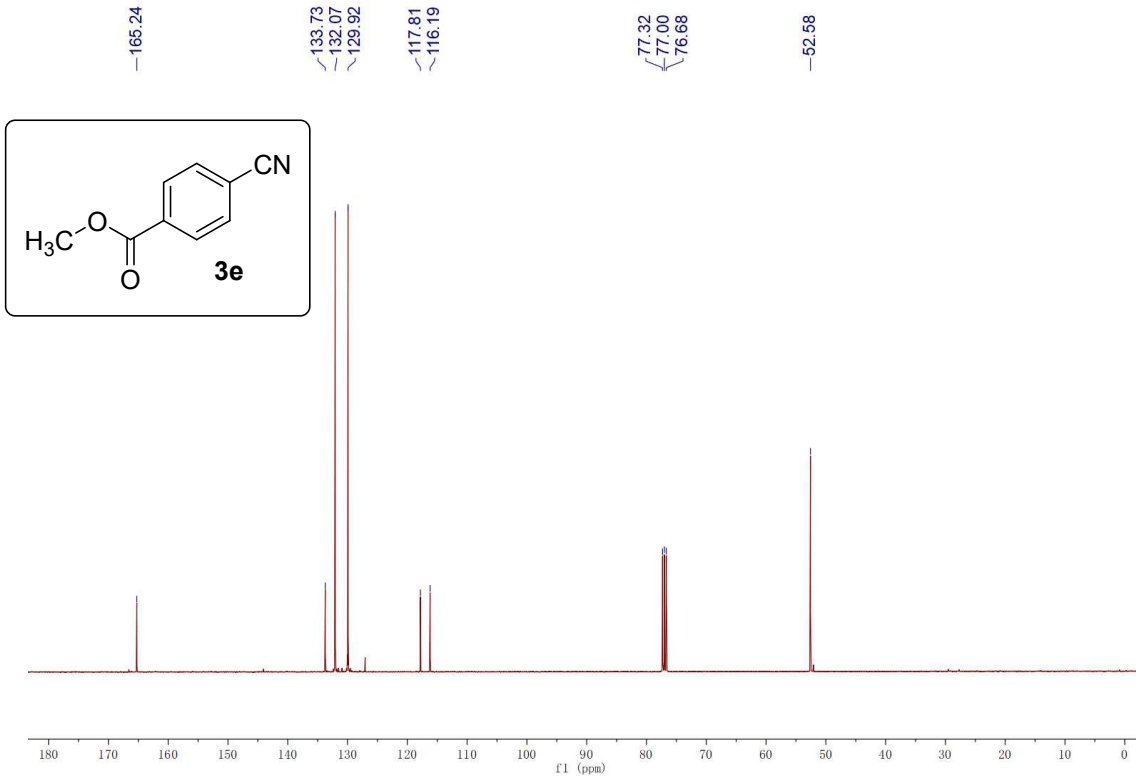
O
O
3e
2.00
2.00
3.00
f1 (ppm)


165.24
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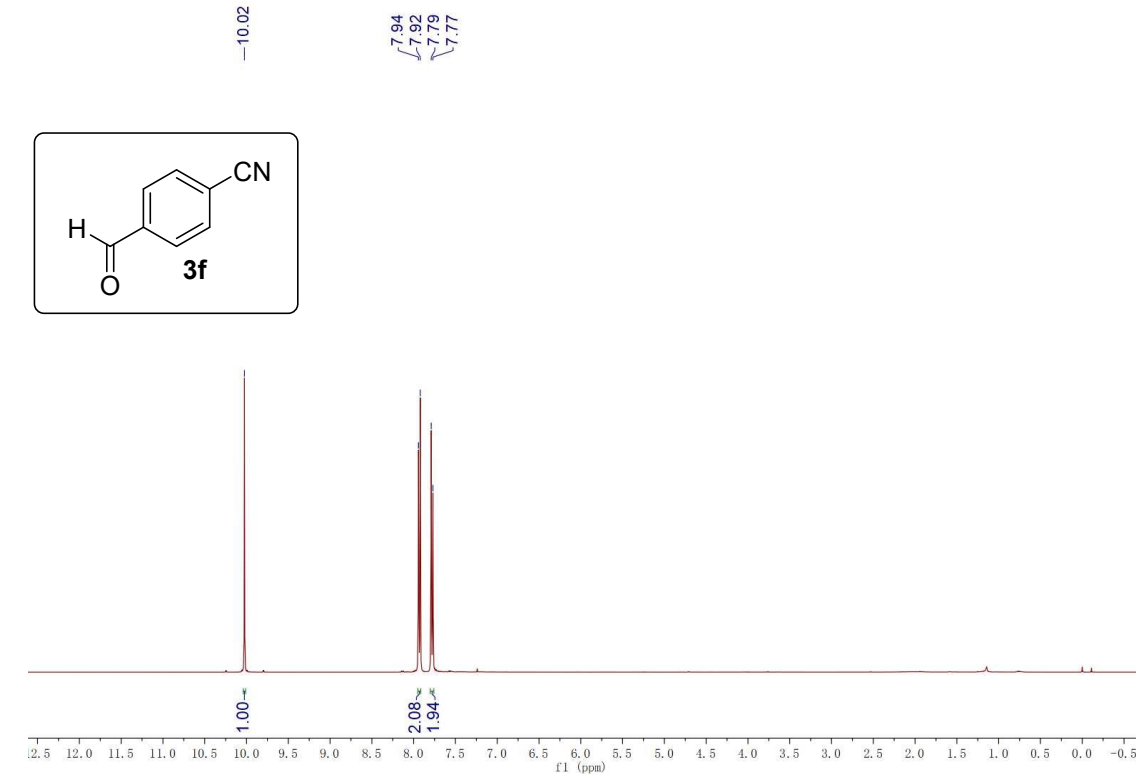
116.19
77.32
77.00
76.68
52.58
CN
H3C
O
O
3e
f1 (ppm)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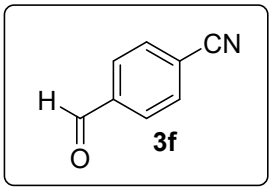
2.08
1.94
f1 (ppm)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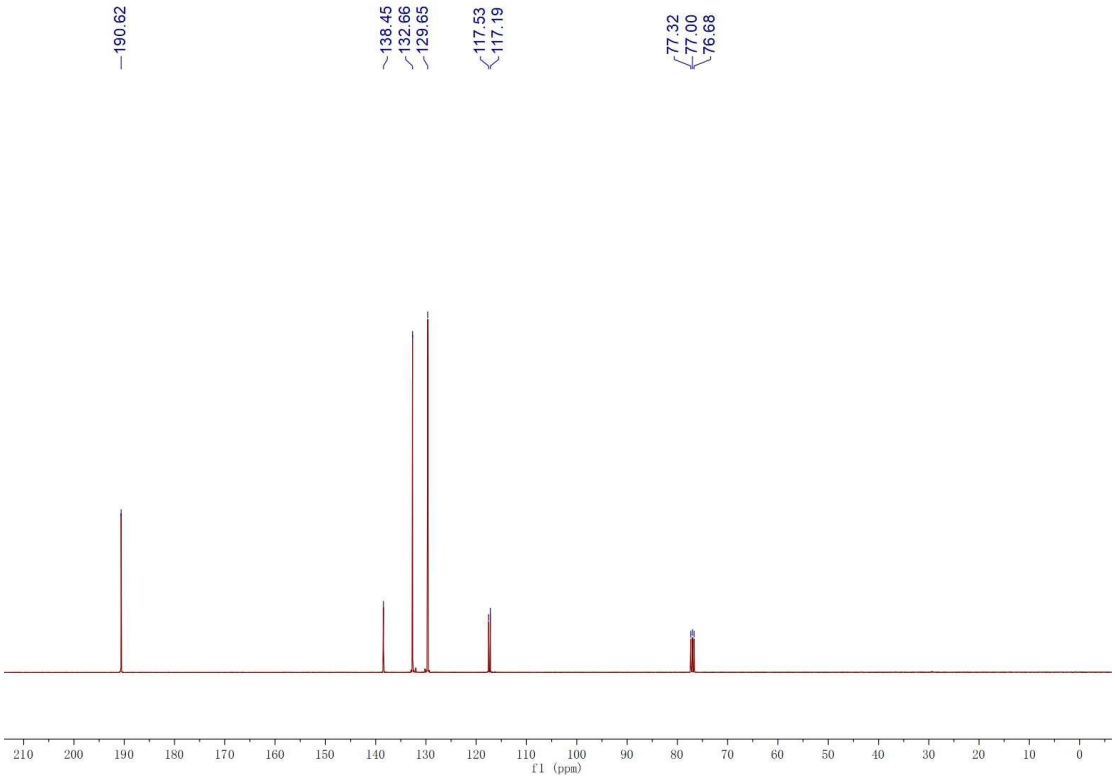
H
O
3f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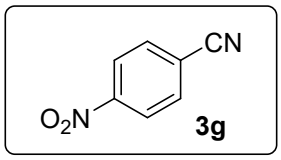
117.53
117.19
77.32
77.00
76.68
f1 (ppm)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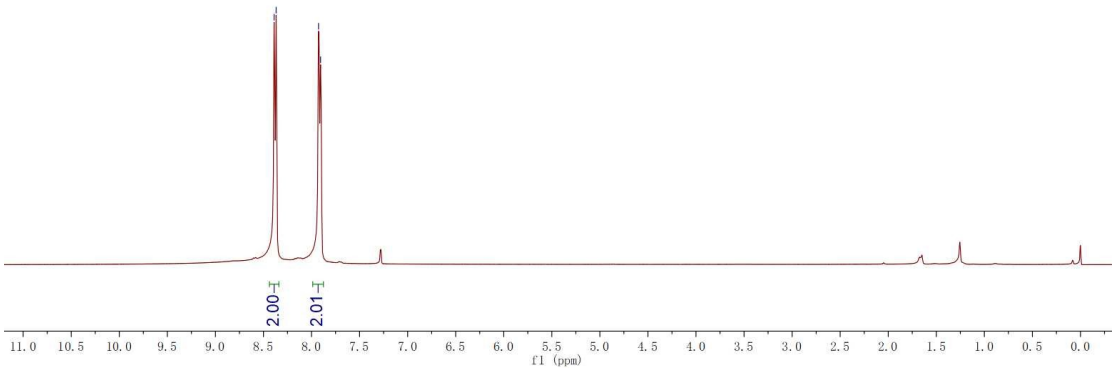
O2N
3g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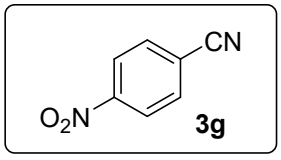
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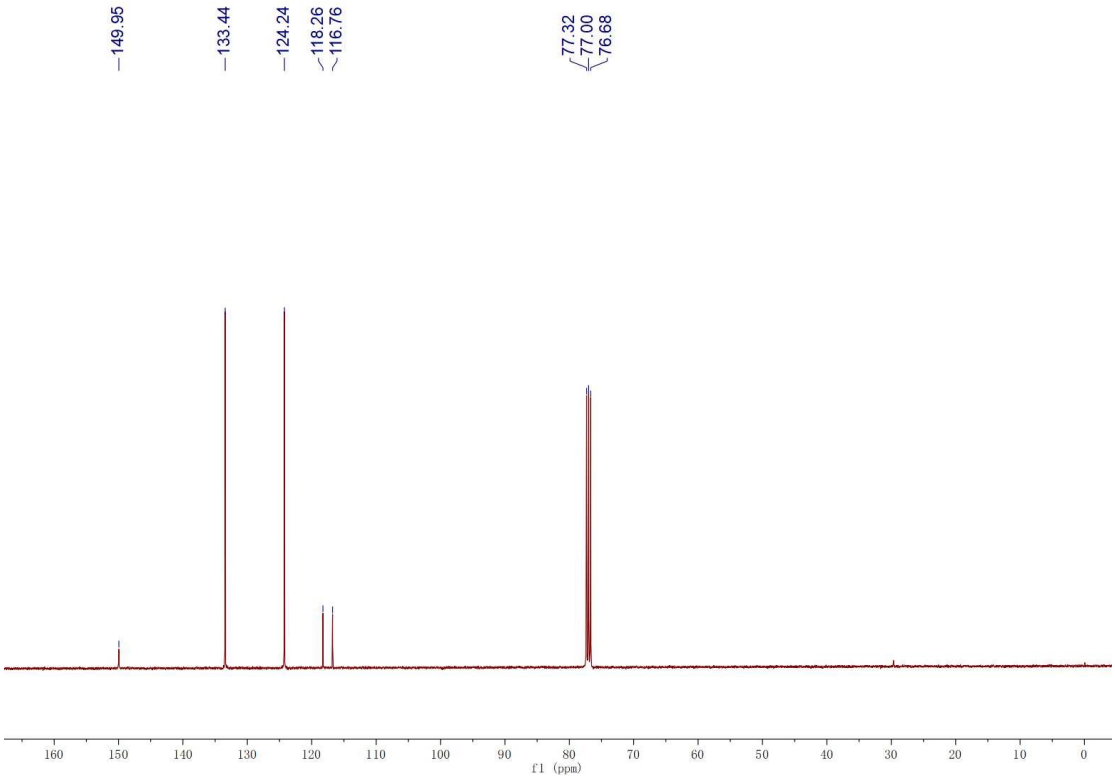
O2N
3g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77.32
77.00
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130
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110
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90
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50
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20
10
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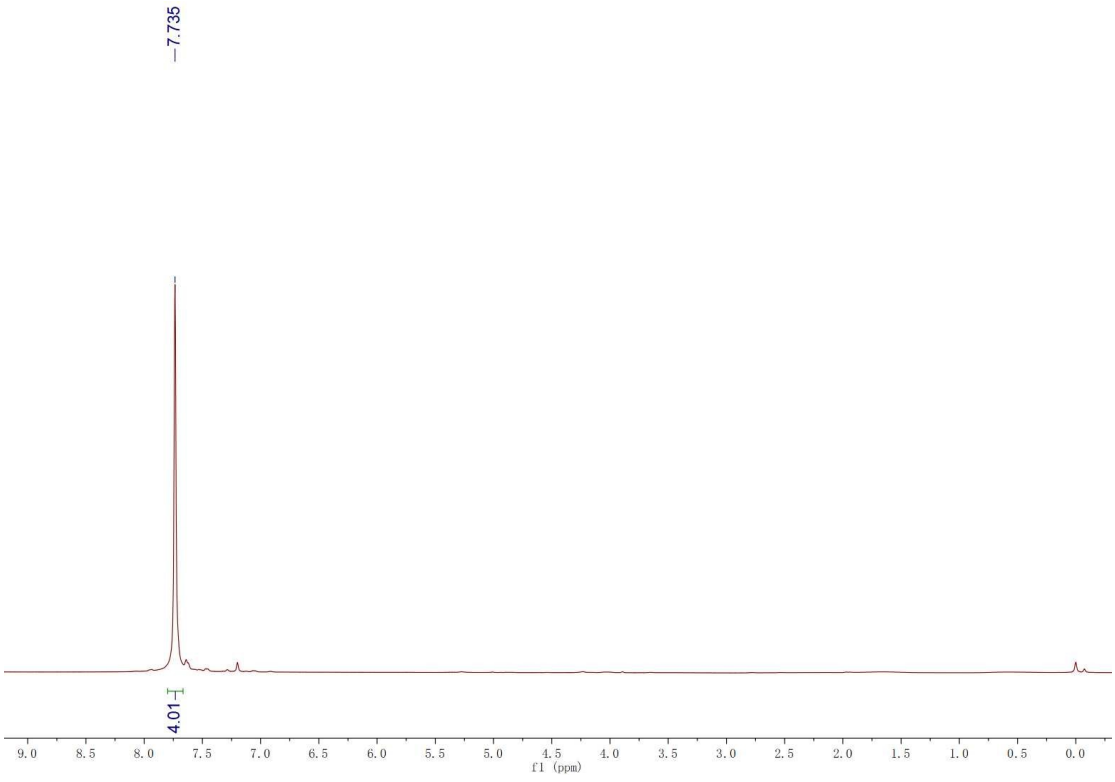
f1 (ppm)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5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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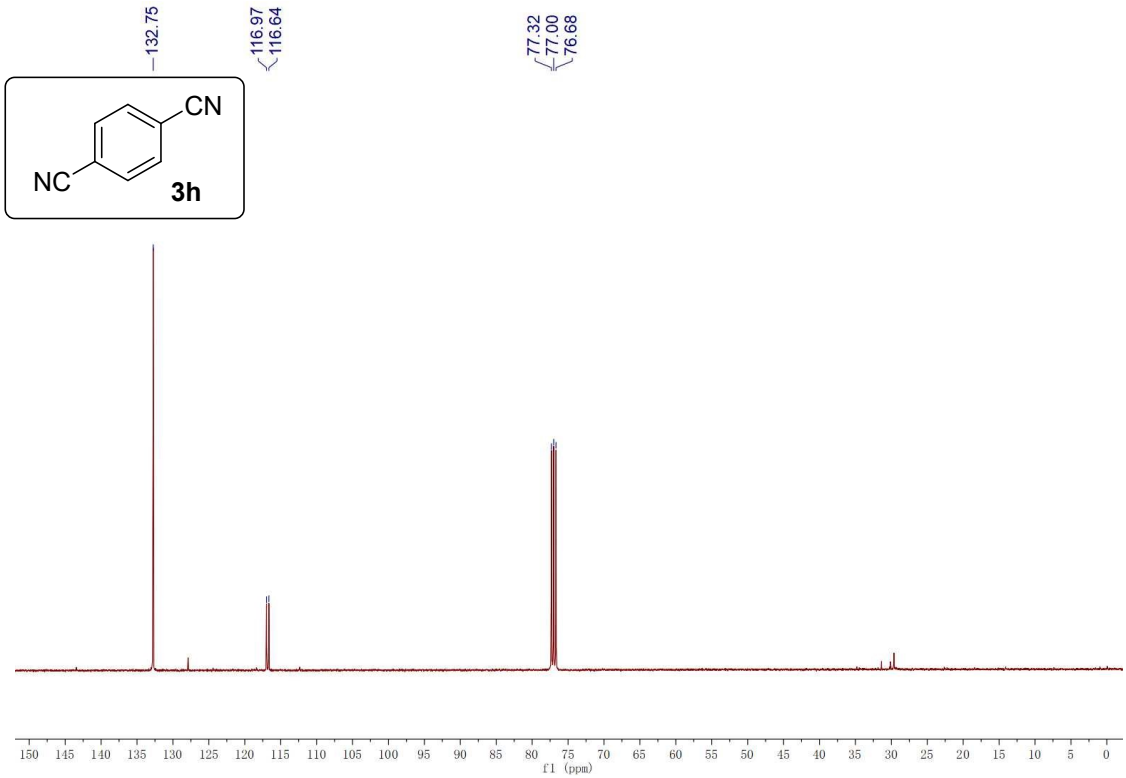
0.0
f1 (ppm)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NC
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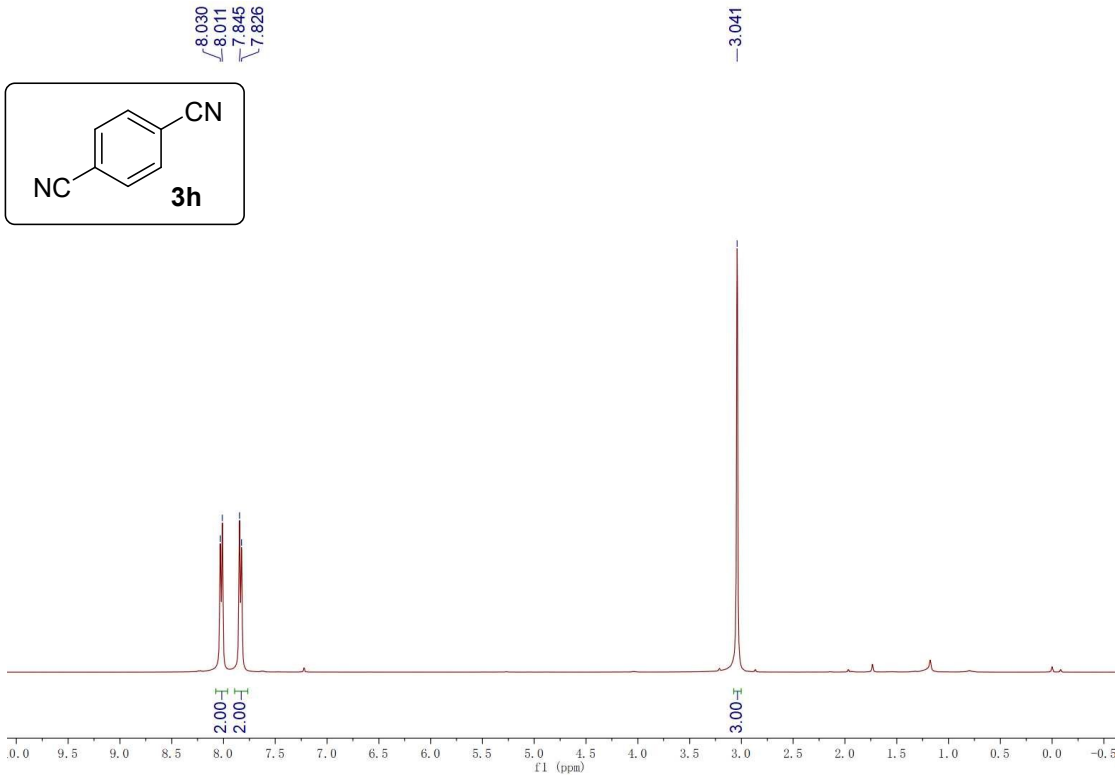
f1 (ppm)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7.826
3.041
CN
NC
3h
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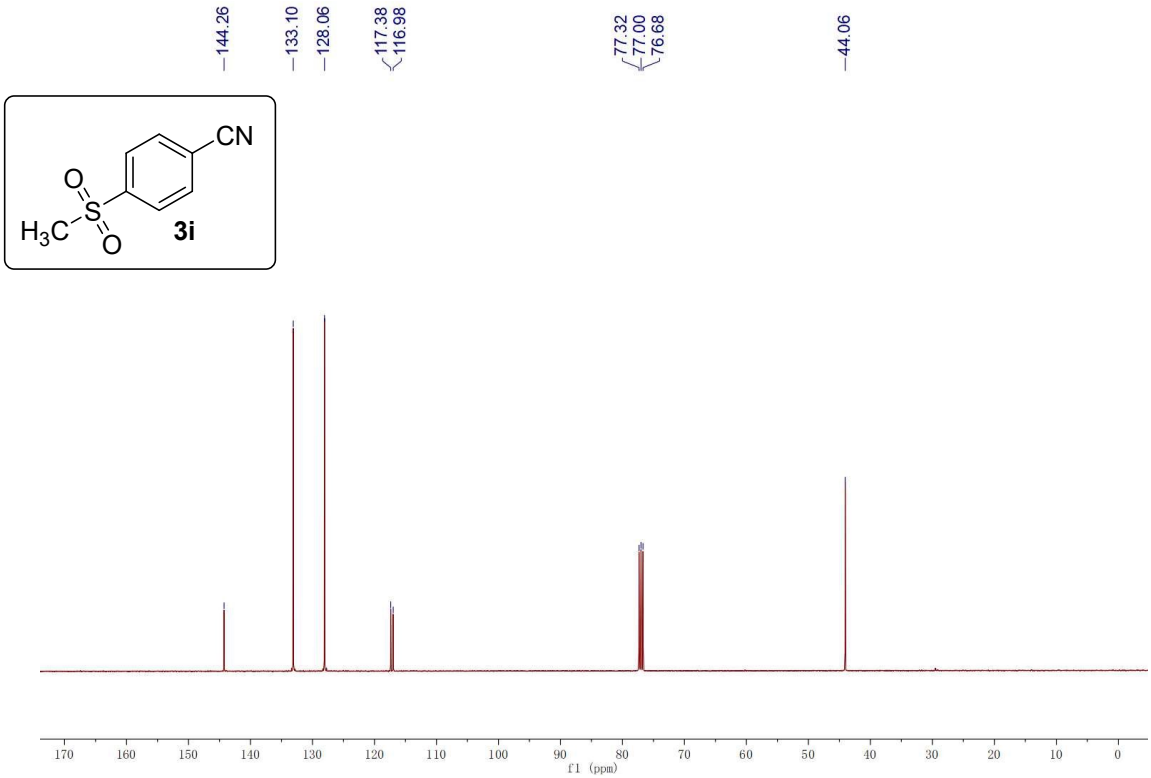
2.00
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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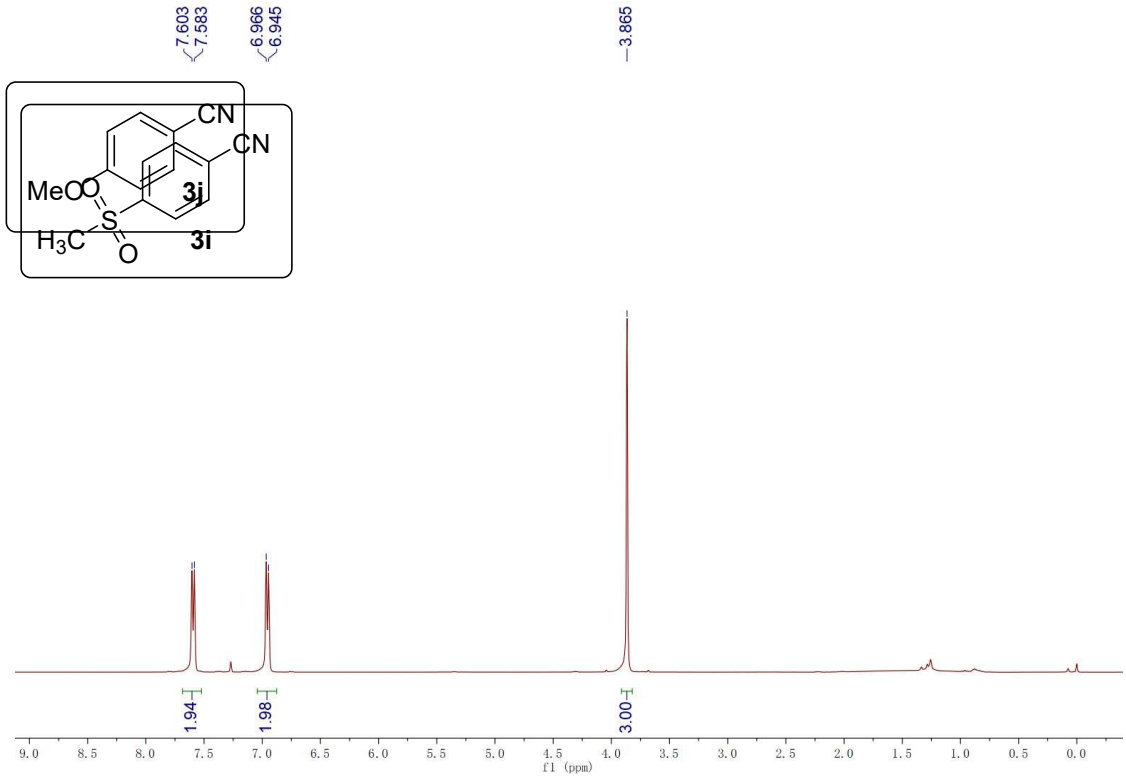
O
S
H3C
O
3i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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MeO
O
3j
S
H3C
O
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1.94
1.98
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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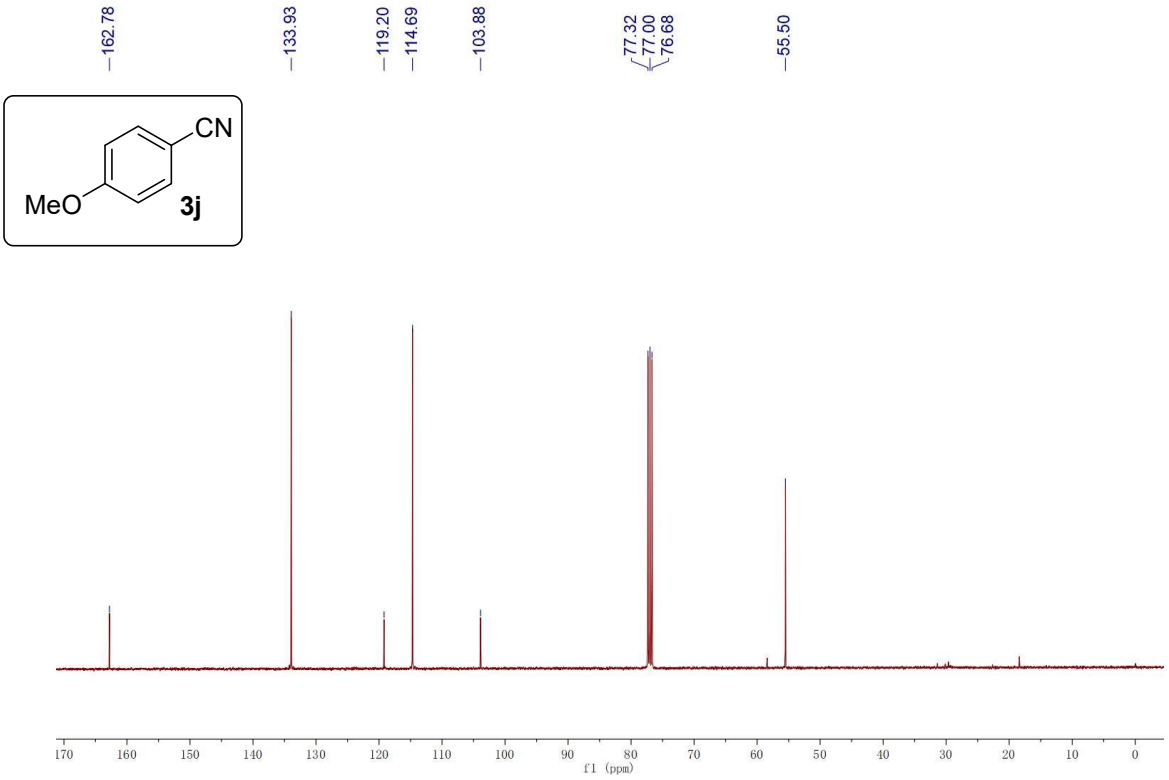
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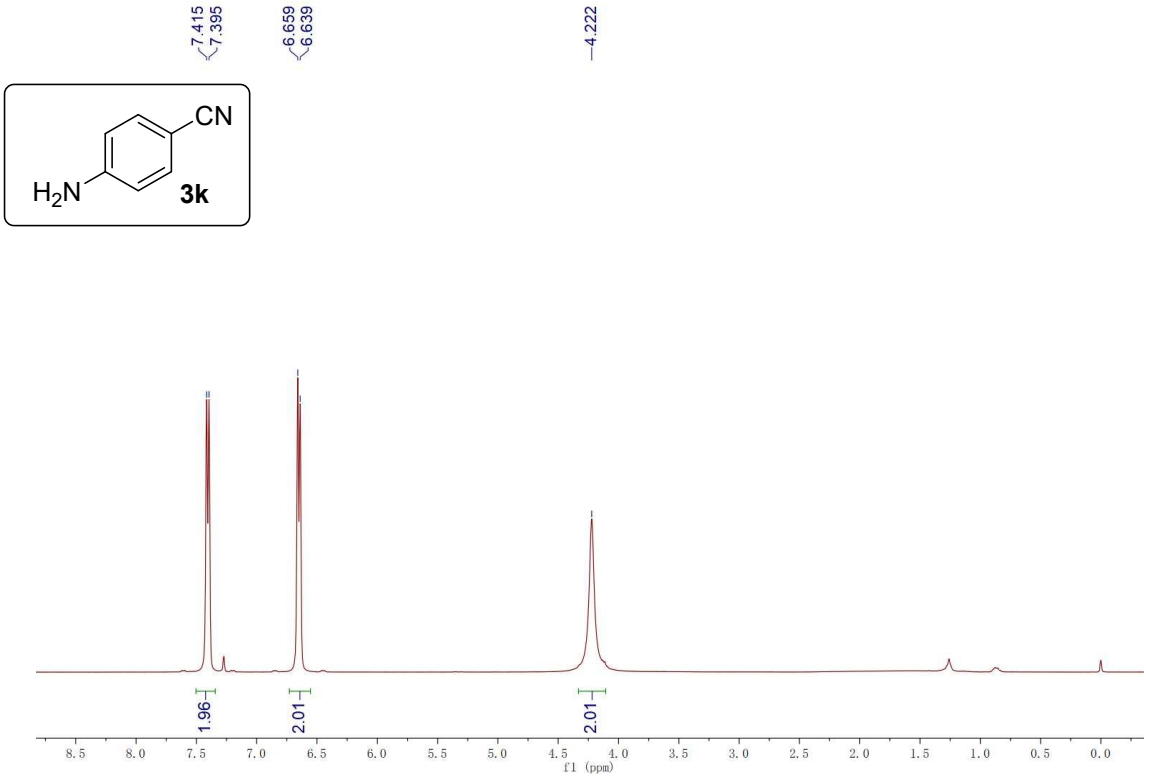
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2.01
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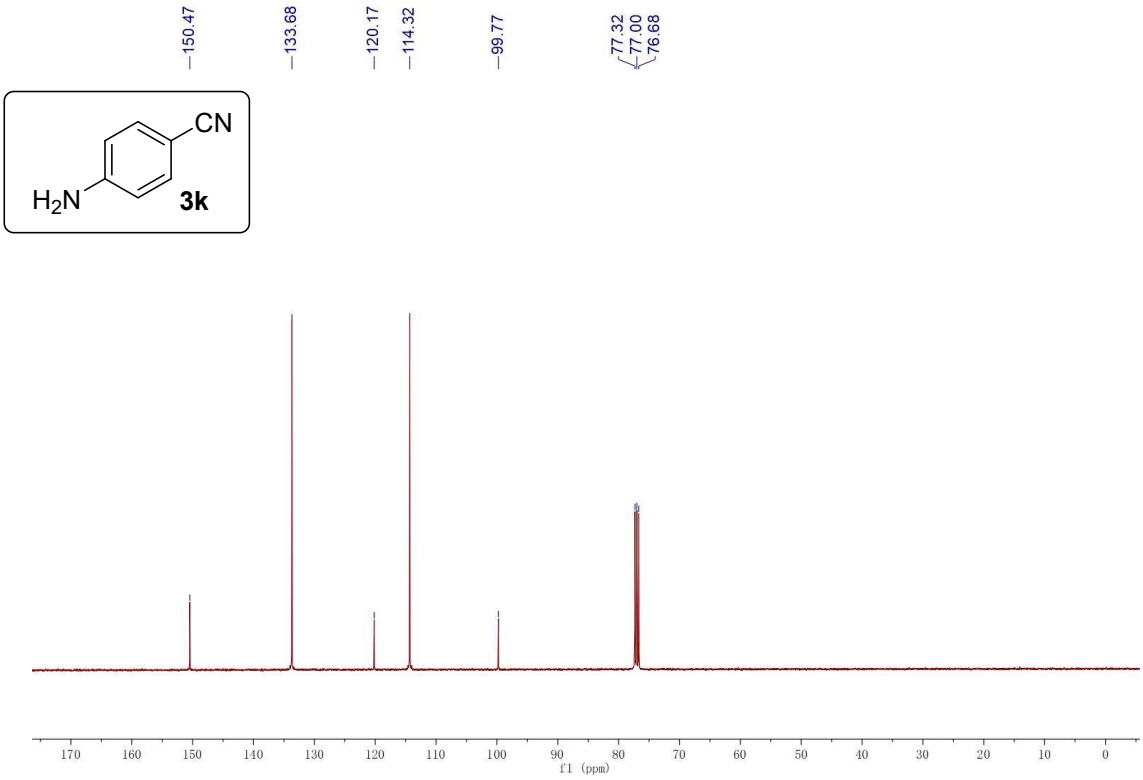
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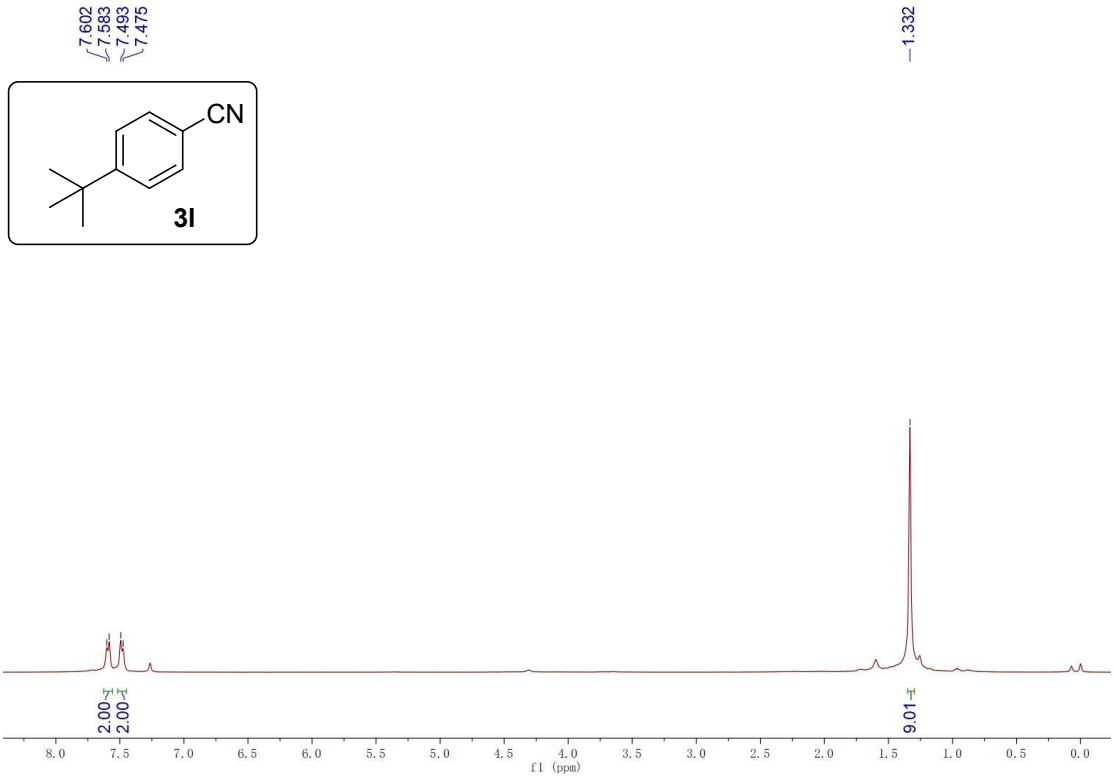
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2.00
9.01
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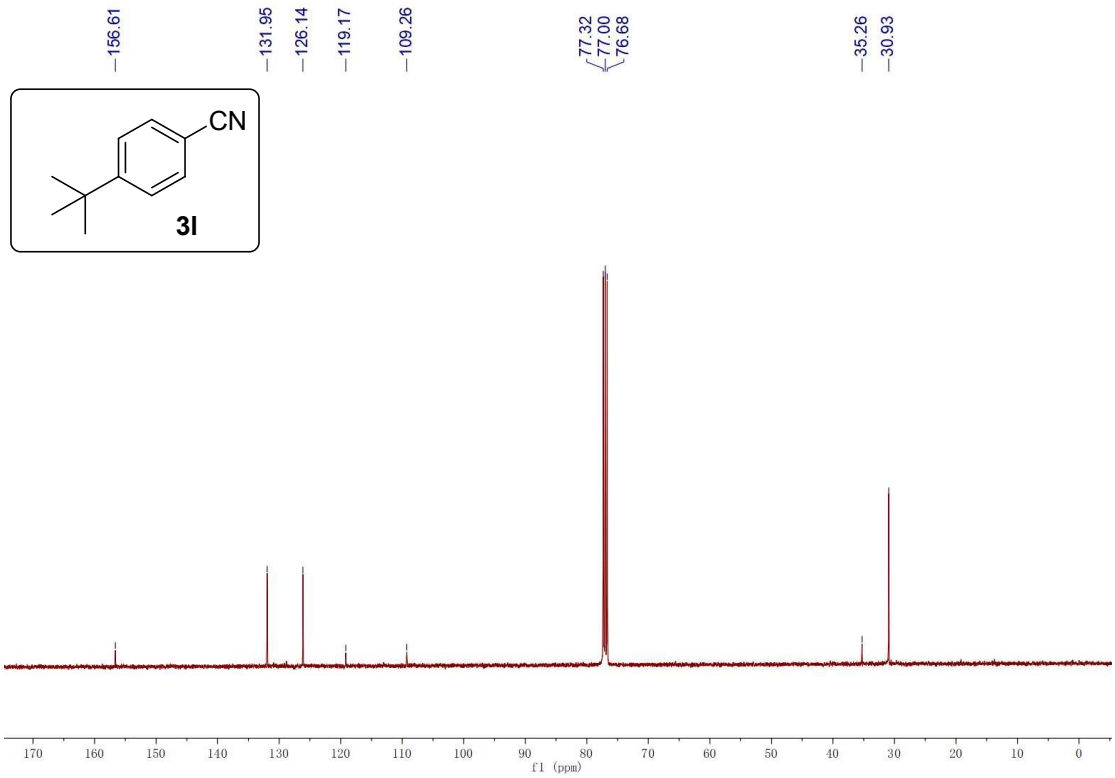
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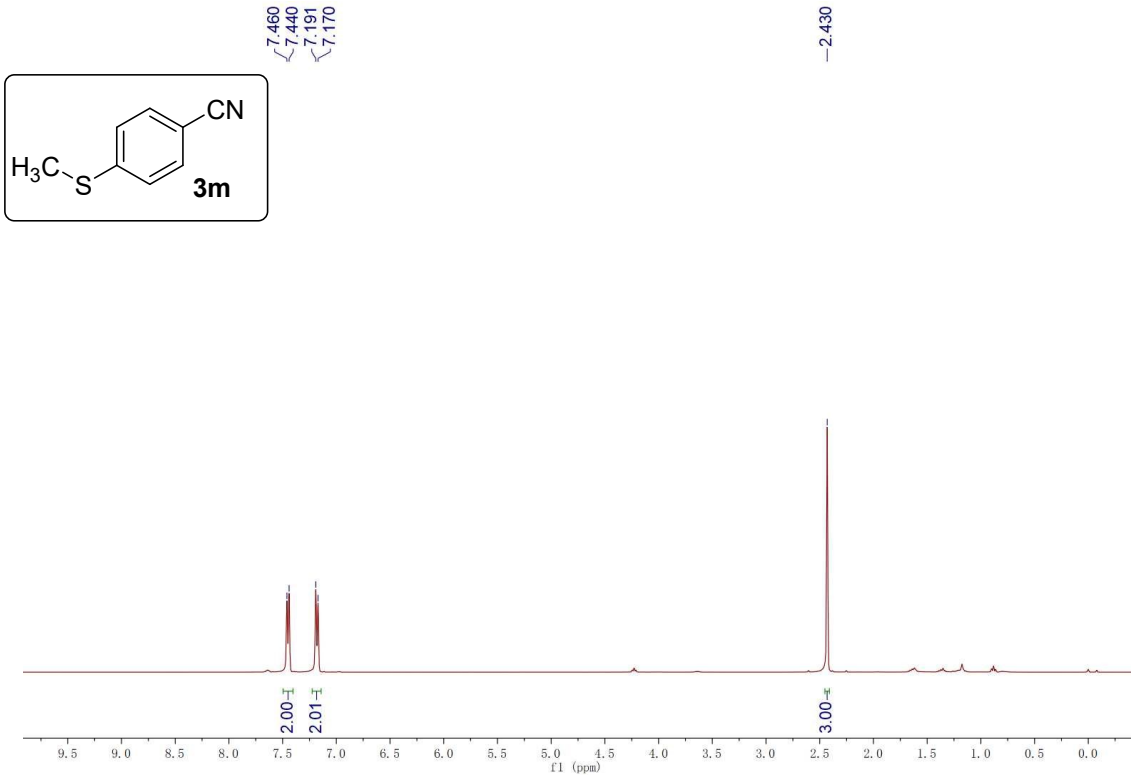
CN
3l
f1 (ppm)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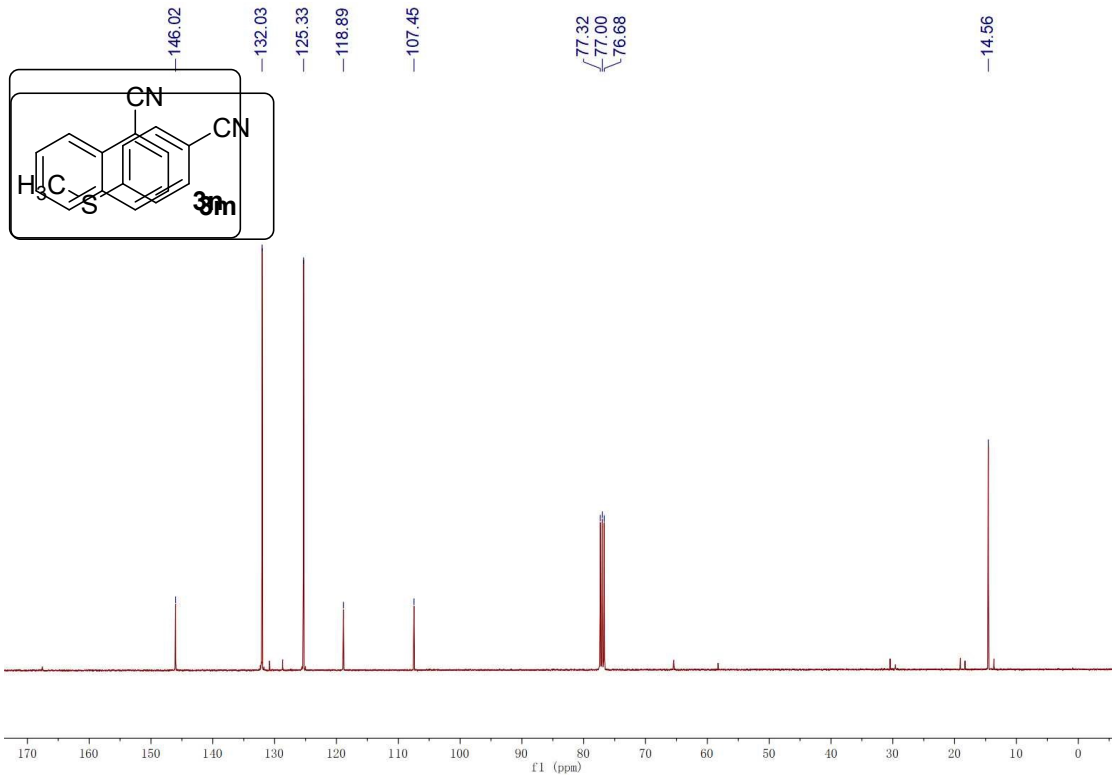
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125.33
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76.68
14.56
CN
CN
H3C
S
3m
f1 (ppm)


8.231
8.210
8.073
8.052
7.920
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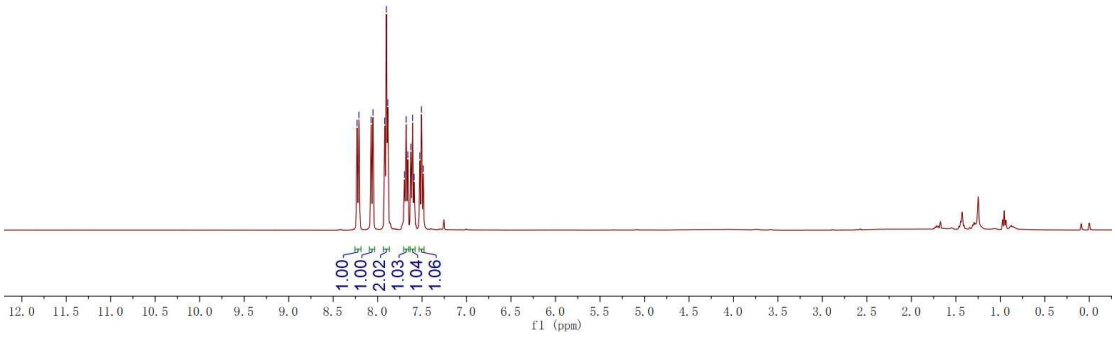
7.506
7.487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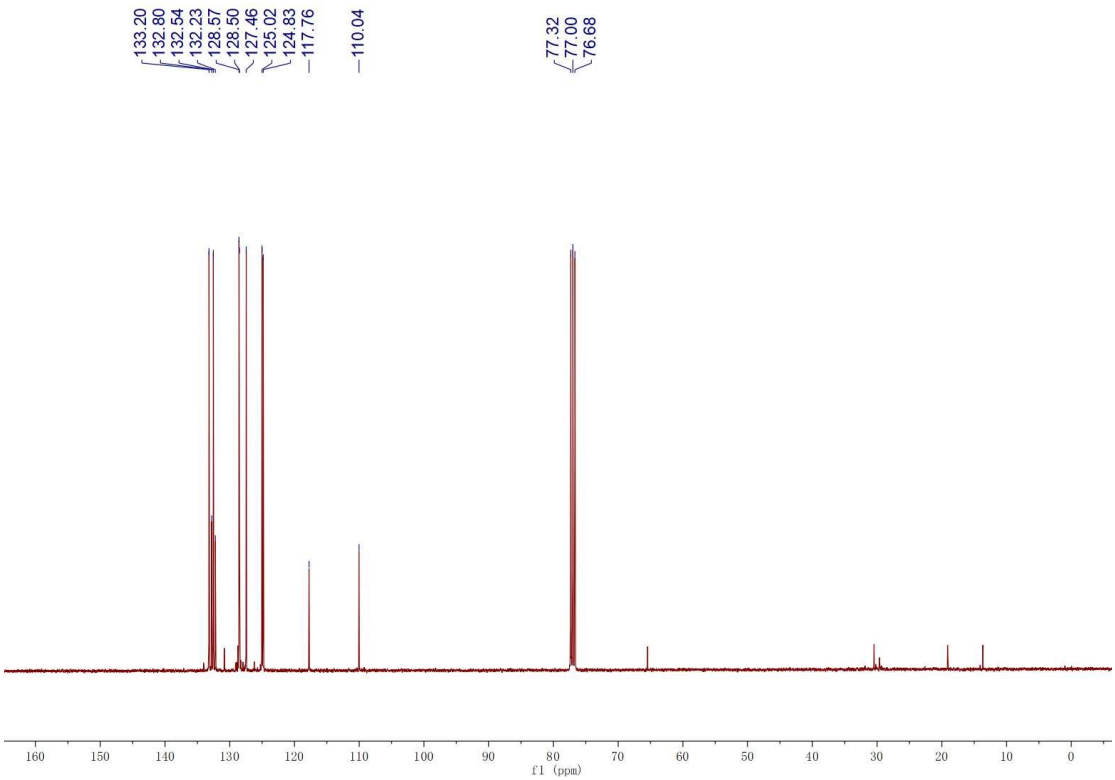
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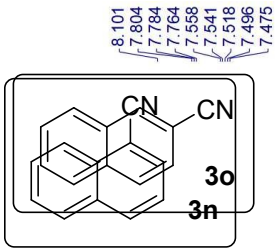
77.00
76.68
f1 (ppm)


CN
CN
3o
3n

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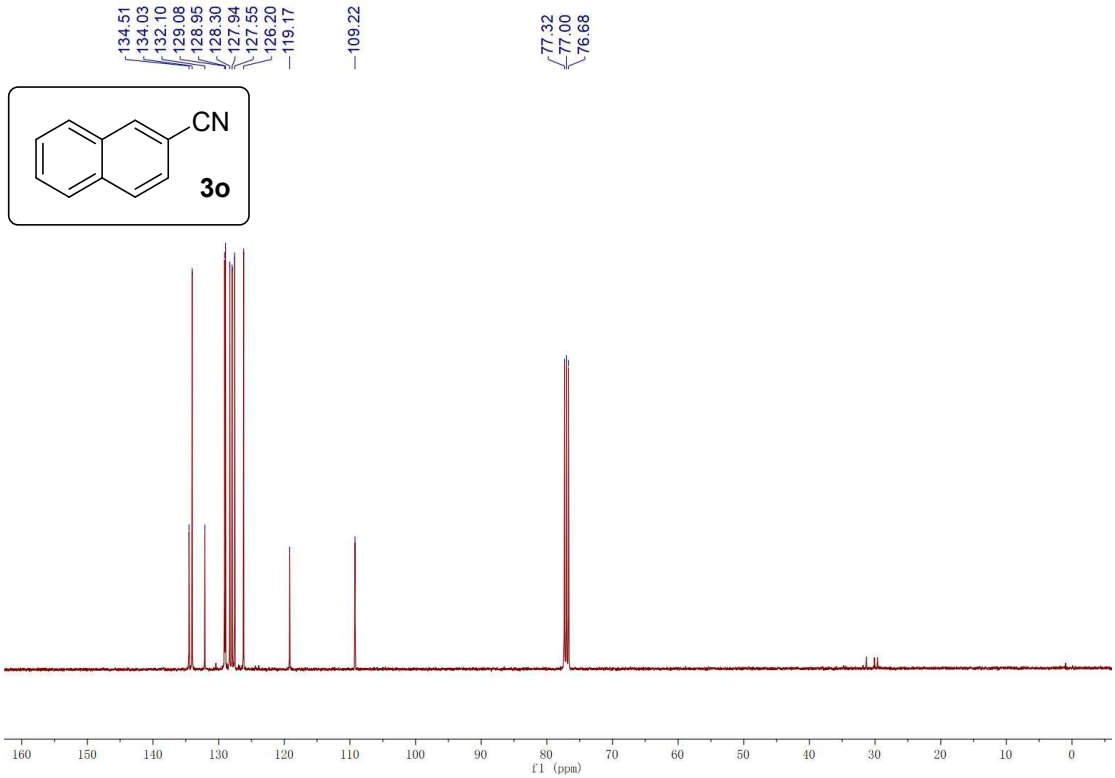
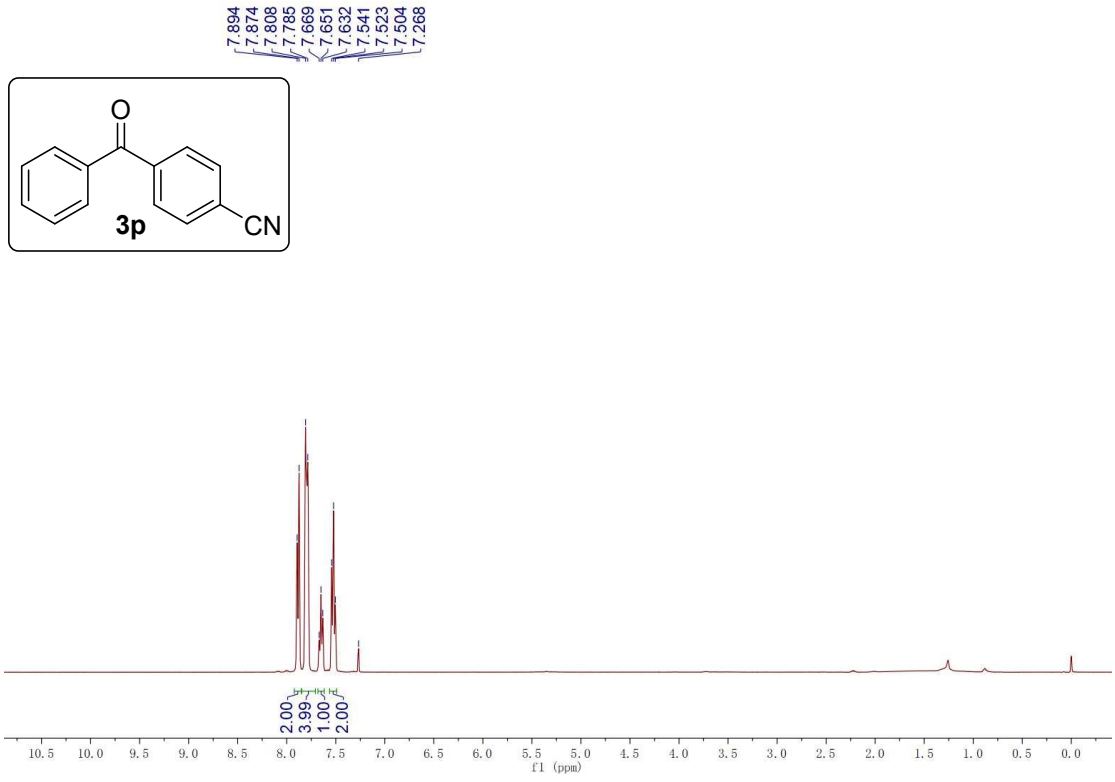
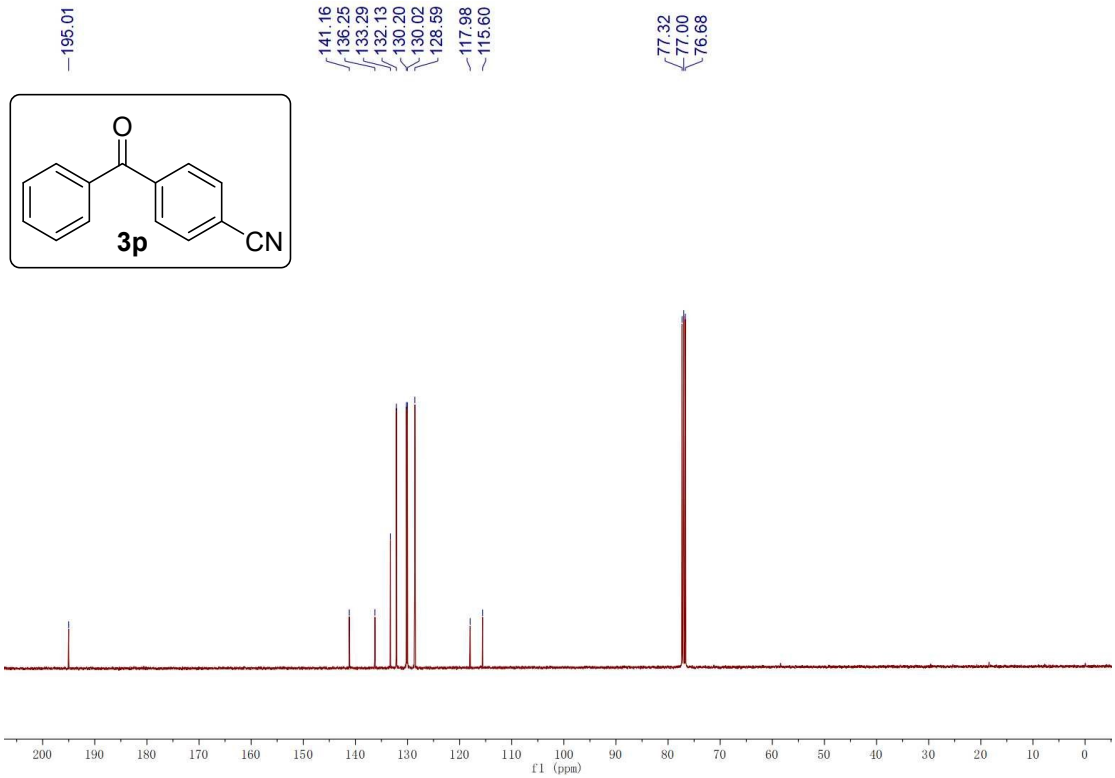
7.518
7.496
7.475
1.00
3.08
3.06
f1 (ppm)


134.51
134.03
132.10
129.08
128.95
128.30
127.94
127.55
126.20
119.17
109.22
77.32
77.00
76.68
CN
3o
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.894
7.874
7.808
7.785
7.669
7.651
7.632
7.541
7.523
7.504
7.268
O
3p
CN
2.00
3.99
1.00
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)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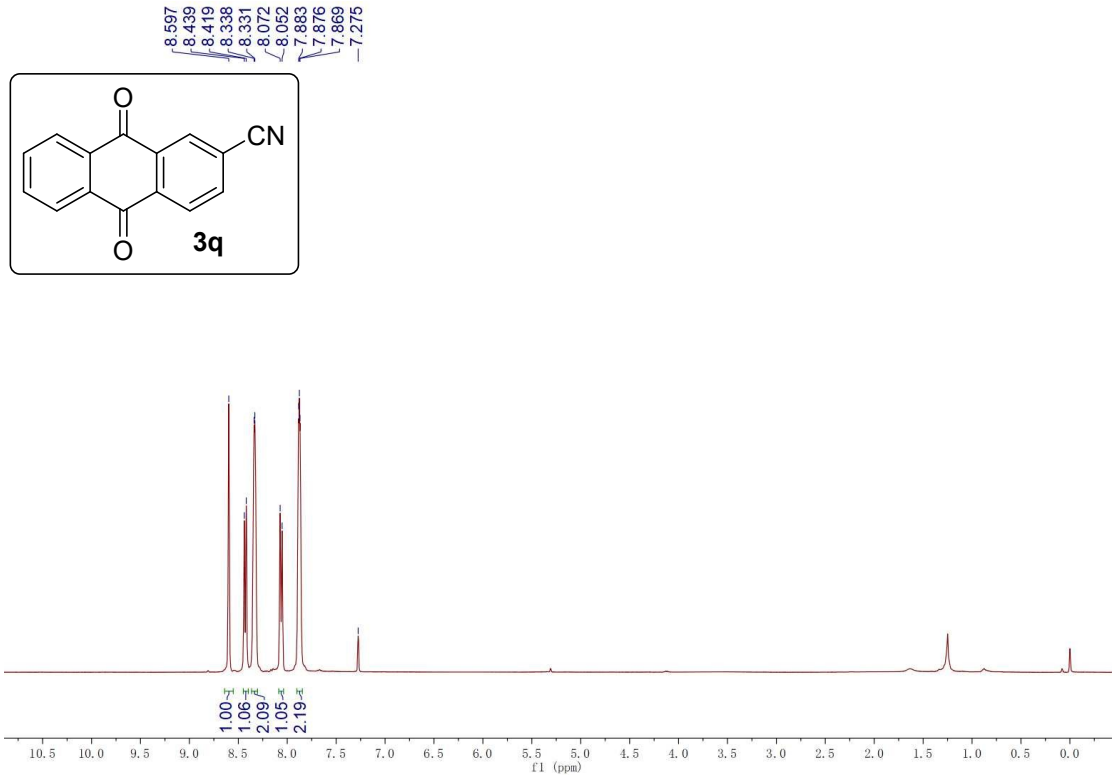
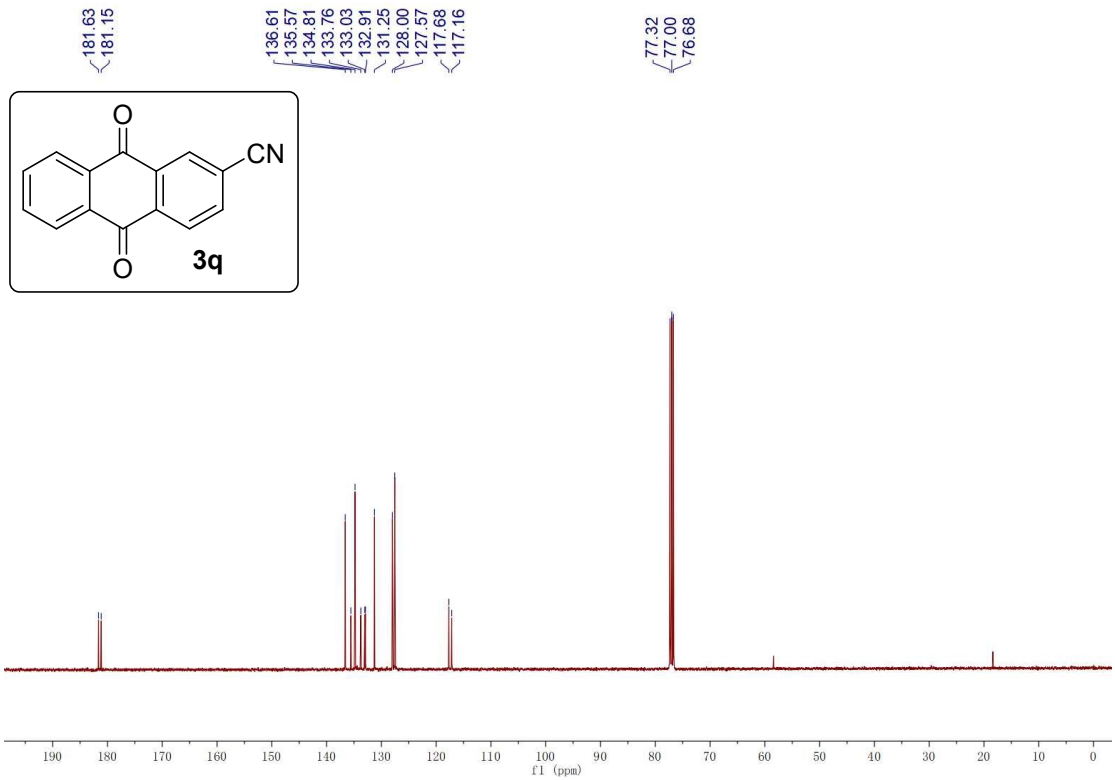
141.16
136.25
133.29
132.13
130.20
130.02
128.59
117.98
115.60
77.32
77.00
76.68
O
CN
3p
f1 (ppm)


8.597
8.439
8.419
8.338
8.331
8.072
8.052
7.883
7.876
7.869
7.275
O
CN
O
3q
1.00
1.06
2.09
1.05
2.19
f1 (ppm)


181.63
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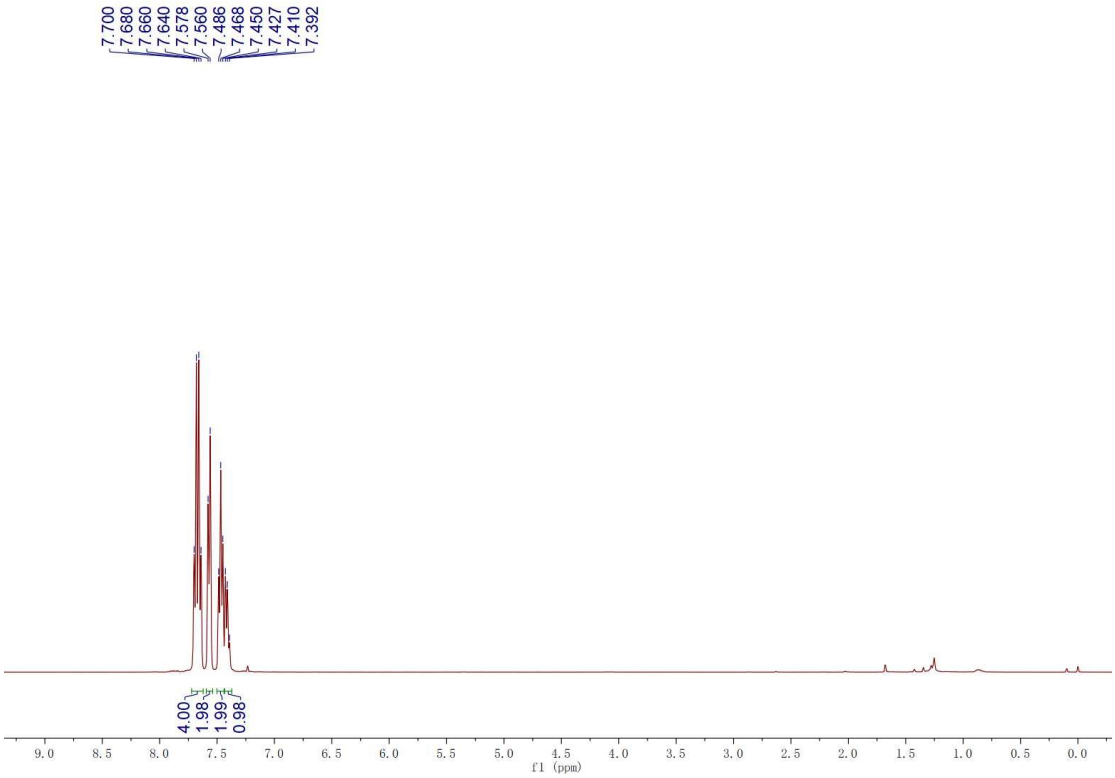
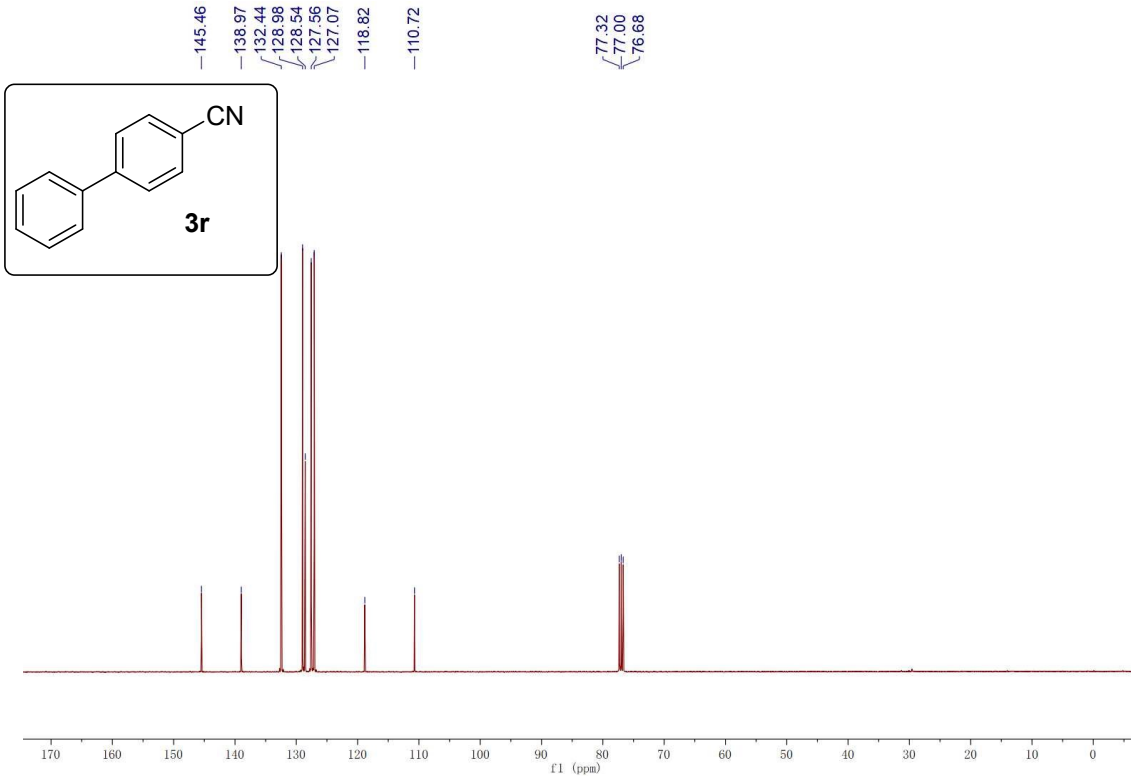
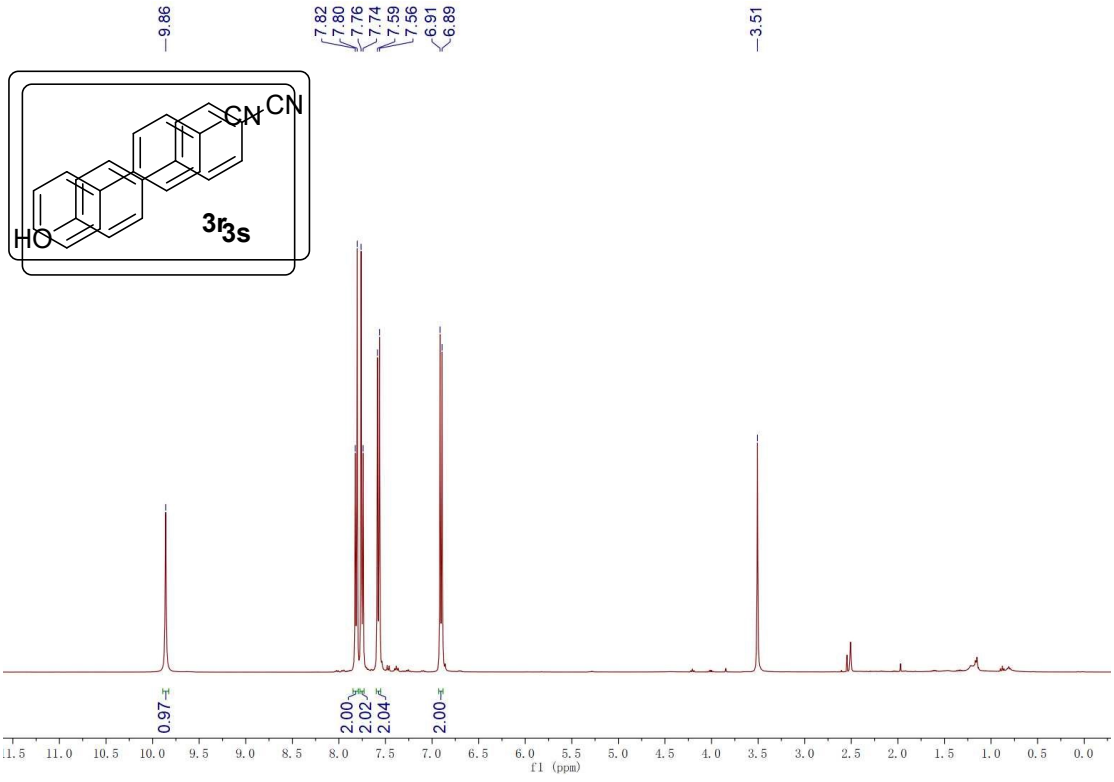
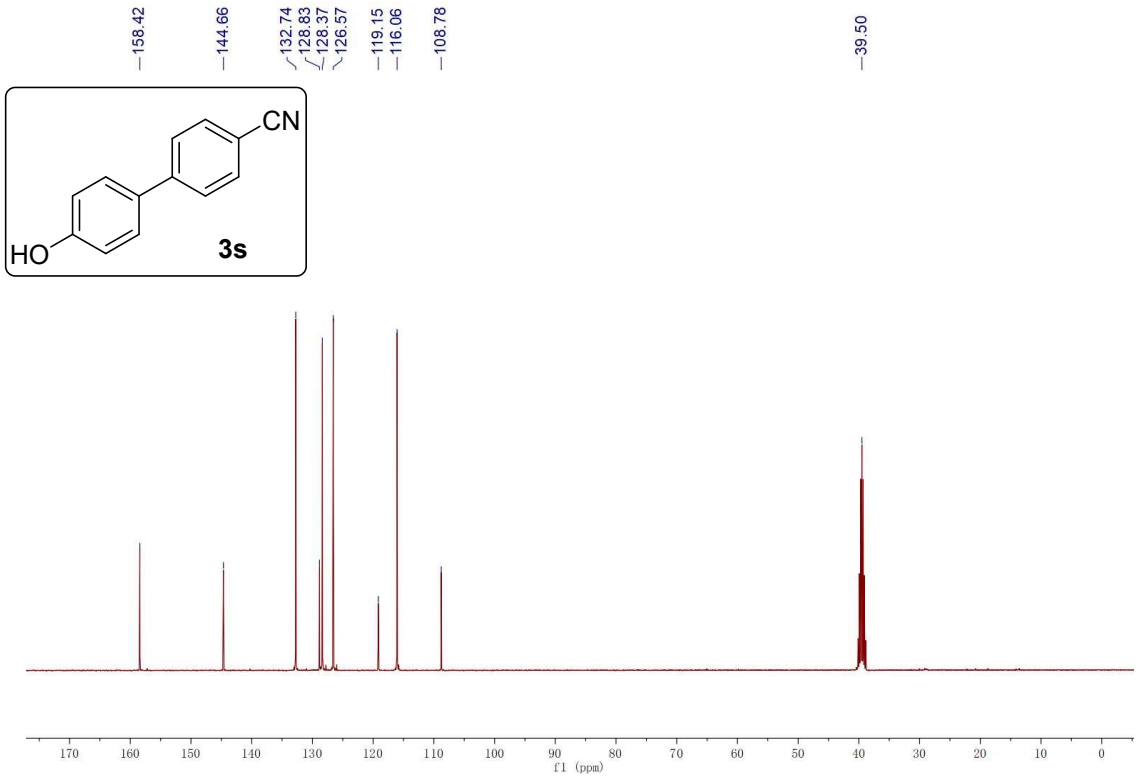
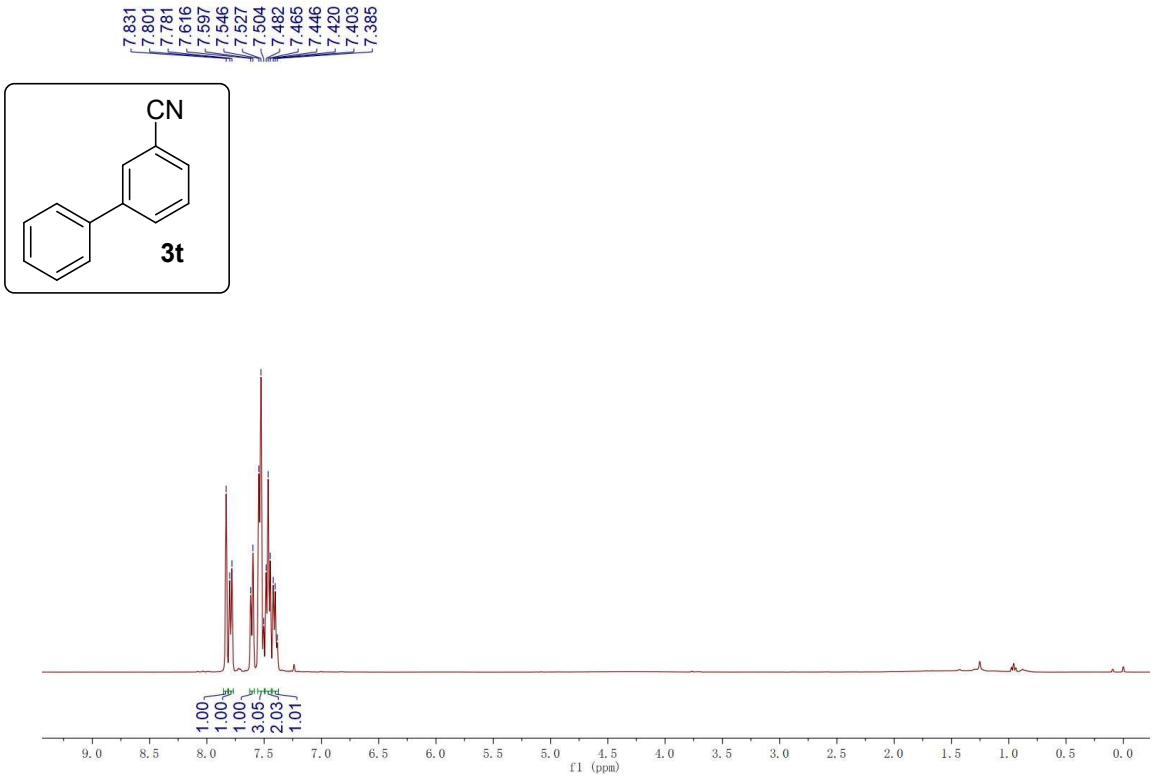
136.61
135.57
134.81
133.76
133.03
132.91
131.25
128.00
127.57
117.68
117.16
77.32
77.00
76.68
O
CN
O
3q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

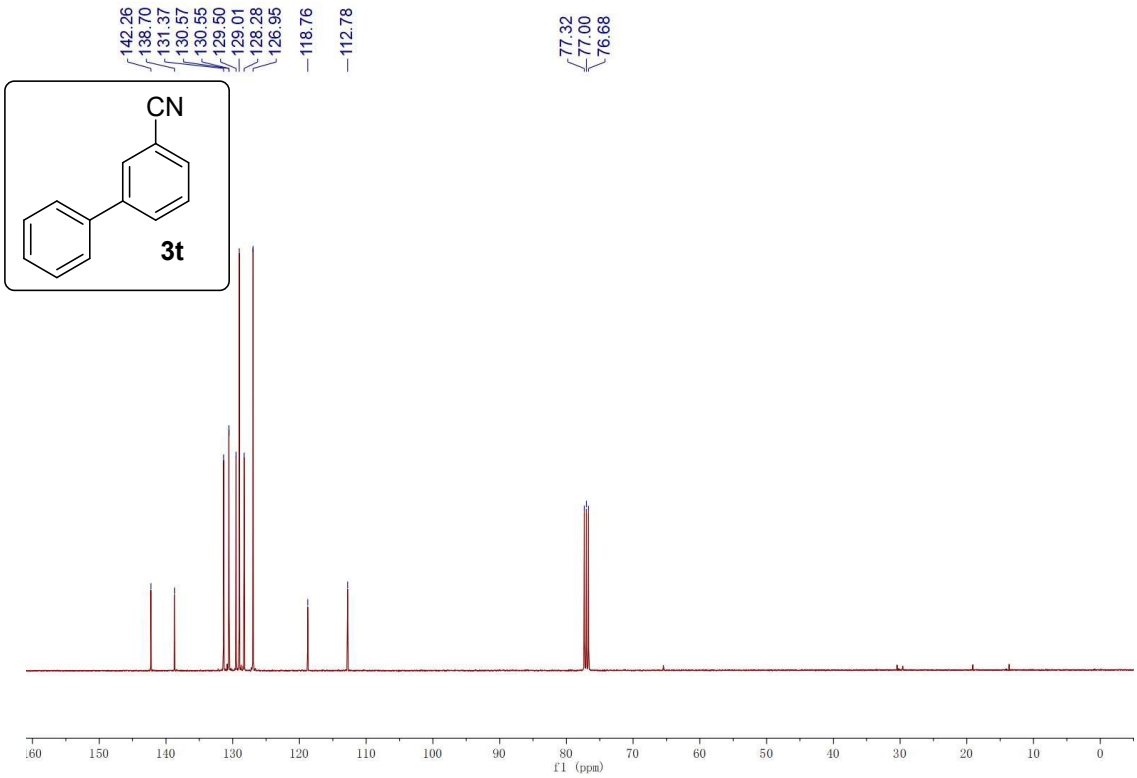

7.700
7.680
7.660
7.640
7.578
7.560
7.486
7.468
7.450
7.427
7.410
7.392
4.00
1.98
1.99
0.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

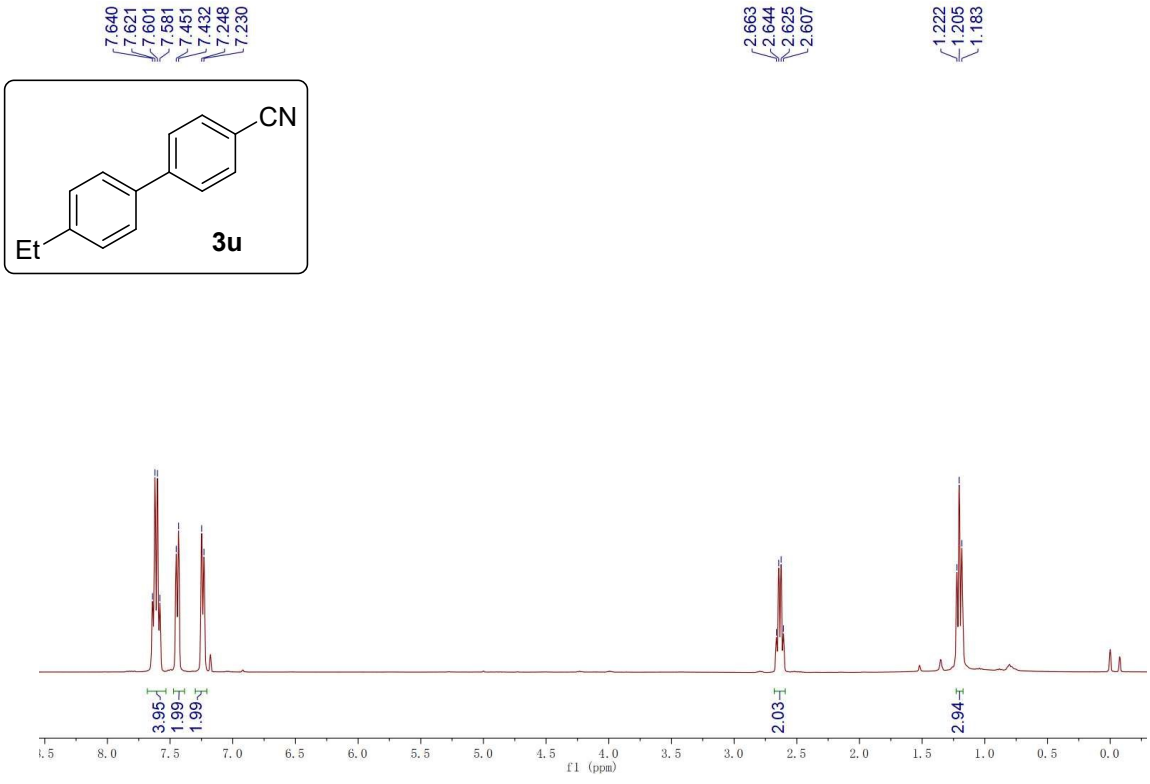

145.46
138.97
132.44
128.98
128.54
127.56
127.07
118.82
110.72
77.32
77.00
76.68
CN
3r
f1 (ppm)

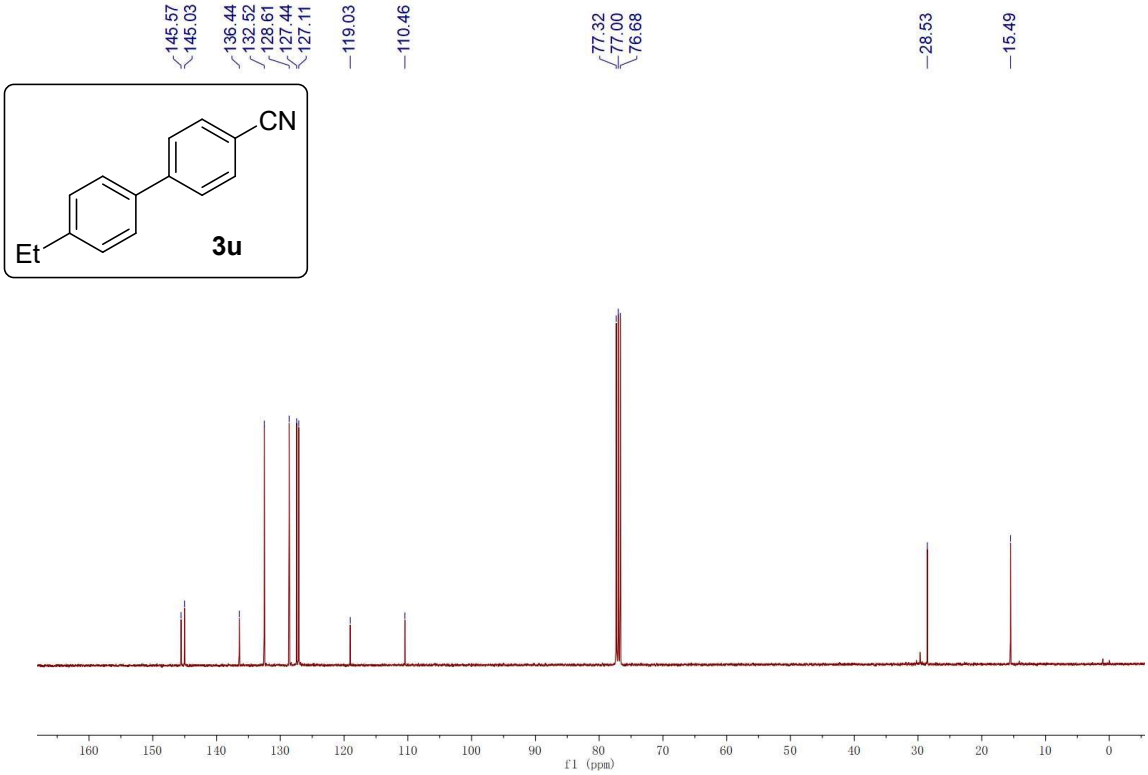

9.86
7.82
7.80
7.76
7.74
7.59
7.56
6.91
6.89
3.51
CN
CN
HO
3r3s
0.97
2.00
2.02
2.04
2.00
f1 (ppm)

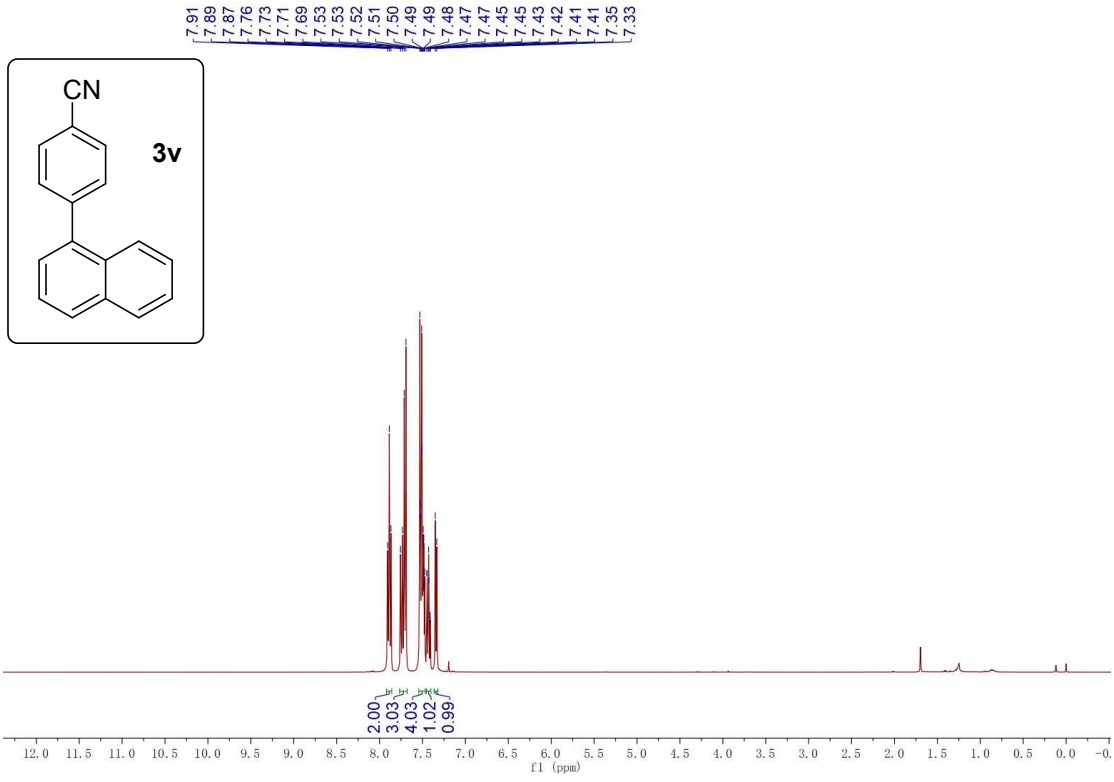

158.42
144.66
132.74
128.83
128.37
126.57
119.15
116.06
108.78
39.50
CN
HO
3s
f1 (ppm)

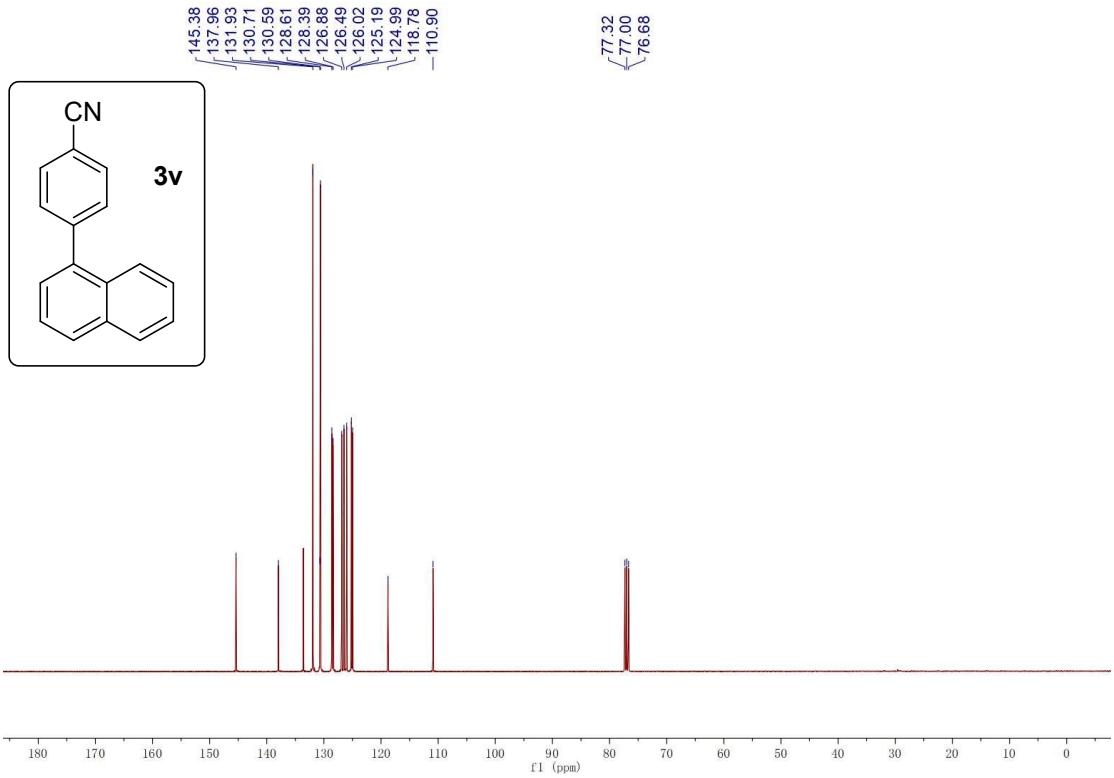

7.831
7.801
7.781
7.616
7.597
7.546
7.527
7.504
7.482
7.465
7.446
7.420
7.403
7.385
CN
3t
1.00
1.00
1.00
3.05
2.03
1.01
f1 (ppm)

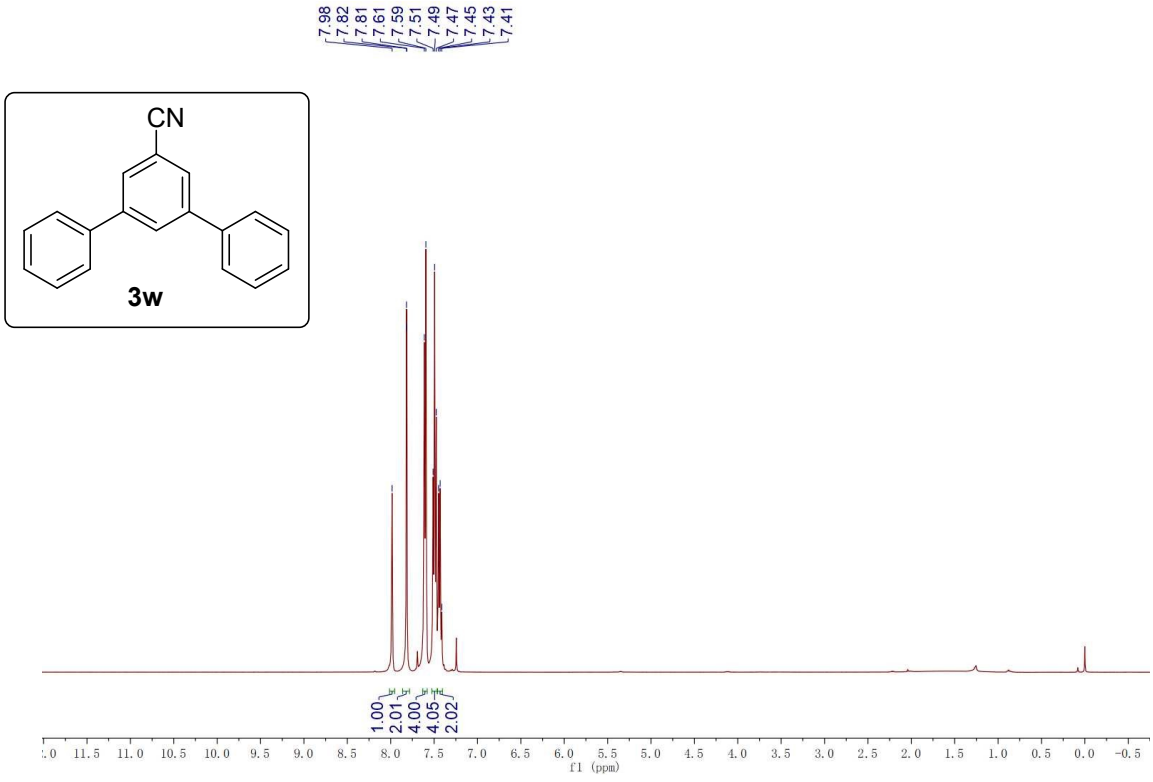

142.26
138.70
131.37
130.57
130.55
129.50
129.01
128.28
126.95
118.76
112.78
77.32
77.00
76.68
CN
3t
f1 (ppm)

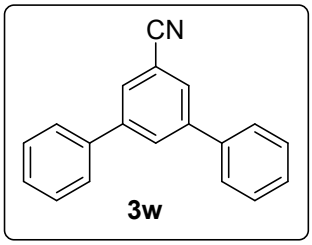

7.640
7.621
7.601
7.581
7.451
7.432
7.248
7.230
2.663
2.644
2.625
2.607
1.222
1.205
1.183
CN
Et
3u
3.95
1.99
1.99
2.03
2.94
f1 (ppm)

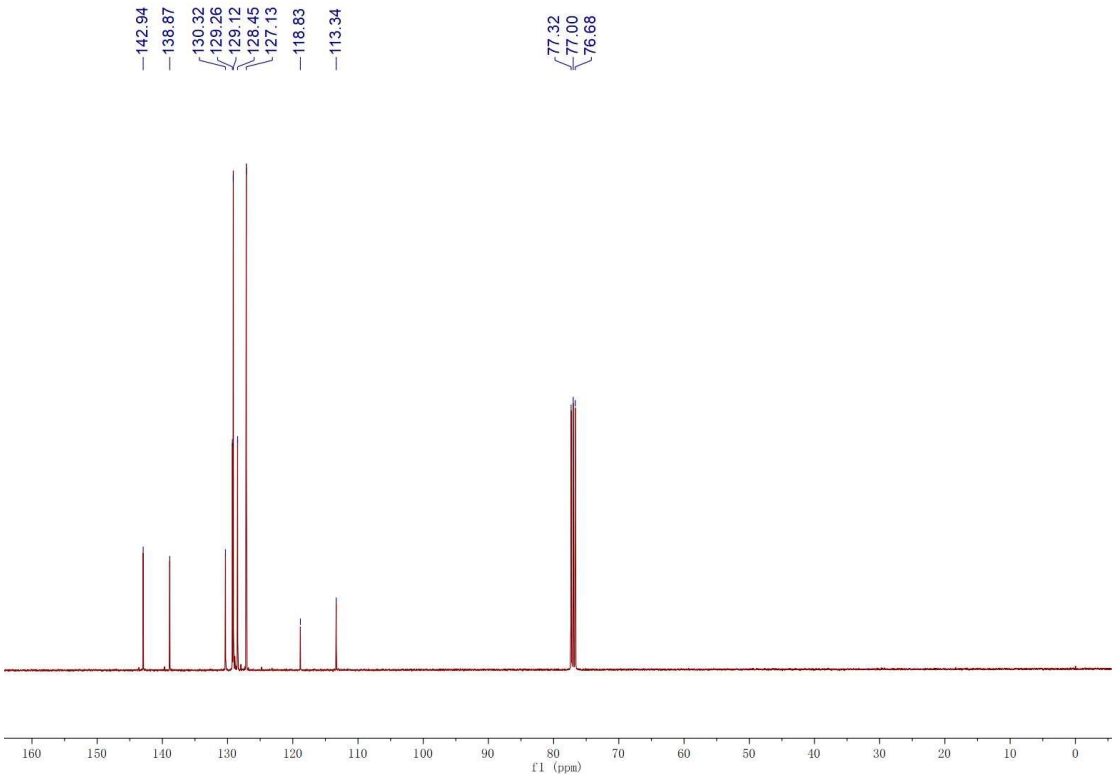

145.57
145.03
136.44
132.52
128.61
127.44
127.11
119.03
110.46
77.32
77.00
76.68
28.53
15.49
CN
Et
3u
f1 (ppm)

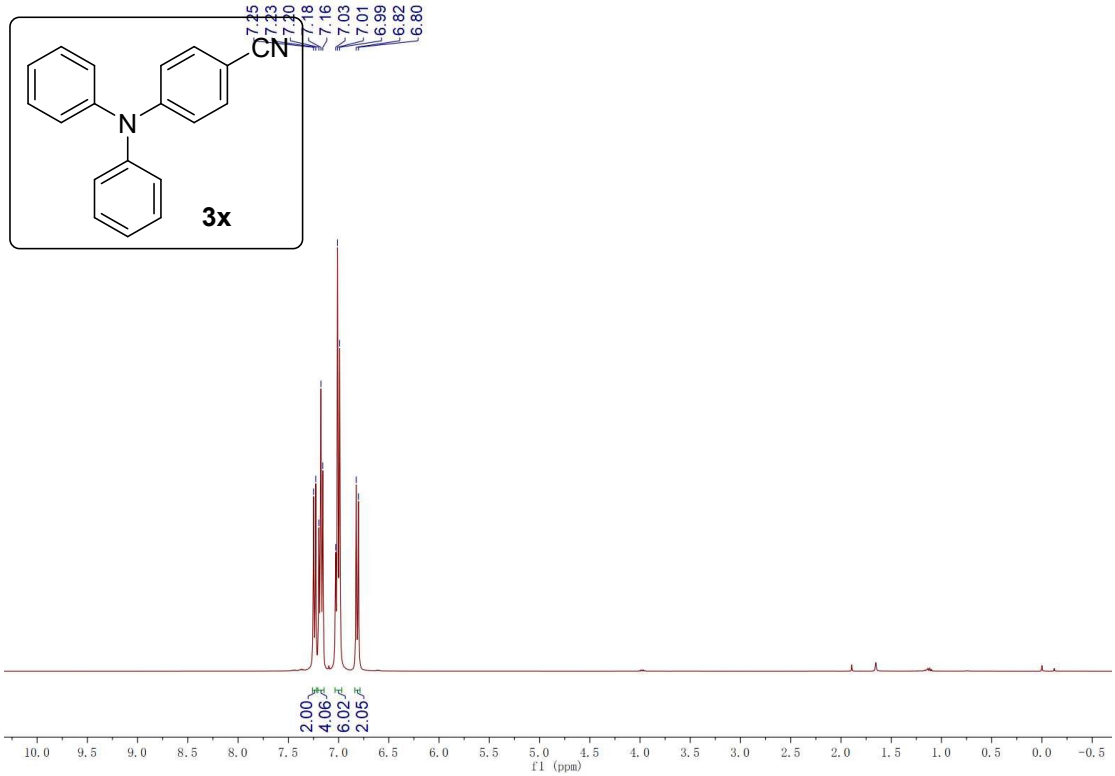

7.91
7.89
7.87
7.76
7.73
7.71
7.69
7.53
7.53
7.52
7.51
7.50
7.49
7.49
7.48
7.47
7.47
7.45
7.45
7.43
7.42
7.41
7.41
7.35
7.33
CN
3v
2.00
3.03
4.03
1.02
0.99
f1 (ppm)

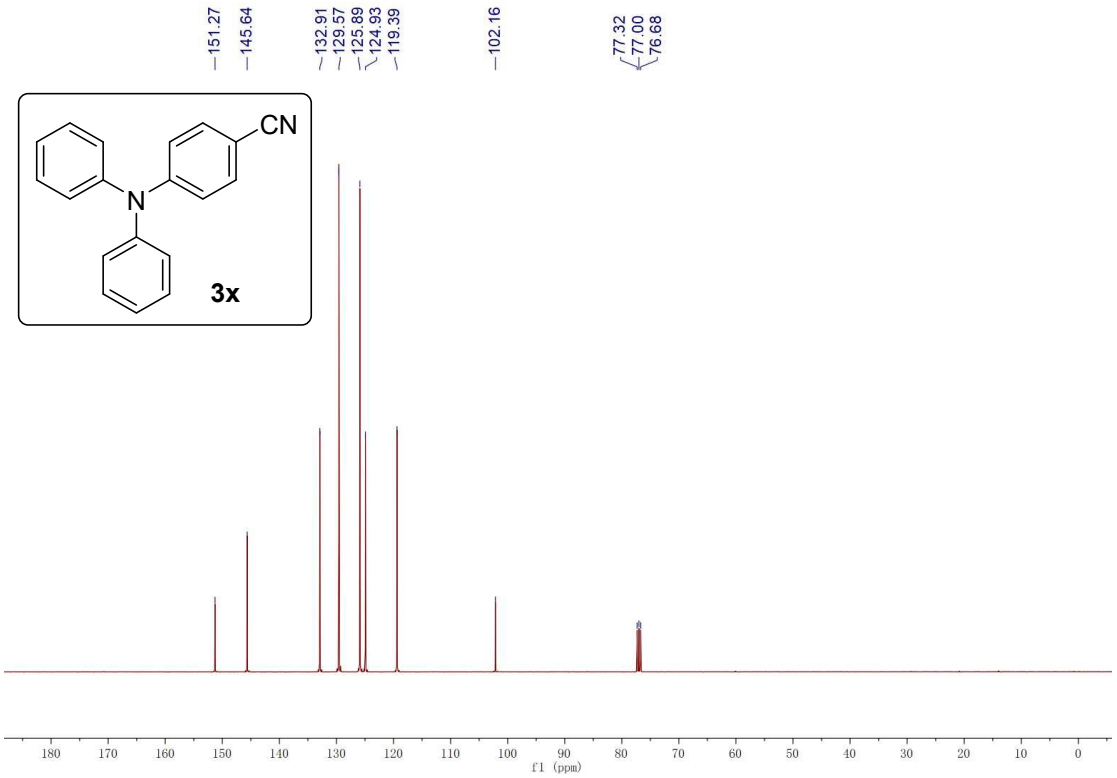

145.38
137.96
131.93
130.71
130.59
128.61
128.39
126.88
126.49
126.02
125.19
124.99
118.78
110.90
77.32
77.00
76.68
CN
3v
f1 (ppm)

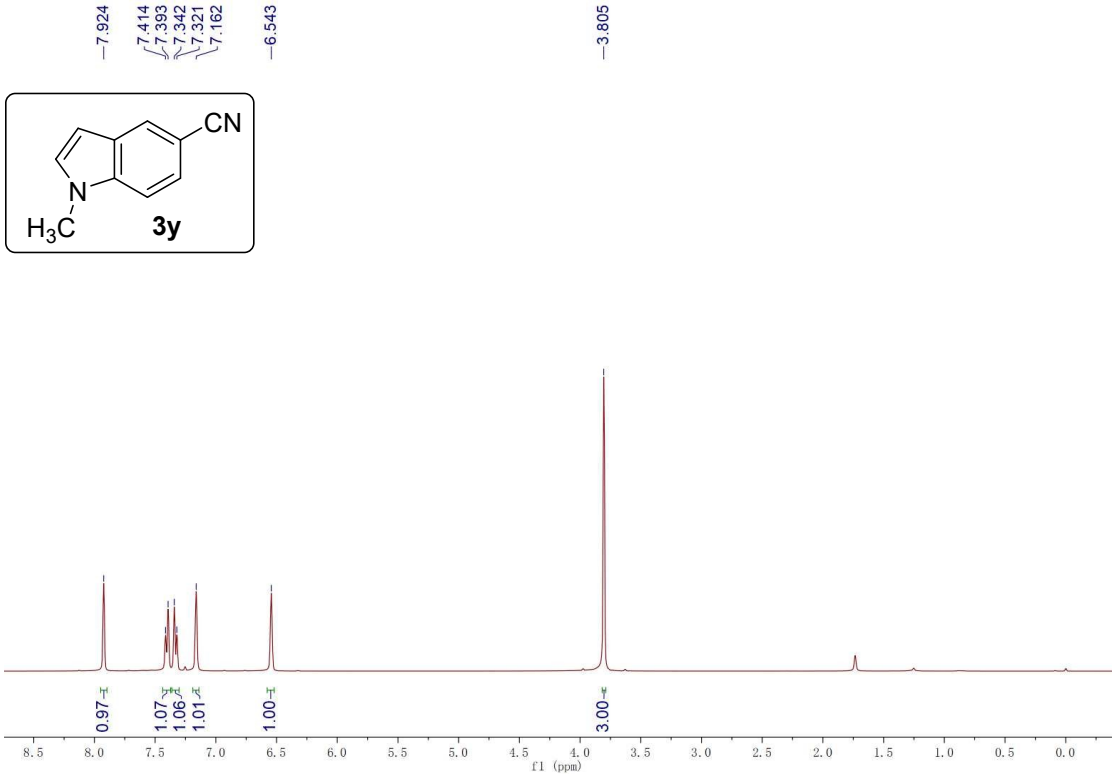

7.98
7.82
7.81
7.61
7.59
7.51
7.49
7.47
7.45
7.43
7.41
CN
3w
1.00
2.01
4.00
4.05
2.02
f1 (ppm)


CN
3w


142.94
138.87
130.32
129.26
129.12
128.45
127.13
118.83
113.34
77.32
77.00
76.68
f1 (ppm)


7.25
7.23
7.20
7.18
7.16
7.03
7.01
6.99
6.82
6.80
CN
N
3x
2.00
4.06
6.02
2.05
f1 (ppm)


151.27
145.64
132.91
129.57
125.89
124.93
119.39
102.16
77.32
77.00
76.68
CN
N
3x
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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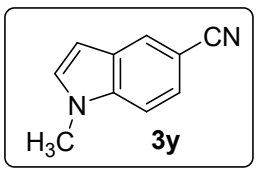
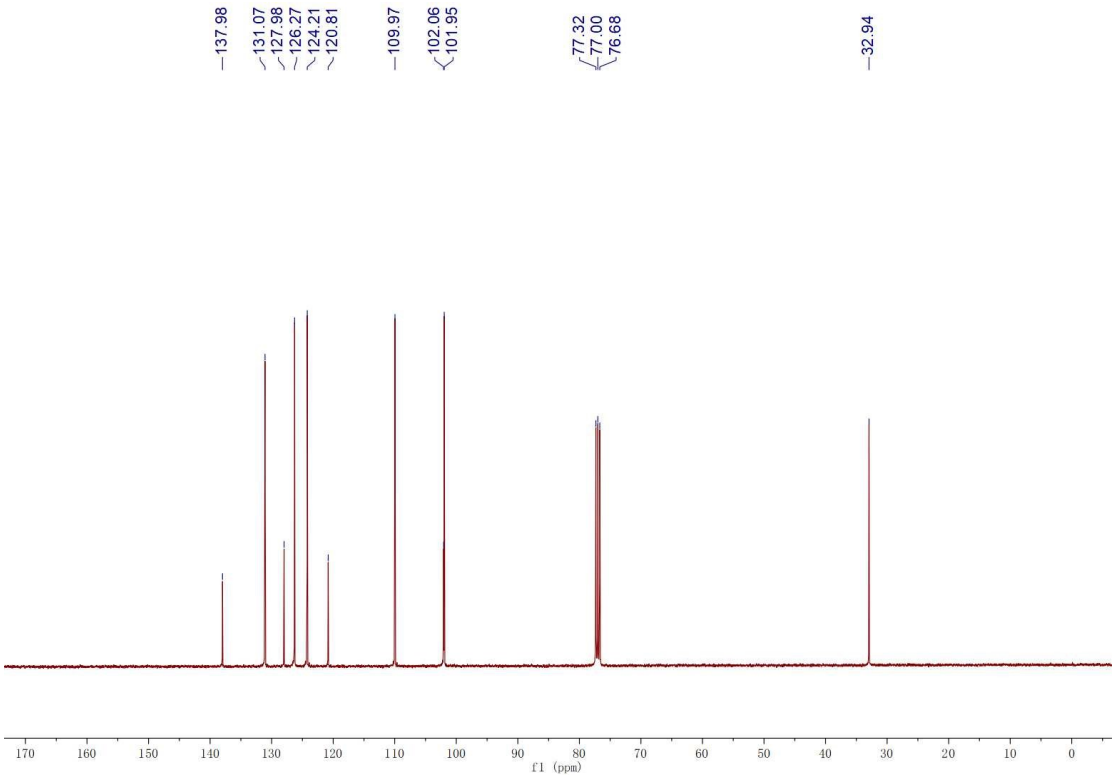
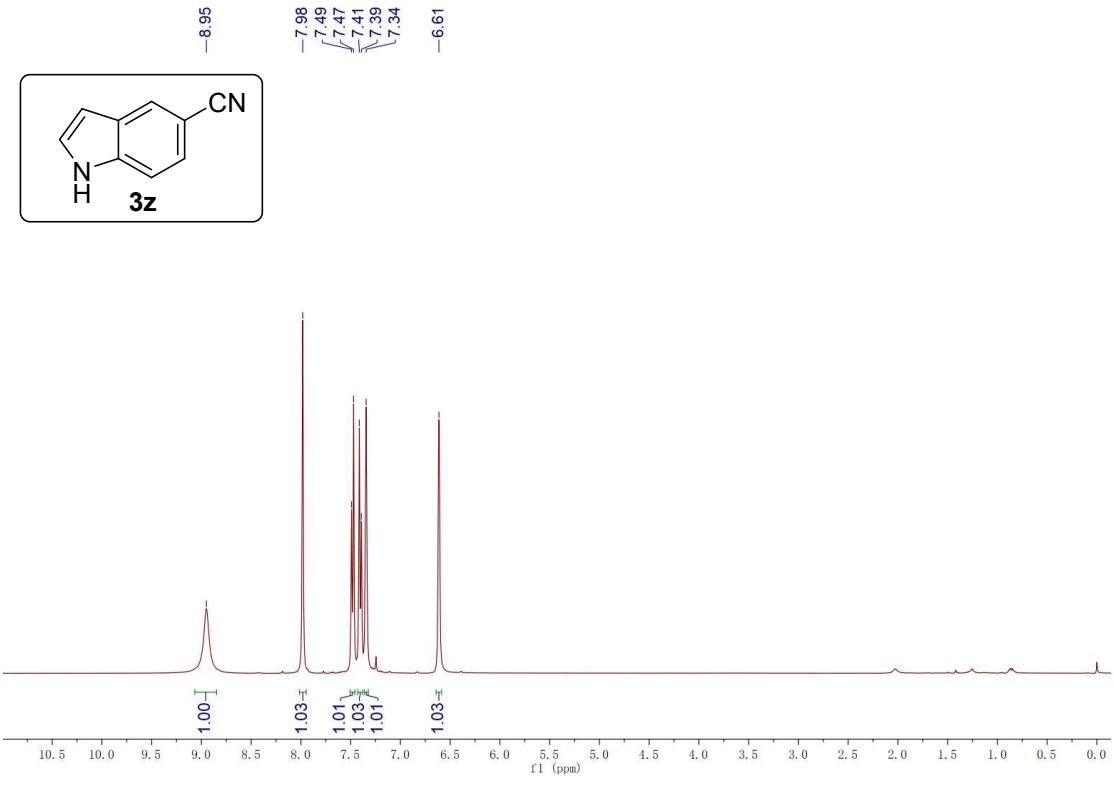
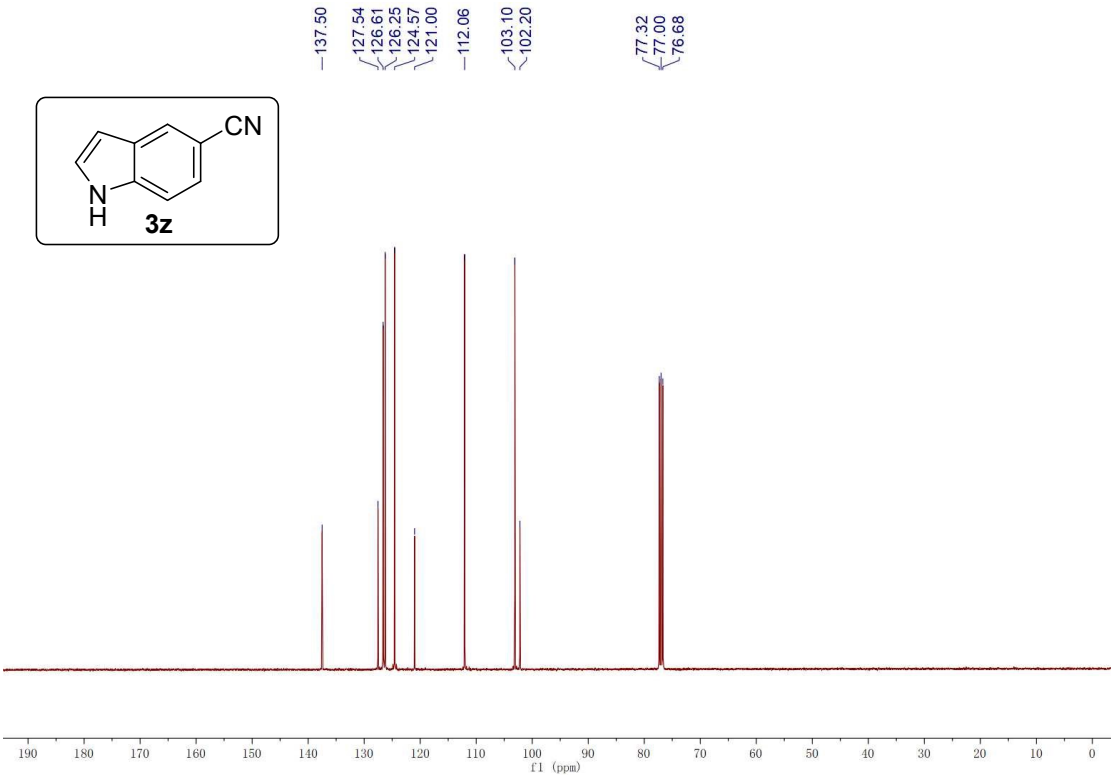
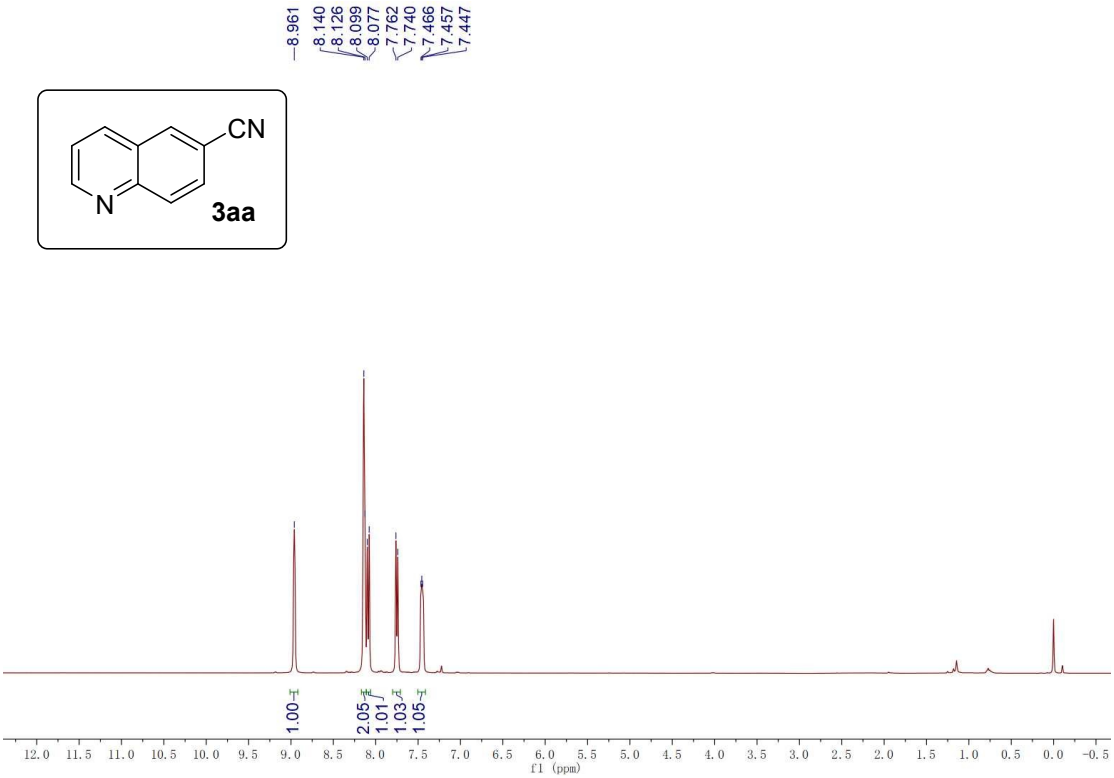
7.414
7.393
7.342
7.321
7.162
6.543
3.805
CN
N
H3C
3y
0.97
1.07
1.06
1.01
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


CN
N
H3C
3y


137.98
131.07
127.98
126.27
124.21
120.81
109.97
102.06
101.95
77.32
77.00
76.68
32.94
f1 (ppm)


8.95
7.98
7.49
7.47
7.41
7.39
7.34
6.61
CN
N
H
3z
1.00
1.03
1.01
1.03
1.01
1.03
f1 (ppm)


137.50
127.54
126.61
126.25
124.57
121.00
112.06
103.10
102.20
77.32
77.00
76.68
CN
N
H
3z
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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7.466
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7.447
CN
N
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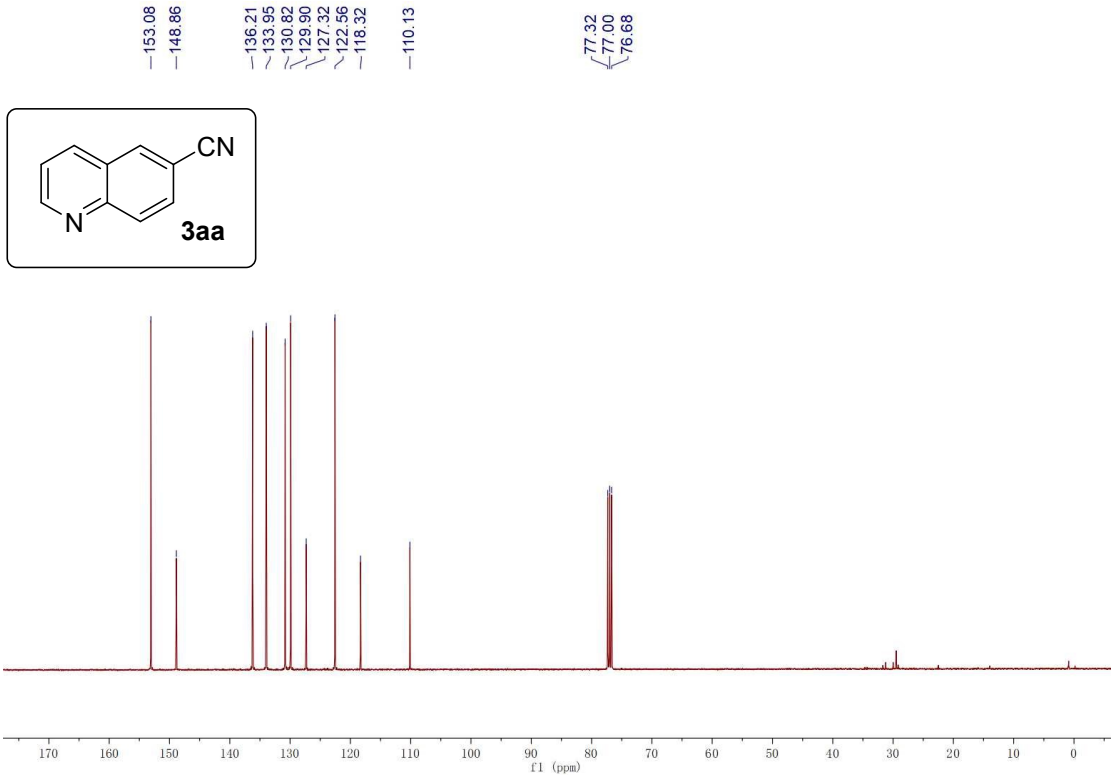
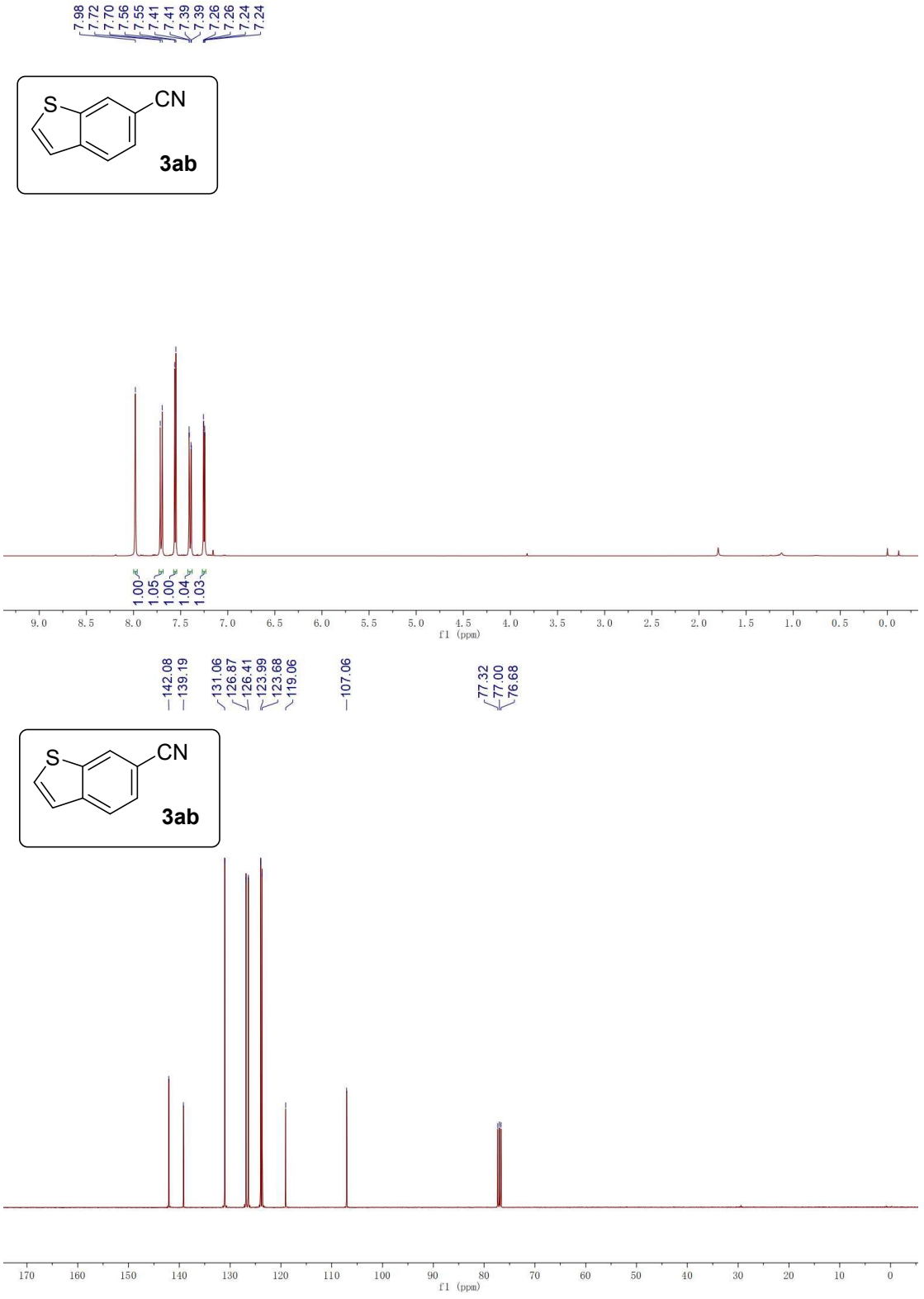
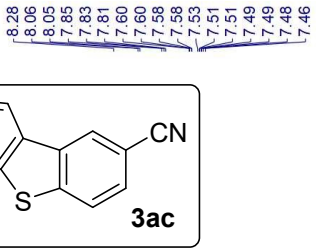
2.05
1.01
1.03
1.05
f1 (ppm)


153.08
148.86
136.21
133.95
130.82
129.90
127.32
122.56
118.32
110.13
77.32
77.00
76.68
CN
N
3aa
f1 (ppm)


7.98
7.72
7.70
7.56
7.55
7.41
7.41
7.39
7.39
7.26
7.26
7.24
7.24
S
CN
3ab
1.00
1.05
1.00
1.04
1.03
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)
142.08
139.19
131.06
126.87
126.41
123.99
123.68
119.06
107.06
77.32
77.00
76.68
S
CN
3ab
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.85
7.83
7.81
7.60
7.60
7.58
7.58
7.53
7.51
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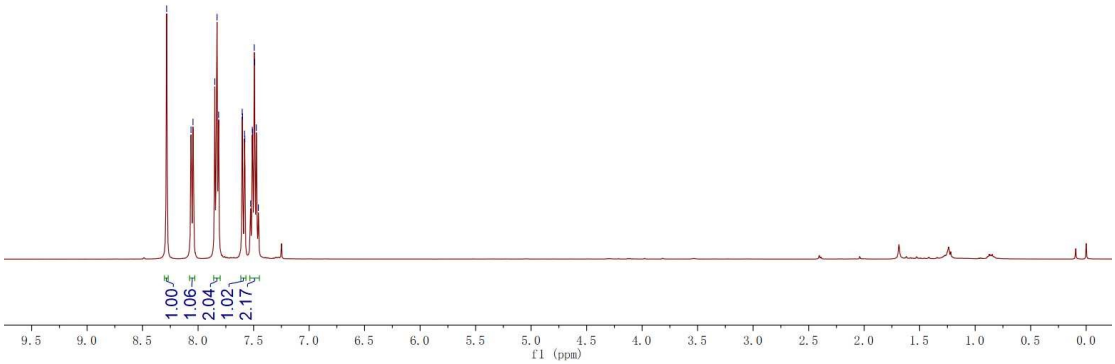
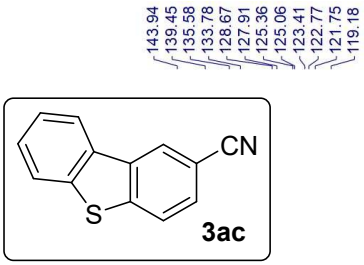
7.49
7.49
7.48
7.46
CN
S
3ac


1.00
1.06
2.04
1.02
2.17
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)


143.94
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135.58
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128.67
127.91
125.36
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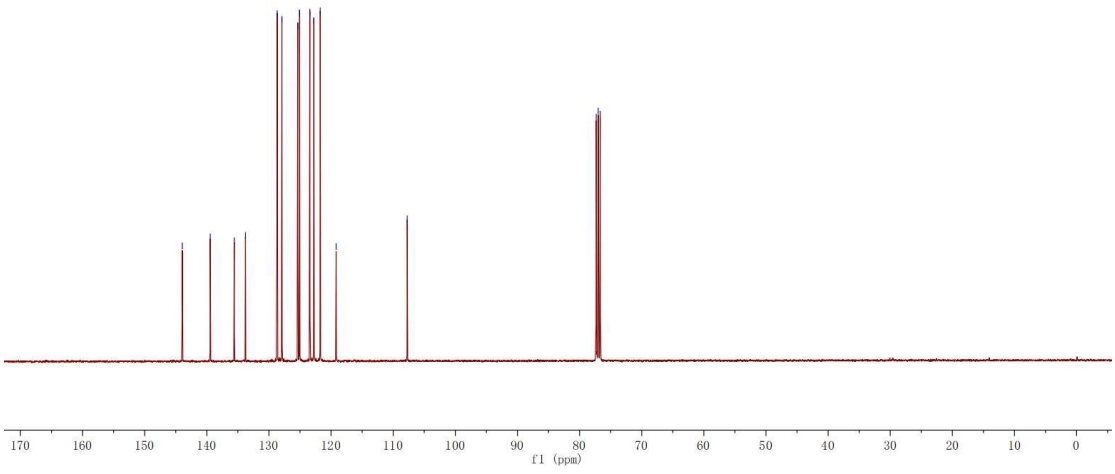
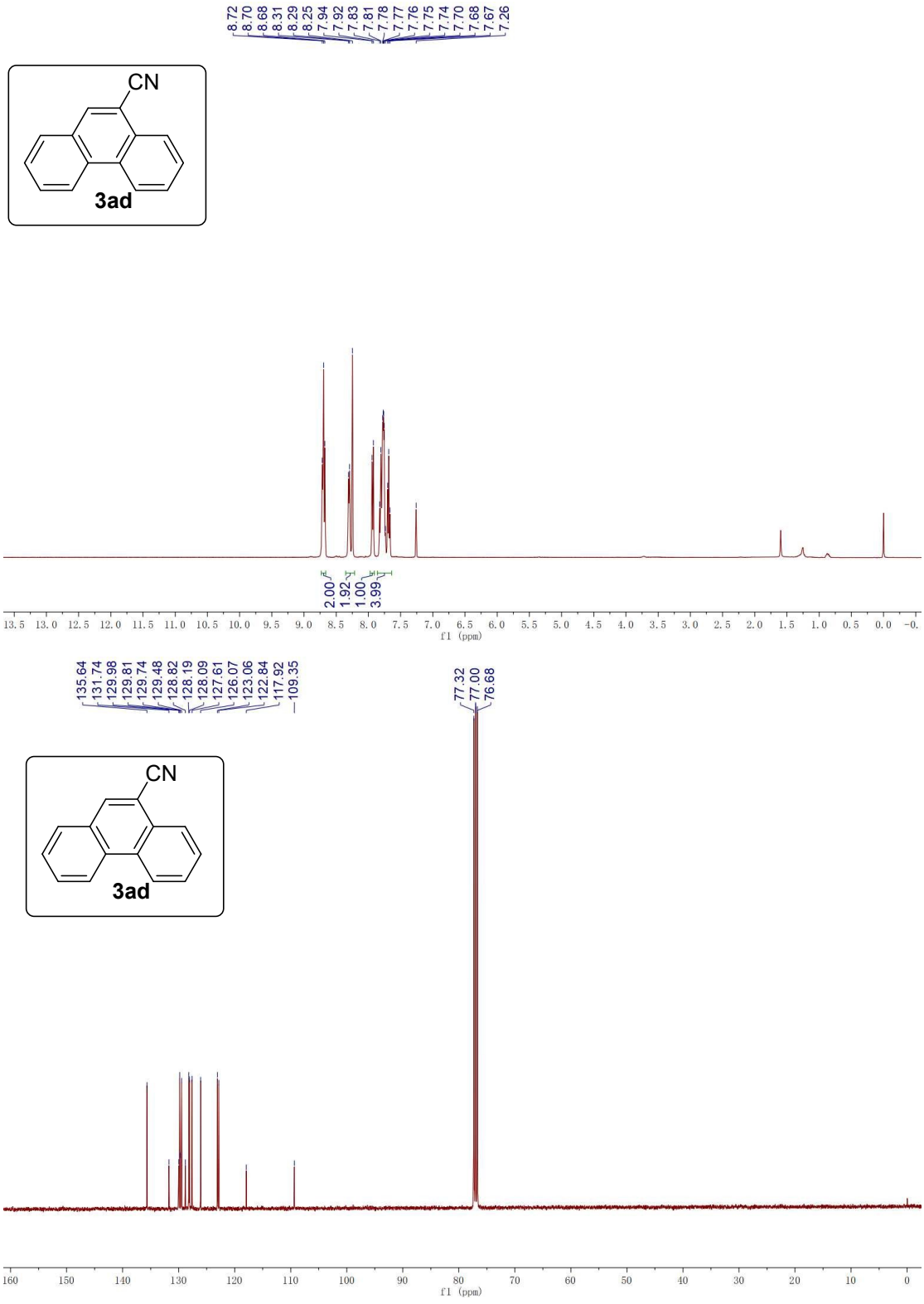
122.77
121.75
119.18
107.74
77.32
77.00
76.68
CN
S
3ac


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.68
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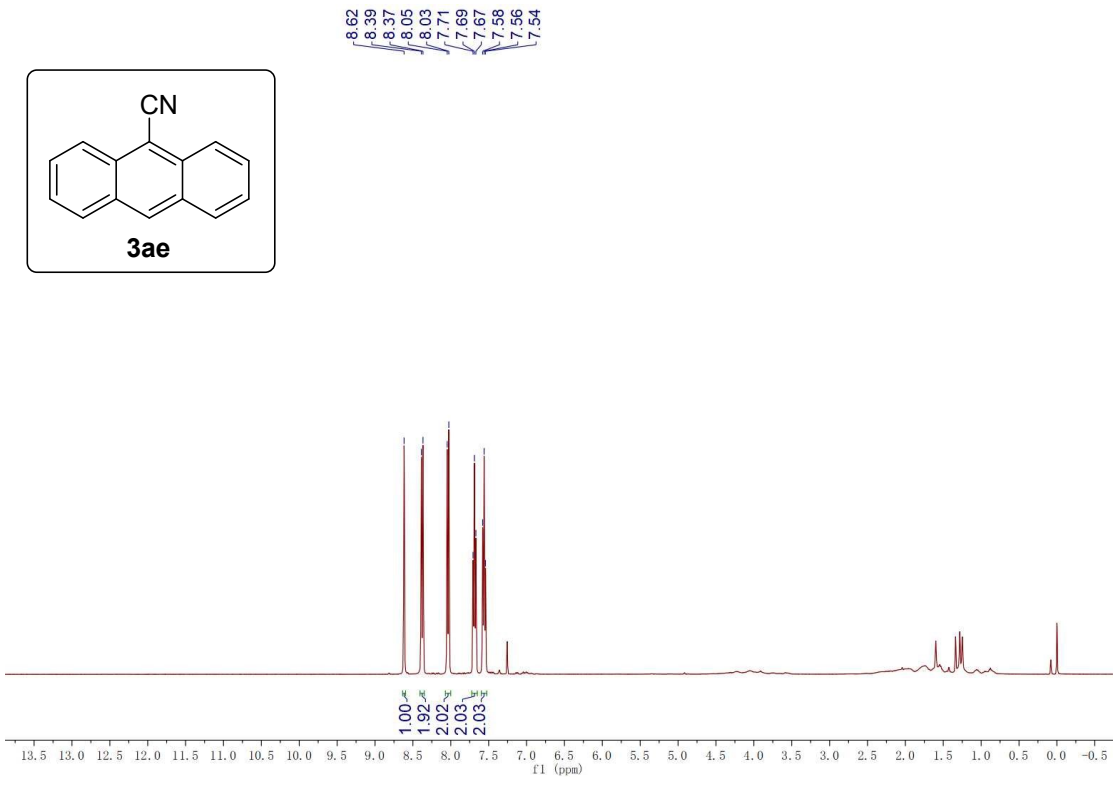
8.29
8.25
7.94
7.92
7.83
7.81
7.78
7.77
7.76
7.75
7.74
7.70
7.68
7.67
7.26
CN
3ad
2.00
1.92
1.00
3.99
f1 (ppm)
135.64
131.74
129.98
129.81
129.74
129.48
128.82
128.19
128.09
127.61
126.07
123.06
122.84
117.92
109.35
77.32
77.00
76.68
CN
3ad
f1 (ppm)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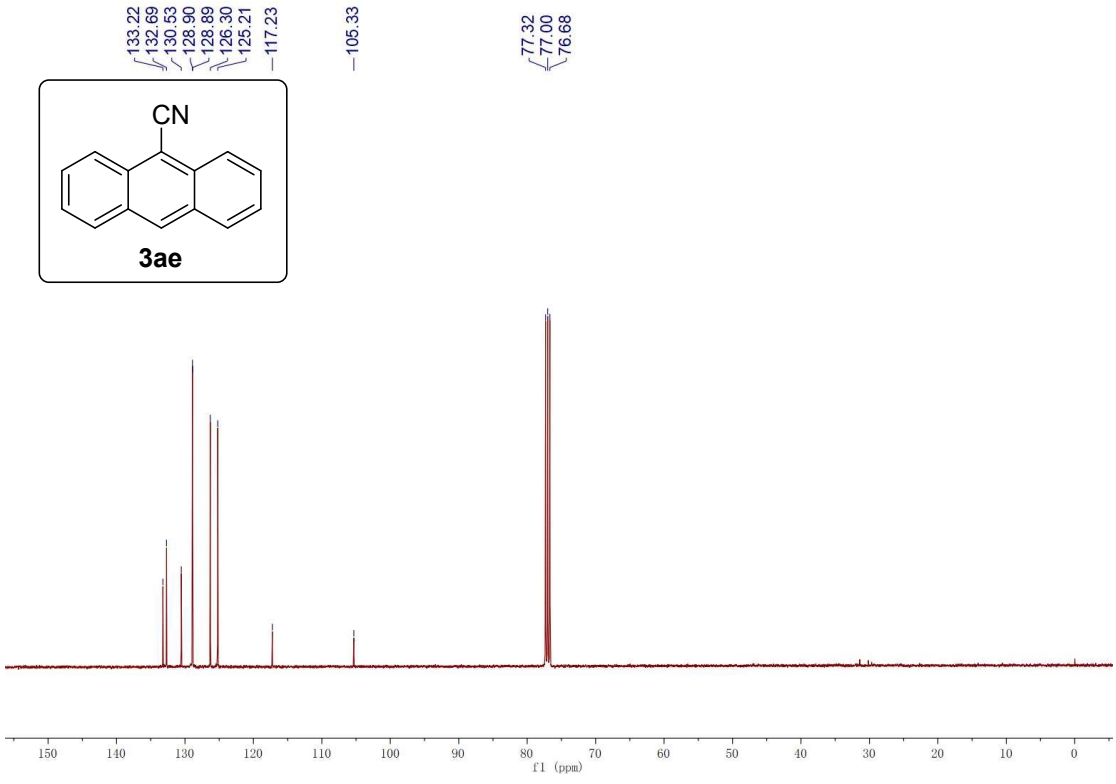
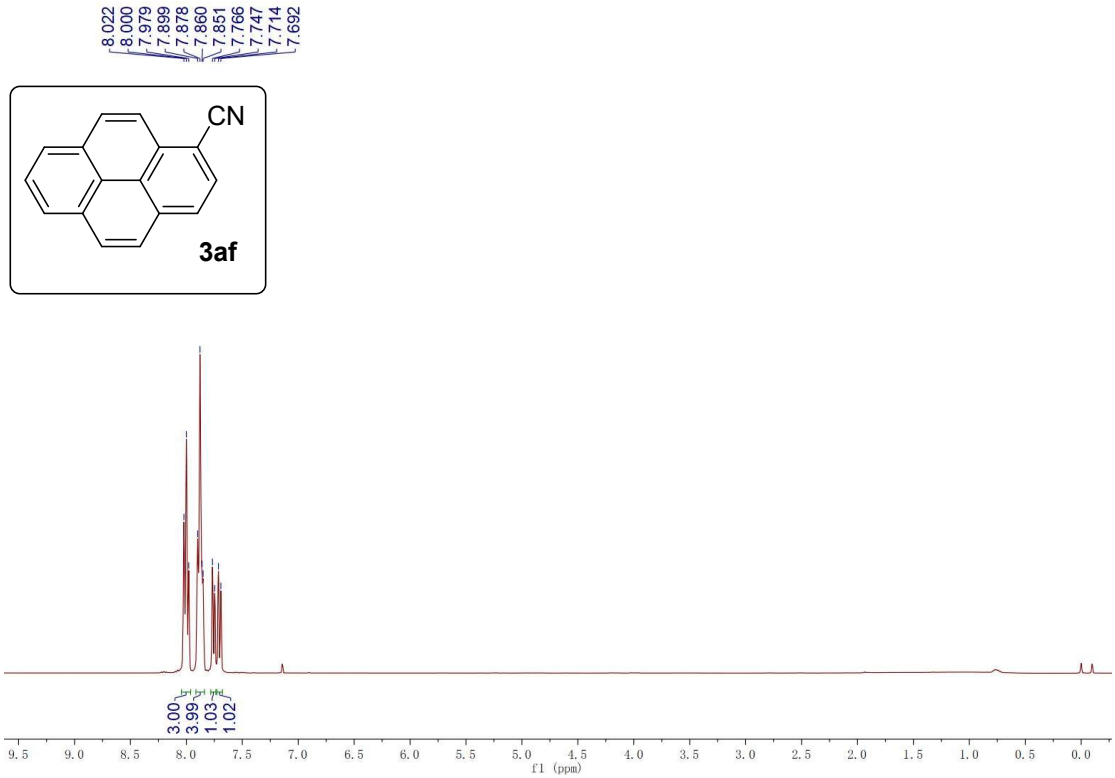
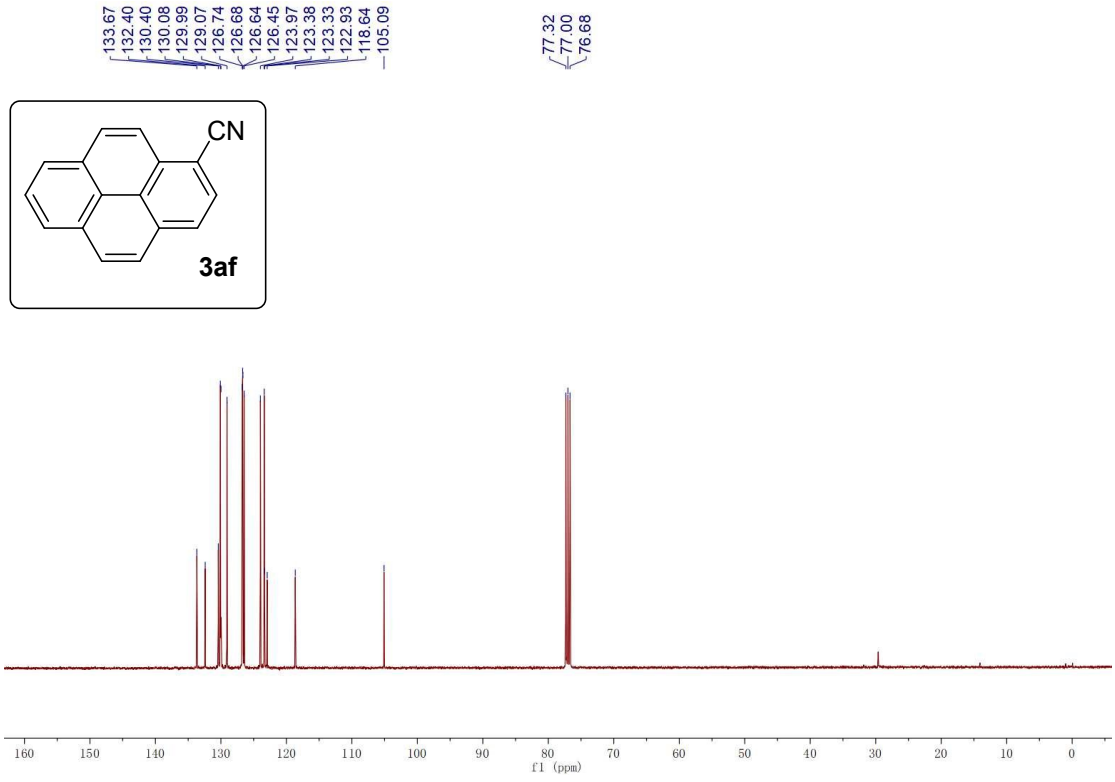
7.67
7.58
7.56
7.54
CN
3ae
1.00
1.92
2.02
2.03
2.03
f1 (ppm)


133.22
132.69
130.53
128.90
128.89
126.30
125.21
117.23
105.33
77.32
77.00
76.68
CN
3ae
f1 (ppm)


8.022
8.000
7.979
7.899
7.878
7.860
7.851
7.766
7.747
7.714
7.692
CN
3af
3.00
3.99
1.03
1.02
f1 (ppm)


133.67
132.40
130.40
130.08
129.99
129.07
126.74
126.68
126.64
126.45
123.97
123.38
123.33
122.93
118.64
105.09
77.32
77.00
76.68
CN
3af
f1 (ppm)