Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

A Novel Electromagnetic Mill Promoted Mechanochemical Solid-State Suzuki–Miyaura Cross-Coupling Reactions Using Ultra-Low Catalyst Loading

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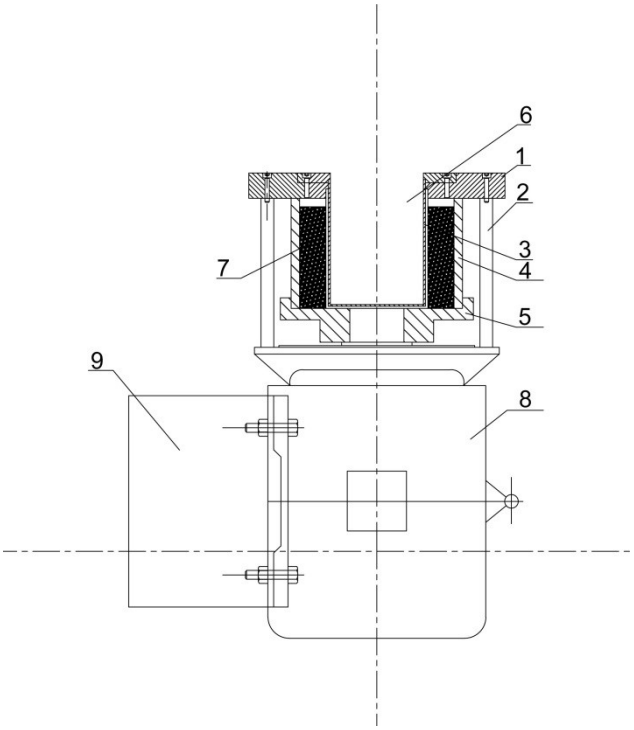
1. General Information

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 Materials 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 vessels in a Magnetic grinding machine. The reaction bottles used were commercially available 10 ml flat bottom flask or customized reaction jar（6.5◊8cm）.The grinding medium is customized ferromagnetic rods（3.5◊0.5mm）. ^{1}H NMR (400 MHz), ^{13}C 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,and the instrument consists of two parts, the working room(left blue part of the picture) and the console(right part of the picture). The left cavity is the main working part. The four square magnets rotate around the cavity to form a rotating magnetic field, which drives the ferromagnetic rod to move. The magnetic field strength is about 0.2T. Unknown compounds synthesized in the manuscript as follows:3p 3q 3u 3w 3x 4a 4b 4f 4l 4n 4o 4p 4s 4t 6c 7b 7c 7d 7e 8b 8d.

Figure S1. Magnetic Ginding equipment



1 Fixed disc

2 Support shaft

3 Jacket

4 Rotating body

5 Rotating seat

6 Grinding space

7 Magnet

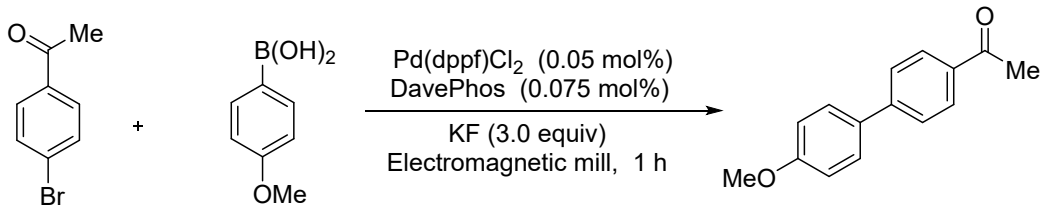
8 Frequency conversion motor

9 Bearing bracket

Figure S2. Plan view of Magnetic Ginding equipment(left blue part)

2. General Procedure for Solid-State Cross-Coupling

1) Procedure I:General solid-state cross –coupling reaction



1a **2a** **3a**

Aryl halide **1a** (199.04mg. 1mmol 1.0equiv), aryl boronic acid **2a** [181.2mg(10mg+171.2mg), 1.2mmol, 1.2 equiv], $Pd(dppf)Cl_2$ (0.4mg. 0.05% mmol) and DavePhos (0.3mg, 0.075%mmol), KF (174.21mg, 3mmol 3.0 equiv) ferromagnetic rods 5g (about a quarter of the volume of the bottle)were placed in a flat bottom flask. Put it in magnetic grinder. After 1 h , the mixture was dissolved in CH_2Cl_2, filtering out ferromagnetic rods. Then remove the inorganic salt from the mixture with water. The organic phase was combined, dried over Na_2SO_4, evaporated and purified by flash chromatography (PE: EA = 10:1) to give compound **3a** (224.0 mg, 99% yield).

Weighting of 0.4 mg $Pd(dppf)Cl_2$ and 0.3mg DavePhos,taking procedure 1 as an example ,frist we weight 4 mg cataltst,3 mg DavePhos and 100 mg 2a into a 100 ml eggplant-shaped flask, than dissolve with 20 ml $CHCl_3$,stir well ,and then spin dry to vacuumize. When we weigh 2a, we first weigh 10 mg of the mixed starting material, which contains 0.4 mg of catalyst and 0.3 mg of ligand, and then weigh 171.2 mg of pure product 2a.

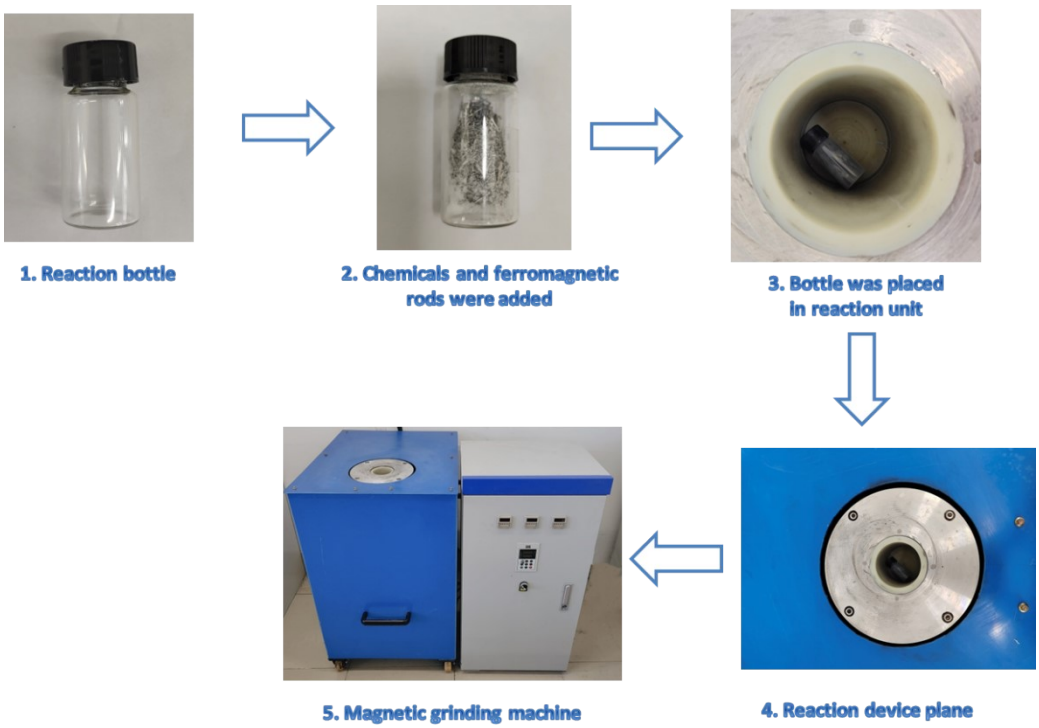
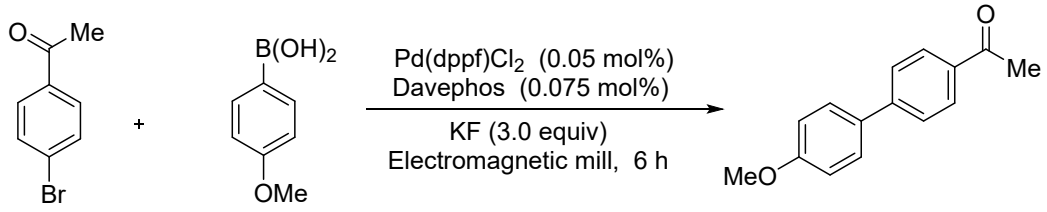


Figure S3. Set-up procedure for the solid-state cross-coupling.

2) Procedure II: Procedure for Solid-State Cross-Coupling at Gram Scale

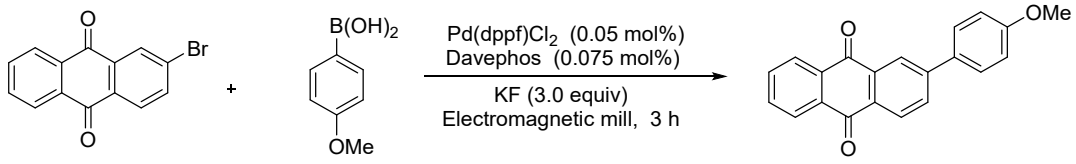


1a **2a** **3a**

A

ryl halide **1a** (2g. 5mmol 1.0equiv), aryl boronic acid **2a** (1.81g, 6.1mmol, 1.2 equiv), Pd(dppf)Cl_2 (1.8 mg. 0.05% mmol) and DavePhos (1.5 mg, 0.075% mmol), KF (0.87g, 1.5mmol 3.0 equiv) ferromagnetic rods 20g (about a quarter of the volume of the jar) were placed in ferromagnetic rods. After 6 h, the mixture was dissolved in CH_2Cl_2, filtering out ferromagnetic rods .Then remove the inorganic salt from the mixture with water. The organic phase was combined, dried over Na_2SO_4, evaporated and purified by flash chromatography (PE:EA = 10:1) to give compound **3a** (2.08g, 92% yield).

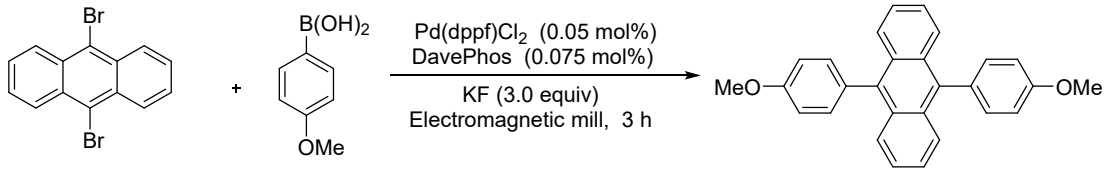
3) Procedure III: Coupling procedure for fluorescent products



1-6a **2a** **6a**

Aryl halide **1-6a** (287.11mg. 1mmol 1.0equiv), aryl boronic acid **2a** (181.2mg, 1.2mmol, 1.2 equiv), Pd(dppf)Cl_2 (0.4 mg. 0.05% mmol) and DavePhos (0.3 mg, 0.075% mmol), KF (174.21g, 3mmol 3.0 equiv) ferromagnetic rods 5g (about a quarter of the volume of the jar) were placed in flat bottom flask. After 3 h, the mixture was dissolved in CH_2Cl_2, filtering out ferromagnetic rods .Then remove the inorganic salt from the mixture with water. The organic phase was combined, dried over Na_2SO_4, evaporated and purified by flash chromatography (PE: EA= 10:1) to give compound yellow solid **6a** (300mg, 95% yield).

4) Procedure IV: Coupling procedure for insoluble compounds



1-7a **2a** **7a**

Aryl halide **1-7a** (168.01mg. 0.5mmol 1.0equiv), aryl boronic acid **2a** (181.2mg, 1.2mmol, 1.2 equiv), Pd(dppf)Cl_2 (0.4 mg. 0.05% mmol) and DavePhos (0.3 mg, 0.075% mmol), KF (174.21g, 3mmol 3.0 equiv) ferromagnetic rods 5g (about a quarter of the volume of the jar) were placed in flat bottom flask. After 1 h, the mixture was dissolved in CH_2Cl_2, filtering out ferromagnetic rods .Then remove the inorganic salt from the mixture with water. The organic phase was combined, dried over Na_2SO_4, evaporated and purified by flash chromatography (PE: EA = 10:1-1:1) to give compound yellow solid **7a** (145mg, 74% yield).

Solubility evaluation of compounds

An compound (7d.7e) and toluene were add vial and stirred for 1 h at room temperature (23°C). Then the mixture was filtered using a syringe filter (diameter; 0.22 um) and concentrated under reduced pressure until the weight of a flask with the obtained solid was not changed. The solubility was evaluated by measuring the weight of the obtained solid. (1-7a, 1-7b, 1-7c solubility [1])

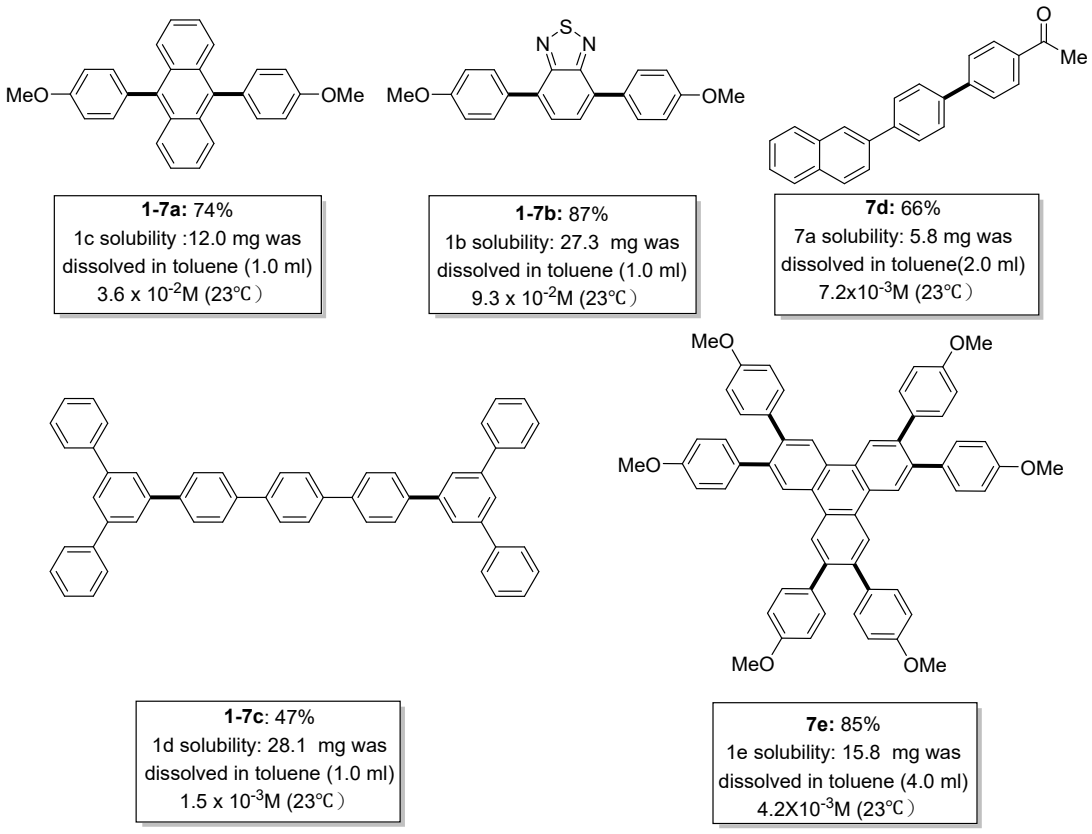
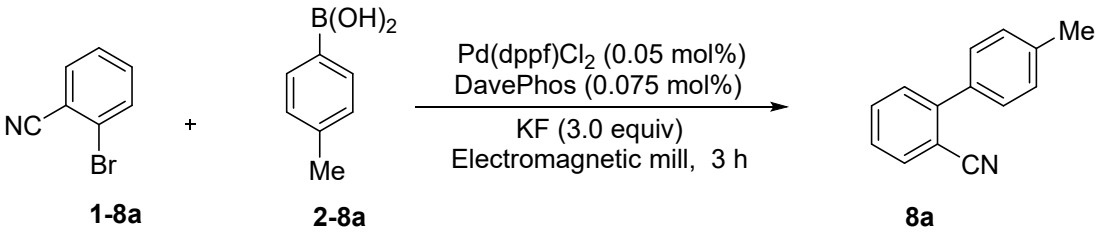


Figure S4.Solubility evaluation of compounds.

4) Procedure V: General procedure for drug molecular coupling



Aryl halide **1-8a** (182.02mg. 1mmol 1.0equiv), aryl boronic acid **2-8a** (163.152mg, 1.5mmol, 1.2 equiv), Pd(dppf)Cl_2 (0.4 mg. 0.05% mmol) and DavePhos (0.3 mg, 0.075% mmol), KF (174.21g, 3mmol 3.0 equiv) ferromagnetic rods 5g (about a quarter of the volume of the jar) were placed flat bottom flask. After 1 h, the mixture was dissolved in CH_2Cl_2, filtering out ferromagnetic rods .Then remove the inorganic salt from the mixture with water. The organic phase was combined, dried over Na_2SO_4, evaporated and purified by flash chromatography (PE: EA = 10:1) to give compound white solid **8a** (139.14mg, 72% yield).

3. Ferromagnetic rods of different specifications

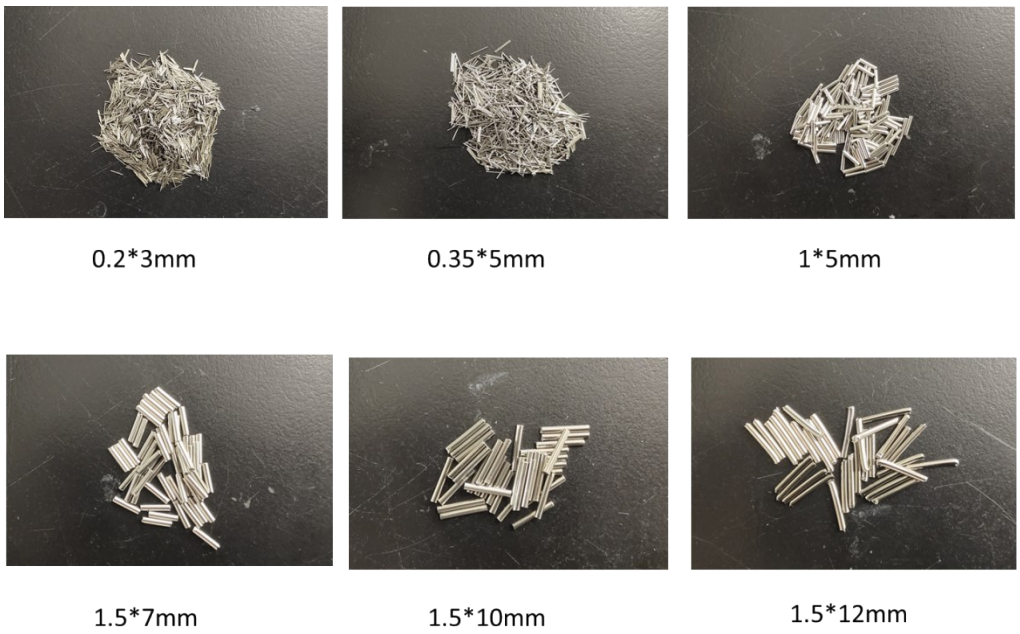


Figure S5. Ferromagnetic rods of different sizes used in experiments

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

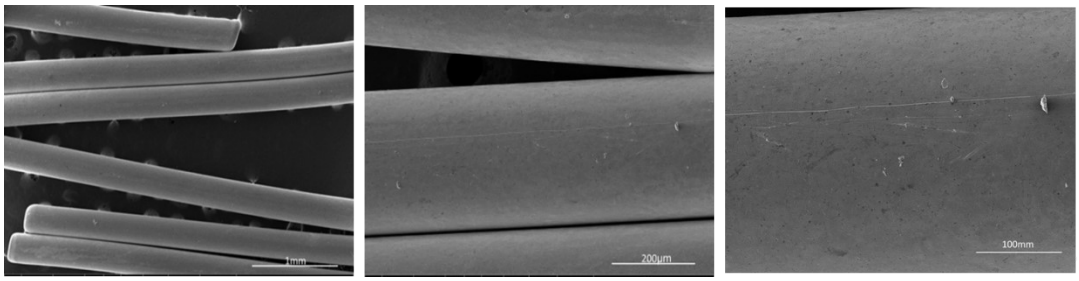
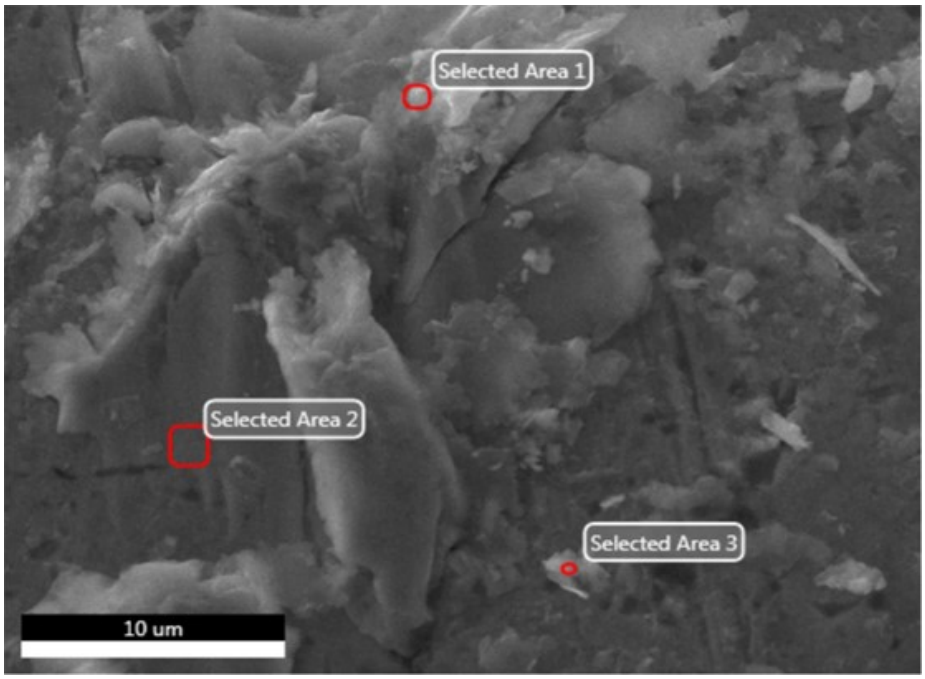
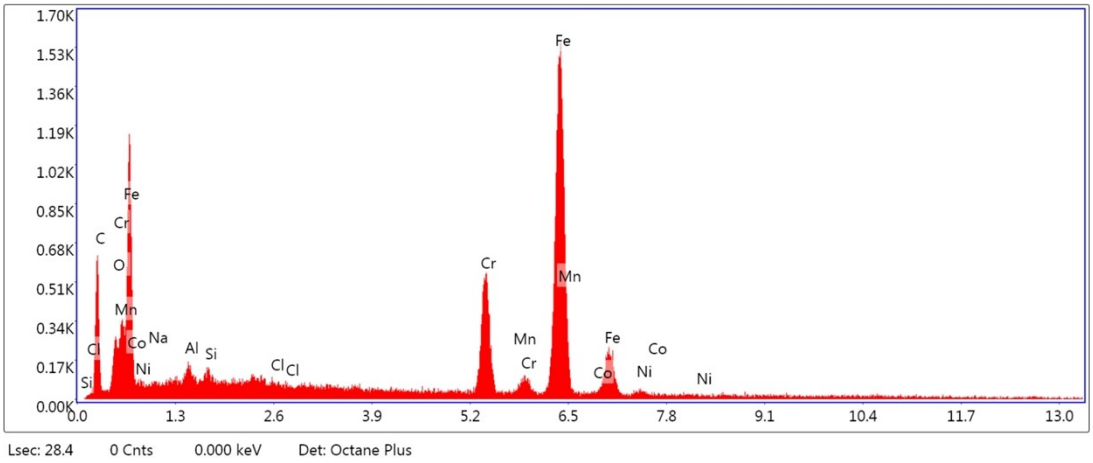


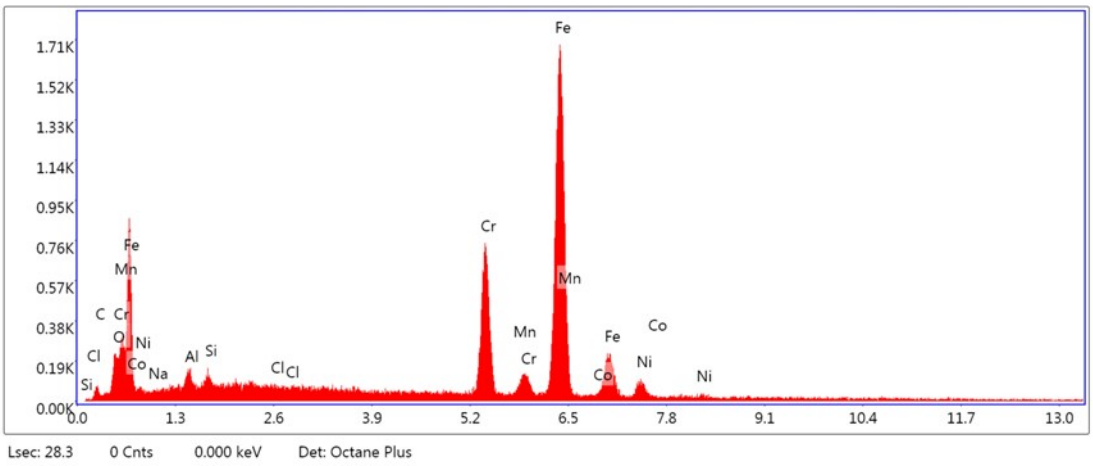
Figure S6. Morphology of ferromagnetic rod under scanning electron microscope



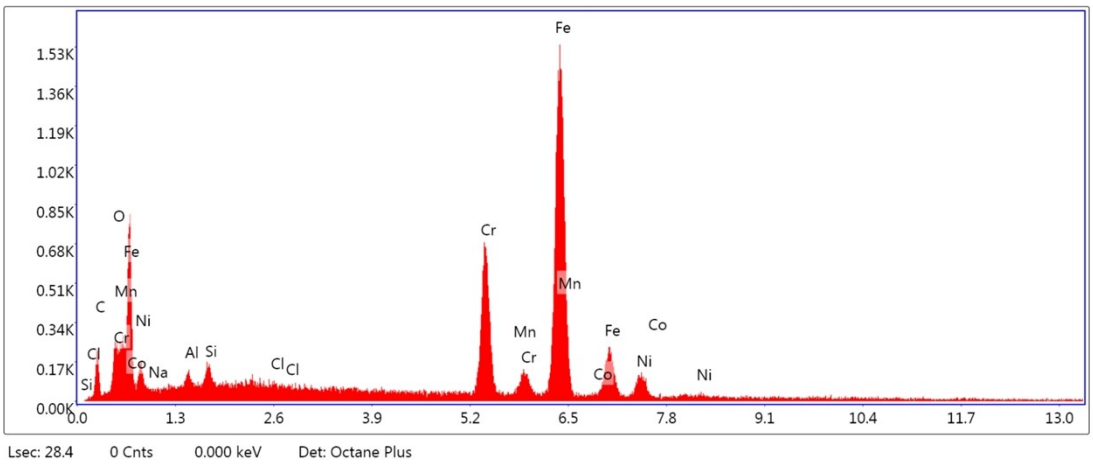
Selected Area 1



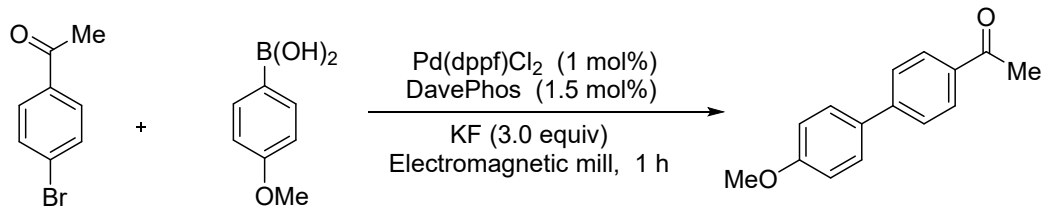
Selected Area 2



Selected Area 3

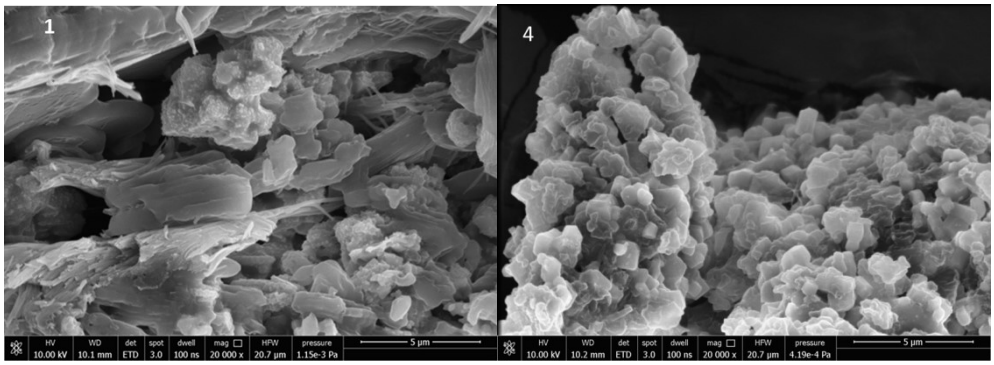


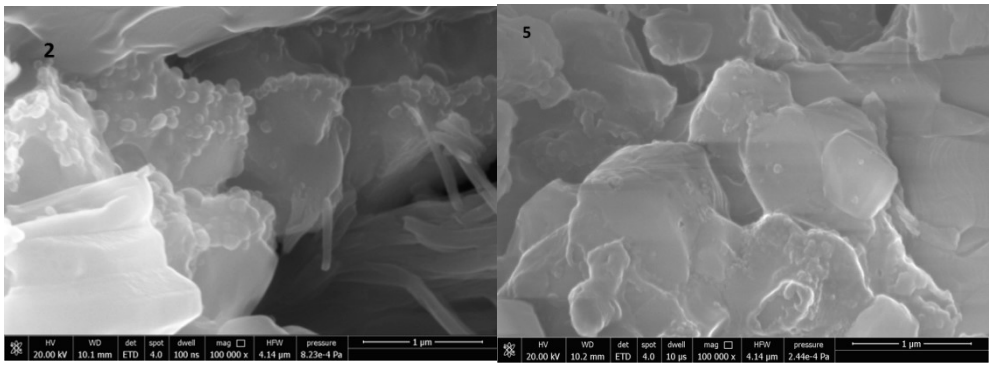
5. SEM analysis for crude product and Mapping images of palladium.



1a **2a** **3a**

Aryl halide 1a (199.04mg. 1mmol 1.0equiv), aryl boronic acid 2a [181.2mg, 1.2mmol, 1.2 equiv], Pd(dppf)Cl_2 (7.3mg. 15% mmol) and DavePhos (3.9mg, 1.5%mmol), KF (174.21mg, 3mmol 3.0 equiv) ferromagnetic rods 5g were placed in a flat bottom flask. Set up a set of control experiment (before the reaction) and one put in the grinder for 1 h (after the reaction). The ferromagnetic rods were separated, and the crude product was ground into powder for SEM analysis and the results as followes:





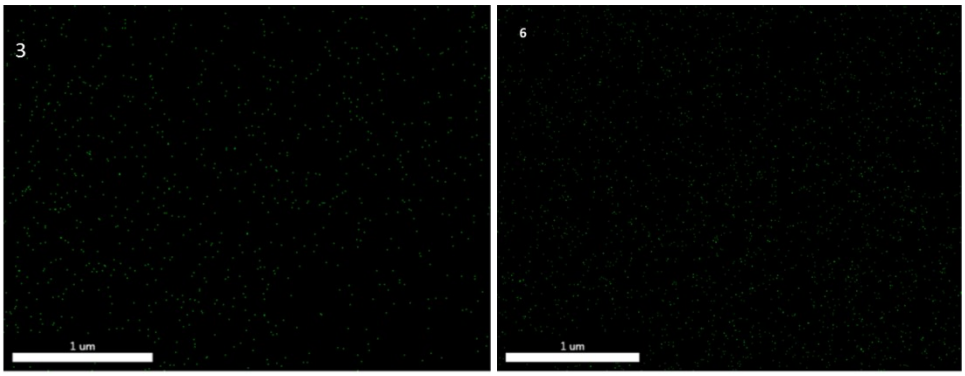
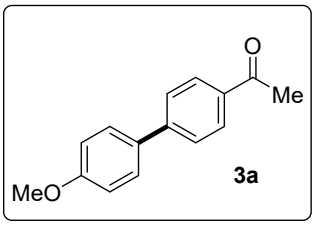


Figure S7. 1 and 2: SEM images of the crude reaction mixtures before the reaction. 3: Mapping images of palladium before the reaction. 4 and 5: SEM images of the crude reaction mixtures (after 1 h with 1 mol% palladium catalyst). 6: Mapping image of palladium after the reaction was completed.

6. Reaction Temperature Confirmed by Electronic temperature measuring gun

The temperature inside the reaction bottle after the solid-state coupling reaction was confirmed by Electronic temperature measuring gun.The crude mixtures were prepared by the following **standard conditions:** 1 mmol of **1a**; 1.2 mmol of **1b**; 0.0005 mmol of $PdCl_2$(dppf); 0.00075 mmol of DavePhos, 3 mmol of KF, 50 Hz; 1 h. The obtained date showed that the temperature was around 75^{o}C.

7. Characterization of Obtained Coupling Products.



1-(4'-methoxy-[1,1'-biphenyl]-4-yl)ethan-1-one

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

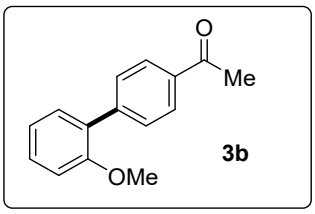
$C_{15}H_{14}O_2$ Melting Point :150.0 °C -153.7 °C

MW: 226.28 g·mol^{-1} **White Solid** **Isolated amounts**: 224.0 mg **Yield**: 99%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.01 (d, *J* =7.6 Hz, 2H), 7.64 (d, *J* =7.6 Hz, 2H), 7.58 (d, *J* =8.0 Hz, 2H), 7.00 (d, *J* =8.0 Hz, 2H), 3.86(s, 3H). 2.63 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.75, 159.84, 145.31, 135.18, 132.16, 128.90, 128.31, 128.55, 114.34, 55.33, 26.60.

HRMS (ESI) Calcd for $C_{15}H_{14}O_2$+H 227.1080, Found 227.1072



1-(2'-methoxy-[1,1'-biphenyl]-4-yl)ethan-1-one

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

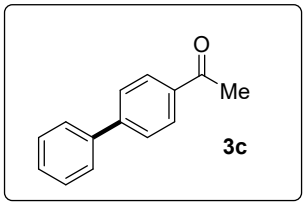
$C_{15}H_{14}O_2$ Melting Point :106.5 °C -106.8 °C

Melting Point were in agreement with the literature[3] (105 °C -106 °C)

MW: 226.28 g·mol^{-1} **White Solid** **Isolated amounts**: 208.18 mg **Yield**: 92%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.00 (d, *J* =7.6 Hz, 2H), 7.64 (d, *J* =7.6 Hz, 2H) 7.36 (q, *J*=9.6 Hz, 2H), 7.07-7.00 (m, 2H), 3.83 (s, 3H), 2.64 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.90, 156.41, 143.56, 135.45, 130.69, 129.70, 129.46, 129.40, 128.06, 120.92, 111.28, 55.54, 26.65.



1-([1,1'-biphenyl]-4-yl)ethan-1-one

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

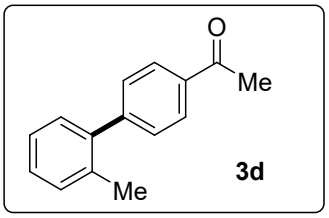
$C_{14}H_{12}O$ Melting Point :120.50 °C - 121.2 °C

Melting Point were in agreement with the literature[4] (117 °C -118 °C)

MW: 196.25g·mol^{-1} **Pale yellow solid** **Isolated amounts**:184.48 mg **Yield**: 94%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.04 (d, *J* =7.6 Hz, 2H), 7.69 (d, *J* =7.6 Hz, 2H) 7.63 (d, *J* =7.2 Hz, 2 H), 7.48 (t, *J* =7.2 Hz, 2H), 7.41(t, *J* =7.2 Hz, 1H), 2.64 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.75, 145.72, 139.79, 135.76, 128.90, 128.87, 128.18, 127.21, 127.17, 26.64.



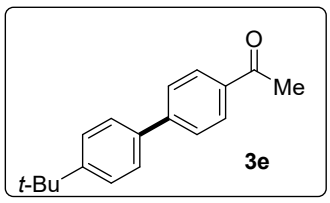
1-(2'-methyl-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[5]
$C_{15}H_{14}O$

MW: 210.28 g·mol^{-1} **Yellow Oil**

Isolated amounts: 203.97 mg **Yield**: 97%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.99 (d, *J* =7.6 Hz, 2H), 7.40 (d, *J* =7.6 Hz, 2H) 7.26-7.19 (m, 4 H), 2.61 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.52, 146.70, 140.50, 135.35, 134.89, 130.34, 129.28,129.24, 128.02, 127.71, 125.75, 26.42, 20.20



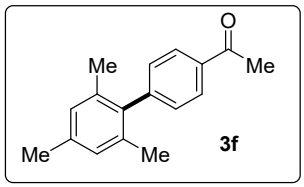
1-(4'-(tert-butyl)-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[6]
$C_{18}H_{20}O$ **Melting Point** :129.9 °C -131.2 °C

MW: 252.38 g·mol^{-1} **White Solid**

Isolated amounts: 239.76 mg **Yield**: 95%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.98 (d, *J* = 7.6 Hz, 2H), 7.64 (d, *J* =8.0 Hz, 2H), 7.55 (d, *J* =7.6 Hz, 2H), 7.47 (d, *J* =7.6 Hz, 2H),2.58 (s, 3H), 1.35 (s, 9H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.76, 151.41, 145.57 136.86, 135.55, 128.87, 126.96, 126.89, 125.91, 34.61, 31.28, 26.65,.



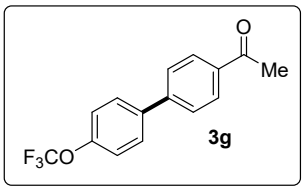
1-(2',4',6'-trimethyl-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[6]
$C_{17}H_{18}O$ Melting Point :93.8 °C -94.5 °C

MW: 238.33 g·mol^{-1} **White Solid**

Isolated amounts: 197.81 mg **Yield**: 83%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.94 (d, *J* =8 Hz, 2H), 7.17 (d, *J* =7.6 Hz, 2H) 6.87(s, 2H), 2.57(s, 3H), 2.25 (s, 3H), 1.90 (s, 6H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.89, 146.49, 137.83, 137.08, 135.41, 129.63, 128.49, 128.15, 26.59, 20.98, 20.60.



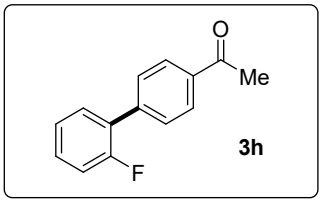
1-(4'-(trifluoromethoxy)-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[7]
$C_{15}H_{11}F_3O_2$ Melting Point :85.9 °C -86.5 °C

MW: 280.25 g·mol^{-1} **White Solid** **Isolated amounts**: 238.21 mg **Yield**: 85%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.02 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* =9.2 Hz, 4H), 7.30 (d, *J* =8.0 Hz, 2H), 2.62 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.43, 149.15(d, *J* =2 Hz), 144.04, 138.39 , 136.00, 128.87, 128.52, 127.02, 121.21, 26.45.

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ -57.82



1-(2'-fluoro-[1,1'-biphenyl]-4-yl)ethan-1-one

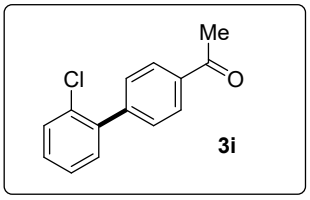
^{1}H and ^{13}C NMR were in agreement with the literature[8]
$C_{14}H_{11}FO$ Melting Point :84.9 °C -85.8 °C **Melting Point were in agreement with the literature[8](84.5** °C **-86.0** °C)

MW: 214.24 g·mol^{-1} **White Solid** **Isolated amounts**: 162.82 mg **Yield**: 76%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.04 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* =8.0 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.37 (q, *J* = 6.0 Hz, 1H), 7.24 (d, *J* = 7.4 Hz, 1H), 7.18 (t, *J* = 9.6 Hz, 1H) ,2.65 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.74, 160.92, 158.45, 140.53, 136.04, 130.58 (d, *J* =3 Hz) 129.87 (d, *J* =8 Hz), 129.18 (d, *J* =3 Hz), 128.45, 127.84 (d, *J* =13 Hz), 124.53 (d,*J*=3 Hz), 116.26 (d, *J* =23 Hz), 26.68.

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ -117.48



1-(2'-chloro-[1,1'-biphenyl]-4-yl)ethan-1-one

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

$C_{14}H_{11}ClO$ Melting Point :52.9 °C -53.9 °C

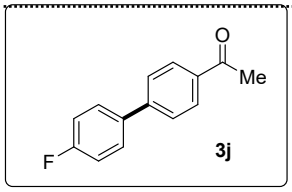
Melting Point were in agreement with the literature[9](52. °C -54 °C)

MW: 230.69 g·mol^{-1} **White Solid** **Isolated amounts**: 177.63 mg **Yield**: 77%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.03 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* =8.0 Hz, 2H), 7.49 (d, *J* = 6.8 Hz, 1H) ,7.34-7.31(m, 3H), 2.65 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.73, 144.08, 139.34, 136.08, 132.25, 131.06, 130.08, 129.71, 129.17, 128.09, 126.96, 26.68

HRMS (ESI) Calcd for $C_{14}H_{11}ClO$+H 231.0572, Found 231.0577



1-(4'-fluoro-[1,1'-biphenyl]-4-yl)ethan-1-one

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

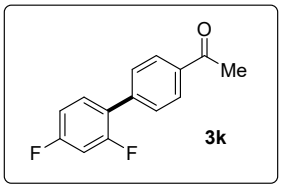
$C_{14}H_{11}FO$ Melting Point :102.3 °C -103.7 °C

MW: 214.24 g·mol^{-1} **White Solid** **Isolated amounts**: 194.96 mg **Yield**: 91%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.02 (d, *J* =8.0 Hz, 2H), 7.64-7.57(m, 4H) 7.15 (t, *J* =8.4 Hz, 2 H), 2.63 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.62, 162.90(d, *J* =246 Hz), 144.63, 135.90 (d, *J* =3 Hz), 135.73, 128.91, 128.82, 126.98,115.85, (d, *J* =22 Hz), 26.62

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ -113.967.



1-(2',4'-difluoro-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[4]
$C_{14}H_{10}F_2O$ Melting Point :81.3 °C -82.5 °C

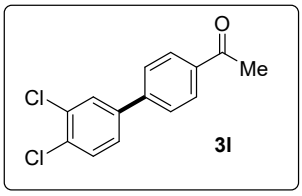
Melting Point were in agreement with the literature(84 °C -93 °C**)**

MW: 230.07 g·mol^{-1} **White Solid** **Isolated amounts**: 204.76 mg **Yield**: 89%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.02 (d, *J* =8.0 Hz, 2H), 7.59 (d, *J* =7.6 Hz, 2H), 7.42 (q, *J* =8 Hz, 1H), 6.99-6.90 (m, 2H), 2.63 (s , 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.58, 162.47 (dd, *J* =297, 12 Hz)159.97 (dd, *J* =298, 12Hz)139.59 (d,*J* =1Hz) 136.07, 131.35 (dd, *J* = 10, 5 Hz) 128.99 (d, *J* = 2Hz), 124.10 (dd,*J* = 14, 4 Hz) 111.81 (dd, *J* = 21, 4 Hz)104.60 (t, *J* = 17Hz), 26.61

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ -109.79, δ -112.94



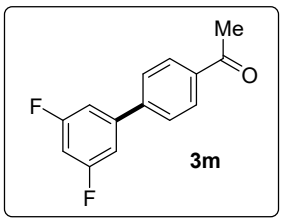
1-(3',4'-dichloro-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[4]

$C_{14}H_{10}Cl_2O$ Melting Point :132.4 °C -132.6 °C

MW: 265.13g·mol^{-1} **White Solid** **Isolated amounts**: 188.24 mg **Yield**: 71%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.02 (d, *J* =8.0 Hz, 2H), 7.68 (s ,1H) 7.61(d, *J* =8.0 Hz, 2 H) , 7.51 (d, *J* =8.4 Hz, 1 H), 7.43 (d, *J* =8.0 Hz, 1 H), 2.64 (s , 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.41, 142.98, 139.69, 136.37, 133.02, 132.39, 130.80, 128.98, 128.94, 126.97, 126.34, 26.62



1-(3',5'-difluoro-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[11]
$C_{14}H_{10}F_2O$ Melting Point :70.3 °C -70.8 °C

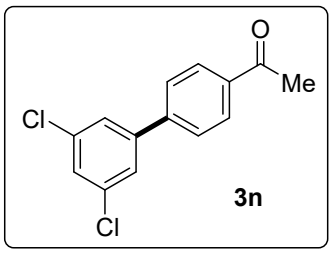
MW: 230.07 g·mol^{-1} **White Solid**

Isolated amounts: 179.45 mg **Yield**: 78%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.02 (d, *J* =7.6 Hz, 2H), 7.61 (d, *J* =7.6 Hz, 2H) 7.11 (d, *J* =7.2 Hz, 2H), 6.81(t, *J* =8.4 Hz, 1H) 2.63 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.40, 163.24(dd, *J*=260,235 Hz),143.06, 143.06, 142.92, 136.67, 128.97, 127.08, 110.07(dd, *J*=26,12Hz), 103.34(t, *J*=25Hz) 26.60.

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ -57.82



1-(3',5'-dichloro-[1,1'-biphenyl]-4-yl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[4].

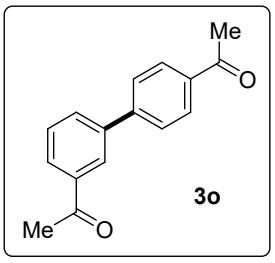
$C_{14}H_{10}Cl_2O$ **Melting Point** :63.5 °C -65.7 °C

Melting Point were in agreement with the literature(64 °C **-**66 °C**)**

MW: 265.13 g·mol^{-1} **White Solid** **Isolated amounts**: 217.69 mg **Yield**: 85%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.04 (d, *J* =8.0 Hz, 2H), 7.63 (d, *J* =8.0 Hz, 2H) 7.48(s, 2 H), 7.39 (s, 1H), 2.65 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.46, 142.84, 142.78, 136.71, 135.48, 129.04, 128.00, 127.22, 125.73, 26.70.



1,1'-([1,1'-biphenyl]-3,4'-diyl)bis(ethan-1-one)
^{1}H and ^{13}C NMR were in agreement with the literature[12]

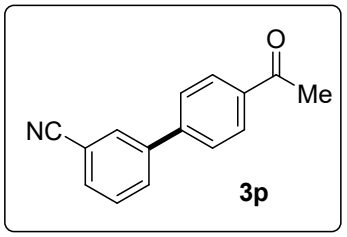
$C_{16}H_{14}O_2$ **Melting Point** :104.9 °C -105.2 °C

MW: 238.10 g·mol^{-1} **White Solid**

Isolated amounts: 188.10 mg **Yield**: 79%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.16 (s, 1H), 7.99 (d, *J* =7.6 Hz, 2H), 7.92 (d, *J* =7.6 Hz, 1H), 7.6 (d, *J* =7.6 Hz, 1H), 7.65 (d, *J* =7.6 Hz, 2H) ,7.51 (t, *J* =7.6 Hz 1H), 2.61(s, 3H), 2.59(s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.83, 197.64, 144.59, 140.35, 137.67, 136.20, 131.74, 129.23, 128.98, 128.09, 127.28, 126.91, 26.76, 26.69.



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

$C_{15}H_{11}NO$ **Melting Point** :132.5 °C -132.7 °C

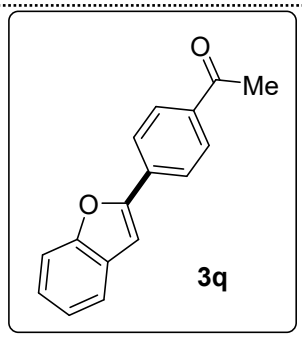
MW: 221.08 g·mol^{-1} **White Solid**

Isolated amounts: 174.65 mg **Yield**: 79%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.06 (d, *J* =8 Hz, 2H), 7.88 (s, 1H), 7.84 (d, *J* =8 Hz, 1H), 7.66 (t, *J* =8.6 Hz, 3H), 7.58 (t, *J* =7.8 Hz, 1H), 2.65(s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.47, 143.18, 141.11, 136.67, 131.55, 130.78, 129.81, 129.13, 127.25, 118.53, 113.19, 26.72.

HRMS (ESI) Calcd for $C_{15}H_{11}NO$+H 222.0922, Found 222.0919



1-(4-(benzofuran-2-yl)phenyl)ethan-1-one

$C_{16}H_{12}O_2$ **Melting Point** :169.0 °C -169.9 °C

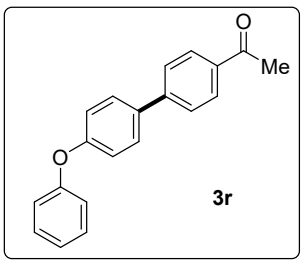
MW: 236.27 g·mol^{-1} **White Solid**

Isolated amounts: 186.65 mg **Yield**: 79%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.04 (d, *J* =8.0 Hz, 2H), 7.95 (d, *J* =8.0 Hz, 2H) 7.62(d, *J* =7.6 Hz, 1H), 7.55(d, *J* =8.0 Hz, 1H) 7.34 (t, *J* =7.6 Hz, 1H) , 7.28-7.24(m , 1H) 7.17 (s, 1H), 2.64(s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.36, 155.17, 154.50, 136.48, 134.57, 128.92, 128.85, 125.13, 124.76, 123.23, 121.31, 111.34, 103.64, 26.65.

HRMS (ESI) Calcd for $C_{16}H_{12}O_2$+H 237.0925, Found 237.0916



1-(4'-phenoxy-[1,1'-biphenyl]-4-yl)ethan-1-one

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

$C_{20}H_{12}O_2$ **Melting Point** :127.8 °C -128.3 °C

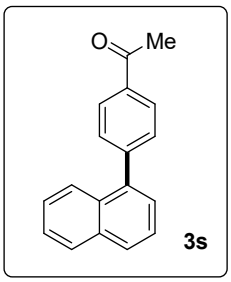
MW: 288.35 g·mol^{-1} **White Solid** **Isolated amounts**: 210.50 mg **Yield**: 73%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.03 (d, *J* =7.6 Hz, 2H), 7.66 (d, *J* =7.2 Hz,

2H) 7.60 (d, *J* =7.2 Hz, 2H) 7.38 (t, *J* =7.4 Hz, 2H), 7.15 (t, *J* =7.4 Hz, 1H), 7.09 (t, *J* =8.0 Hz, 4H), 2.64 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.72, 157.74, 156.66, 145.01, 135.51, 134.58, 129.83, 128.93, 128.57, 126.81, 123.66, 119.22, 118.91, 26.63.

HRMS (ESI) Calcd for $C_{20}H_{12}O_2$+H 289.1230, Found 289.1229



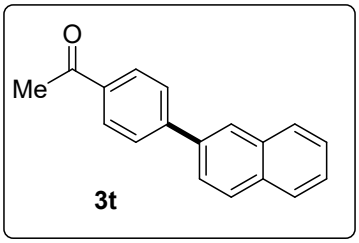
1-(4-(naphthalen-1-yl)phenyl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[9]
$C_{18}H_{14}O$ Melting Point :100.2 °C -101.2 °C

Melting Point were in agreement with the literature(96 °C -98 °C)

MW: 246.31 g·mol^{-1} **White Solid** **Isolated amounts**: 224.14 mg **Yield**: 91%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.10 (d, *J* =7.6 Hz, 2H), 7.92 (t, *J* =9.2 Hz, 2H), 7.85 (d, *J* =8.4 Hz, 1H), 7.61 (d, *J* =7.6 Hz, 2H), 7.57-7.50 (m, 2H) ,7.45 (q, *J* =5.2 Hz 2H), 2.69 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.90, 145.77, 138.97, 135.93, 133.74, , 131.15, 130.30, 128.40, 128.35, 128.33, 126.91, 126.36, 125.98, 125.54, 125.32, 26.74.



1-(4-(naphthalen-2-yl)phenyl)ethan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[13]
$C_{18}H_{14}O$ Melting Point :127. °C -130.7 °C

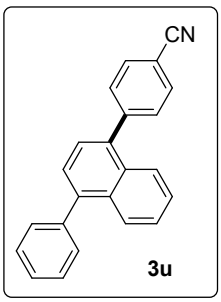
MW: 246.31 g·mol^{-1} **White Solid**

Isolated amounts: 221.70 mg **Yield**: 90%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.08 (d, *J* =9.2 Hz, 2H), 7.96-7.88 (m, 3H) 7.82 (d, *J* =7.6Hz, 2H) 7.76 (d, *J* =8.4Hz, 1H) 7.56-7.50(m, 2H), 2.66 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.80, 145.64, 137.08, 135.78, 133.49, 132.96, 128.67, 128.31, 127.65, 127.42, 126.53, 126.46, 126.34, 125.13, 26.69.

HRMS (ESI) Calcd for $C_{18}H_{14}O$+H 247.1128, Found 247.1123



4-(4-phenylnaphthalen-1-yl)benzonitrile

$C_{23}H_{15}N$ **Melting Point** :146.5 °C -148.0 °C

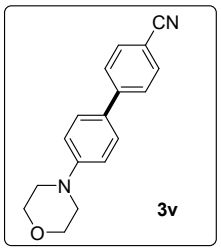
MW: 305.38 g·mol^{-1} **Yellow Solid**

Isolated amounts: 171.01 mg **Yield**: 56%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.01-7.99 (m, 1H), 7.856-7.81(m, 3H), 7.67 (d, *J* =8.0 Hz, 2H),7.53-7.44(m, 9H),

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 145.69, 140.97, 140.31, 137.65, 133.37, 132.60, 132.14, 131.91, 131.22, 130.84, 130.00, 128.35, 127.49, 126.67, 126.52, 126.42, 126.33, 126.20, 125.50, 118.92, 111.09

HRMS (ESI) Calcd for $C_{23}H_{15}N$+H 306.1286, Found 306.1283



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

$C_{17}H_{16}N_2O$ **Melting Point** :183.6 °C -187.0 °C

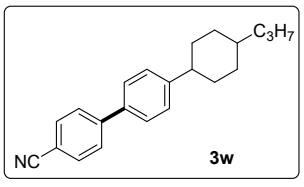
MW: 264.33 g·mol^{-1} **Grey Solid**

Isolated amounts: 162.24mg **Yield**: 61%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.65 (q, *J* =6.8 Hz, 4H), 7.53 (q, *J* =7.6 Hz, 2H), 6.99 (d, *J* =7.6 Hz, 2H), 3.88 (s, 4H), 3.24(s,4H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 151.40, 145.07, 132.49, 129.80, 127.90, 126.68, 119.16, 115.44,109.64, 66.69, 48.54.

HRMS (ESI) Calcd for $C_{17}H_{16}N$+H 265.1340, Found 265.1341



4'-(4-propylcyclohexyl)-[1,1'-biphenyl]-4-carbonitrile

$C_{22}H_{25}N$ **Melting Point** :127.8.0 °C -130.5 °C

MW: 303.45g·mol^{-1} **White Solid**

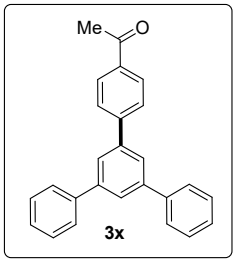
Isolated amounts: 267.03 mg **Yield**: 88%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (q, *J*=6.8 Hz, 4H), 7.53(d, *J* =7.2 Hz, 2H), 7.33(d, *J* =7.2 Hz, 2H), 2.54 (t, *J* =12 Hz, 1H), 1.92 (t, *J* =13.2 Hz, 4H), 1.49 (q, *J* =12.4 Hz, 2H), 1.40-1.33(m, 3H), 1.24 (q, *J* =7.6 Hz, 2H), 1.08 (q, *J* =12 Hz, 2H),

0.92 (t, *J* =7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.67, 145.54, 136.54, 132.49, 127.58, 127.42, 127.06, 119.02, 110.42, 44.29, 39.64, 36.93, 34.21, 33.44, 20.00, 14.39.

HRMS (ESI) Calcd for $C_{22}H_{25}N$+H 304.2060, Found 304.2065



1-(5'-phenyl-[1,1':3',1''-terphenyl]-4-yl)ethan-1-one

$C_{26}H_{20}O$ **Melting Point** :143.6 °C -145.3 °C

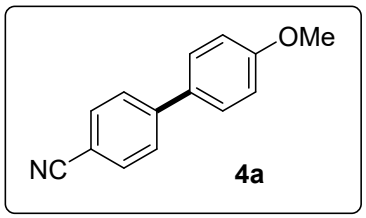
MW: 348.45 g·mol^{-1} **White Solid**

Isolated amounts: 233.46 mg **Yield**: 67%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.08 (d, *J* =7.2 Hz, 2H),7.84(s, 1H), 7.80 (d, *J* =8.0 Hz, 4H) 7.71(d, *J* =7.6 Hz, 4H), 7.51 (t, *J* =7.4 Hz, 4H), 7.42 (d, *J* =7.2 Hz, 2H), 2.67(s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.73, 145.64, 142.57, 140.96, 140.80, 136.02, 128.96, 128.89, 127.70, 127.42, 127.31, 136.06, 125.16, 26.70.

HRMS (ESI) Calcd for $C_{26}H_{20}O$ +H 349.1595, Found 349.1592



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

$C_{14}H_{11}NO$ **Melting Point** :103.1 °C -104.1 °C

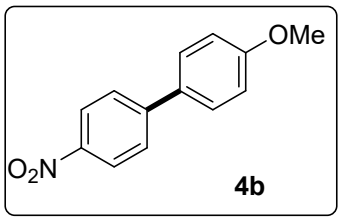
MW: 209.25 g·mol^{-1} **White Solid**

Isolated amounts: 192.51 mg **Yield**: 92%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.66 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 2H), 3.85 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):160.02, 144.95, 132.37, 131.20, 128.17, 126.88, 118.96, 114.36, 109.84, 55.21

HRMS (ESI) Calcd for $C_{14}H_{11}NO$ +H 210.0917, Found 210.0919



4-methoxy-4'-nitro-1,1'-biphenyl

$C_{13}H_{11}NO_3$ **Melting Point** :103.6 °C -104.3 °C

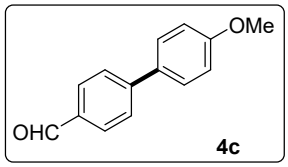
MW: 229.24 g·mol **Yellow Solid**

Isolated amounts: 164.71 mg **Yield**: 64%

^{1}H NMR (400 MHzCDCl$_3$, δ ppm):8.27 (d, *J*=8.0 Hz, 2H), 7.69 (d, *J*=8.0 Hz, 2H), 7.58 (d, *J* =8.0 Hz, 2H), 7.02 (d, *J* =7.6 Hz, 2H), 3.88 (s, 3H),

^{13}C NMR (100 MHz, CDCl$_3$, δ ppm):160.38, 147.15, 146.46, 131.00, 128.53, 127.02, 124.11, 114.55, 55.39.

HRMS (ESI) Calcd for $C_{13}H_{11}NO_3$+H230.0817, Found 230.0817



4'-methoxy-[1,1'-biphenyl]-4-carbaldehyde

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

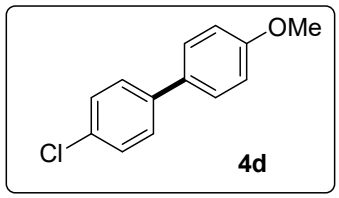
$C_{14}H_{12}O_2$ **Melting Point** :102.1 °C -102.4 °C

Melting Point were in agreement with the literature[14]（101 °C -102 °C）

MW: 212.25 g·mol^{-1} **White Solid** **Isolated amounts**: 199.52 mg **Yield**: 94%

^{1}H NMR (400 MHz, CDCl$_3$, δ ppm):10.02, (s, 1H), 7.91 (d, *J* =7.6 Hz, 2H), 7.70(d, *J* =7.6 Hz, 2H), 7.58 (d, *J*=7.6Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 2H), 3.85 (s, 3H).

^{13}C NMR (100 MHz, CDCl$_3$, δ ppm):191.84, 160.00, 146.66, 134.54, 131.90, 130.23, 128.41, 126.94, 114.38, 55.30.



4-chloro-4'-methoxy-1,1'-biphenyl

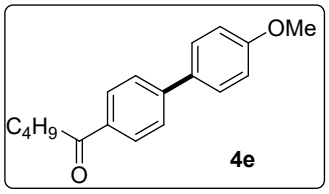
^{1}H and ^{13}C NMR were in agreement with the literature[15]

$C_{13}H_{11}ClO$ **Melting Point** :113.8 °C -114.4 °C

MW: 218.68 g·mol^{-1} **White Solid** **Isolated amounts**: 194.63 mg **Yield**: 89%

^{1}H NMR (400 MHz, CDCl$_3$, δ ppm):7.46 (d, *J*=7.0 Hz, 4H), 7.36(d, *J*=7.6 Hz, 2H), 6.96 (d , *J*=7.6 Hz, 2H), 3.83 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.29, 139.19, 132.60, 132.40, 128.79, 127.96, 127.88, 114.25, 55.31.



1-(4'-methoxy-[1,1'-biphenyl]-4-yl)pentan-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[16]

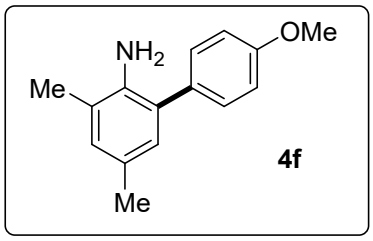
$C_{18}H_{20}O_2$ **Melting Point** :119.4 °C -119.9 °C

Melting Point were in agreement with the literature[15] (121 °C −124 °C)

MW: 268.36 g·mol^{-1} **White Solid** **Isolated amounts**:214.52 mg **Yield**: 90%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.99 (d, *J*=7.6Hz, 2H), 7.61 (d, *J*=8.0, 2H), 7.55 (d, *J* = 7.6 Hz, 2H), 6.98 (d, *J*=7.6 Hz, 2H), 3.83 (s, 3H), 2.96 (t, *J*=7.6, 2H), 1.77-1.69 (m, 2H), 1.46-1.37 (m 2H), 0.96, (t, *J* =7.4, 3H),

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):199.98, 159.74, 144.94, 135.04, 132.11, 128.57, 128.20, 126.43,114.26, 55.22, 38.22, 26.48, 22.43, 13.90.



4'-methoxy-3,5-dimethyl-[1,1'-biphenyl]-2-amine
$C_{15}H_{17}NO$ **Melting Point** :66.1 °C -68.2 °C

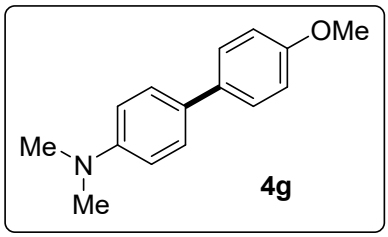
MW: 227.31 g·mol^{-1} **Brown Solid**

Isolated amounts: 170.48 mg **Yield**: 75%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.34 (d, *J* =7.6 Hz, 2H), 6.95 (d, *J* =7.6 Hz, 2H), 6.86 (s,1 H) ,6.08 (s,1H) 3.81 (s, 3H), 3.51 (s, 2H), 2.24, (s, 3H), 2.17 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):158.53, 139.14, 132.08, 130.18, 128.66, 127.04, 122.48, 114.02, 55.15, 20.30, 17.79 .

HRMS (ESI) Calcd for $C_{15}H_{17}NO$ +H 228.1392, Found 228.1388



4'-methoxy-N,N-dimethyl-[1,1'-biphenyl]-4-amine
^{1}H and ^{13}C NMR were in agreement with the literature[17]

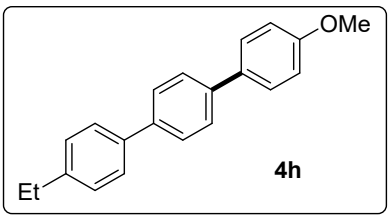
$C_{15}H_{17}NO$ **Melting Point** :151.5 °C -153.1 °C

MW: 227.31 g·mol^{-1} **Brown Solid**

Isolated amounts: 163.66 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm) 7.48(t, *J* =9.2Hz, 4H), 6.94 (d, *J* =8.0Hz, 2H), 6.79 (d, *J*=8.0 Hz, 2H), 3.83 (s, 3H), 2.97 (s, 6H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):158.20, 149.56, 133.92, 129.11, 127.28, 114.07, 112.88, 55.31, 40.66.



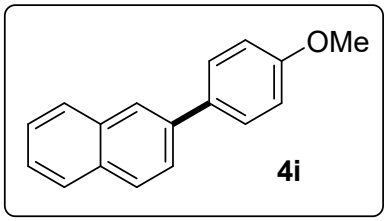
4-ethyl-4''-methoxy-1,1':4',1''-terphenyl
^{1}H and ^{13}C NMR were in agreement with the literature[18]

$C_{21}H_{20}O$ **Melting Point** :233.9 °C -235.8 °C **MW**: 288.39 g·mol^{-1} **White Solid**

Isolated amounts: 236.48 mg **Yield**: 82%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.64 (t, *J* = 9.6 Hz, 4H), 7.58 (t, *J* = 6.4 Hz, 4H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.00 (d, *J*=8.0 Hz, 2H), 3.87 (s, 3H), 2.72 (q, *J* = 7.6Hz, 2H), 1.30 (t, *J* = 7.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.13, 143.37, 139.43, 139.40, 138.10, 133.26, 128.30, 128.00, 127.27, 126.97, 126.88, 114.21, 55.34, 28.52, 15.59 .



2-(4-methoxyphenyl)naphthalene
^{1}H and ^{13}C NMR were in agreement with the literature[19]

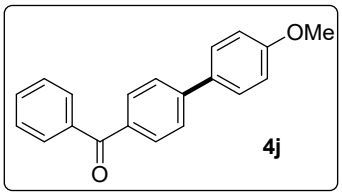
$C_{17}H_{14}O$ **Melting Point** :136.3 °C -136.8 °C

MW: 234.30 g·mol^{-1} **White Solid**

Isolated amounts: 217.90 mg **Yield**: 93%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):8.02, (s, 1H), 7.90 (q, *J* =6.4 Hz, 2H), 7.75(d, *J*=8.8 Hz, 1H), 7.69 (d, *J*=7.6 Hz, 2H), 7.54-7.47 (m, 2H),7.05 (d, *J*=7.6 Hz, 2H) 3.89 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.17, 138.07, 13.69, 133.54, 132.24, 128.37, 128.30, 128.01, 127.58, 126.19, 125.60, 125.38, 124.97, 114.25, 55.32.



(4'-methoxy-[1,1'-biphenyl]-4-yl)(phenyl)methanone
^{1}H and ^{13}C NMR were in agreement with the literature[20]
$C_{20}H_{16}O_2$ Melting Point :158.9 °C -163.8 °C

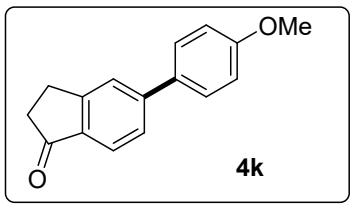
Melting Point were in agreement with the literature[20]

(158.4 °C -162.7 °C)

MW: 288.35 g·mol^{-1} **Brown Solid** **Isolated amounts**: 242.21 mg **Yield**: 84%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.88 (d, *J* = 7.6 Hz, 2H), 7.84 (d, *J* = 7.6 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H) 7.50 (t, *J* = 7.2 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 3.87 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):183.32, 159.82, 144.80, 137.80, 135.51, 132.26, 130.77, 129.93, 128.35, 128.24, 126.32, 114.37, 55.35.



5-(4-methoxyphenyl)-2,3-dihydro-1H-inden-1-one
^{1}H and ^{13}C NMR were in agreement with the literature[21]

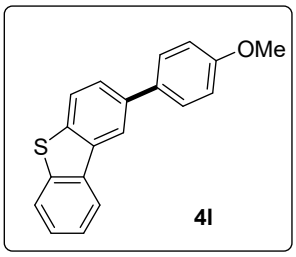
$C_{16}H_{14}O_2$ Melting Point : 151.0 °C -151.6 °C

MW: 238.39 g·mol^{-1} **Yellow Solid** **Isolated amounts**: 202.63 mg **Yield**: 85%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.78 (d, *J* =8.0 Hz, 1H),7.61 (s,1H), 7.56 (t, *J* =7.6 Hz, 3H), 6.99 (d, *J* =7.6 Hz, 2H), 3.85 (s,3H) 3.16 (t, *J* =5 Hz, 2H), 2.71 (t, *J* = 5 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):206.52, 159.88, 155.88, 147.14, 135.32, 132.40, 128.49, 126.13, 124.35, 123.94, 114.30, 55.30, 36.44, 25.78

HRMS (ESI) Calcd for $C_{16}H_{14}O_2$+H 239.1076, Found 239.1072



2-(4-methoxyphenyl)dibenzo[b,d]thiophene

$C_{19}H_{14}OS$ **Melting Point** :92.9 °C -95.2 °C

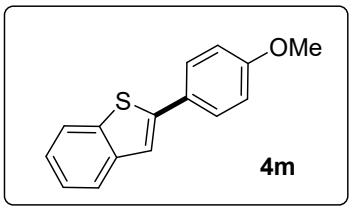
MW: 290.38 g·mol^{-1} **Brown Solid**

Isolated amounts: 209.07 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):8.35 (s, 1H), 8.25-8.23 (m, 1H), 7.90 (d, *J* =8.4Hz, 2H), 7.68(d, *J*=8.4Hz, 3H), 7.52-7.50 (m, 2H), 7.07 (d, *J* = 7.6 Hz, 2H), 3.90 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.02, 139.79, 137.71, 137.34, 125.95, 135.44, 133.49, 128.22, 126.67, 125.74, 124.25, 122.81, 122.77, 121.49, 119.36, 114.18, 55.2

HRMS (ESI) Calcd for $C_{19}H_{14}OS$ +H 291.0841 , Found 291.0841



2-(4-methoxyphenyl)benzo[b]thiophene
^{1}H and ^{13}C NMR were in agreement with the literature[22]

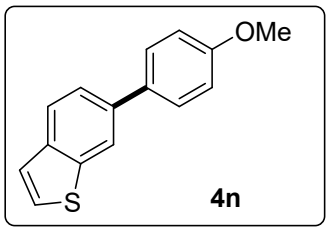
$C_{15}H_{12}OS$ **Melting Point** :191.2 °C -192.1 °C

MW: 240.32 g·mol^{-1} **White Solid**

Isolated amounts: 180.24 mg **Yield**: 75%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.80 (d, *J* =7.6, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* =7.6 Hz, 2H), 7.43(s, 1H), 7.35-7.25 (m, 2H), 6.96 (d, *J*=8 Hz, 2H), 3.85 (s,3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.74, 144.10, 140.85, 139.13, 127.71, 127.00, 124.42, 123.91, 123.22, 122.15, 118.16, 114.31, 55.38.



6-(4-methoxyphenyl)benzo[b]thiophene

$C_{15}H_{12}OS$ **Melting Point** :134.8 °C -137.2 °C

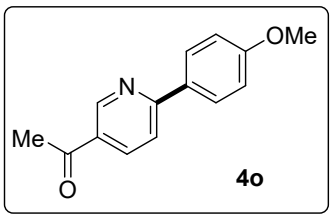
MW: 240.32 g·mol^{-1} **White Solid**

Isolated amounts: 213.78 mg **Yield**: 89%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.99 (s, 1H), 7.92 (d, *J*=8.4 Hz, 1H), 7.61 (d, *J* =8.0 Hz, 2H), 7.57 (d, *J* =8.4 Hz, 1H), 7.48 (d, *J* =5.2Hz, 1H), 7.38 (d, *J* =5.2Hz, 1H), 7.02 (d, *J* =8.0 Hz, 2H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.00, 140.18, 138.15, 137.28, 133.82, 128.36, 126.92, 123.99, 123.65, 122.61, 121.45, 114.21, 55.34.

HRMS (ESI) Calcd for $C_{15}H_{12}OS$ +H 241.0688, Found 241.0687



1-(6-(4-methoxyphenyl)pyridin-3-yl)ethan-1-one

$C_{14}H_{13}NO_2$ **Melting Point** :137.2 °C -138.5 °C

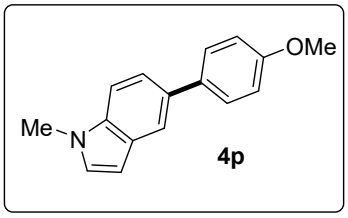
MW: 227.26 g·mol^{-1} **White Solid**

Isolated amounts: 106.81 mg **Yield**: 47%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):9.18 (s, 1H), 8.24 (d, *J* =8.4 Hz, 1H), 8.04(d, *J*=8.0 Hz, 2H), 7.77 (d, *J* =8.4Hz, 2H),7.01(d, *J* =8.0 Hz, 2H), 3.88 (s, 3H).2.64 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):196.47, 161.33, 160.50, 150.10, 136.25, 130.62, 129.88, 128.78, 119.18, 114.27, 55.38, 26.66

HRMS (ESI) Calcd for $C_{14}H_{13}NO_2$ +H 228.1027, Found228.1025



5-(4-methoxyphenyl)-1-methyl-1H-indole

$C_{16}H_{15}NO$ **Melting Point** :140.3 °C -142.0 °C

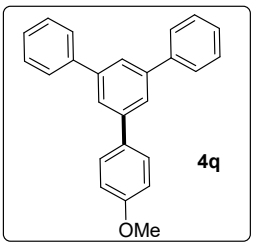
MW: 237.30 g·mol^{-1} **Yellow Solid**

Isolated amounts: 132.89 mg **Yield**: 56%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.88, (s, 1H), 7.66 (d, *J* =7.6Hz, 2H), 7.52 (d, *J*=8.4 Hz, 1H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.12 (s, 1 H),7.06 (d, *J*=7.6 Hz, 2H), 6.60 (s, 1 H), 3.91 (s, 3 H), 3.83 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):158.33, 135.86, 135.16, 132.39, 129.33, 128.87, 128.22, 121.08. 118.78, 114.01, 109.32, 101.08, 55.25, 32.80.

HRMS (ESI) Calcd for $C_{16}H_{15}NO$ +H 283.1233 , Found 283.1232



4-methoxy-5'-phenyl-1,1':3',1''-terphenyl

^{1}H and ^{13}C NMR were in agreement with the literature[23]

$C_{25}H_{20}O$ Melting Point :134.0 °C -135.3 °C

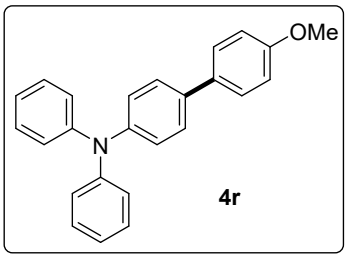
Melting Point were in agreement with the literature[20]

(133 °C−134 °C)

MW: 336.43 g·mol^{-1} **White Solid** **Isolated amounts**: 272.51 mg **Yield**: 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.81 (s, 3H) 7.75 (d, *J* =7.6 Hz, 4H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* =7.4 Hz, 4H), 7..44 (t, *J* =7.2 Hz, 2H), 7.07(d, *J* =7.6 Hz, 2H), 3.90 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.29, 142.25, 141.85, 141.17, 133.54, 128.78, 127.48, 127.31, 124.71, 124.58, 114.22, 55.30.



4'-methoxy-N,N-diphenyl-[1,1'-biphenyl]-4-amine

^{1}H and ^{13}C NMR were in agreement with the literature[24]

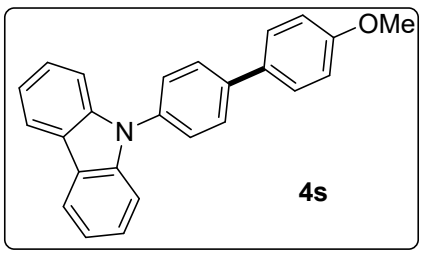
$C_{25}H_{21}NO$ Melting Point :129.2 °C -130.4 °C

MW: 351.45 g·mol^{-1} **Green Solid**

Isolated amounts: 224.93 mg **Yield**: 64%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.49 (d, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 7.6 Hz, 2H), 7.24(t, *J* = 6.6 Hz, 4H), 7.11(d, *J* = 8.0 Hz, 6H), 7.00 (t, *J* = 7.4 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 3.82 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):158.74, 147.69, 146.52, 134.92, 133.18, 129.20, 127.63, 127.29, 124.17, 122.70, 114.12, 55.28.



9-(4'-methoxy-[1,1'-biphenyl]-4-yl)-9H-carbazole

$C_{25}H_{19}NO$ Melting Point :262.6 °C -263.1 °C

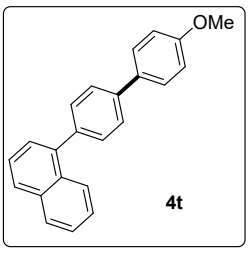
MW: 349.43 g·mol^{-1} **Brown Solid**

Isolated amounts: 251.59mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.17 (d, *J* =8.0 Hz, 2H), 7.78 (d, *J* = 7.2 Hz, 2H), 7.63 (t, *J* =8.0 Hz, 4H), 7.49-7.41(m, 4H), 7.31 (t, *J* =7.2 Hz, 2H), 7.05(d, *J* =7.6Hz, 2H), 3.90 (s,3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.37, 140.84, 139.89, 136.19, 132.74, 128.15, 127.98, 127.29, 125.90, 123.32, 120.28, 119.87, 114.35, 55.37 .

HRMS (ESI) Calcd for $C_{25}H_{19}NO$+H 350.1548, Found 350.1545



1-(4'-methoxy-[1,1'-biphenyl]-4-yl)naphthalene

$C_{23}H_{18}O$ **Melting Point** :122.7 °C -123.0 °C

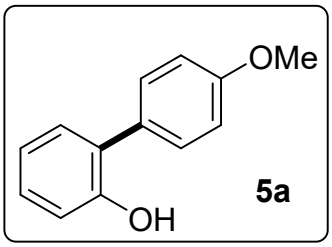
MW: 310.40 g·mol^{-1} **White Solid**

Isolated amounts: 192.45 mg **Yield**: 62%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):8.01 (d, *J* =8.4 Hz, 1H), 7.94 (q, *J* =8.0 Hz, 1H), 7.89(d, *J* =8.0Hz, 1H), 7.70 (d, *J*=7.6 Hz, 2H),7.65(d, *J* =7.6 Hz, 2H), 7.59-7.45 (m, 6 H), 7.04 (d, *J* =7.6 Hz, 2H) 3.89 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.18, 139.88, 139.66, 139.06, 133.79, 133.29, 131.57, 130.44, 128.27, 128.11, 127.61, 126.90, 126.51, 126.02, 125.77, 125.40, 114.25, 55.34.

HRMS (ESI) Calcd for $C_{23}H_{18}O$+H 31.3435, Found 311.3436



4'-methoxy-[1,1'-biphenyl]-2-ol

^{1}H and ^{13}C NMR were in agreement with the literature[25]

$C_{13}H_{12}O_2$ **Melting Point** : 63.8 °C -64.2 °C

Melting Point were in agreement with the literature[25]

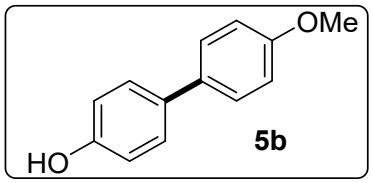
(66 °C -67 °C)

MW: 200.34 g·mol^{-1} **Colorless prisms** **Isolated amounts**:144.24 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.37 (d, *J* =7.6 Hz, 2H), 7.21(d, *J* =10.8 Hz, 2H), 6.96 (q , *J* =6.4 Hz, 2H), 5.36 (s, 1H). 3.80 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.07, 152.40, 130.20, 130.17, 129.19,

128.68, 127.76, 120.70, 115.63, 114.51, 55.23



4'-methoxy-[1,1'-biphenyl]-4-ol
^{1}H and ^{13}C NMR were in agreement with the literature[26]

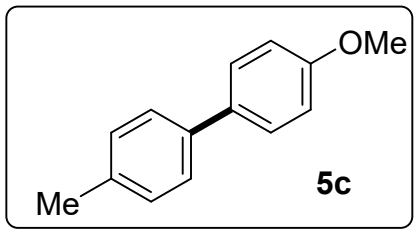
$C_{13}H_{12}O_2$ **Melting Point** :169.6 °C -170.4 °C

MW: 200.34 g·mol^{-1} **White Solid**

Isolated amounts: 152.26 mg **Yield**: 76%

^{1}H NMR (400 MHz, DMSO d-6, δ ppm):9.47 (s, 1H), 7.49(d, *J* =7.6 Hz, 2H),7.42 (d, *J* =7.6 Hz, 2H), 6.97(d, *J* =7.6 Hz, 2H), 6.83 (d, *J*=7.6 Hz, 2H), 3.77 (s, 3H).

^{13}C NMR (100 MHz, DMSO d-6 δ ppm):158.54, 156.97, 133.20, 131.18, 127.68 127.46, 116.09, 114.67, 55.54



4-methoxy-4'-methyl-1,1'-biphenyl
^{1} H and ^{13} C NMR were in agreement with the literature[5].

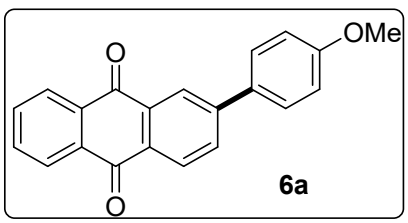
$C_{14}H_{14}O$ **Melting Point** :107.0 °C -107.7 °C

MW: 198.27 g·mol^{-1} **White Solid**

Isolated amounts: 109.05 mg **Yield**: 55%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.51 (d, *J*=7.2 Hz, 2H), 7.45(d, *J* =7.6 Hz, 2H), 7.22(d, *J* =7.2Hz, 2H), 6.96 (d, *J* =7.6 HZ, 2H), 3.84 (s, 3H), 2.38 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):158.86, 137.91, 136.32, 133.69, 129.40, 127.92,126.55, 114.10, 55.31, 21.04.



2-(4-methoxyphenyl)-4a,9a-dihydroanthracene-9,10-dione
^{1}H and ^{13}C NMR were in agreement with the literature[27]

$C_{21}H_{15}O_3$ **Melting Point** :175.8 °C -176.7 °C

MW: 314.34 g·mol^{-1} **Yellow Solid**

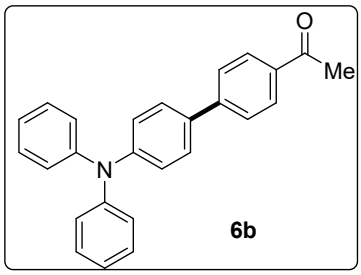
Isolated amounts: 298.62 mg **Yield**: 95%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):8.48 (s, 1H), 8.33 (d, *J* = 7.2 Hz, 3H), 7.97 (d, *J*

= 8.0 Hz, 1H), 7.81-7.80 (m, 2H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):183.32, 182.83, 160.36, 146.37, 134.12, 133.95, 133.84, 133.64, 133.57, 131.66, 131.51, 131.21, 128.48. 128.03, 127.22, 127.15, 124.79, 114.54, 55.40

HRMS (ESI) Calcd for $C_{21}H_{15}O_3$+H 315.1025, Found 315.1021



1-(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)ethan-1-one

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

$C_{26}H_{21}NO$ **Melting Point** :105.8 °C -106.3 °C

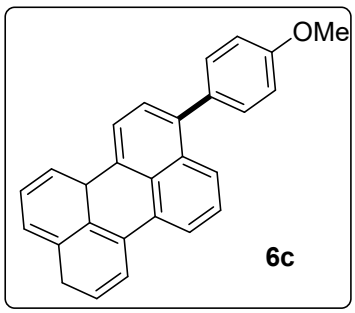
MW: 363.46 g·mol^{-1} **Green Solid**

Isolated amounts: 210.80 mg **Yield**: 58%

^{1}H NMR (400 MHz, DMSO, δ ppm): 7.91 (d, *J* =8.0 Hz, 2H), 7.56, (d, *J* =7.6 Hz, 2H), 7.41 (d, *J* =8.0 Hz, 2H), 7.19 (t, *J* =7.4 Hz, 4H), 7.05(d, *J* =8.4 Hz, 6H), 6.97 (t, *J* =7.2 Hz, 2H), 2.53(s, 3H).

^{13}C NMR (100 MHz, DMSO, δ ppm): 197.65, 148.09, 147.31, 145.11, 135.20, 133.01, 129.32, 128.91, 127.85, 126.41, 124.70, 123.29, 123.20, 26.60.

HRMS (ESI) Calcd for $C_{26}H_{21}NO$+H 364.700, Found 364.1701



9-(4-methoxyphenyl)-3,6a-dihydroperylene

$C_{27}H_{20}O$ **Melting Point** :255.3 °C -257.0 °C

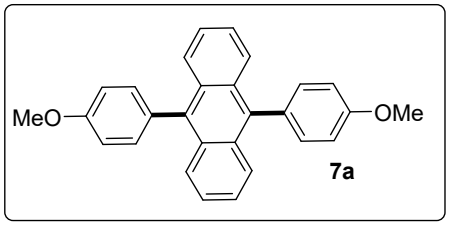
MW: 360.46 g·mol^{-1} **Yellow Solid**

Isolated amounts: 273.95 mg **Yield**: 76%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):8.19 (t, *J* =5.8 Hz, 4H), 7.79 (d, *J* =8.4 Hz, 1H), 7.68(d, *J* =8.0Hz, 2H), 7.50-7.39(m, 6H), 7.05(d, *J*=8.0Hz, 2H), 3.90 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):158.96, 139.59, 134.65, 133.06, 131.41, 131.33, 131.26, 131.00, 130.26, 129.05, 128.60 ,127.70, 127.67, 127.59, 126.57, 126.55, 126.37, 126.10, 120.28, 120.23, 119.96, 119.92, 113.78, 55.34.

HRMS (ESI) Calcd for $C_{27}H_{20}O$+H 361.1585, Found 361.1592



7a

9,10-bis(4-methoxyphenyl)anthracene

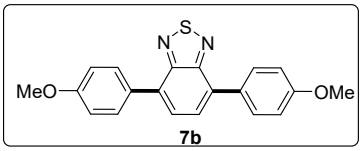
^{1}H and ^{13}C NMR were in agreement with the literature[28]

$C_{28}H_{22}O_2$ **Melting Point** :277.9 °C -279.1 °C

MW: 390.48 g·mol^{-1} **Yellow Solid** **Isolated amounts**: 144.0 mg **Yield**: 74%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.75-7.73(m, 4H), 7.39 (d, *J*=7.6 Hz, 4H), 7.33 (d, *J* =7.2 Hz, 4H), 7.14 (d, *J* =7.6 Hz, 4H), 3.96 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.26, 158.97, 140.46, 136.72, 132.37, 131.12, 130.23, 128.66, 127.56, 127.02, 124.87, 123.38, 113.83, 113.73, 55.38



7b

4,7-bis(4-methoxyphenyl)benzo[c][1,2,5]thiadiazole

$C_{20}H_{18}N_2O_5$ **Melting Point** :196.7 °C -197.0 °C

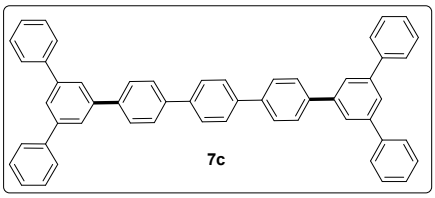
MW: 348.42 g·mol^{-1} **Yellow Solid**

Isolated amounts: 151.56 mg **Yield**: 87%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.92(d, *J* =7.6 Hz, 4H), 7.71(s, 2H) 7.08 (d, *J* =7.6 Hz, 4H), 3.89 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):159.71, 154.16, 132.28, 130.34, 129.96, 127.37, 114.06, 55.38.

HRMS (ESI) Calcd for $C_{20}H_{18}N_2O_5$+H 349.1009, Found 349.1011


7c

5',5''''-diphenyl-

1,1':3',1'':4'',1''':4''',1'''':4'''',1''''':3''''',1'''''-sepiphenyl

$C_{54}H_{38}$ **Melting Point** :293.6 °C −297.2 °C

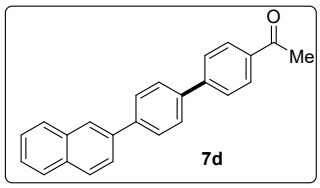
MW: 686.90 g·mol^{-1} **White Solid**

Isolated amounts: 216.37 mg **Yield**: 63%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.85 (s 4H), 7.83-7.78 (m, 14H) 7.73(d, *J* =7.6 Hz, 2H), 7.50 (t, *J*=7.4 Hz, 8H), 7.41 (t, *J*=7.4 Hz, 4H),

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.43, 141.77, 141.11, 140.12, 139.82, 139.64, 139.86, 127.77, 127.58, 127.48, 127.45, 127.36, 125.31, 125.03.

HRMS (ESI) Calcd for $C_{54}H_{38}$+H 687.3060, Found 687.3052



1-(4'-(naphthalen-2-yl)-[1,1'-biphenyl]-4-yl)ethan-1-one

$C_{24}H_{18}O$ **Melting Point** :228.7 °C -229.2 °C

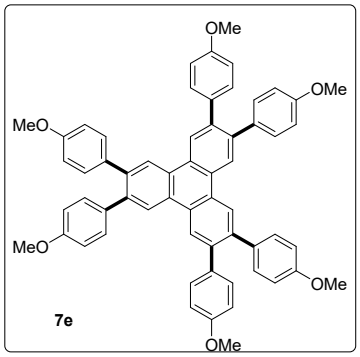
MW: 322.41 g·mol^{-1} **White Solid**

Isolated amounts: 109.70 mg **Yield**: 66%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.11(s, 1H), 8.07 (d, *J* =7.6 Hz, 2H), 7.94, (t, *J* =9.2 Hz, 2 H),7.89 (d, *J* =7.2 Hz, 1H), 7.85 (d, *J* =7.6 Hz, 2H), 7.78 (t, *J* =10.6 Hz, 5 H), 7.55-7.49 (m,2H), 2.66(s , 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 197.75, 145.21, 140.99, 138.73, 137.65, 135.86, 133.63, 132.72, 128.99, 128.57, 128.22, 127.91, 127.72, 127.66, 127.08, 126.41, 126.12, 125.80, 125.30, 26.71.

HRMS (ESI) Calcd for $C_{24}H_{18}O$+H 323.1436, Found 323.1436



2,3,6,7,10,11-hexakis(4-methoxyphenyl)triphenylene

$C_{60}H_{48}O_6$ **Melting Point** :259.0 °C -260.1 °C

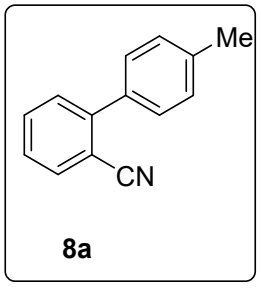
MW: 865.04 g·mol^{-1} **White Solid**

Isolated amounts: 367.29 mg **Yield**: 85%

^{1}H NMR (400 MHz, DMSO d-6, δ ppm):8.71 (s, 5H), 7.27 (d, *J* =8.0 Hz, 12H), 6.89 (d, *J*=8.0 Hz, 12H), 3.77 (s, 18H).

^{13}C NMR (100 MHz, DMSO d-6, δ ppm):158.64, 139.69, 133.74, 131.45, 128.45, 125.82, 114.06, 55.52

HRMS (ESI) Calcd for $C_{60}H_{48}O_6$+H 865.3525, Found 865.3529



8a

4'-methyl-[1,1'-biphenyl]-2-carbonitrile

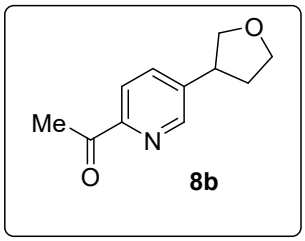
^{1}H and ^{13}C NMR were in agreement with the literature[29]

$C_{14}H_{11}N$

MW: 193.25 g·mol^{-1} **White oil** **Isolated amounts**: 139.14 mg **Yield**: 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.70 (d, *J* =7.6 Hz, 1H), 7.58 (t, *J* =7.6 Hz, 1H), 7.45 (t, *J*=8.2 Hz, 3H)，7.37(t, *J* =7.6Hz, 1H)，7.27(d, *J* =7.6 Hz, 2H), 2.38 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):145.22, 138.44, 135.04, 133.48, 132.61, 129.76, 129.23, 128.40, 127.10, 118.71, 110.87, 21.05.



8b

1-(5-(tetrahydrofuran-3-yl)pyridin-2-yl)ethan-1-one

$C_{11}H_{13}NO_2$ **Melting Point** :117.8 °C -118.9 °C

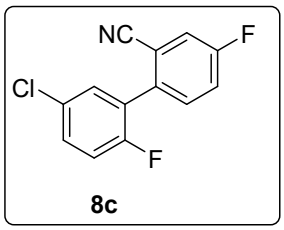
MW: 191.23 g·mol^{-1} **Yellow Solid**

Isolated amounts: 120.47 mg **Yield**: 63%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.81（s, 1H）8.05 (d, *J* =10.4 Hz, 1H), 7.87 (d, *J* =8.0 Hz, 2H), 7.56 (s, 1H), 6.77(s, 1H), 2.73 (s, 3H）

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):199.42, 1551.80, 145.98, 144.44, 139.86, 133.19, 131.62, 122.61, 121.78, 108.20, 25.64.

HRMS (ESI) Calcd for $C_{11}H_{13}NO_2$+H 192.1027, Found 192.1025



8c

5'-chloro-2',4-difluoro-[1,1'-biphenyl]-2-carbonitrile

^{1}H and ^{13}C NMR were in agreement with the literature[30]

$C_{13}H_6ClF_2N$ **Melting Point** :117.8 °C -118.9 °C

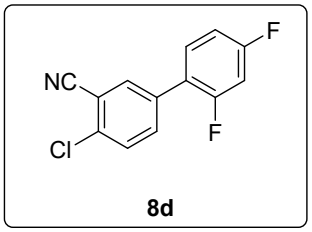
MW: 249.64 g·mol^{-1} **Yellow Solid**

Isolated amounts: 199.71 mg **Yield**: 80%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):7.48(t, *J* =9.2 Hz, 2H), 7.39 (q, *J* =9.6 Hz, 3H), 7.17 (t, *J* =9 Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):161.08 (d, *J* =387Hz)，158.59 (d, *J* =384 Hz), 134.40 (d, *J* =4 Hz)，132.79 (dd, *J* =9, 1 Hz)，130.90， 130.85, 130.82, 129.54 (d, *J* =3 Hz), 126.28 (d, *J* =16 Hz)，120.28 (dd, *J* =3, 1 Hz)，117.58(d *J*= 24 Hz), 116.41(d, *J*=3 Hz), 114.28(d, *J* =9 Hz)

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ-110.55, δ-117.54



8d

4-chloro-2',4'-difluoro-[1,1'-biphenyl]-3-carbonitrile

$C_{13}H_6ClF_2N$

MW: 249.64 g·mol^{-1} **Colorless Oil**

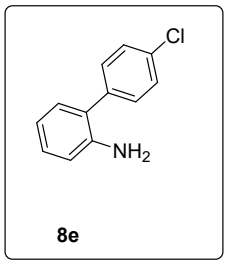
Isolated amounts: 217.18 mg **Yield**: 87%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.80 (s,1H）7.68(d, *J* =8.4 Hz, 1H), 7.59, (d , *J* =8.4 Hz, 1H), 7.39(q, *J* =8.0 Hz, 1H),7.03-6.93 (m, 2H)

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):162.54 (dd, *J* =332, 12Hz), 160.04 (dd, *J* =332, 12Hz), 136.07, 134.36, 134.05 (dd, *J* =13, 3Hz), 131.03 (dd, *J* =9, 4Hz), 130.18, 121.95 (dd, *J* =13, 4Hz), 115.68, 113.66, 112.22(dd, *J* =21, 4Hz), 104.81(t, *J* = 26 Hz)

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): δ-108.41, δ-113.19

HRMS (ESI) Calcd for $C_{13}H_6ClF_2N$ +H 250.0238, Found 250.0235



8e

4'-chloro-[1,1'-biphenyl]-2-amine

^{1}H and ^{13}C NMR were in agreement with the literature[31]

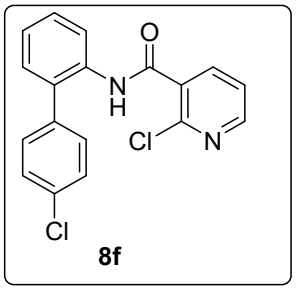
$C_{12}H_{10}ClN$

MW: 230.67 g·mol^{-1} **Yellow Oil**

Isolated amounts: 186.84 mg **Yield**: 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.40-7.36（m, 4H）,7.14(t, *J*=7.6 Hz, 1H), 7.07, (d, *J*=7.2 Hz, 1H), 6.81 (t, *J*=7.6 Hz, 1H), 6.73 (d, *J* =8.0 Hz, 1H), 3.66(s,2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):143.25, 137.73, 132.82, 130.26, 130.15, 128.78, 128.65, 126.01, 118.55, 115.55.



8f

2-chloro-N-(4'-chloro-[1,1'-biphenyl]-2-yl)nicotinamide

^{1}H and ^{13}C NMR were in agreement with the literature[32]

$C_{18}H_{12}Cl_2N_2O$ **Melting Point** :140.4 °C -141.6 °C

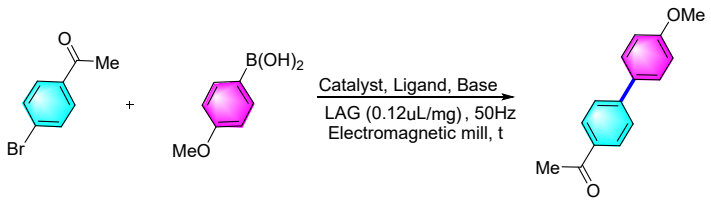
MW: 343.21 g·mol^{-1} **White Solid**

Isolated amounts: 302.02 mg **Yield**: 88%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.35-8.29 (m, 2H),8.04(s, 1H), 8.03, (d, *J* =7.6 Hz, 1H), 7.38-7.34 (m, 3H), 7.25 (d, *J* =7.2 Hz, 3H), 7.19-7.18 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):162.50, 151.17, 146.58, 139.96, 136.19, 134.30, 134.17, 132.29, 131.03, 130.71, 130.17, 129.19, 128.79, 125.33, 122.82, 122.18.

8. Optimization of the Reaction Conditions.



1a **2a** **3a**

Entry	Catalyst	Ligand	Base	LAG	time/h	Yield/%[b]
1	$Pd(OAc)_2$ (3 mol%)	DavePhos	CsF	-	3	82
2	$Pd(OAc)_2$ (0.5mol%)	DavePhos	CsF	-	3	93
3	$Pd(OAc)_2$ (0.1 mol%)	DavePhos	CsF	-	3	95
4	$Pd(OAc)_2$ (0.05 mol%)	DavePhos	CsF	-	3	95
5	$Pd(OAc)_2$ (0.02 mol%)	DavePhos	CsF	-	3	56
6	$Pd(OAc)_2$ (0.01 mol%)	DavePhos	CsF	-	3	32
7	-	DavePhos	CsF	-	3	-
8	$Pd(OAc)_2$ (0.05 mol%)	DavePhos	K_2CO_3	-	3	76
9	$Pd(OAc)_2$ (0.05 mol%)	DavePhos	KOAc	-	3	73
10	$Pd(OAc)_2$ (0.05 mol%)	DavePhos	Cs_2CO_3	-	3	50
11	$Pd(OAc)_2$ (0.05 mol%)	DavePhos	KF	-	3	97
12	$Pd(OAc)_2$ (0.05 mol%)	dppf	KF	-	3	86
13	$Pd(OAc)_2$ (0.05 mol%)	xphos	KF	-	4	84
14	$Pd(OAc)_2$ (0.05 mol%)	PCy_3	KF	-	5	73
15	$Pd(OAc)_2$ (0.05 mol%)	PPh_3	KF	-	5	88
16	$Pd(OAc)_2$ (0.05 mol%)	PhDavePhos	KF	-	3	81
17	$Pd(OAc)_2$ (0.05 mol%)	Ruphos	KF	-	3	82
18	$Pd(OAc)_2$ (0.05 mol%)	1,1'-Bis(diisopropyl-phosphino)ferrocene	KF	-	3	79
19	$PdCl_2$ (0.05 mol%)	DavePhos	KF	-	1	79
20	**$Pd(dppf)Cl_2$ (0.05 mol%)**	**DavePhos**	**KF**	**-**	**1**	**99**
21	$Pd_2(dba)_3$ (0.05 mol%)	DavePhos	KF	-	3	79
22	$Pd(dba)_2$ (0.05 mol%)	DavePhos	KF	-	3	56
23	$PdCl_2(MeCN)_2$ (0.05 mol%)	DavePhos	KF	-	1	90
24	$Pd(dppf)Cl_2$ (0.05 mol%)	-	KF	-	1	85
25	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	1,5-cod	1	25
26	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	MeCN	1	92
27	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	toluene	1	93
28	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	DMSO	1	85
29	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	THF	1	98
30	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	DME	1	99
31	$Pd(dppf)Cl_2$ (0.05 mol%)	DavePhos	KF	Cyclohexene	1	77

9. References

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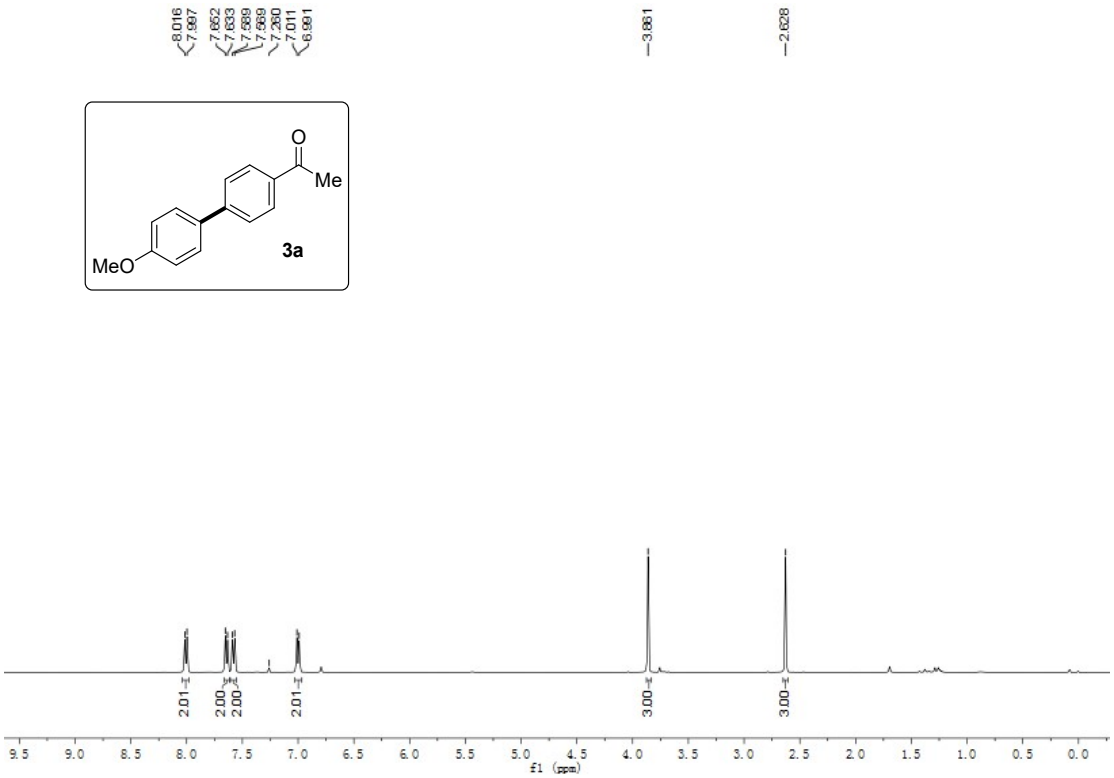
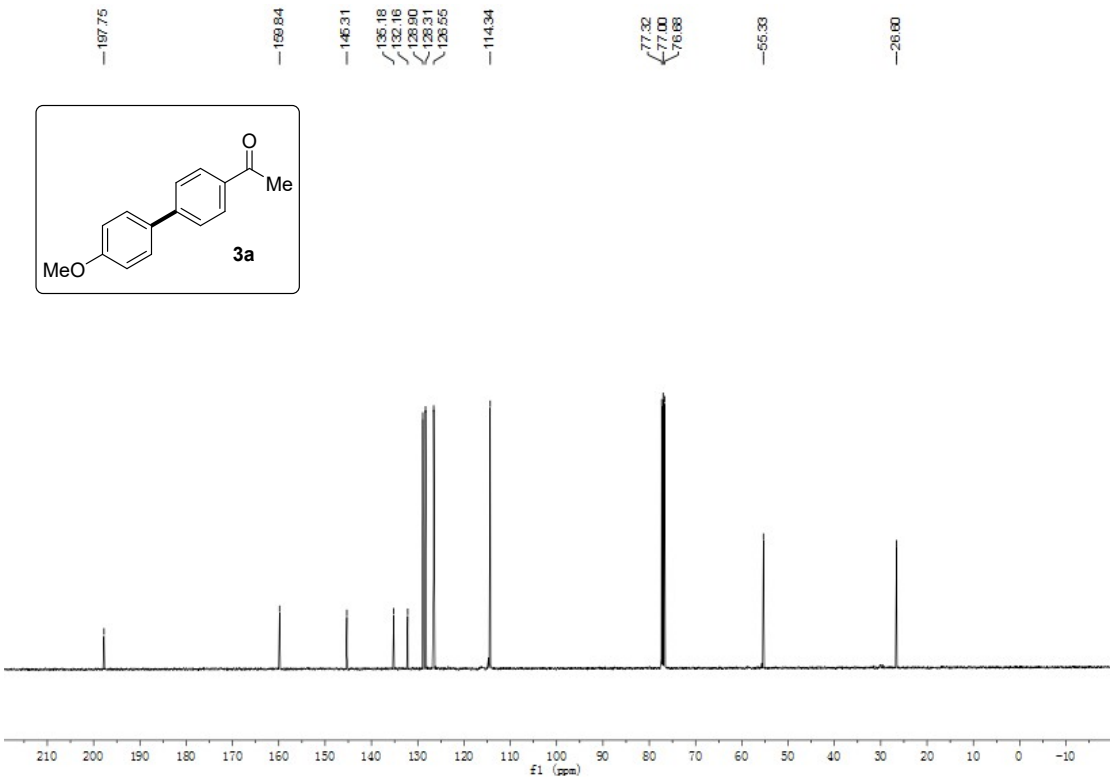
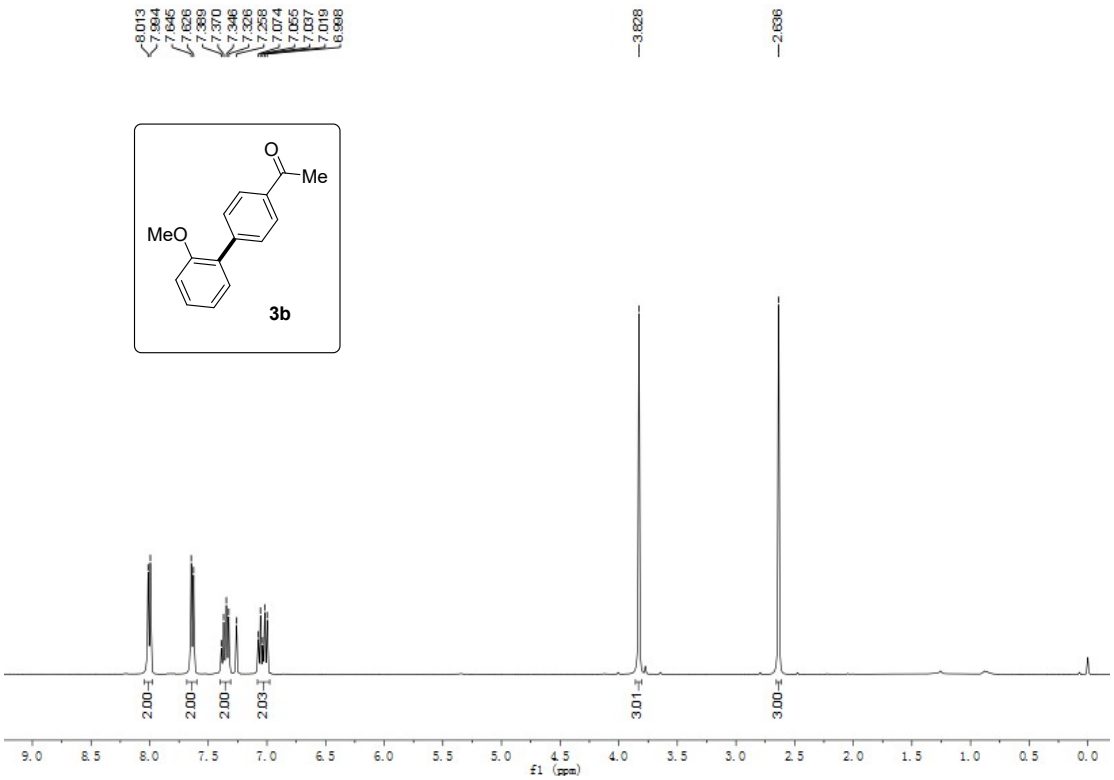
10. Copies of the ^{1}H NMR, ^{13}C NMR



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3.00
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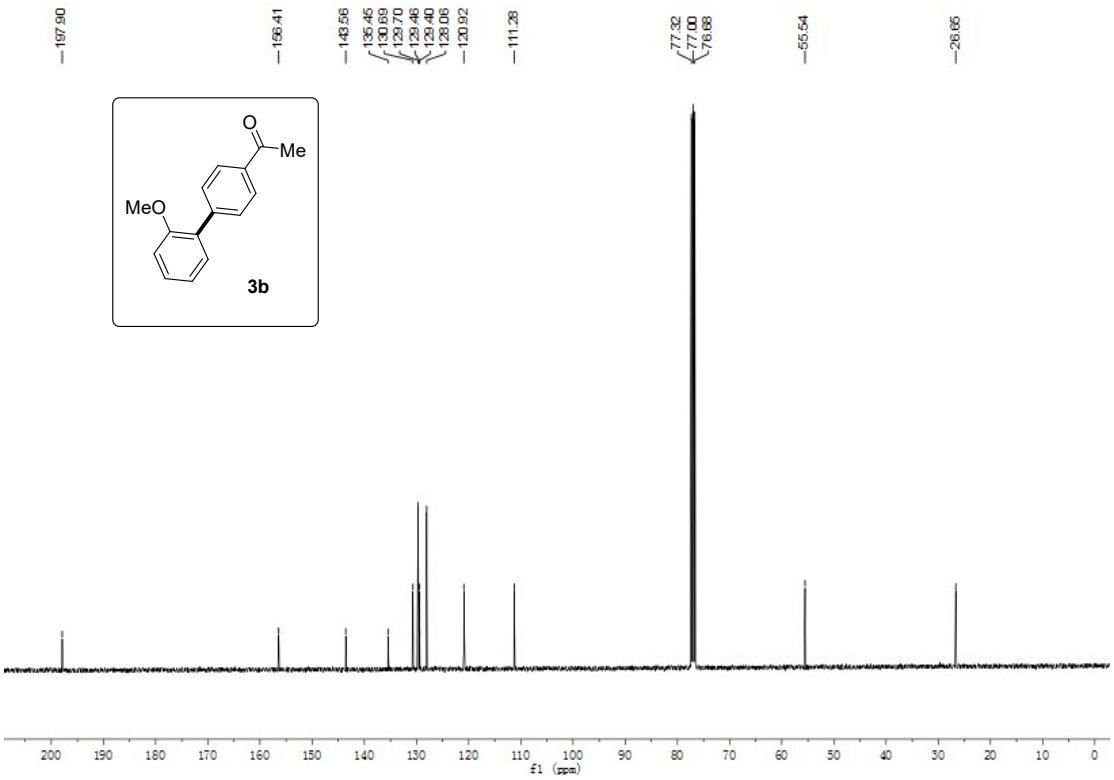
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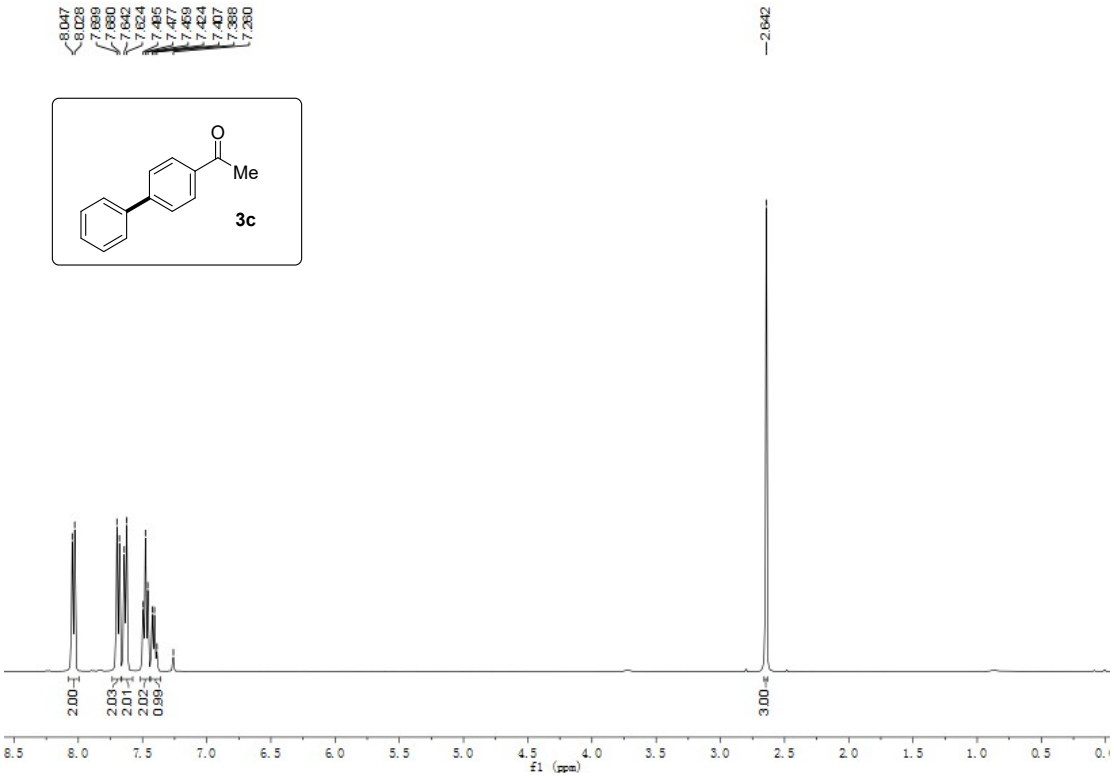
f1 (ppm)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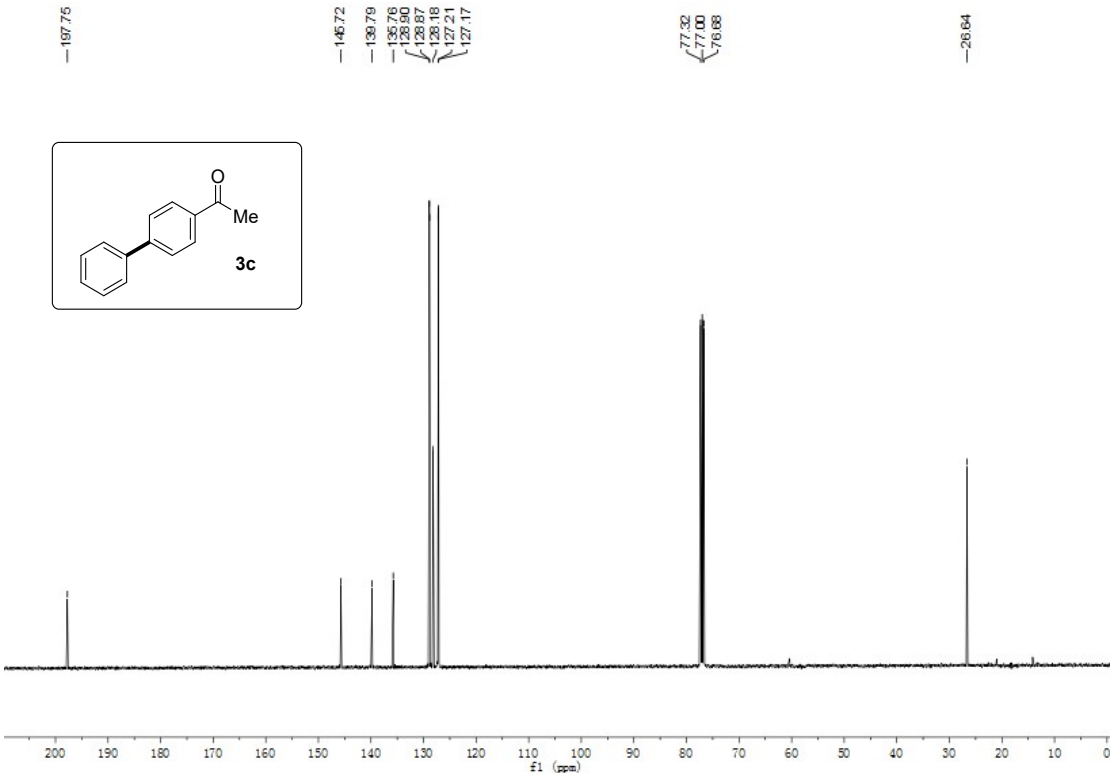
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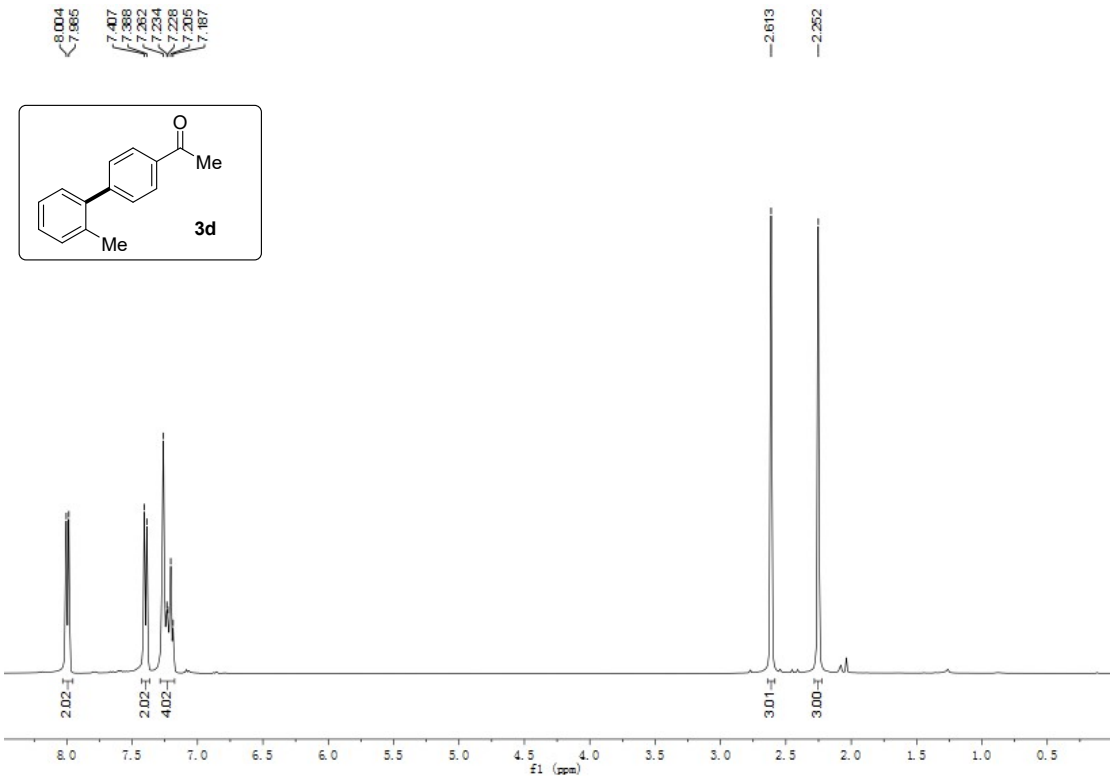
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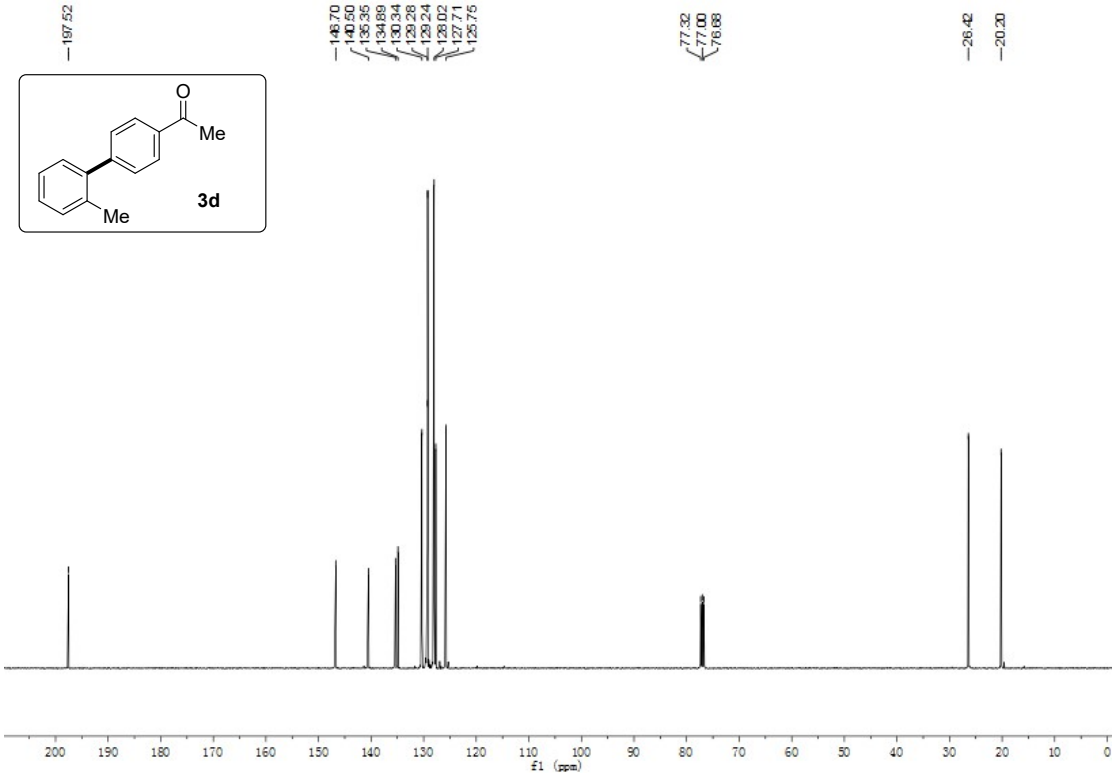
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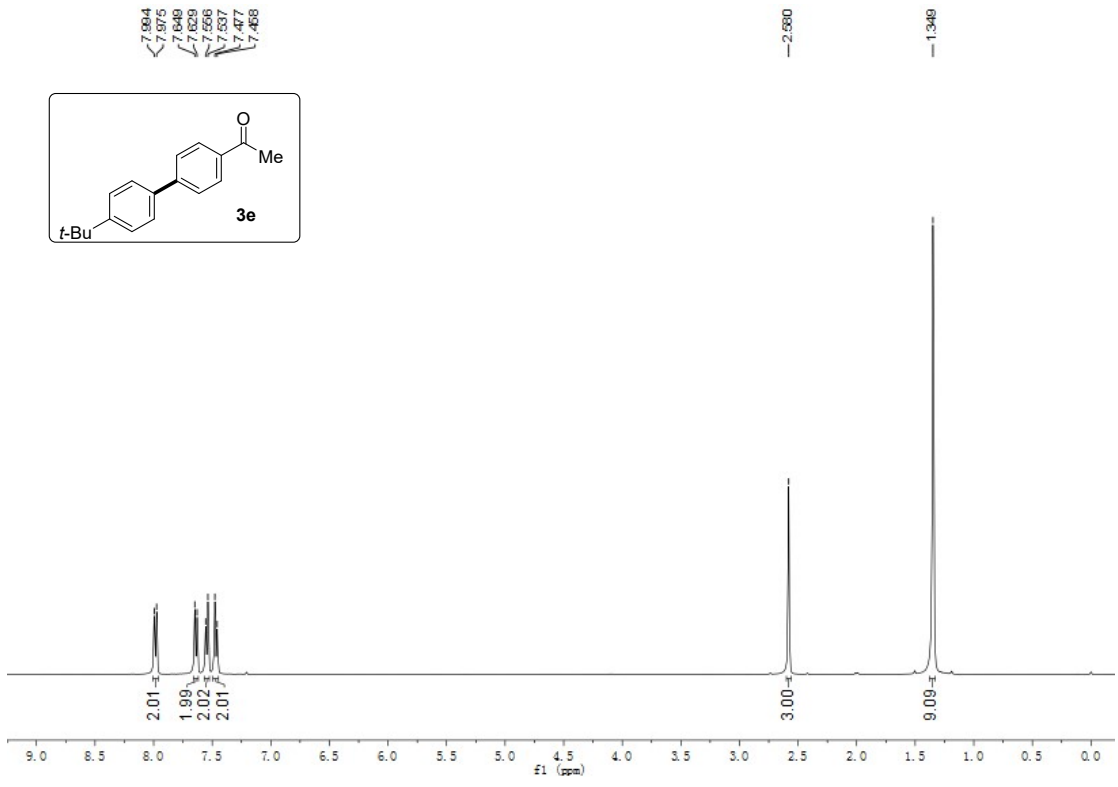
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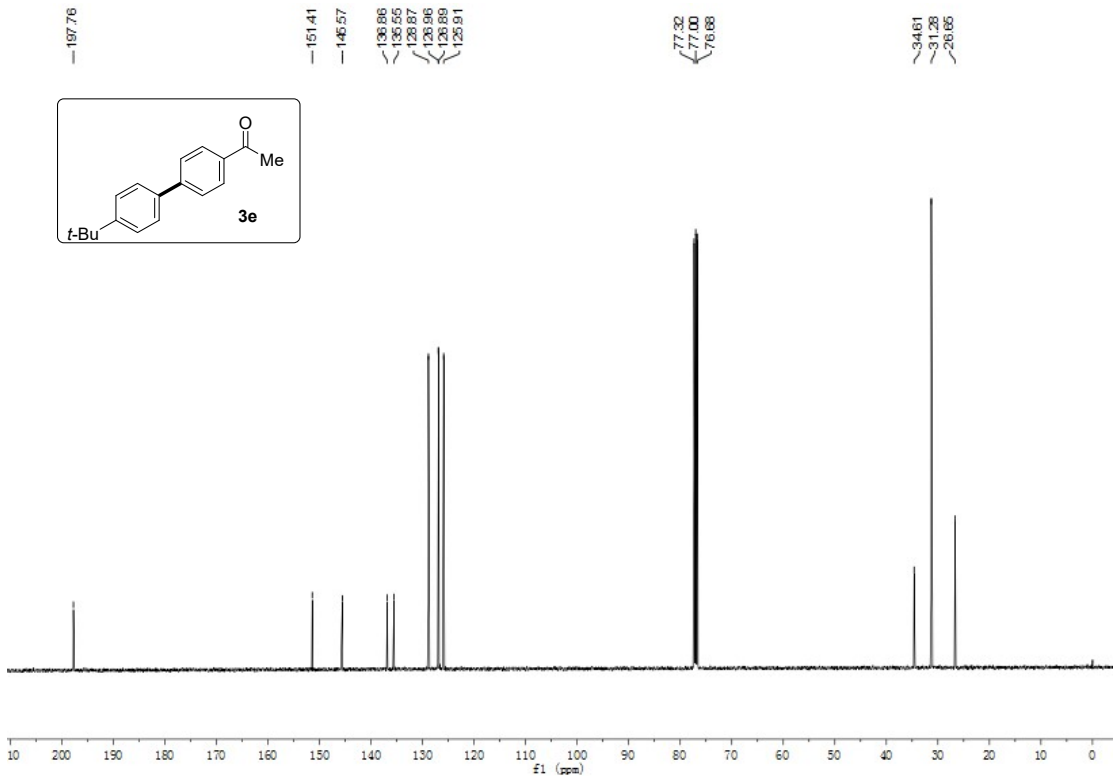
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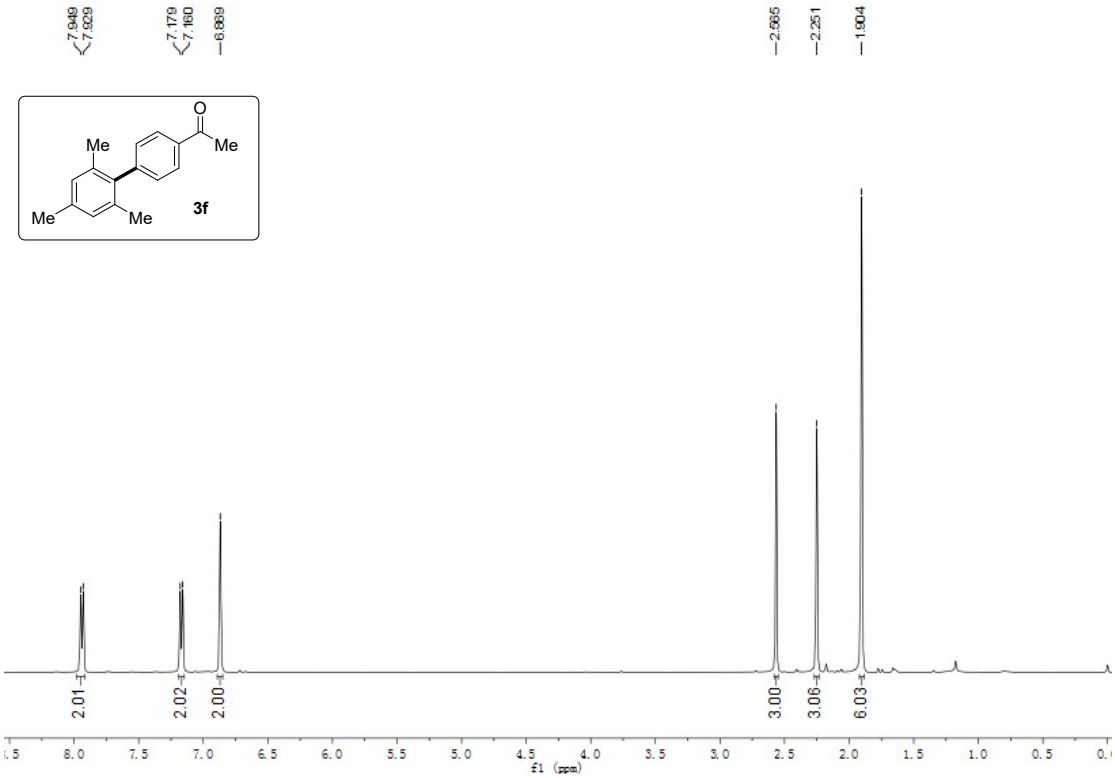
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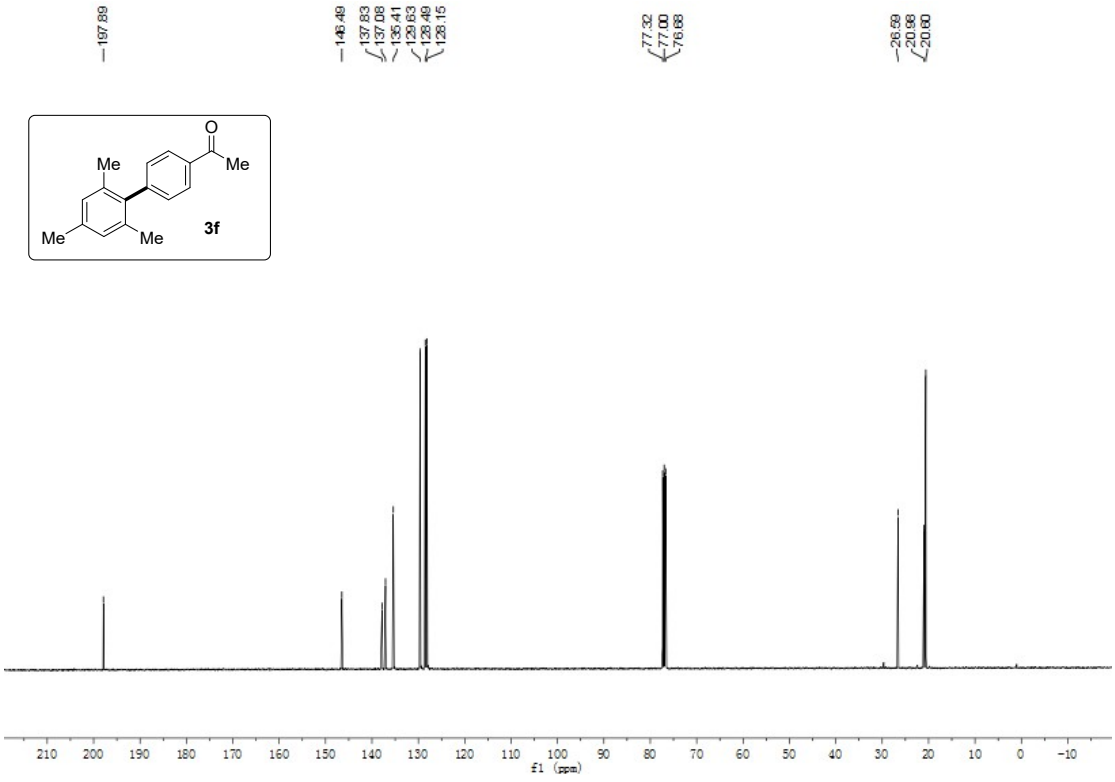
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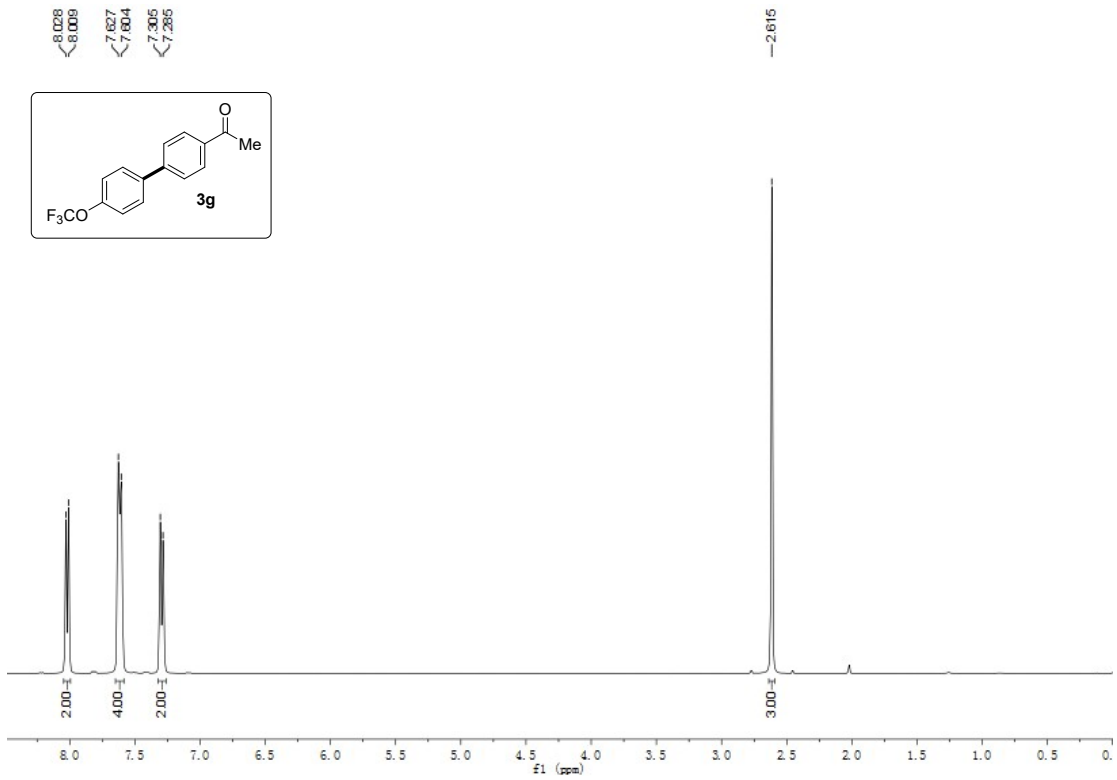
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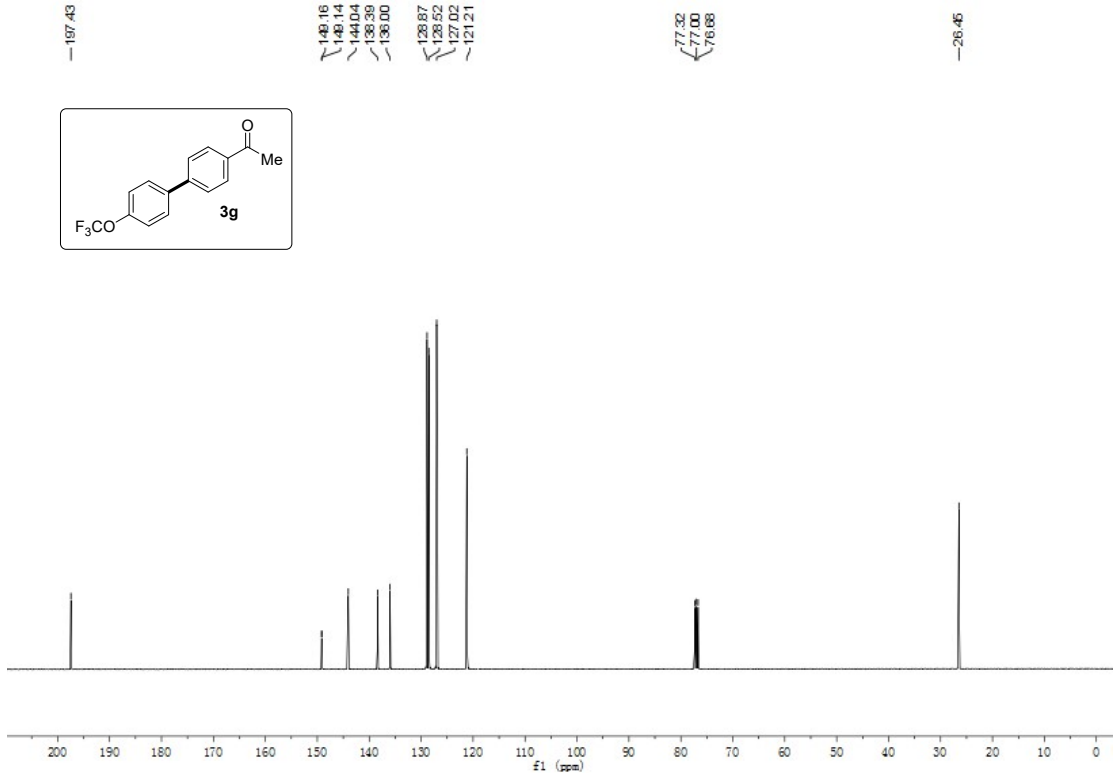
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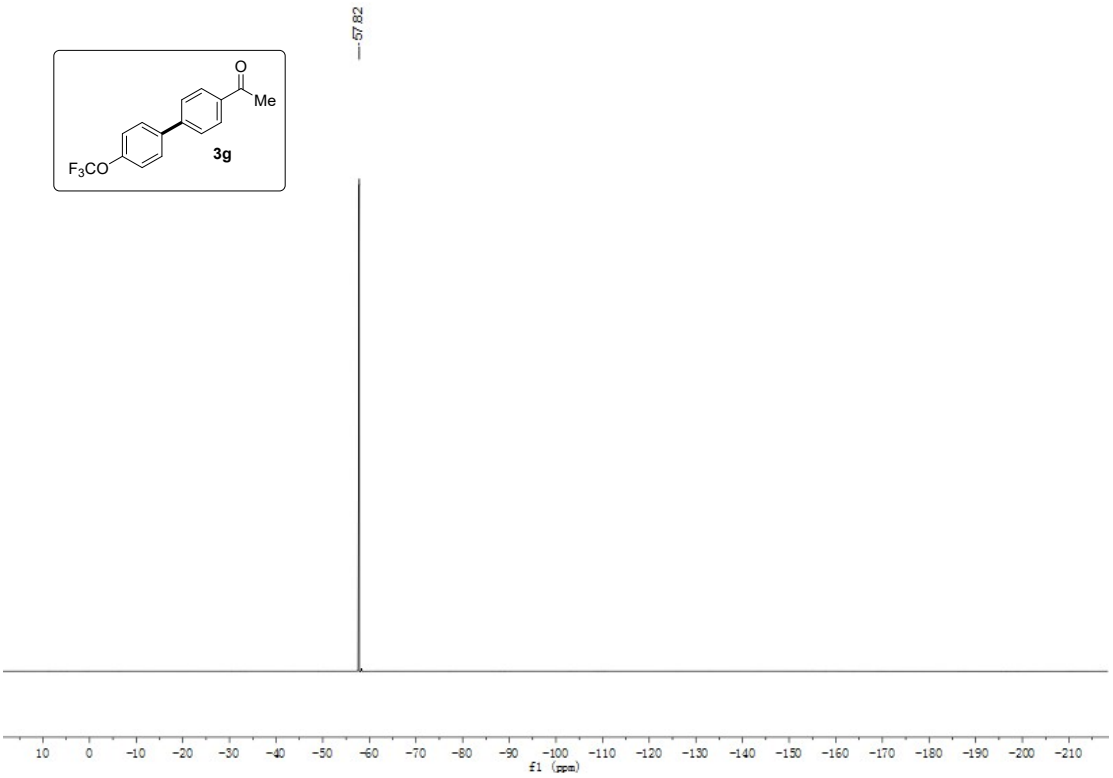
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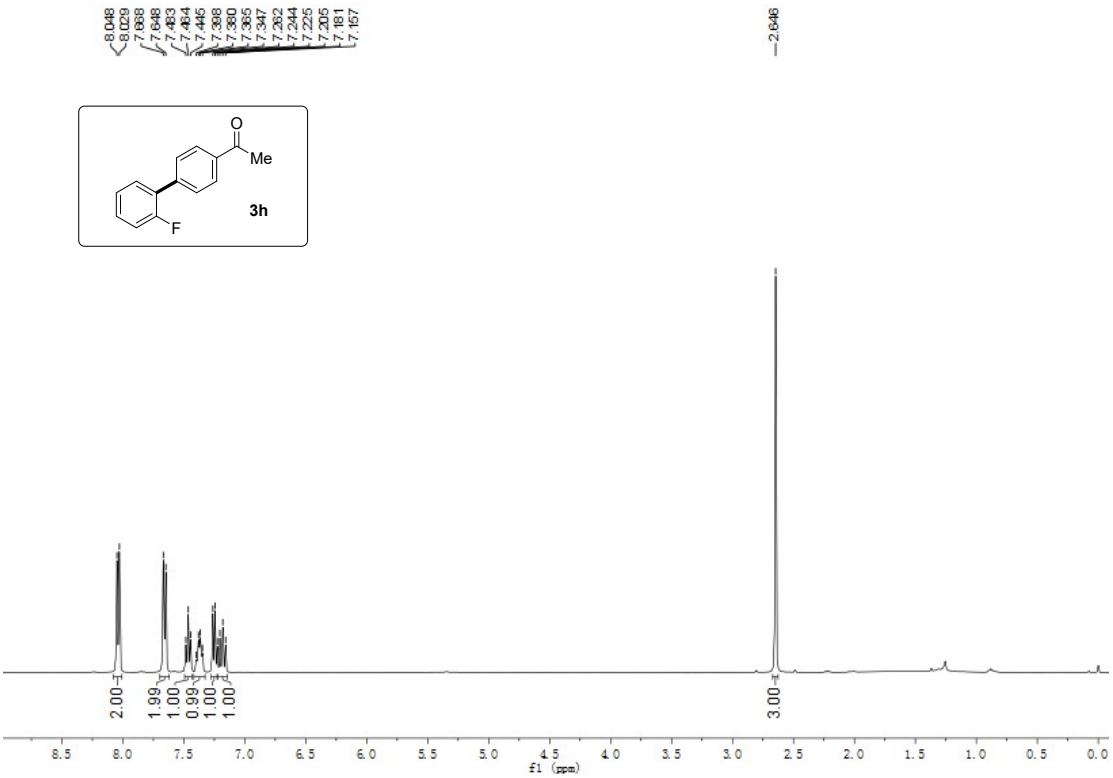
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1.00
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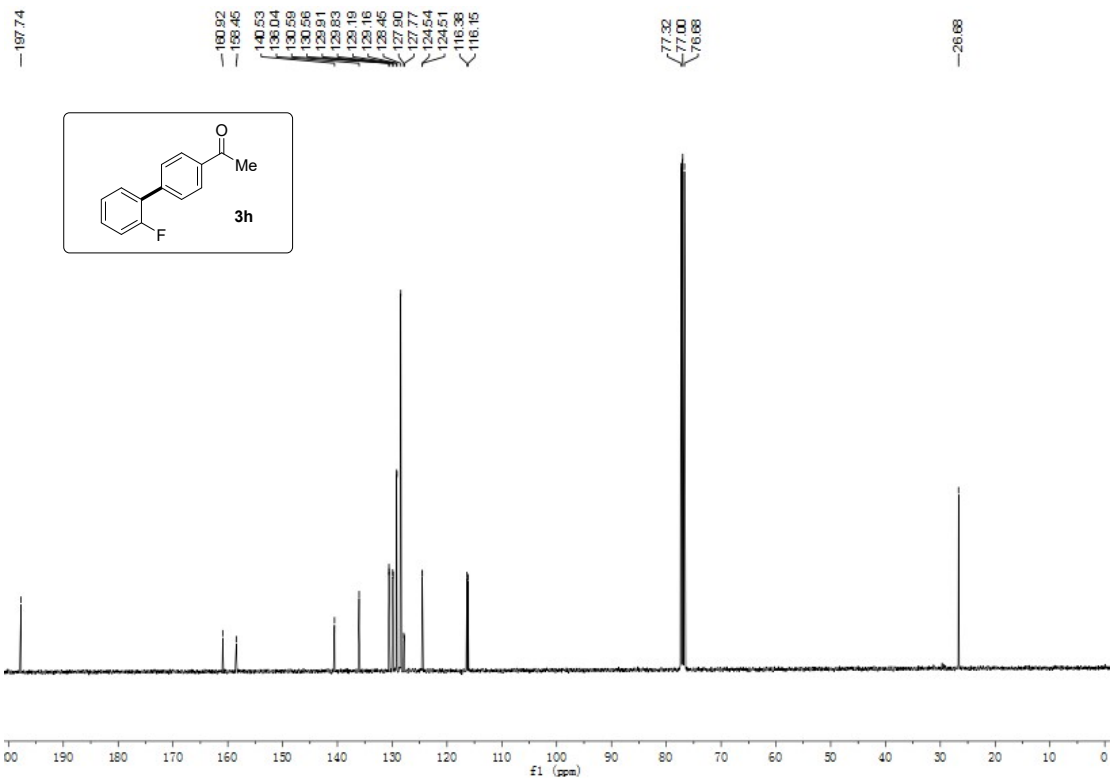
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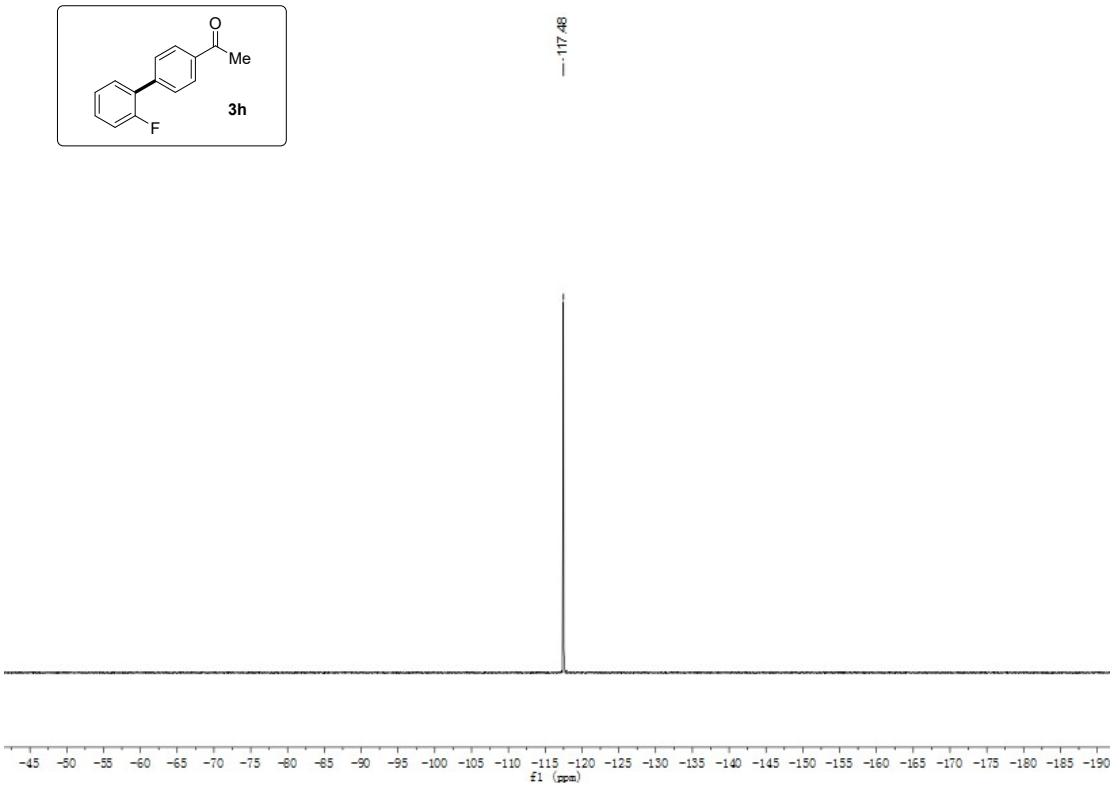
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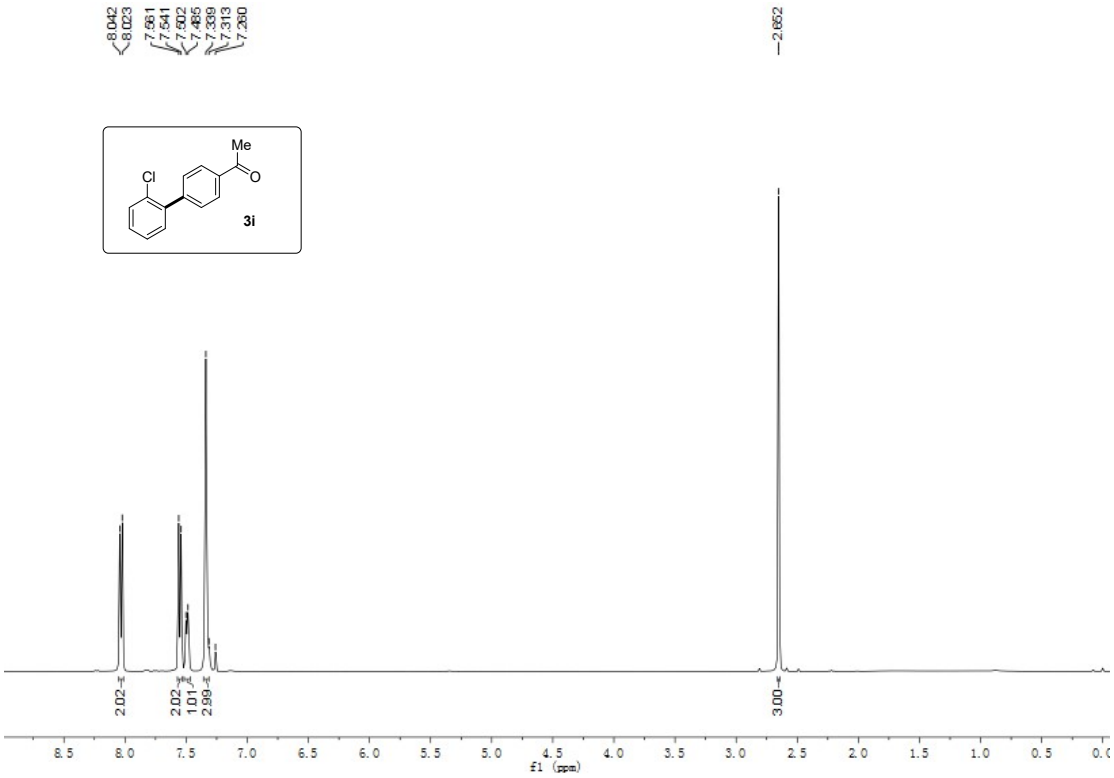
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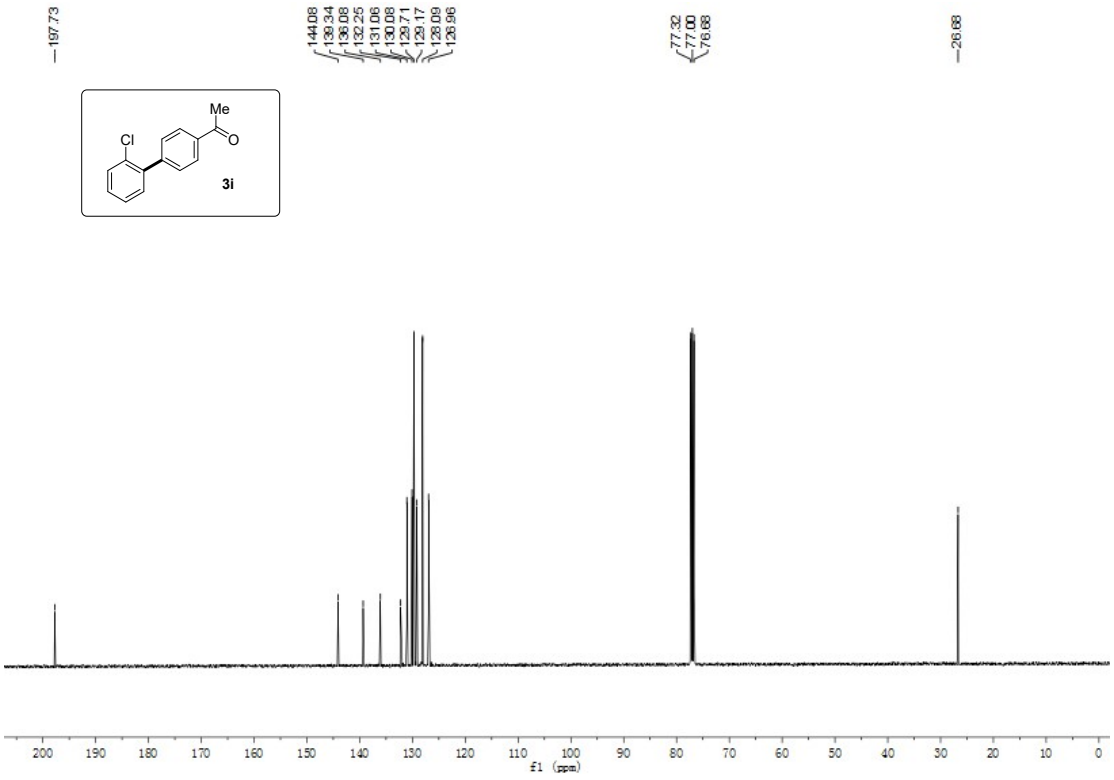
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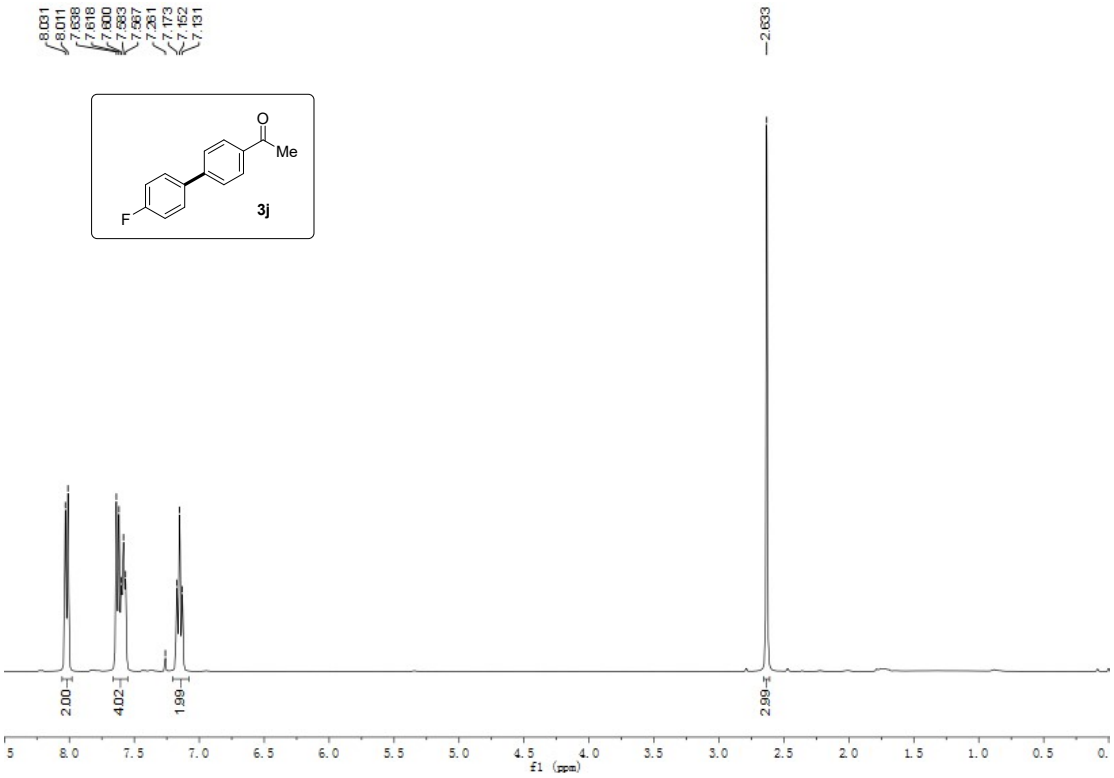
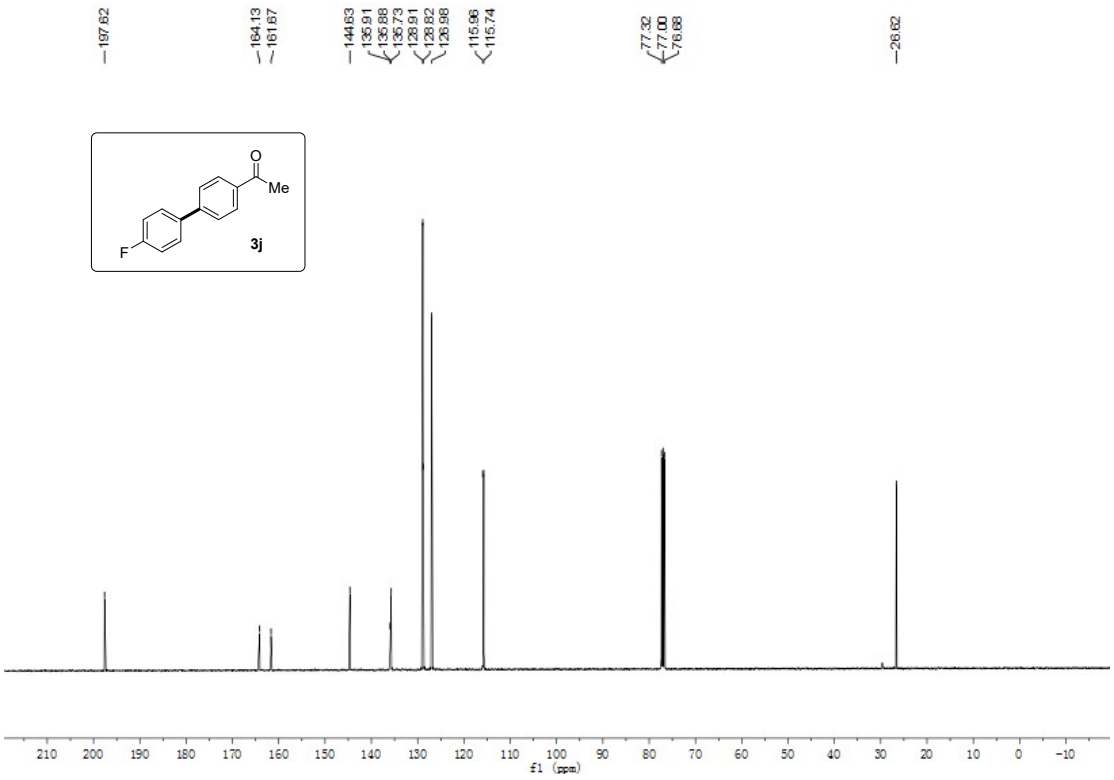
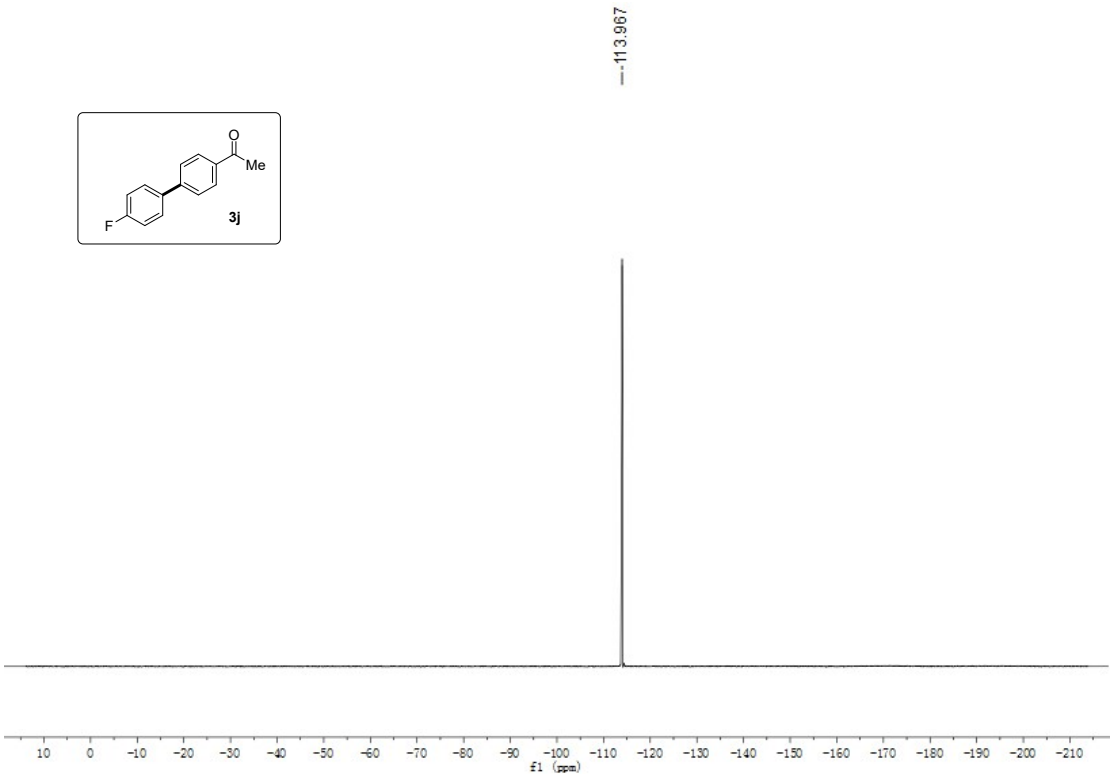
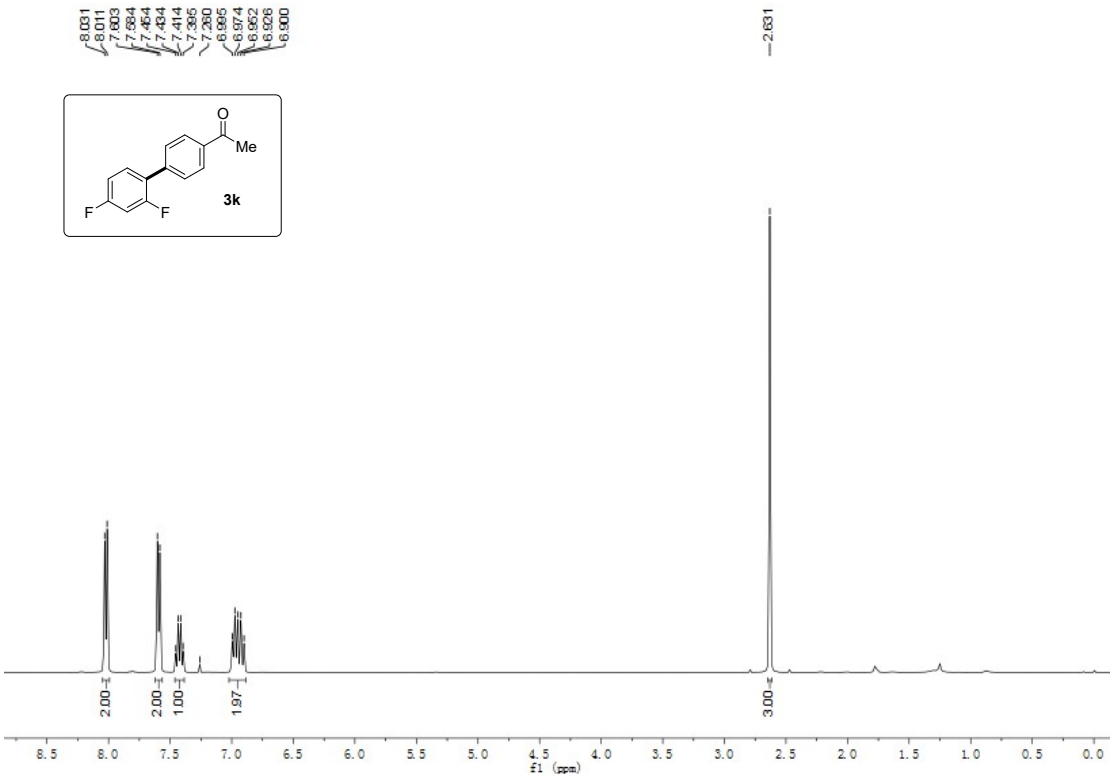
3i
f1 (ppm)


8.031
8.011
7.638
7.618
7.600
7.583
7.567
7.261
7.173
7.152
7.131
2.633
O
Me
F
3j
2.00
4.02
1.99
2.99
f1 (ppm)


197.62
164.13
161.67
144.63
135.91
135.88
135.73
128.91
128.82
126.98
115.96
115.74
77.32
77.00
76.68
26.62
O
Me
F
3j
f1 (ppm)


-113.967
O
Me
F
3j
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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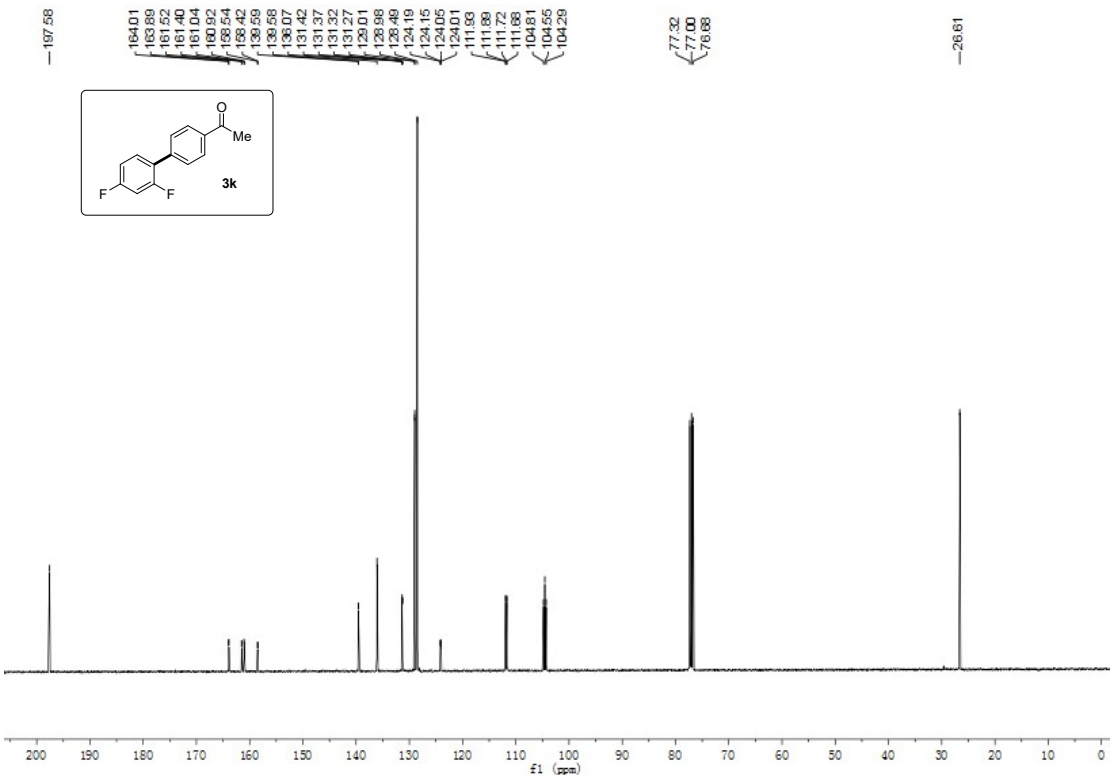
8.011
7.603
7.584
7.464
7.434
7.414
7.395
7.260
6.995
6.974
6.962
6.926
6.900
2.631
O
Me
F
F
3k
2.00
2.00
1.00
1.97
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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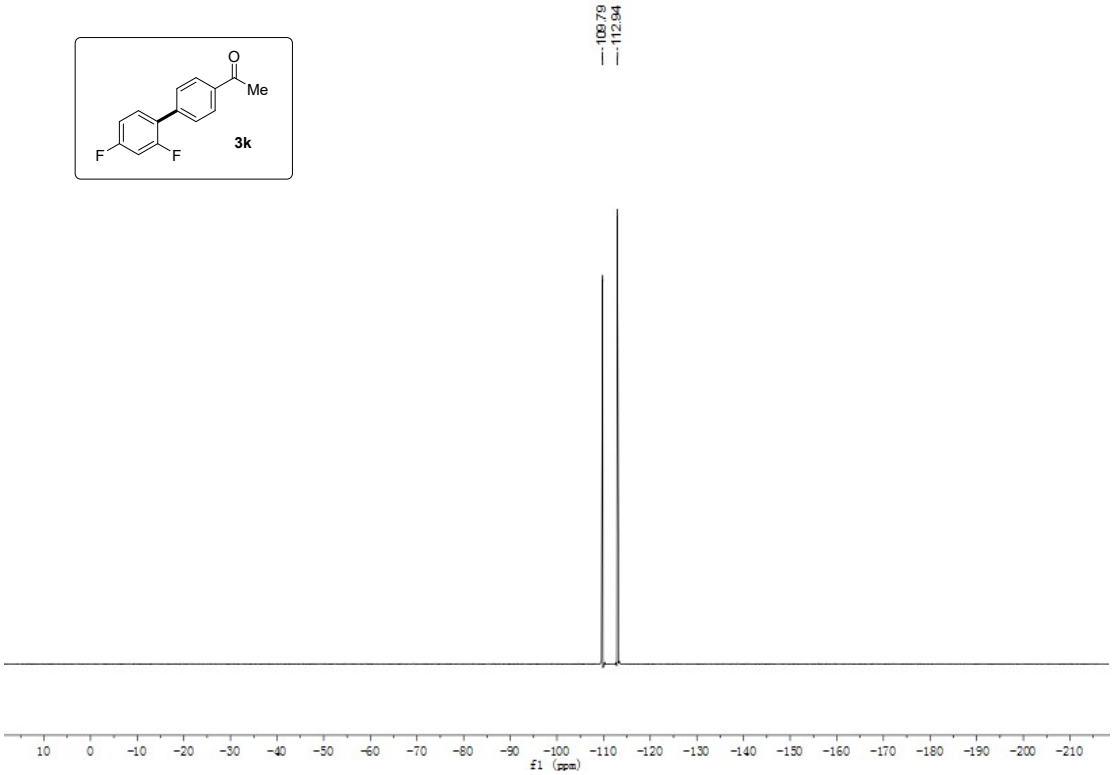
163.89
161.52
161.40
161.04
160.92
158.54
158.42
139.59
139.58
136.07
131.42
131.37
131.32
131.27
129.01
128.98
128.48
124.19
124.15
124.05
124.01
111.93
111.88
111.72
111.68
104.81
104.55
104.29
77.32
77.00
76.68
26.61
O
Me
F
F
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


109.79
112.94
O
Me
F
F
3k
10
0
-10
-20
-30
-40
-50
-60
-70
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-120
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-140
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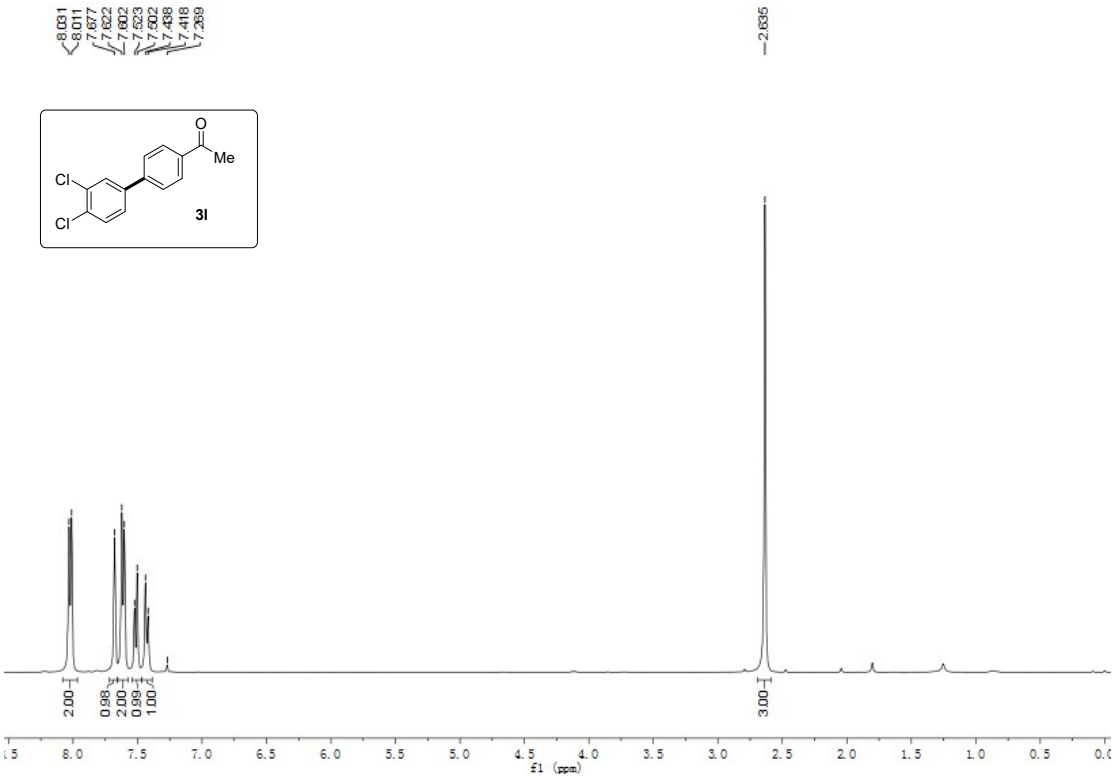
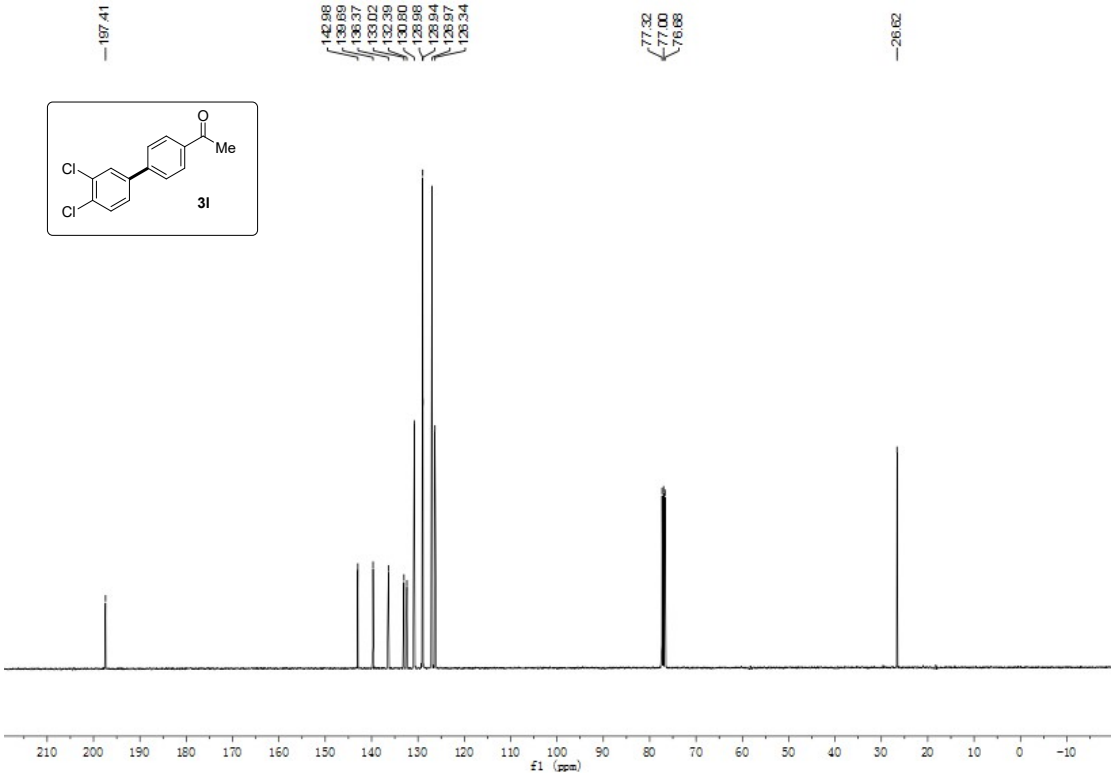
-160
-170
-180
-190
-200
-210
f1 (ppm)


8.031
8.011
7.677
7.622
7.602
7.523
7.502
7.438
7.418
7.269
2.635
O
Me
Cl
Cl
3l
2.00
0.98
2.00
0.99
1.00
3.00
f1 (ppm)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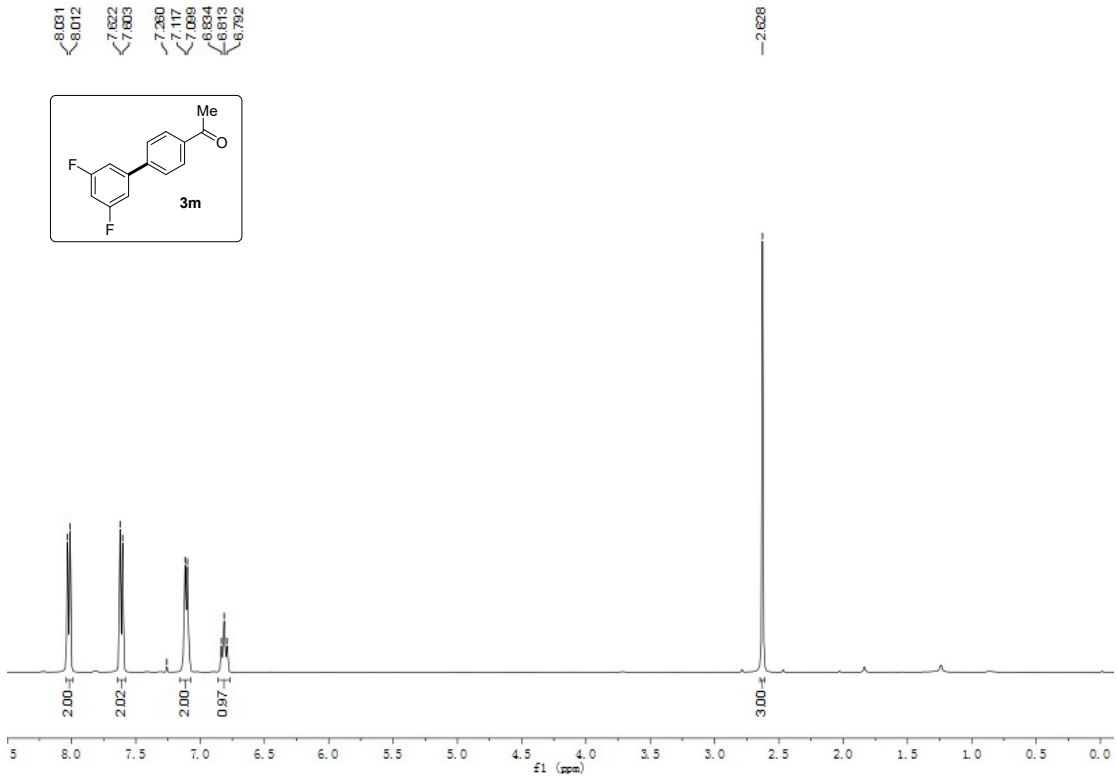
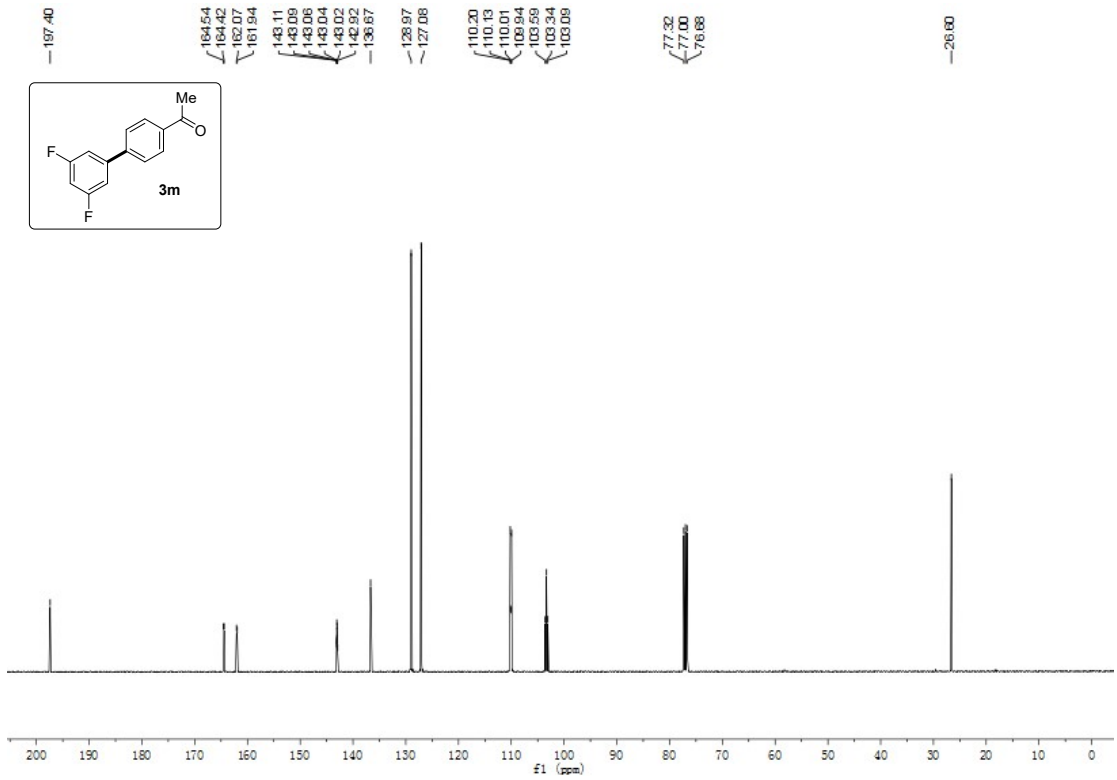
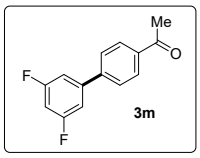
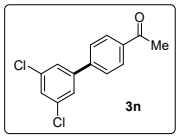
142.98
139.69
138.37
133.02
132.39
130.80
128.98
128.94
128.97
126.34
77.32
77.00
76.68
26.62
O
Me
Cl
Cl
3l
f1 (ppm)


8.031
8.012
7.622
7.603
7.260
7.117
7.099
6.834
6.813
6.792
2.628
Me
O
F
F
3m
2.00
2.02
2.00
0.97
3.00
f1 (ppm)

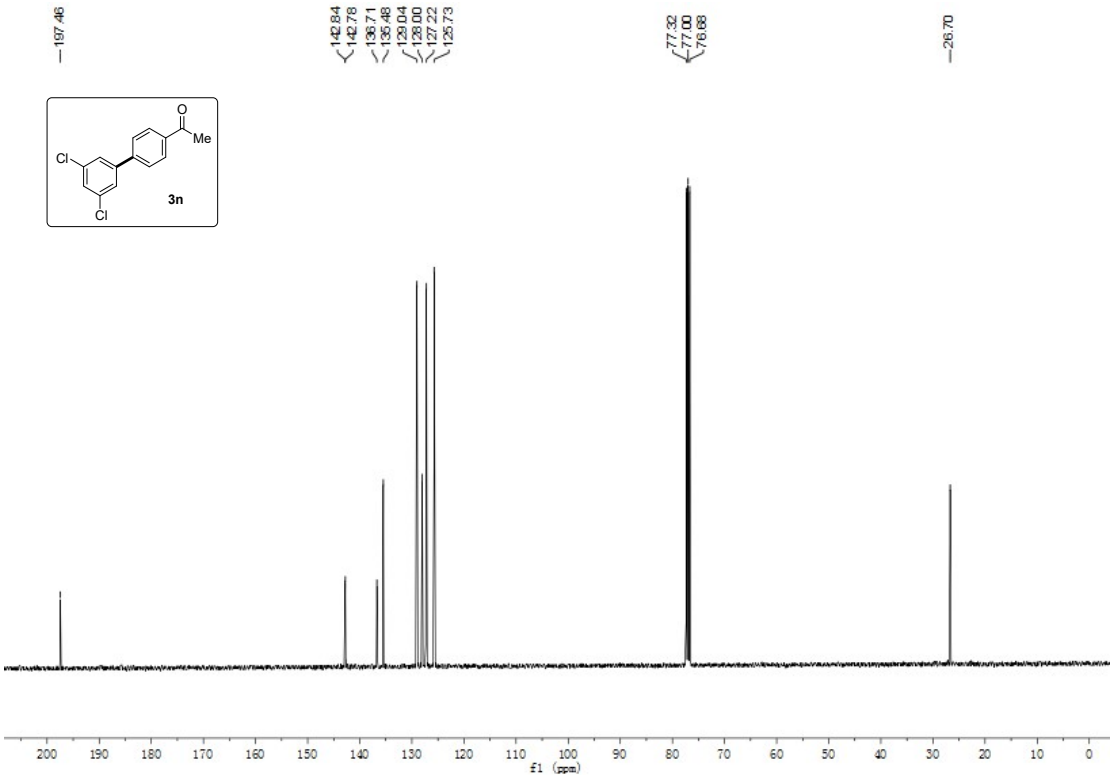

197.40
164.54
164.42
162.07
161.94
143.11
143.09
143.06
143.04
143.02
142.92
136.67
128.97
127.08
110.20
110.13
110.01
109.94
103.59
103.34
103.09
77.32
77.00
76.68
26.60
Me
O
F
F
3m
f1 (ppm)

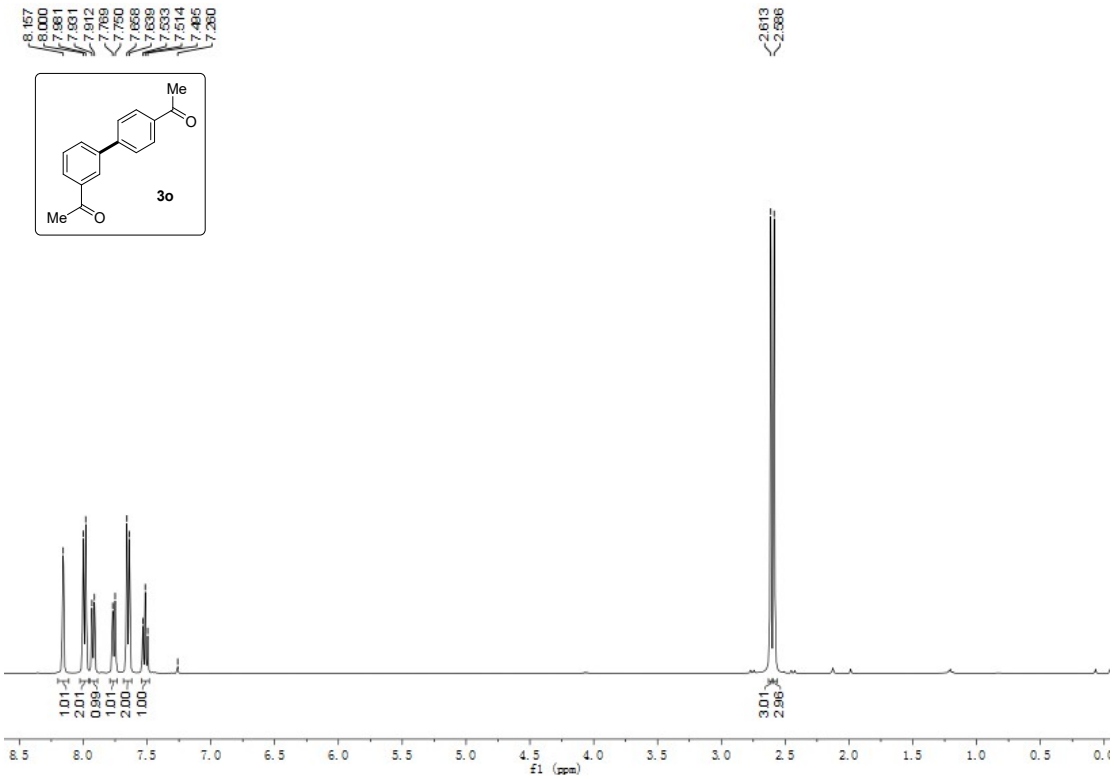

Me
O
F
F
3m

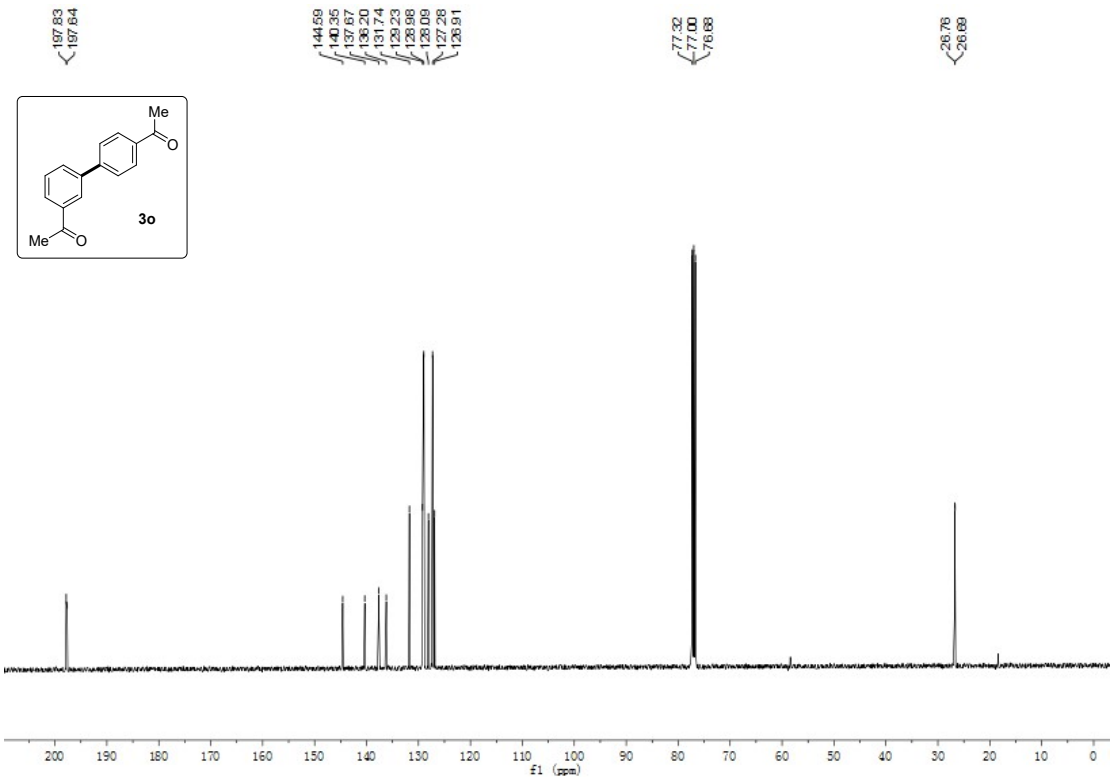
-109.028
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

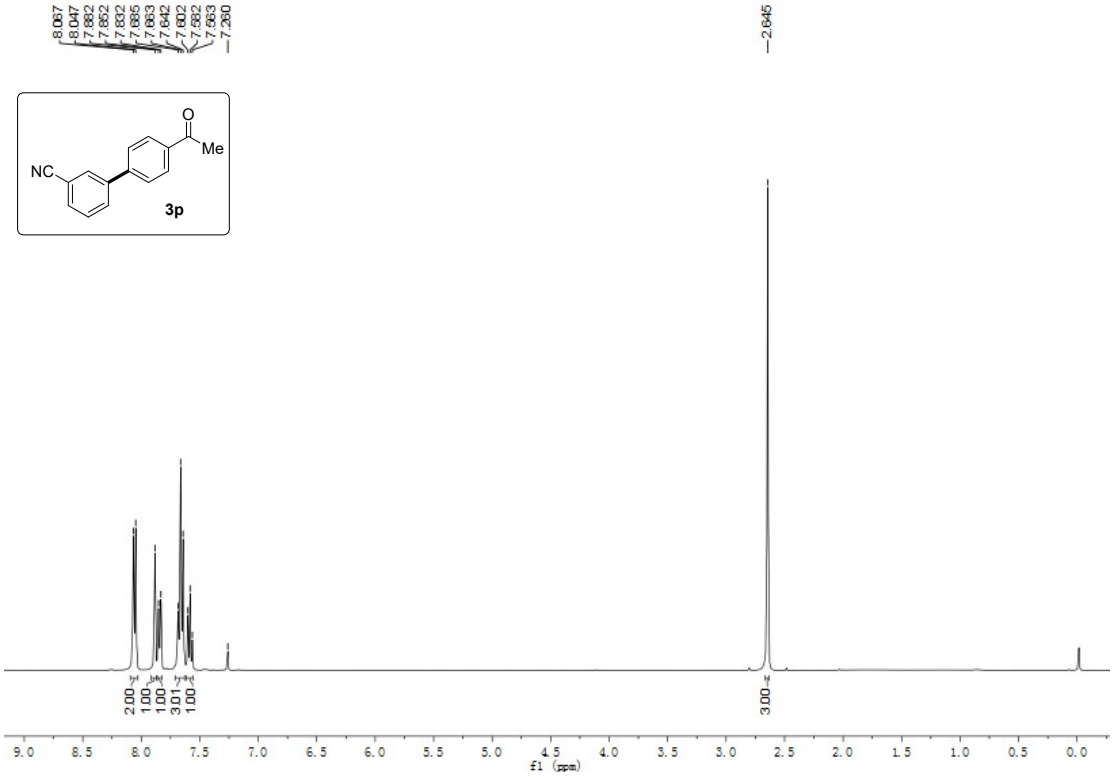

O
Me
Cl
Cl
3n

8.050
8.030
7.638
7.618
7.484
7.365
2.648
2.01
2.08
2.00
1.00
3.00
.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)


197.46
142.84
142.78
136.71
135.48
129.04
128.00
127.22
125.73
77.32
77.00
76.68
26.70
O
Me
Cl
Cl
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.157
8.000
7.981
7.931
7.912
7.769
7.750
7.658
7.639
7.533
7.514
7.405
7.260
2.613
2.596
Me
O
Me
O
3o
1.01
2.01
0.99
1.01
2.00
1.00
3.01
2.96
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
f1 (ppm)


197.83
197.64
144.59
140.35
137.67
136.20
131.74
129.23
128.98
128.09
127.28
126.91
77.32
77.00
76.68
26.78
26.69
Me
O
Me
O
3o
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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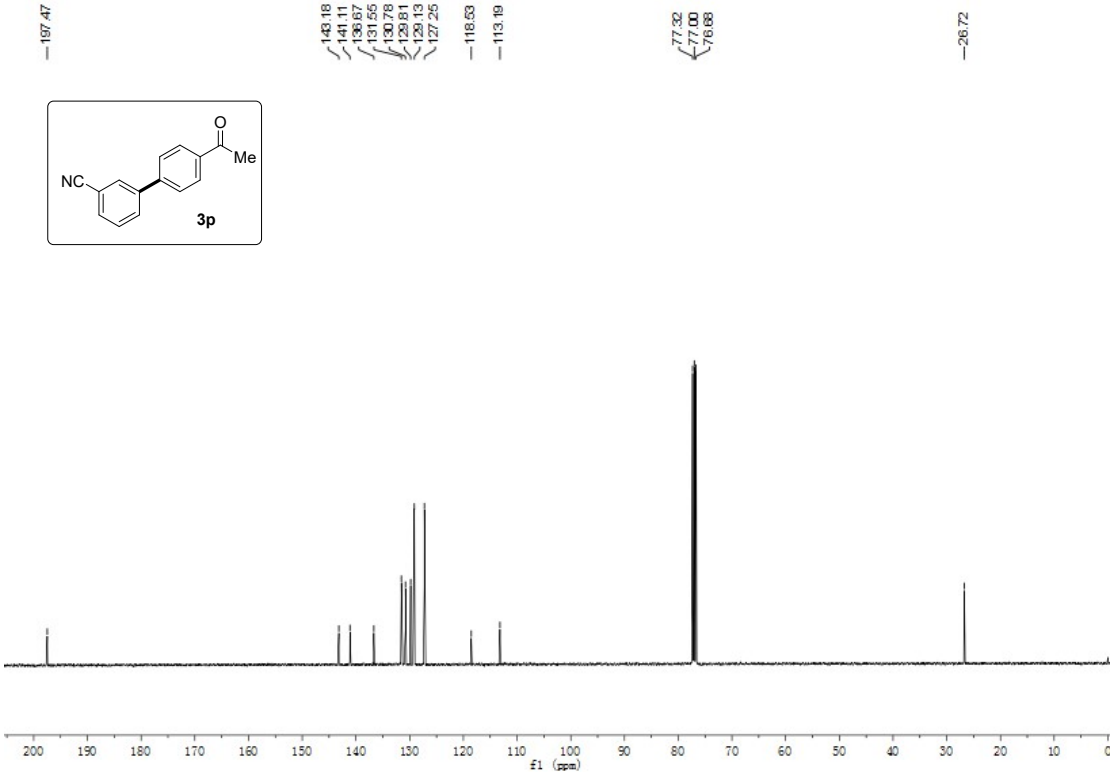
8.047
7.882
7.862
7.832
7.685
7.663
7.642
7.602
7.582
7.563
7.260
2.645
O
Me
NC
3p
2.00
1.00
1.00
3.01
1.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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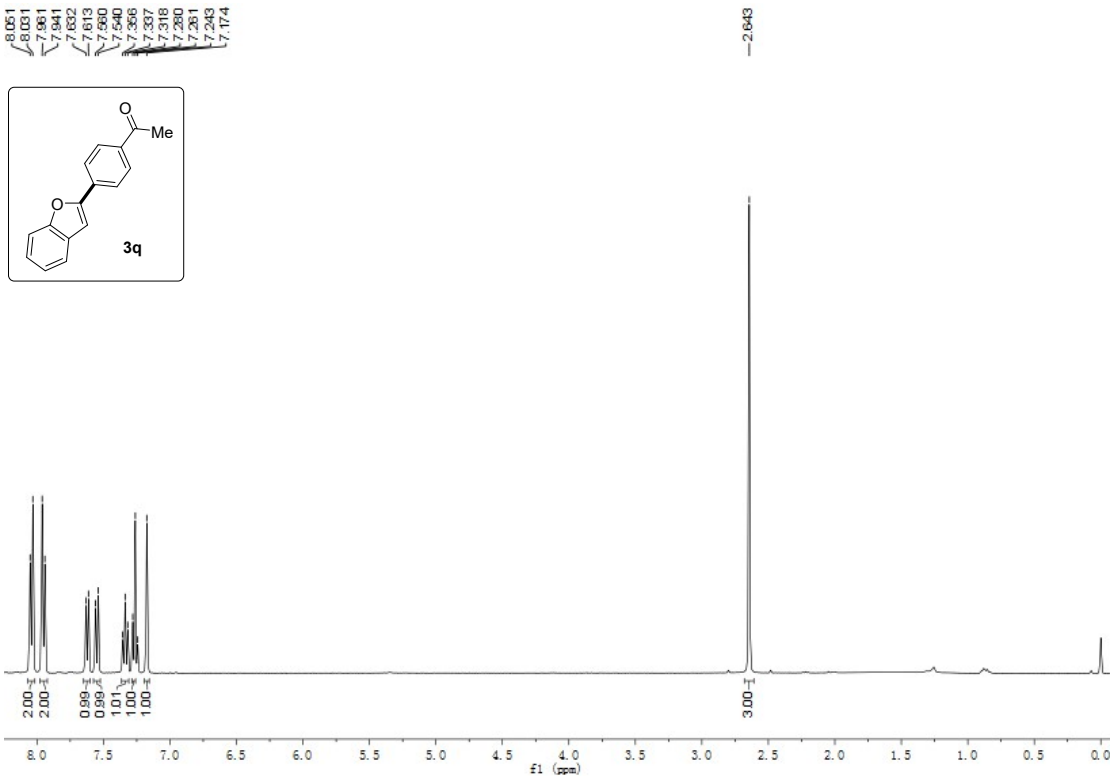
141.11
136.67
131.55
130.78
129.81
129.13
127.25
118.53
113.19
77.32
77.00
76.68
26.72
O
Me
NC
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.031
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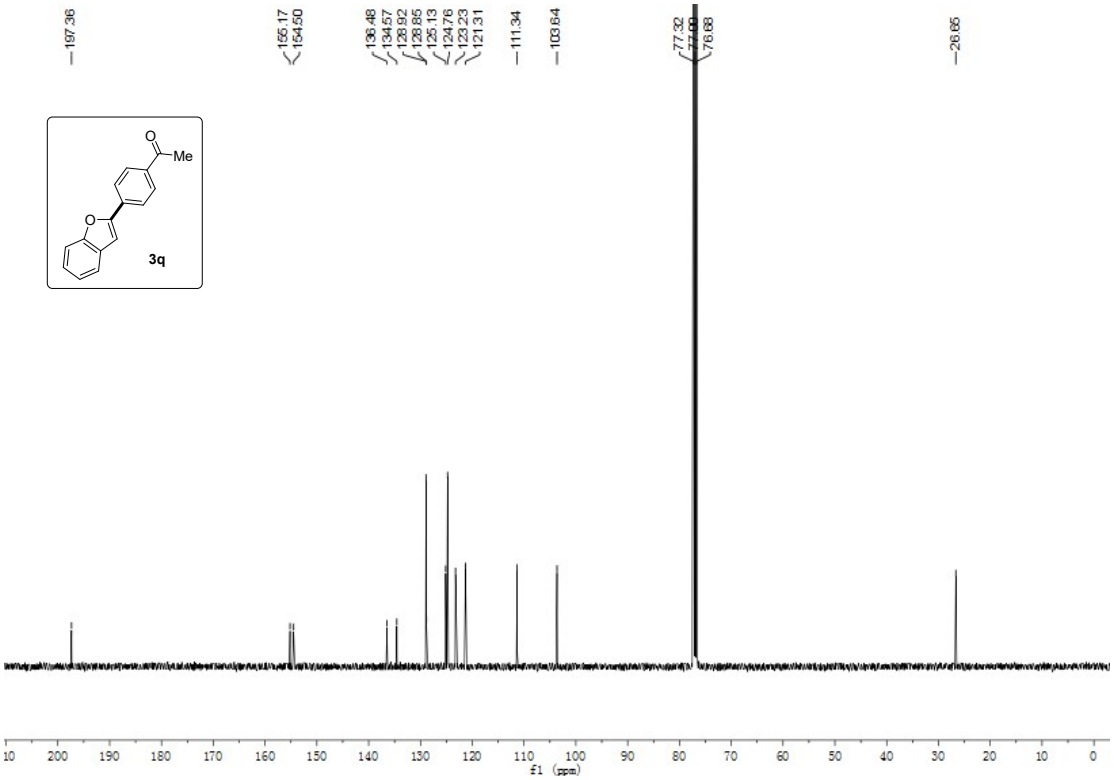
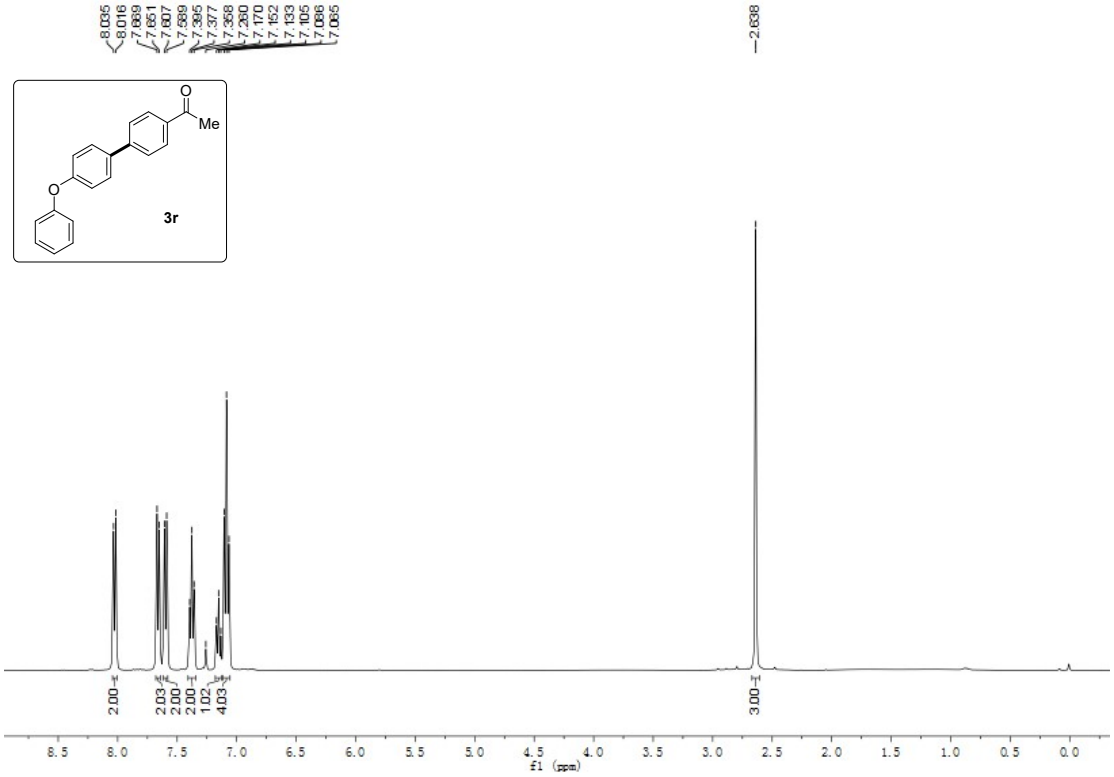
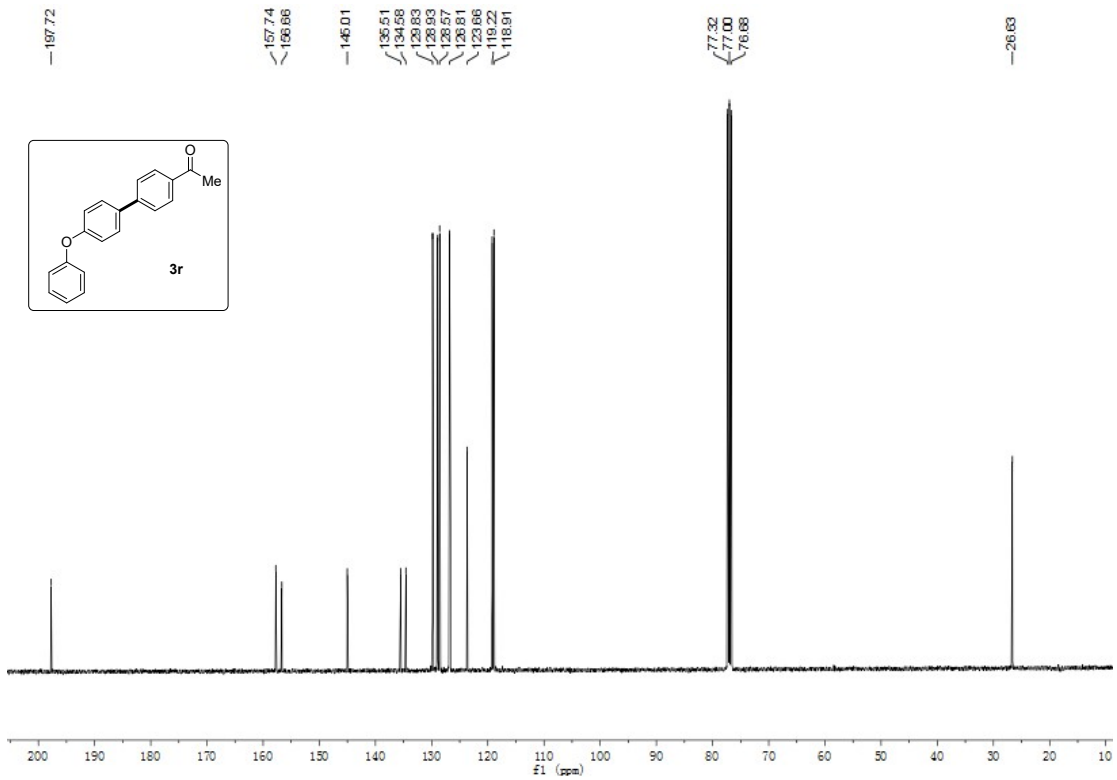
7.941
7.632
7.613
7.560
7.540
7.356
7.337
7.318
7.280
7.261
7.243
7.174
2.643
O
Me
O
3q
2.00
2.00
0.99
0.99
1.01
1.00
1.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


197.36
155.17
154.50
136.48
134.57
128.92
128.85
125.13
124.76
123.23
121.31
111.34
103.64
77.32
77.00
76.68
26.65
Me
O
O
3q
f1 (ppm)


8.035
8.016
7.669
7.651
7.607
7.589
7.395
7.377
7.368
7.260
7.170
7.152
7.133
7.105
7.086
7.065
2.638
Me
O
O
3r
2.00
2.03
2.00
2.00
1.02
4.03
3.00
f1 (ppm)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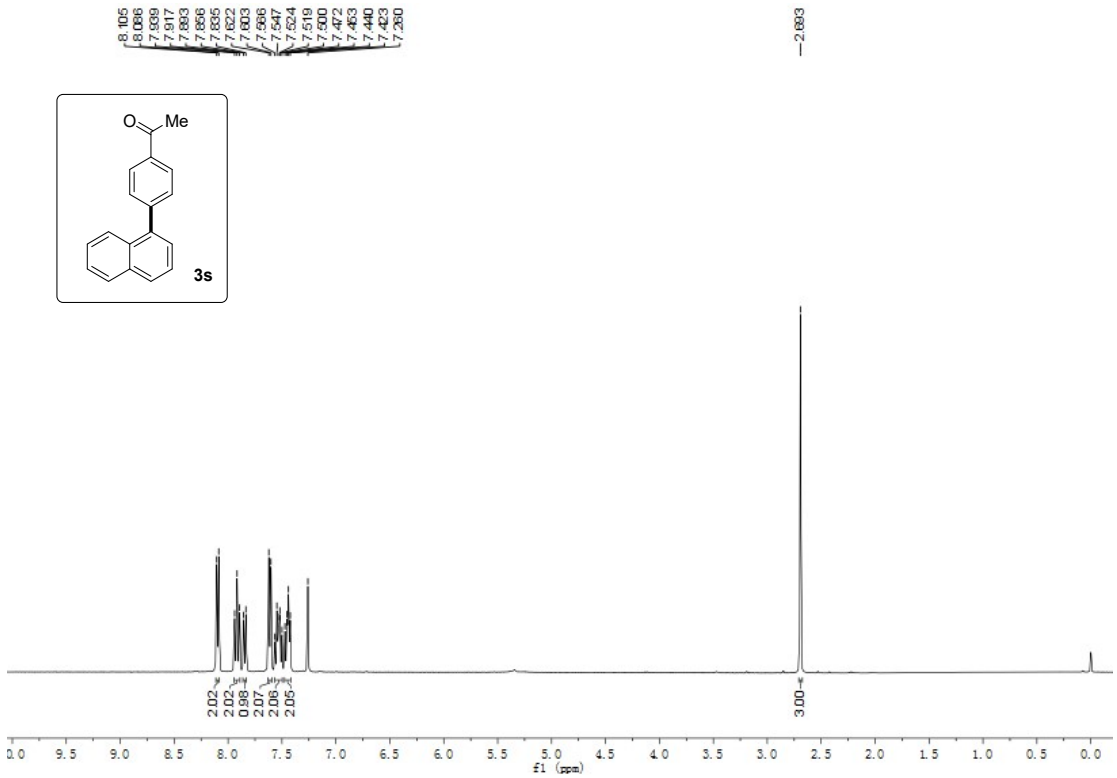
145.01
135.51
134.58
129.83
128.93
128.57
126.81
123.66
119.22
118.91
77.32
77.00
76.68
26.63
O
Me
O
3r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.086
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7.917
7.893
7.856
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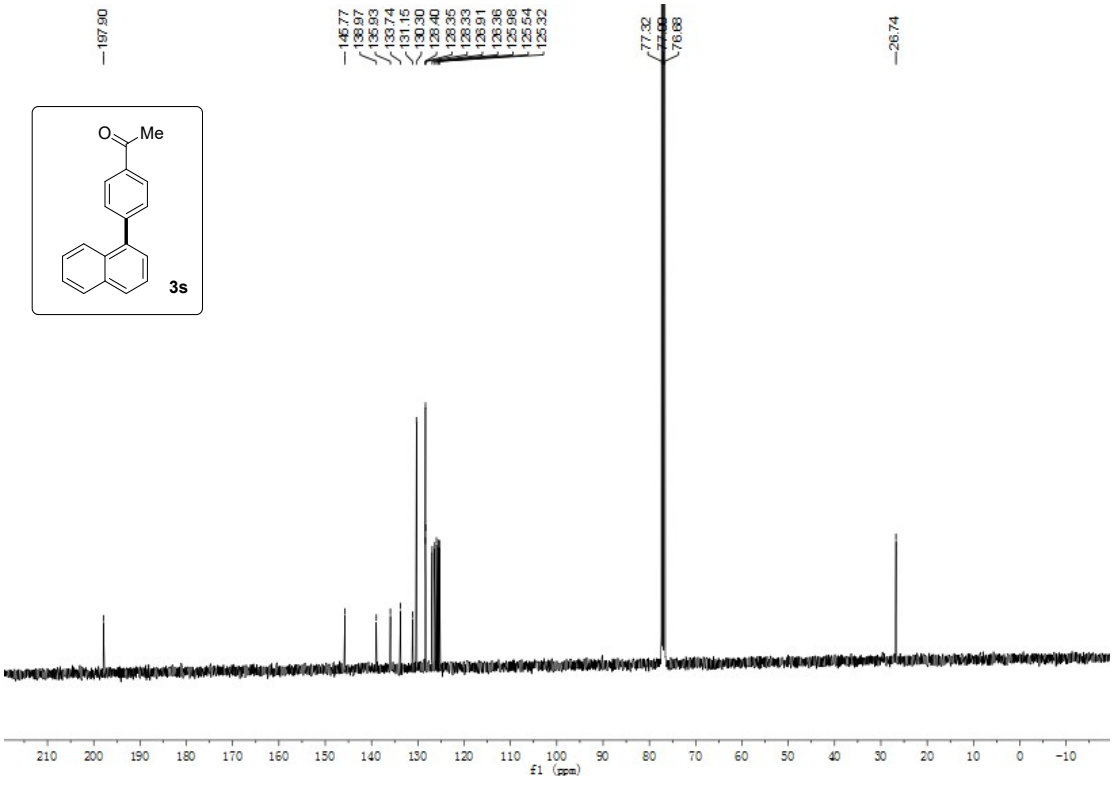
7.622
7.603
7.566
7.547
7.524
7.519
7.500
7.472
7.453
7.440
7.423
7.260
2.693
O
Me
3s
2.02
2.02
0.98
2.07
2.06
2.05
3.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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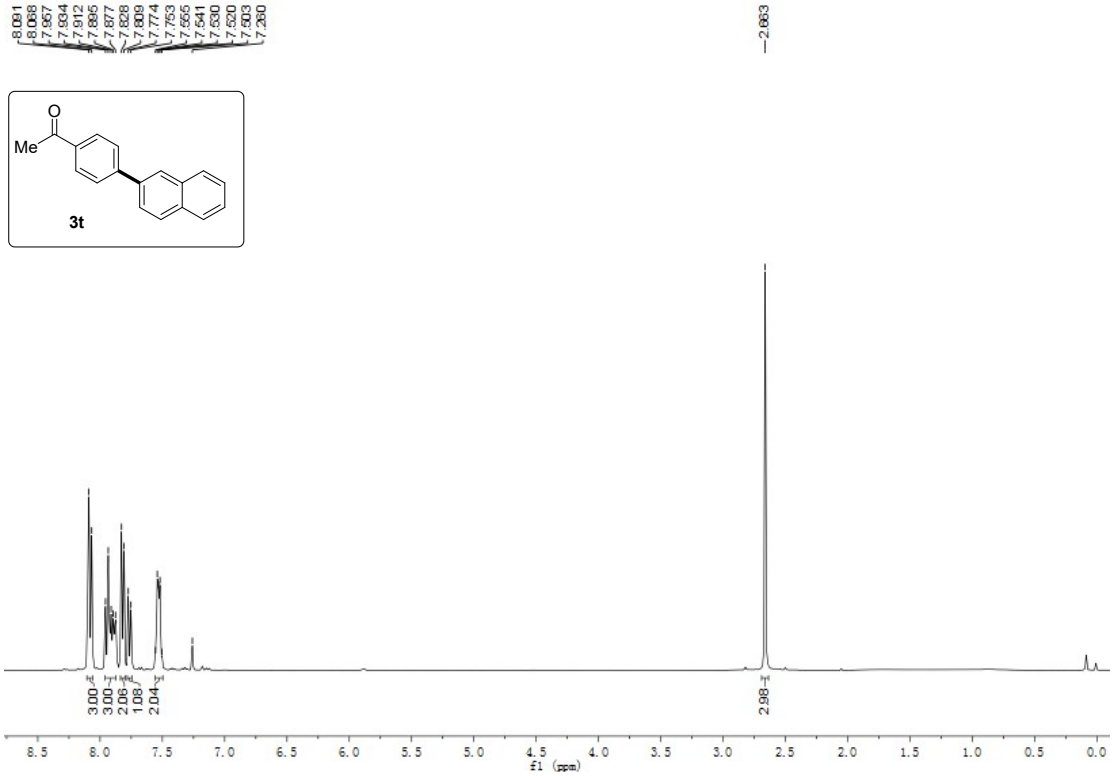
133.74
131.15
130.30
129.40
128.35
128.33
126.91
126.36
125.98
125.54
125.32
77.32
77.00
76.68
26.74
O
Me
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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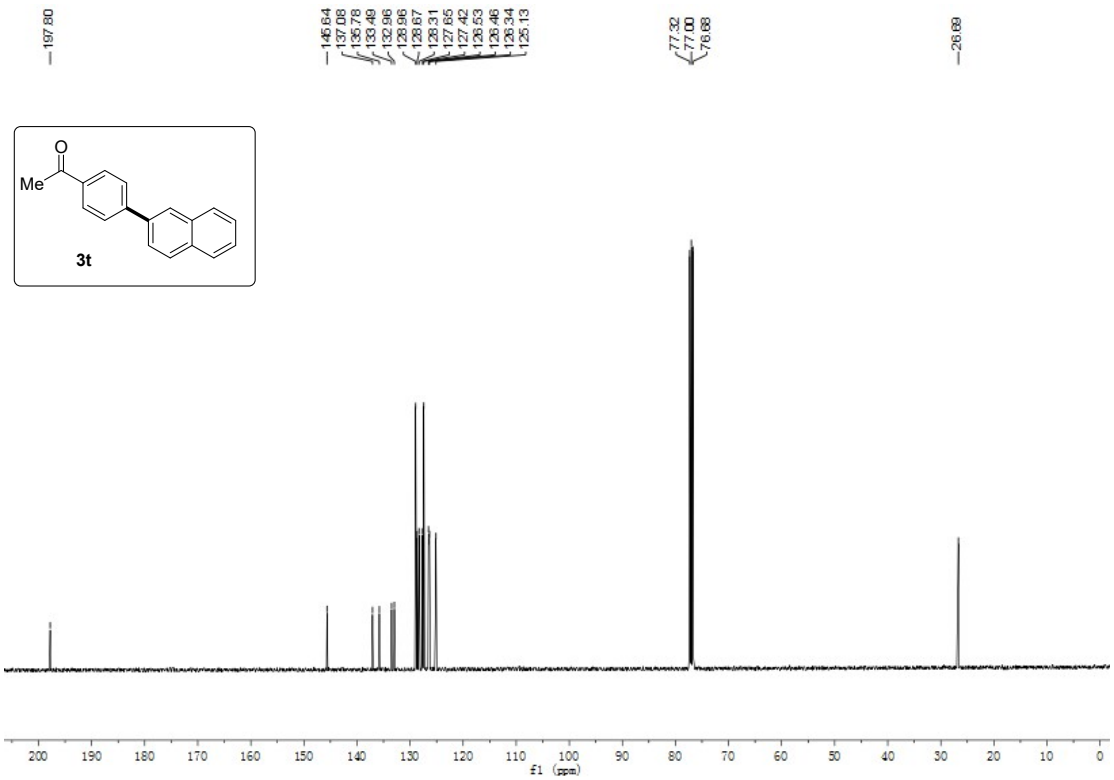
7.912
7.895
7.877
7.828
7.809
7.774
7.753
7.555
7.541
7.530
7.520
7.503
7.260
2.663
O
Me
3t
3.00
3.00
2.06
1.08
2.04
2.98
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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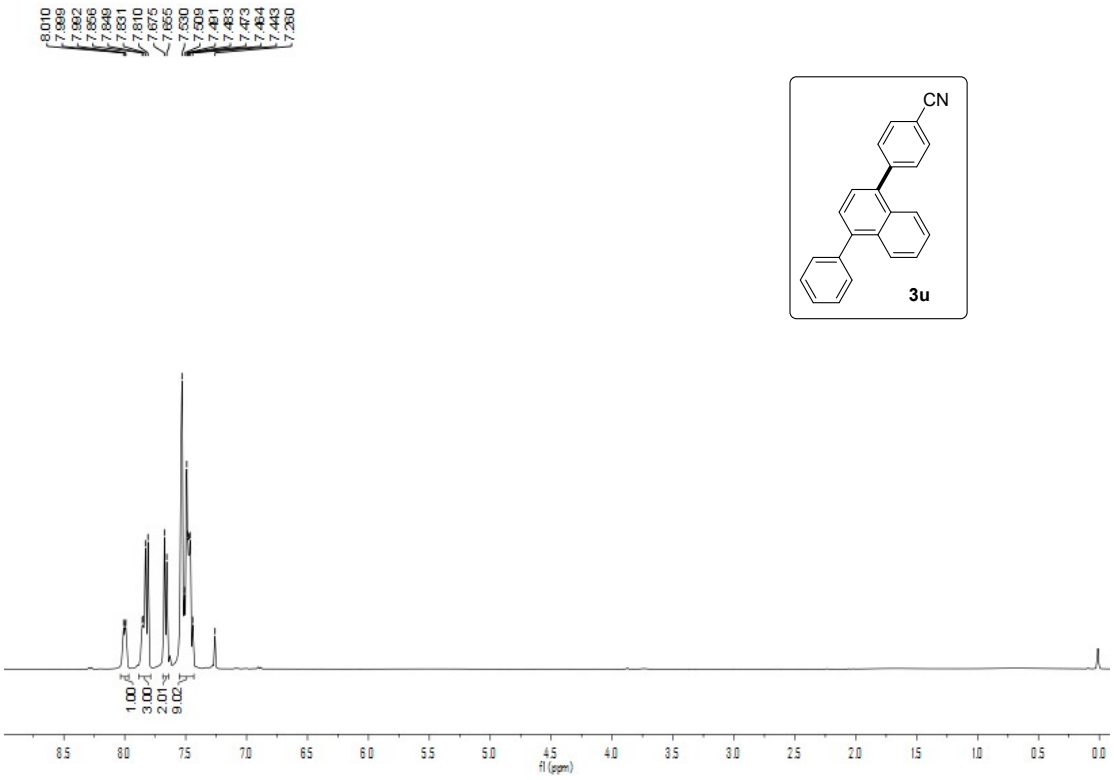
135.78
133.49
132.96
128.96
128.67
128.31
127.65
127.42
126.53
126.46
126.34
125.13
77.32
77.00
76.68
26.69
O
Me
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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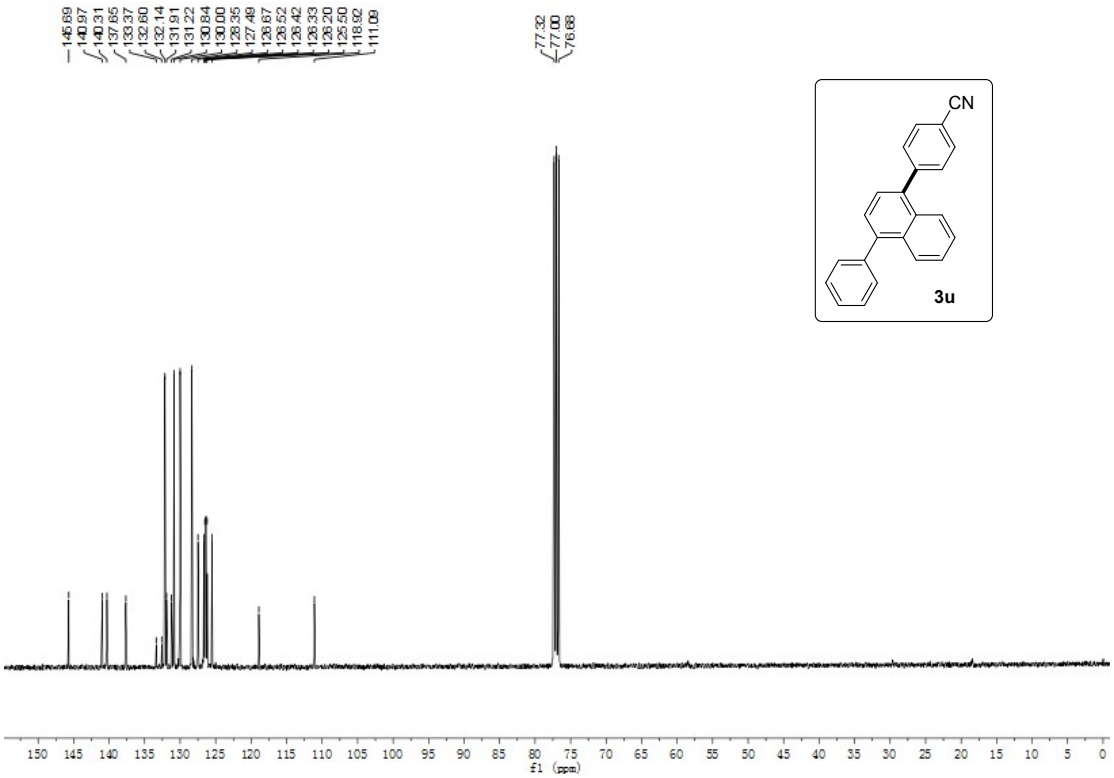
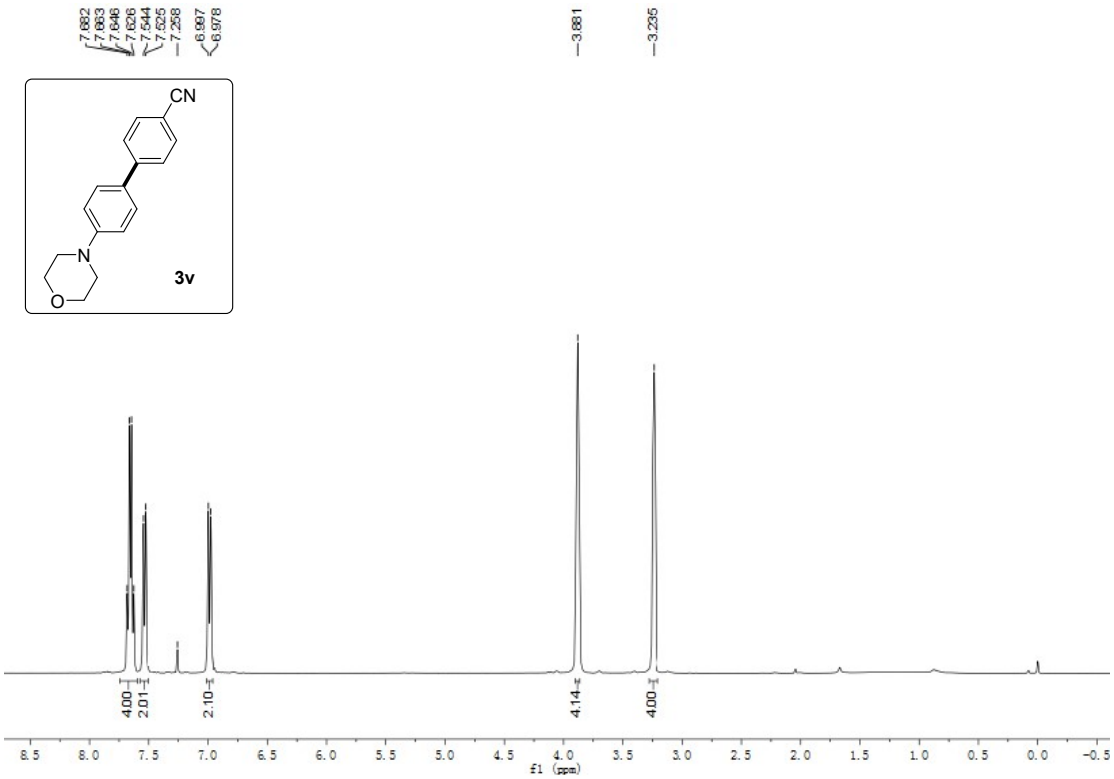
7.992
7.856
7.849
7.831
7.810
7.675
7.655
7.530
7.509
7.481
7.463
7.473
7.464
7.443
7.260
CN
3u
1.00
3.00
2.01
9.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


145.69
140.97
140.31
137.65
133.37
132.60
132.14
131.91
131.22
130.84
130.00
128.35
127.49
126.67
126.52
126.42
126.33
126.20
125.50
118.92
111.09
77.32
77.00
76.68
CN
3u
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.863
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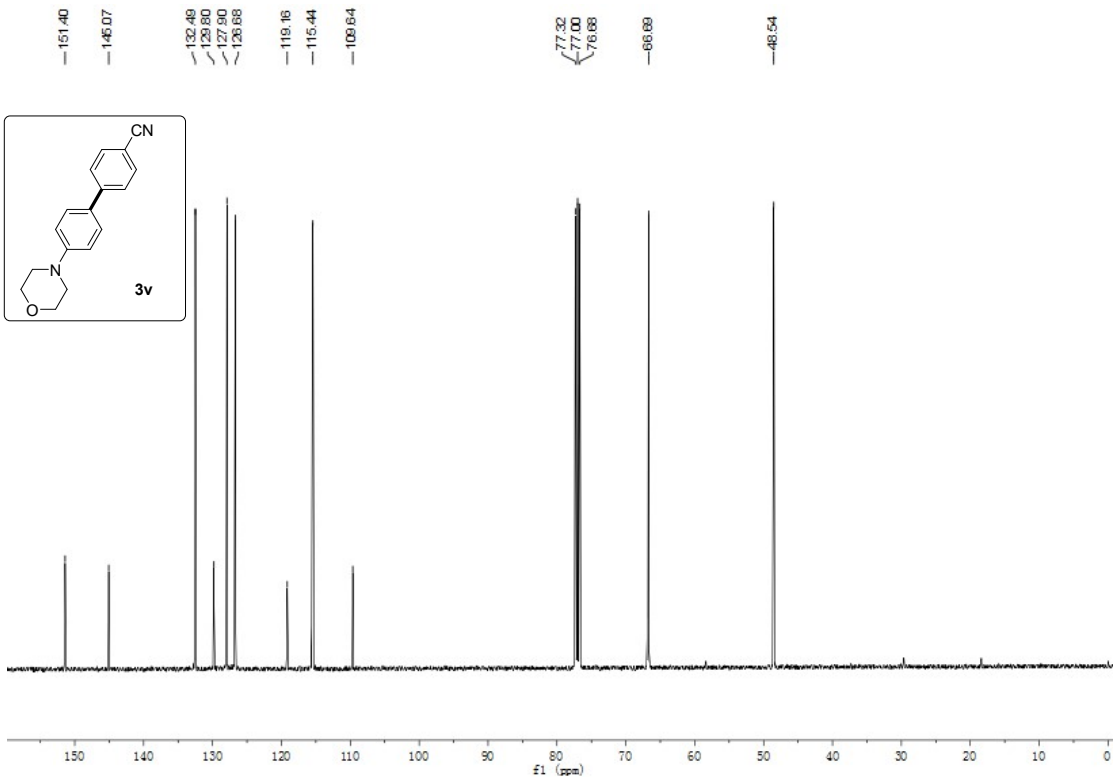
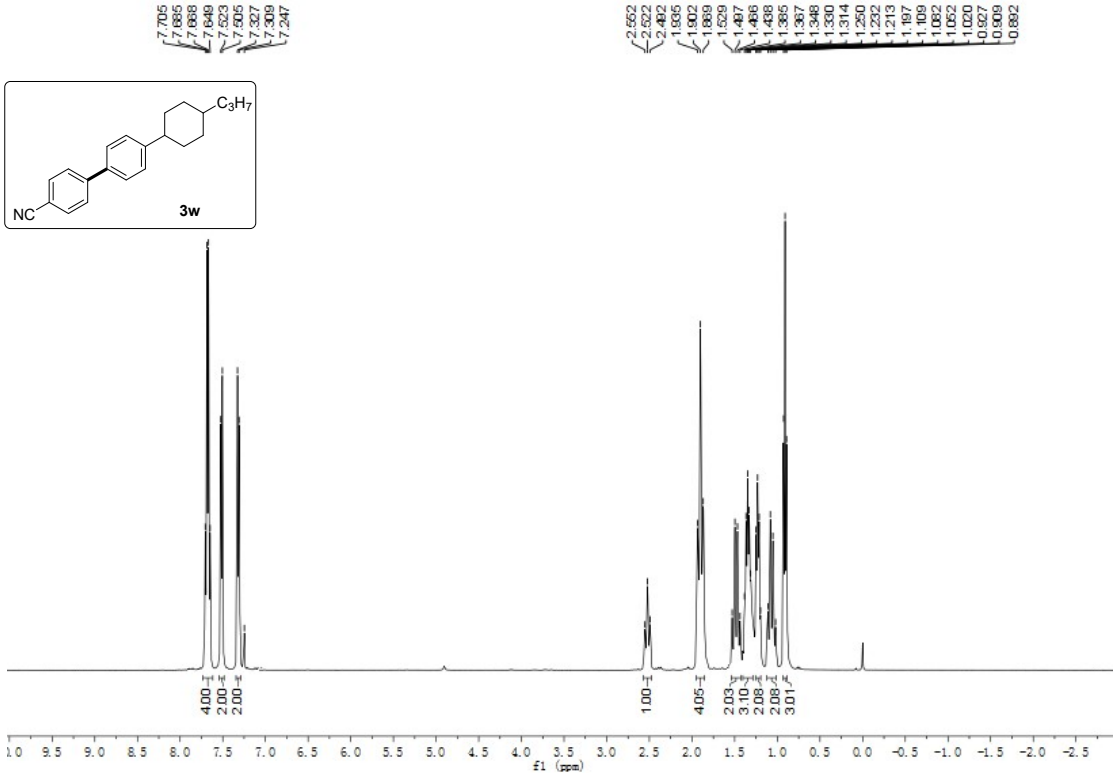
7.626
7.544
7.525
7.258
6.987
6.978
3.881
3.235
CN
N
O
3v
4.00
2.01
2.10
4.14
4.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


151.40
145.07
132.49
129.80
127.90
126.68
119.16
115.44
109.64
77.32
77.00
76.68
66.89
48.54
CN
N
O
3v
f1 (ppm)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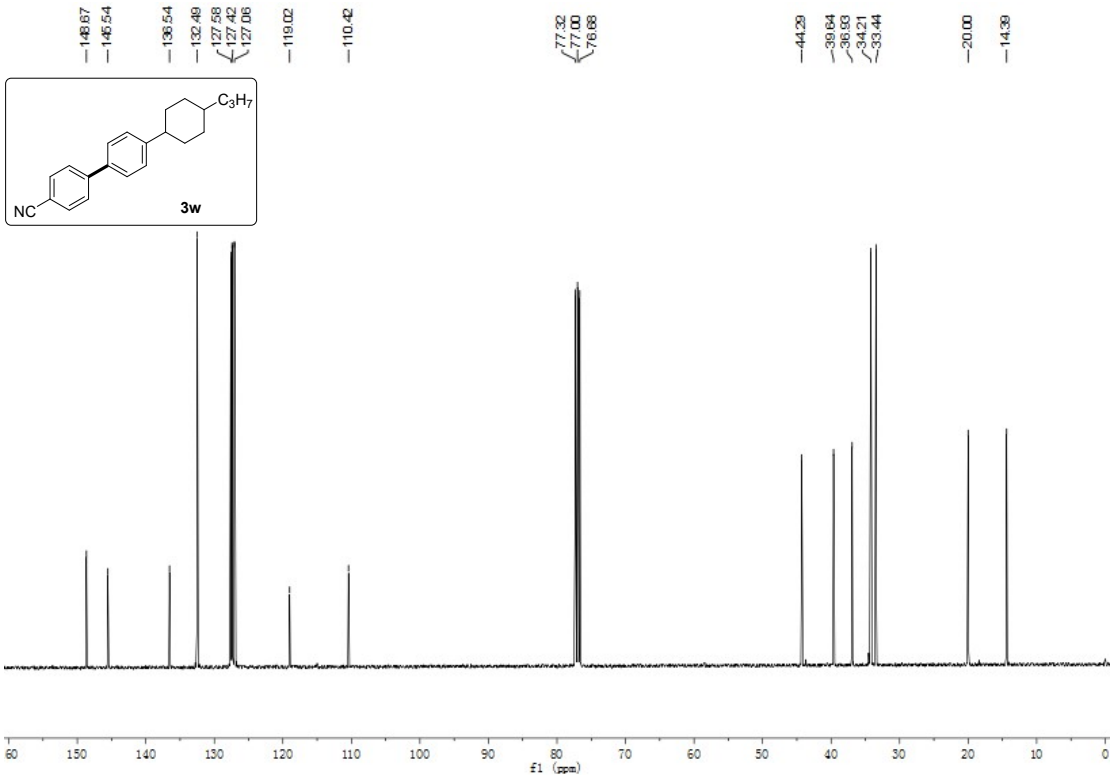
7.668
7.649
7.523
7.505
7.327
7.309
7.247
2.552
2.522
2.492
1.935
1.902
1.869
1.529
1.497
1.456
1.438
1.385
1.367
1.348
1.330
1.314
1.250
1.232
1.213
1.197
1.109
1.082
1.052
1.020
0.927
0.909
0.892
C3H7
NC
3w
4.00
2.00
2.00
1.00
4.05
2.03
3.10
2.08
2.08
3.01
f1 (ppm)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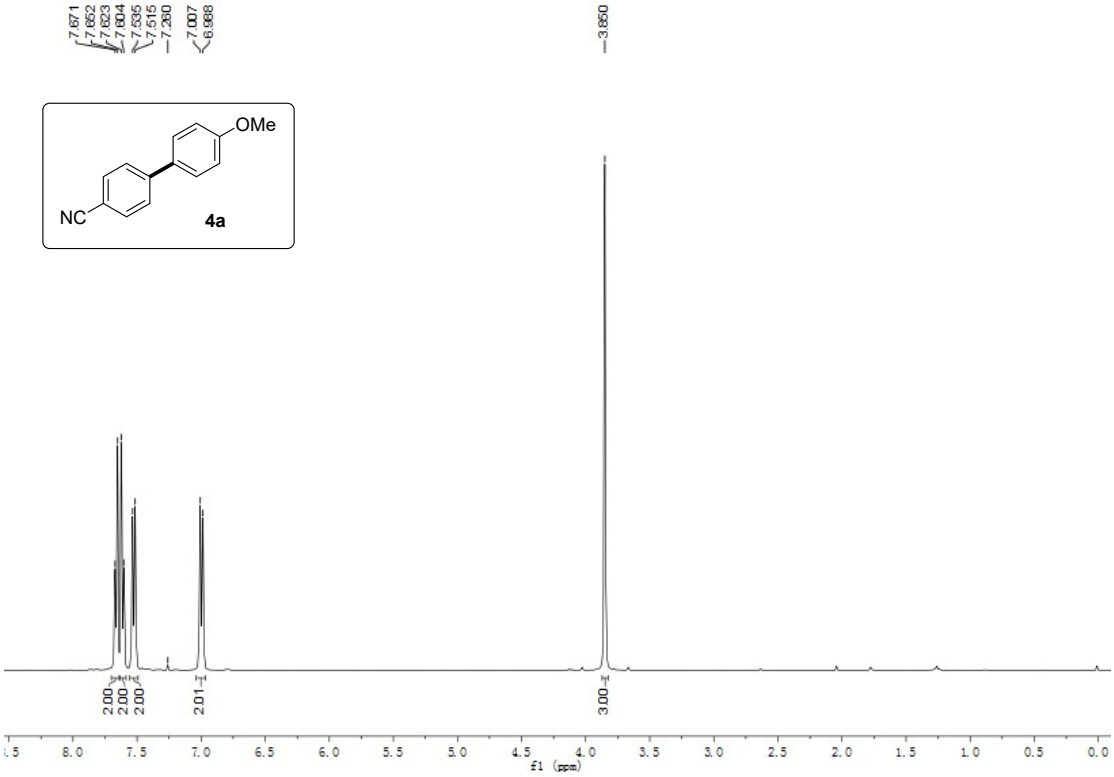
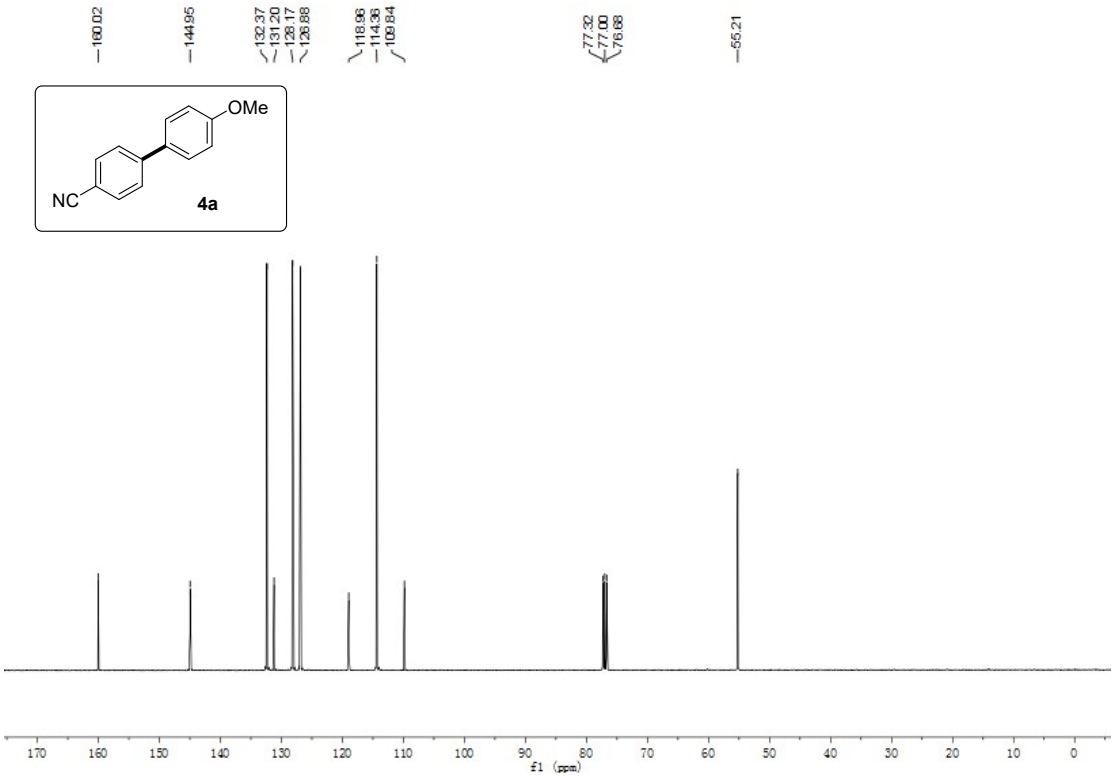
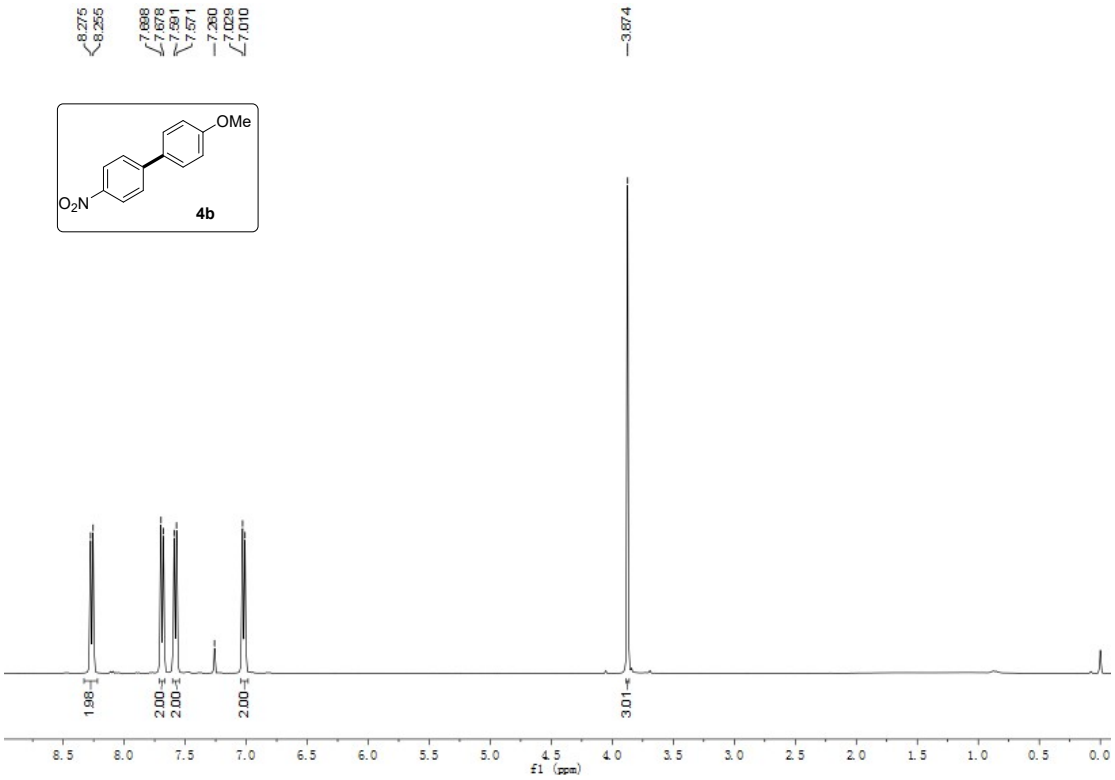
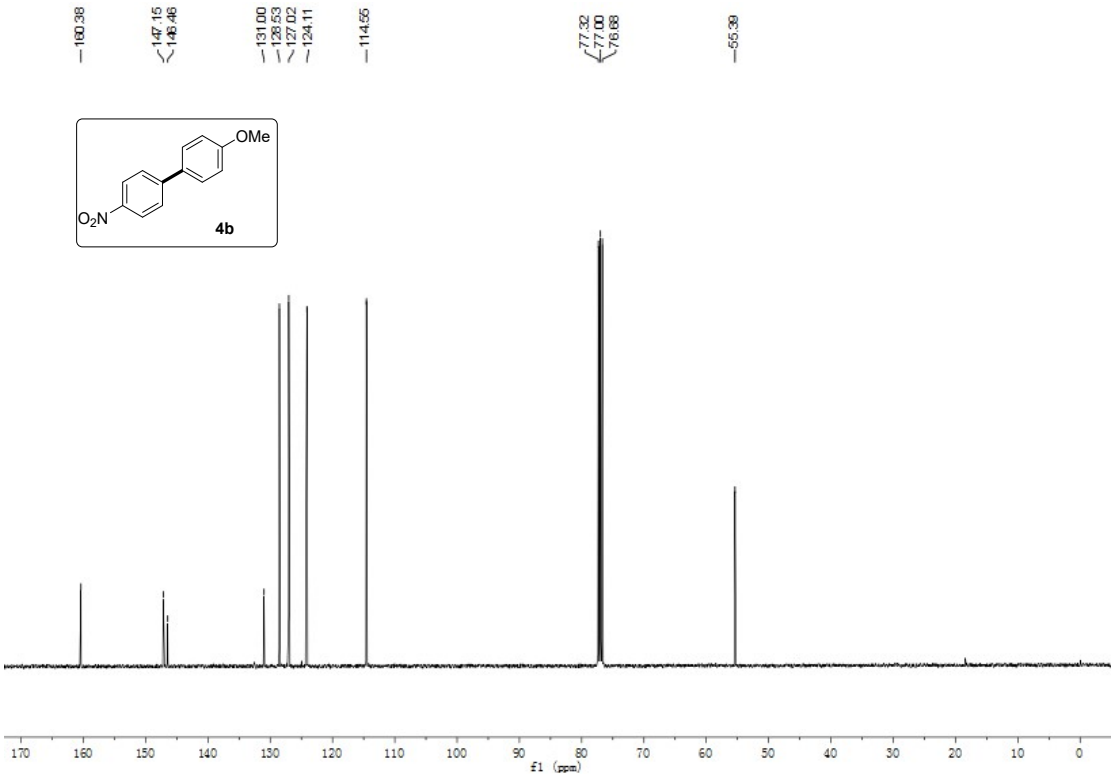
145.54
136.54
132.49
127.58
127.42
127.06
119.02
110.42
77.32
77.00
76.68
44.29
39.64
36.93
34.21
33.44
20.00
14.39
C3H7
NC
3w
f1 (ppm)


7.671
7.662
7.623
7.604
7.535
7.515
7.260
7.007
6.988
3.850
OMe
NC
4a
2.00
2.00
2.00
2.01
3.00
f1 (ppm)


160.02
144.95
132.37
131.20
128.17
126.88
118.96
114.36
109.84
77.32
77.00
76.68
55.21
OMe
NC
4a
f1 (ppm)


8.275
8.255
7.698
7.678
7.591
7.571
7.260
7.029
7.010
3.874
OMe
O2N
4b
1.98
2.00
2.00
2.00
3.01
f1 (ppm)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147.15
146.46
131.00
128.53
127.02
124.11
114.55
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77.00
76.68
55.39
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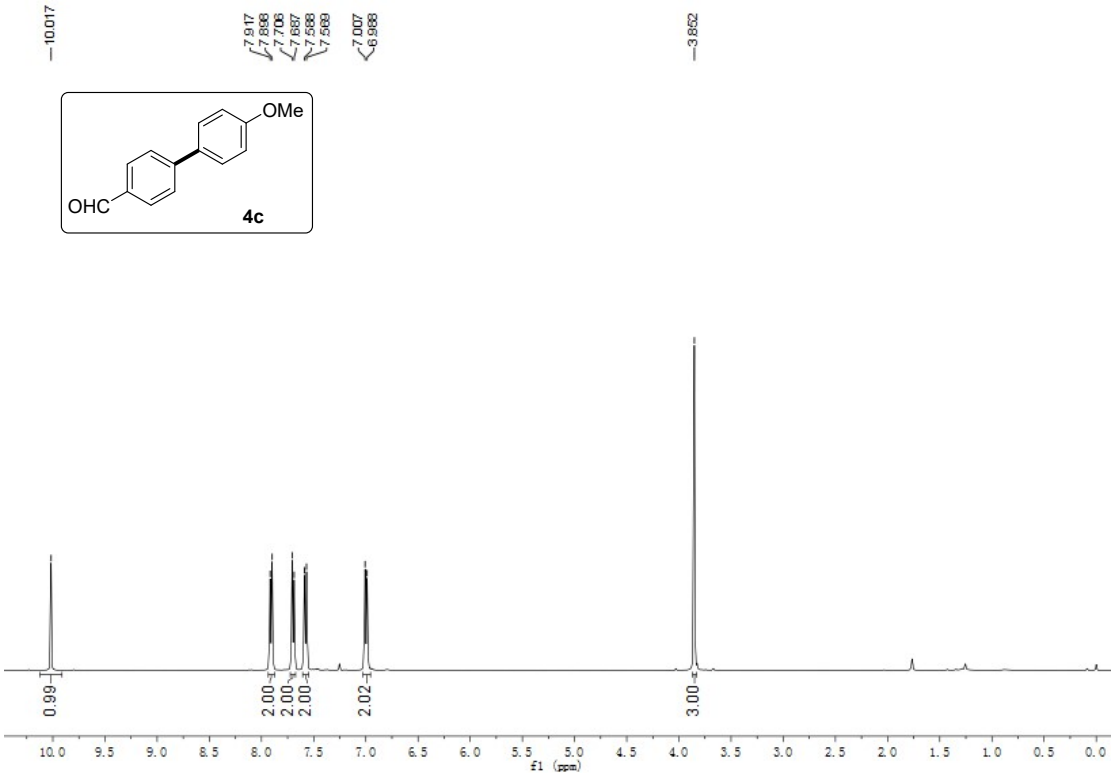
O_2N
4b
f1 (ppm)


10.017
7.917
7.898
7.706
7.687
7.588
7.569
7.007
6.988
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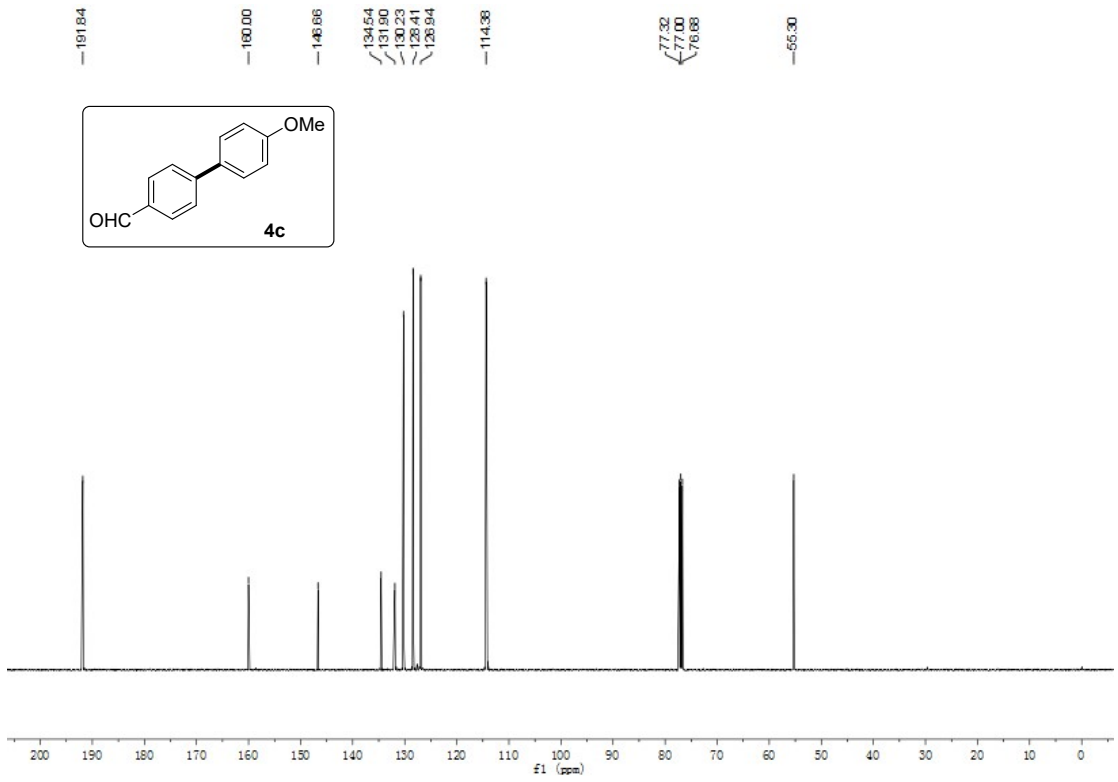
OMe
OHC
4c
0.99
2.00
2.00
2.00
2.02
3.00
f1 (ppm)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160.00
146.66
134.54
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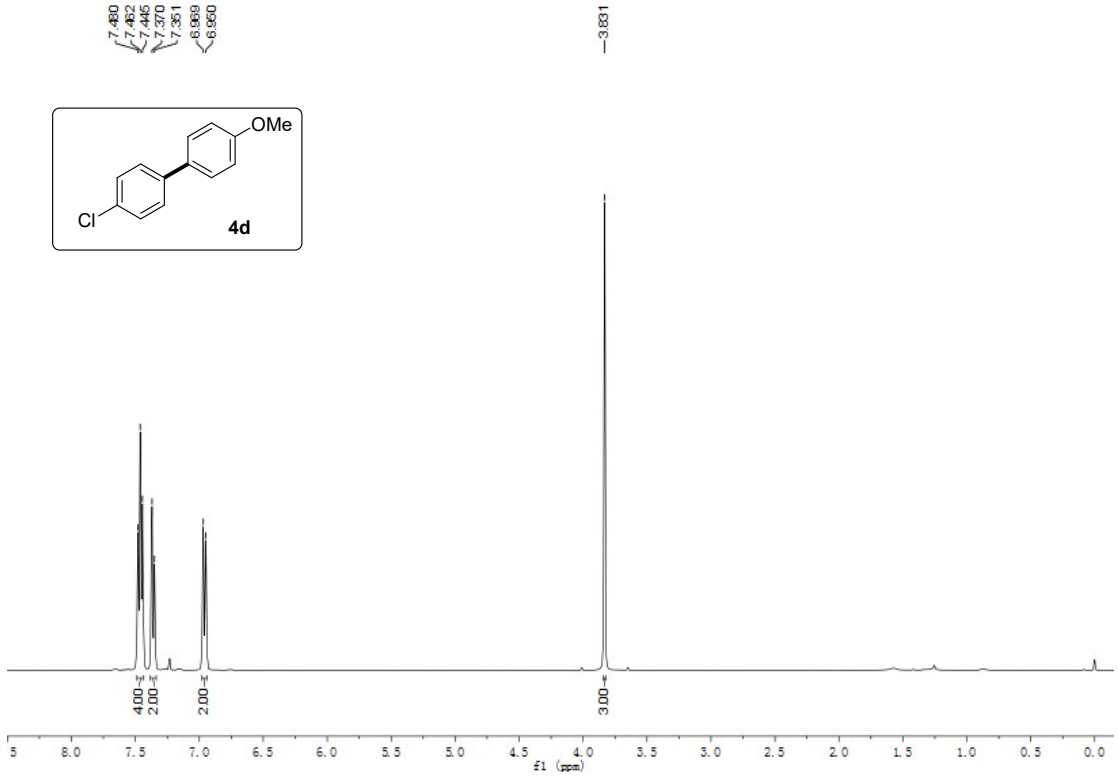
126.94
114.38
77.32
77.00
76.68
55.30
OMe
OHC
4c
f1 (ppm)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7.462
7.445
7.370
7.351
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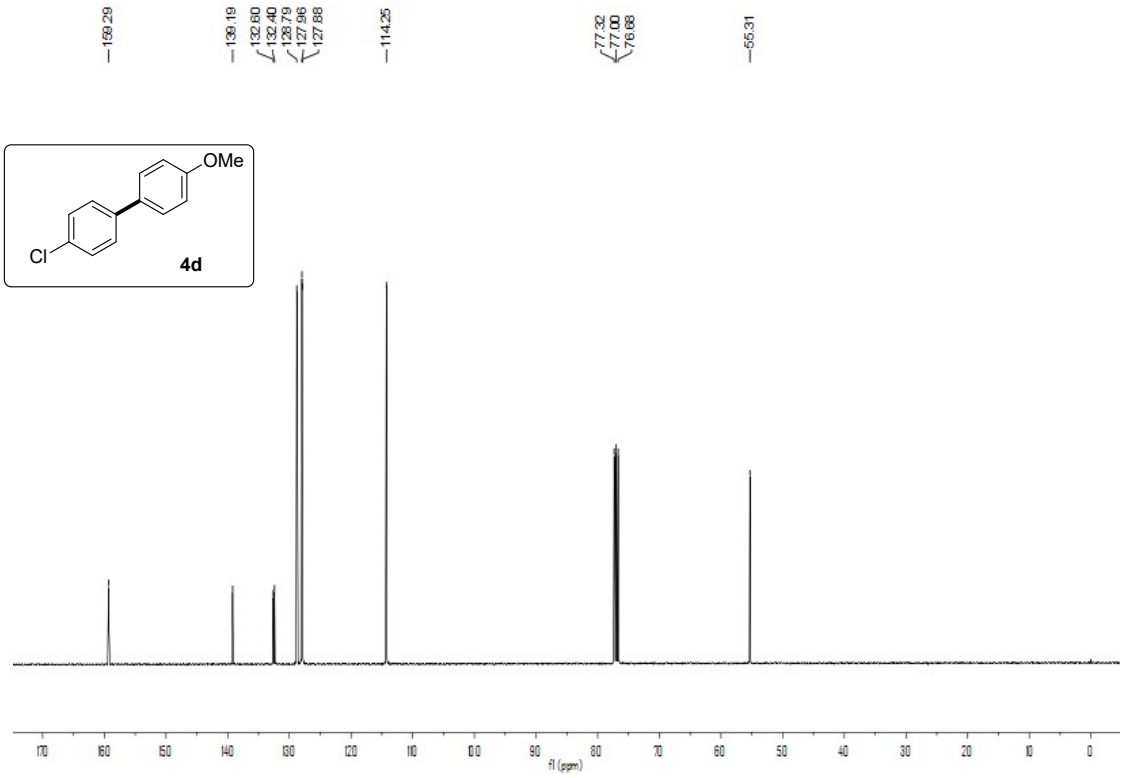
6.950
3.831
OMe
Cl
4d
4.00
2.00
2.00
3.00
f1 (ppm)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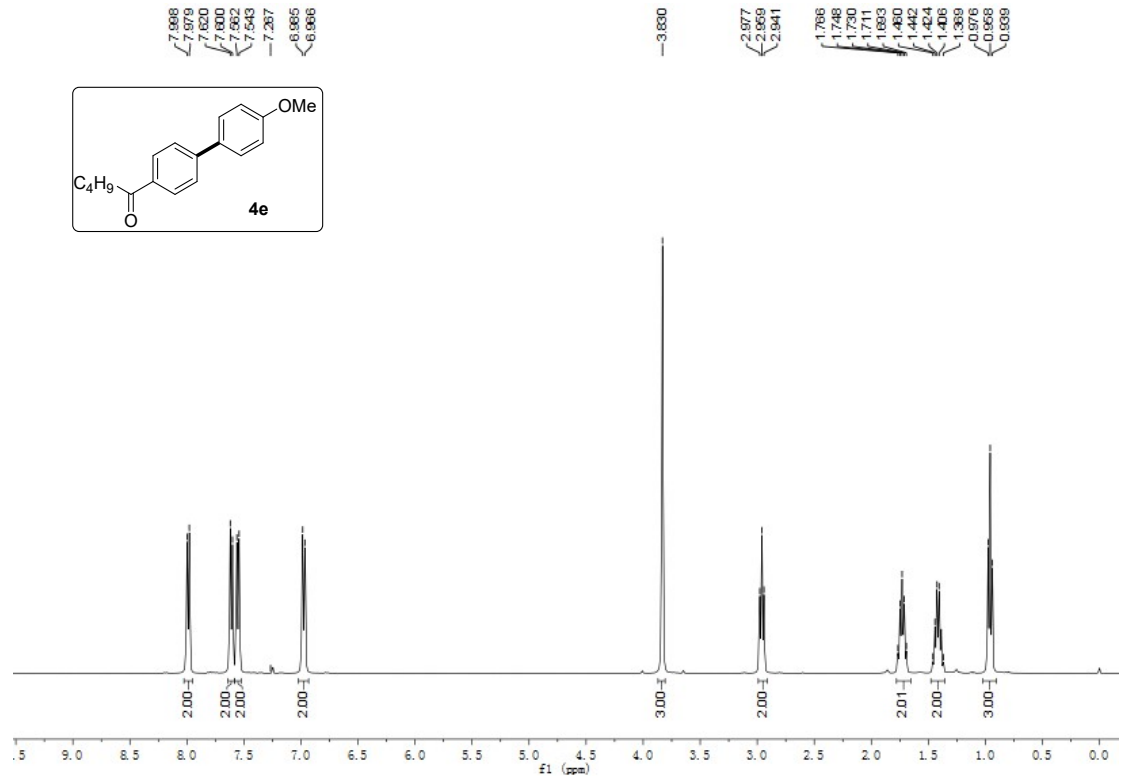
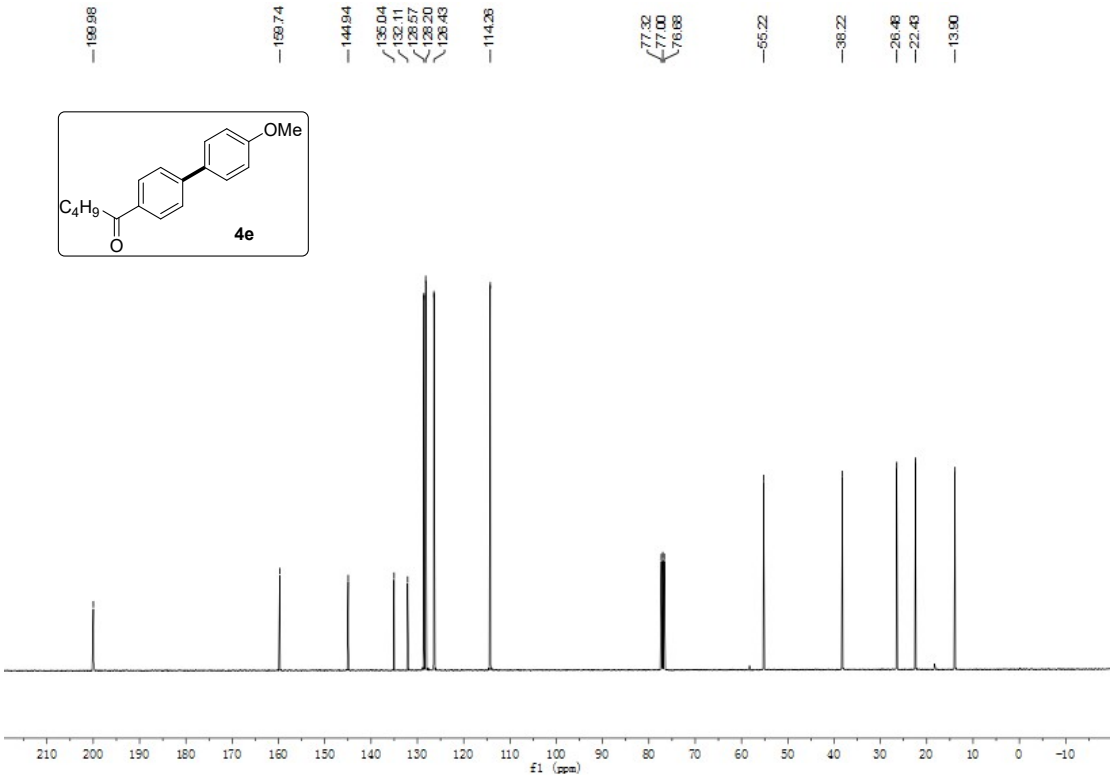
139.19
132.60
132.40
128.79
127.96
127.88
114.25
77.32
77.00
76.68
55.31
OMe
Cl
4d
f1 (ppm)


7.998
7.979
7.620
7.600
7.582
7.543
7.267
6.985
6.966
3.830
2.977
2.959
2.941
1.796
1.748
1.730
1.711
1.693
1.450
1.442
1.424
1.406
1.389
0.976
0.958
0.939
OMe
C4H9
O
4e
2.00
2.00
2.00
2.00
3.00
2.00
2.01
2.00
3.00
f1 (ppm)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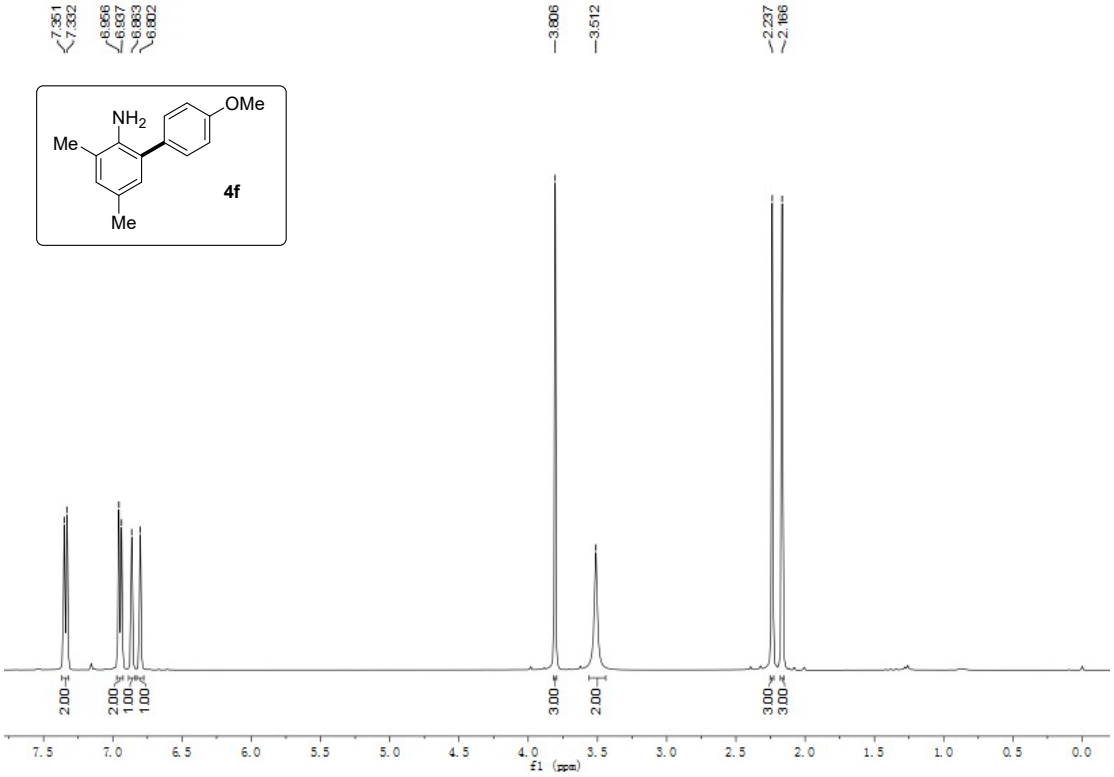
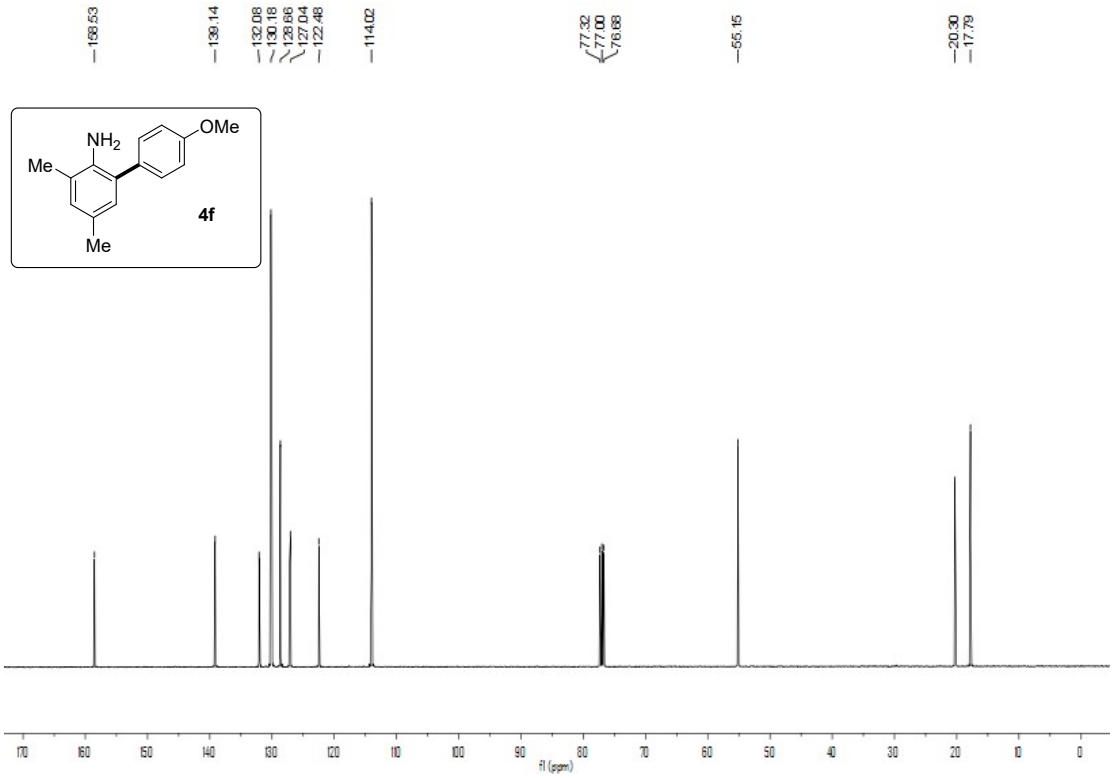
159.74
144.94
135.04
132.11
128.57
128.20
126.43
114.26
77.32
77.00
76.68
55.22
38.22
26.48
22.43
13.90
OMe
C_4H_9
O
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.361
7.332
6.956
6.937
6.883
6.802
3.606
3.512
2.237
2.166
NH2
OMe
Me
Me
4f
2.00
2.00
1.00
1.00
3.00
2.00
3.00
3.00
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)


158.53
139.14
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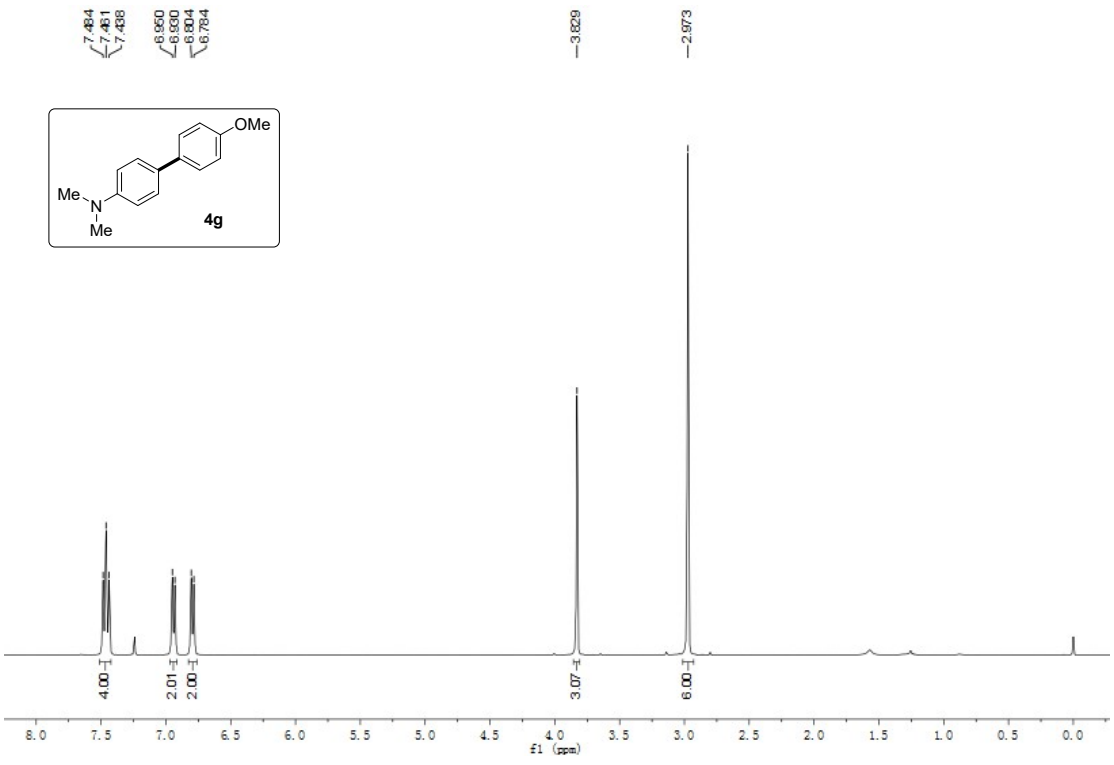
130.18
128.66
127.04
122.48
114.02
77.32
77.00
76.68
55.15
20.30
17.79
NH2
OMe
Me
Me
4f
f1 (ppm)


7.464
7.461
7.438
6.950
6.930
6.804
6.784
3.829
2.973
OMe
Me
N
Me
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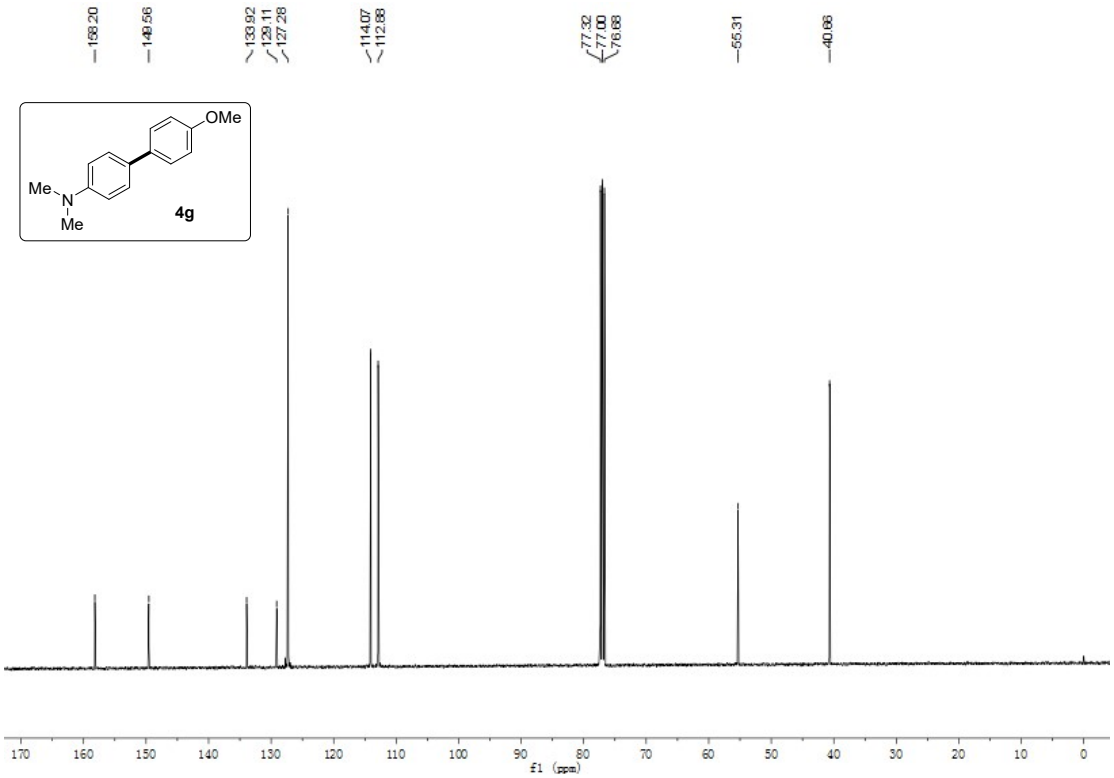
2.01
2.00
3.07
6.00
f1 (ppm)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76.68
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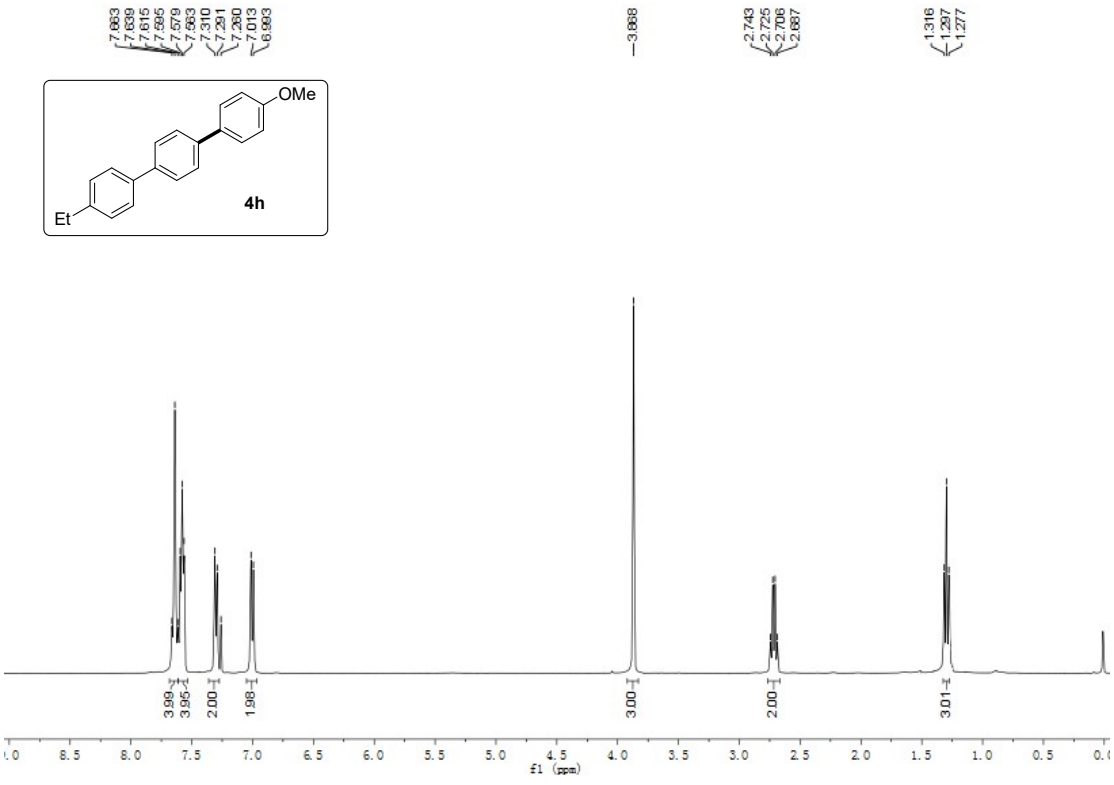
Me
4g
f1 (ppm)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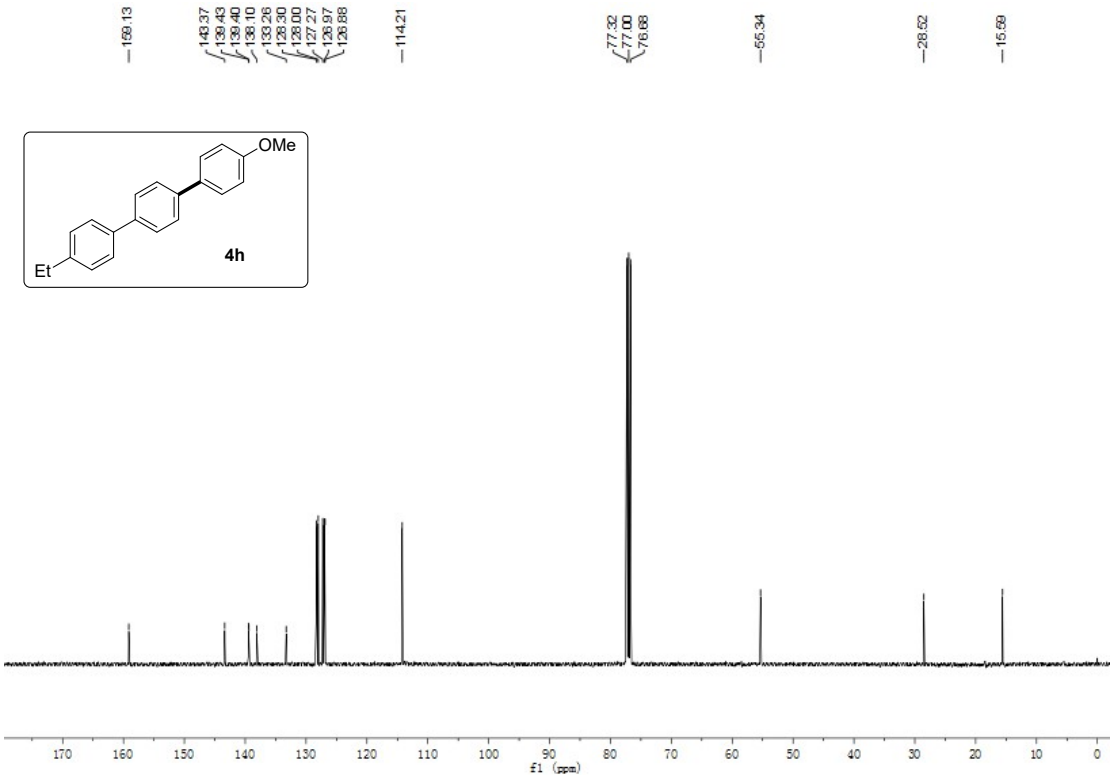
7.615
7.595
7.579
7.563
7.310
7.291
7.280
7.013
6.993
3.868
2.743
2.725
2.706
2.687
1.316
1.297
1.277
OMe
Et
4h
3.99
3.95
2.00
1.98
3.00
2.00
3.01
f1 (ppm)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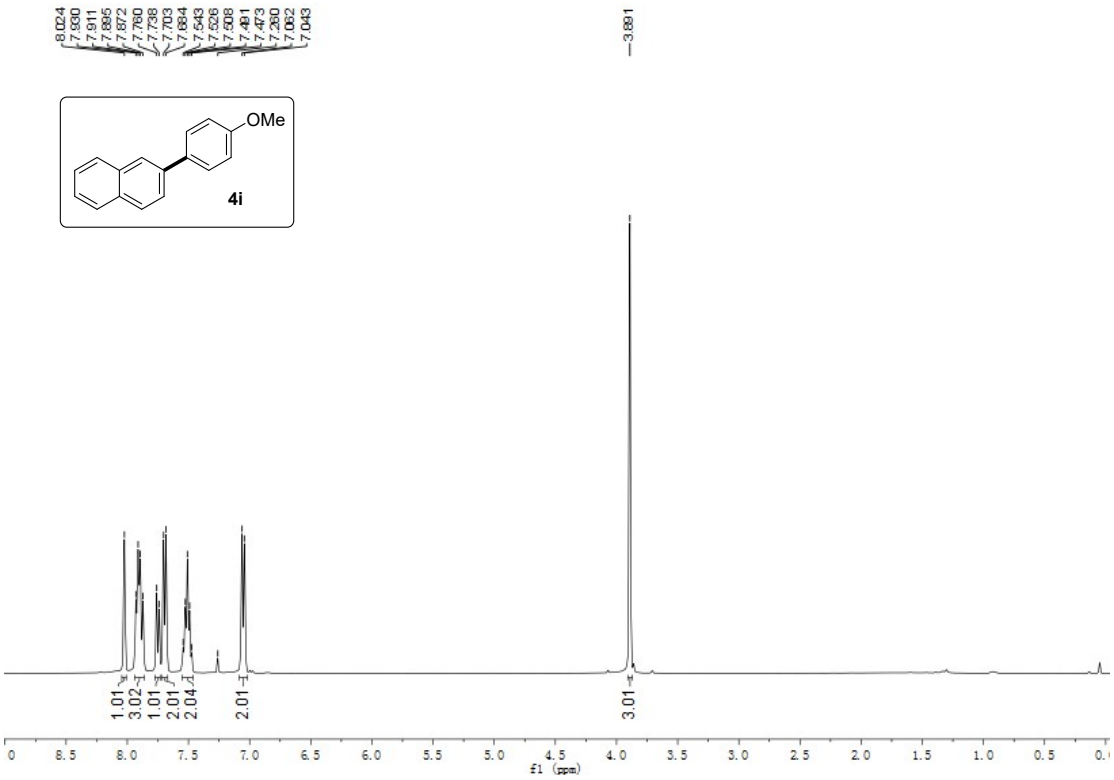
143.37
139.43
139.40
138.10
133.26
128.30
128.00
127.27
126.97
126.88
114.21
77.32
77.00
76.68
55.34
28.52
15.69
OMe
Et
4h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.911
7.895
7.872
7.760
7.738
7.703
7.684
7.543
7.526
7.508
7.491
7.473
7.260
7.062
7.043
3.891
OMe
4i
1.01
3.02
1.01
2.01
2.04
2.01
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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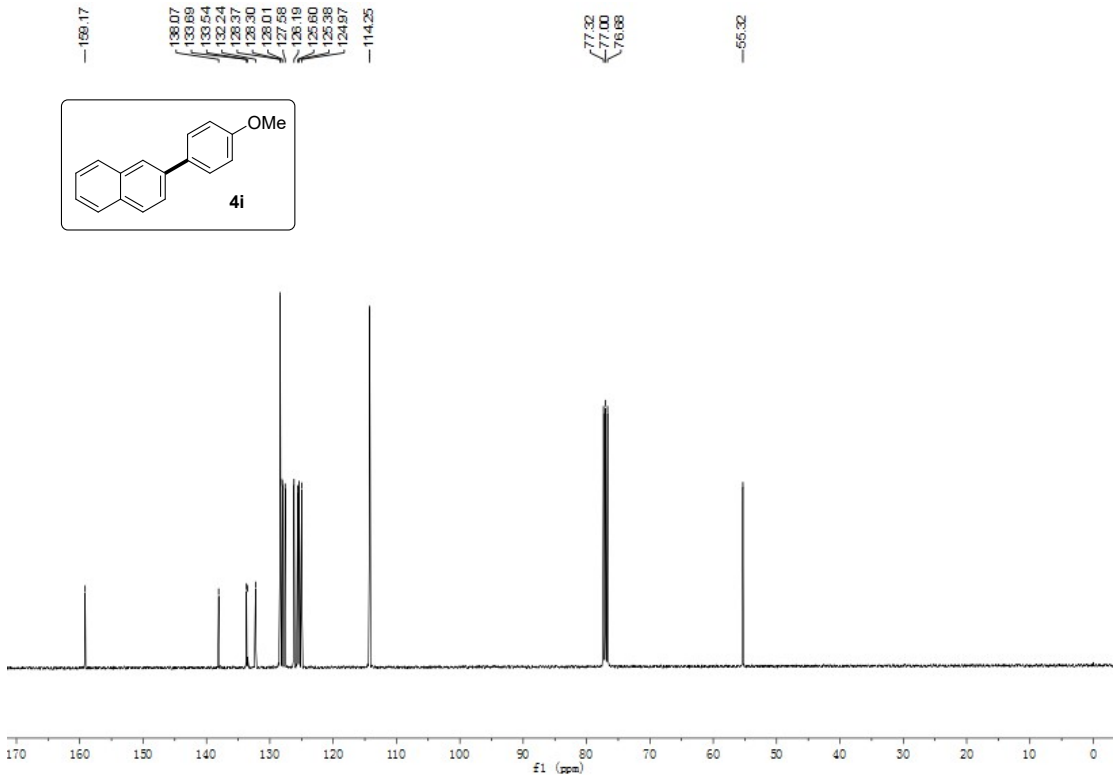
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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138.07
133.69
133.54
132.24
128.37
128.30
128.01
127.58
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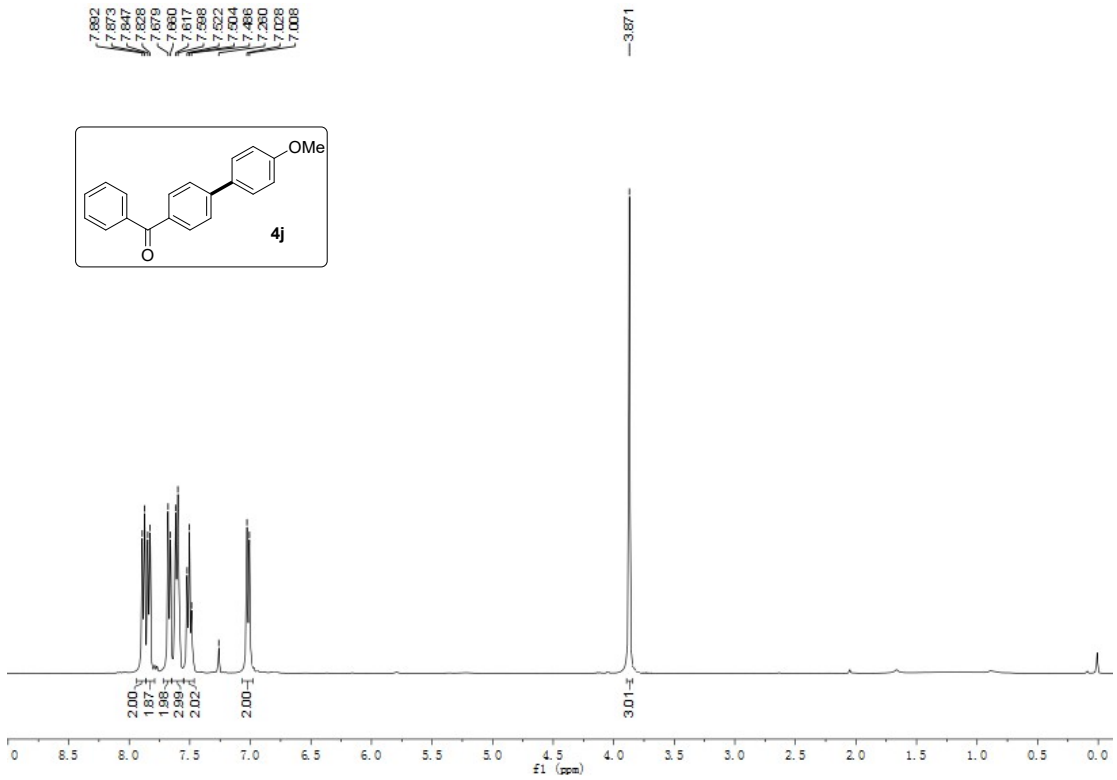
125.60
125.38
124.97
114.25
77.32
77.00
76.68
55.32
OMe
4i
f1 (ppm)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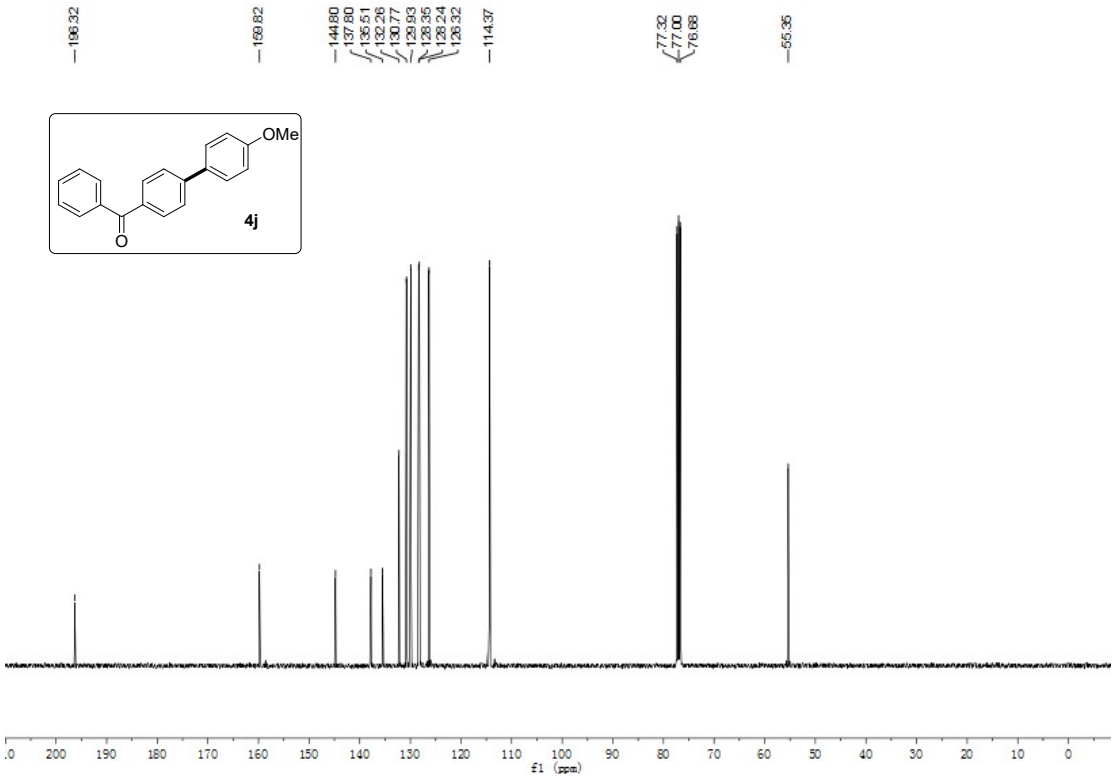
7.660
7.617
7.598
7.522
7.504
7.486
7.260
7.028
7.008
3.871
OMe
O
4j
2.00
1.87
1.98
2.99
2.02
2.00
3.01
f1 (ppm)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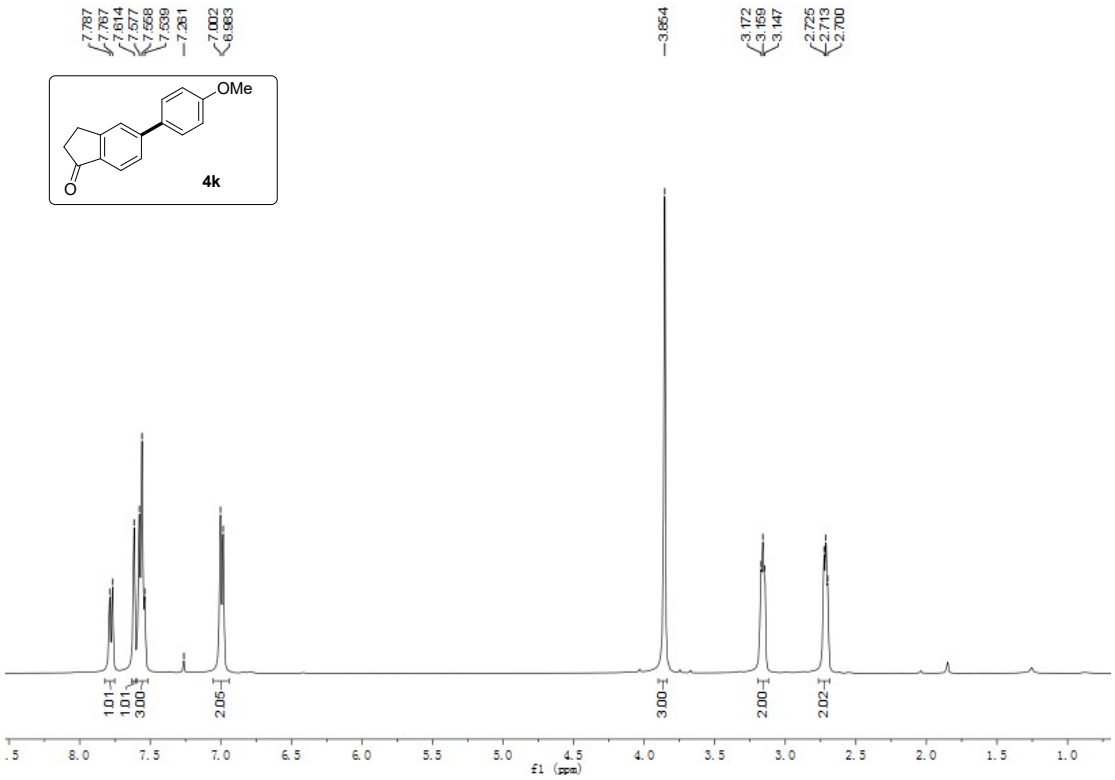
132.26
130.77
129.93
128.35
128.24
126.32
114.37
77.32
77.00
76.68
55.35
OMe
O
4j
f1 (ppm)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7.539
7.261
7.002
6.983
3.854
3.172
3.159
3.147
2.725
2.713
2.700
OMe
O
4k
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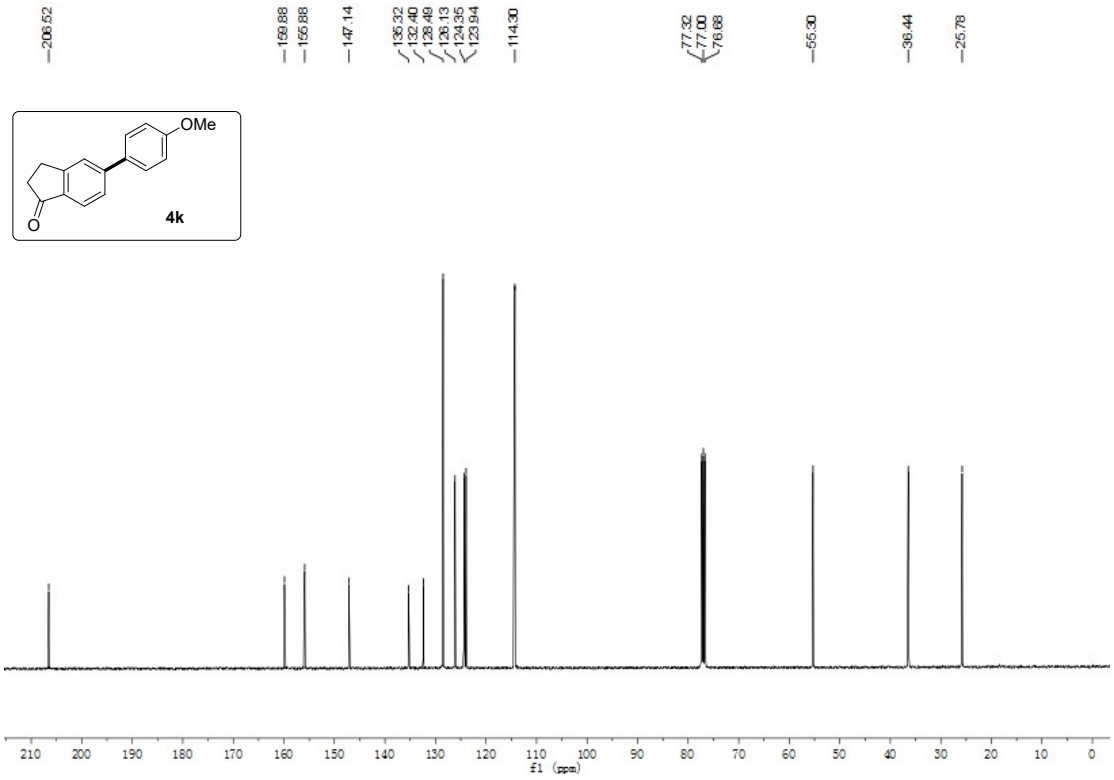
1.01
3.00
2.05
3.00
2.00
2.02
f1 (ppm)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136.32
132.40
128.49
126.13
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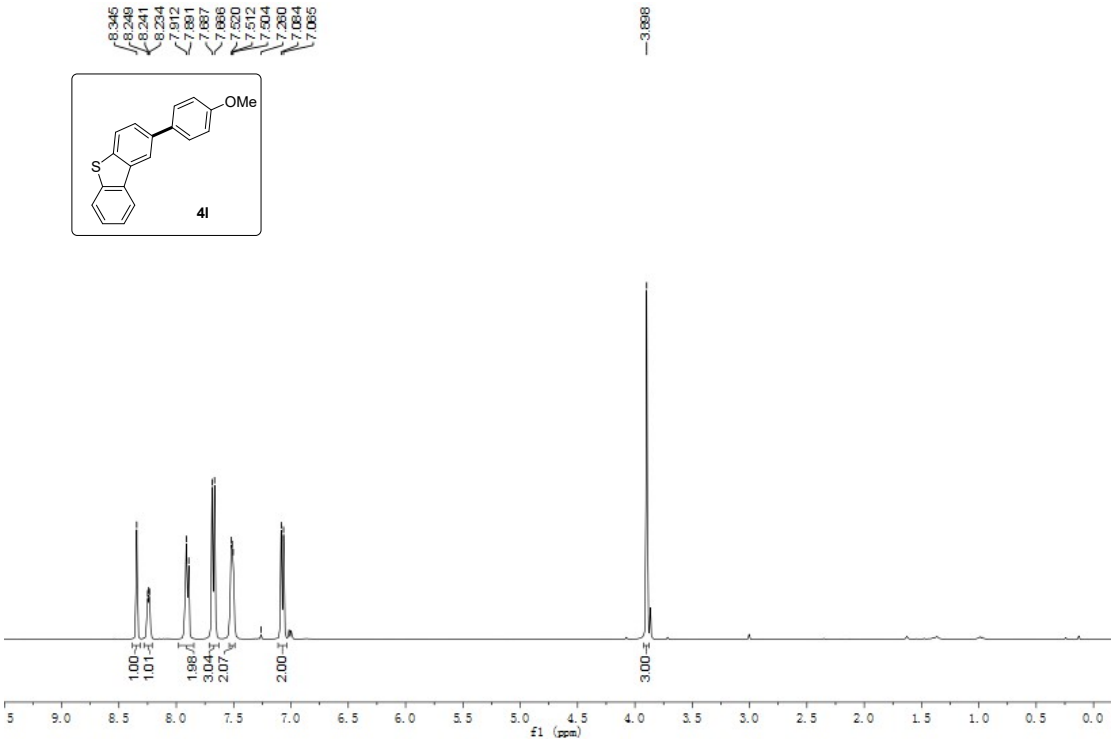
76.68
55.30
36.44
25.78
OMe
O
4k
f1 (ppm)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8.241
8.234
7.912
7.891
7.887
7.886
7.520
7.512
7.504
7.260
7.084
7.065
3.898
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S
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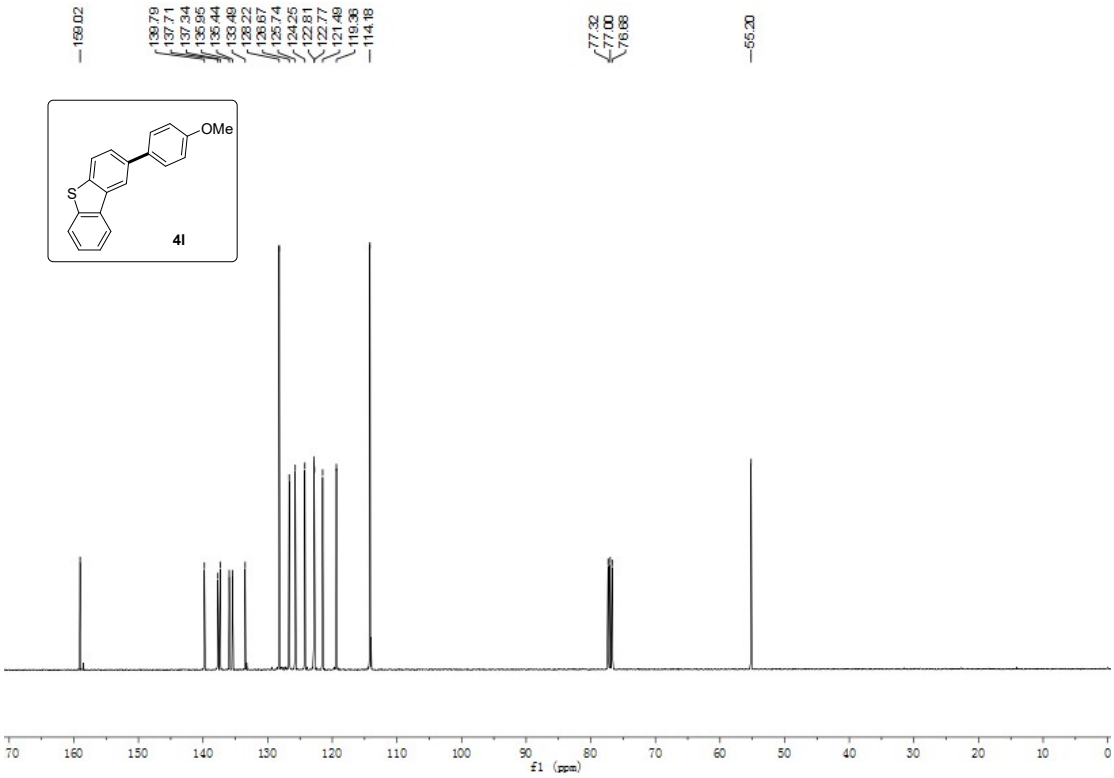
1.01
1.98
3.04
2.07
2.00
3.00
f1 (ppm)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135.44
133.49
128.22
126.67
125.74
124.25
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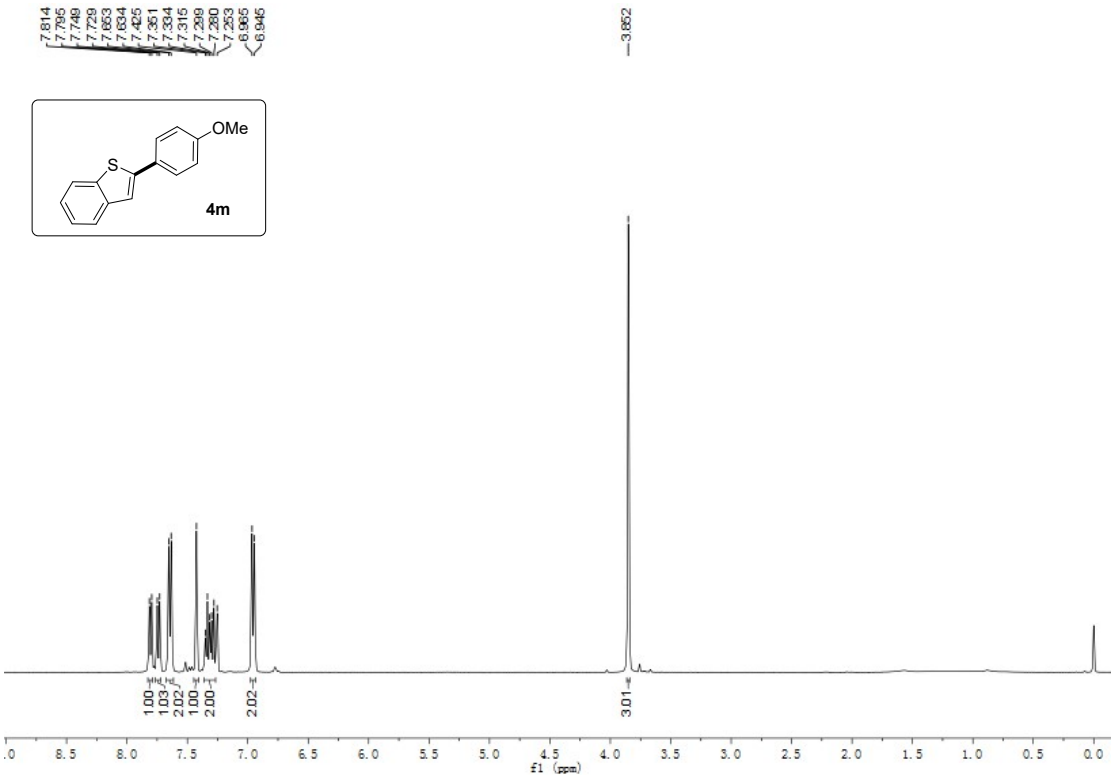
119.36
114.18
77.32
77.00
76.68
55.20
OMe
S
4l
f1 (ppm)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7.729
7.653
7.634
7.425
7.351
7.334
7.315
7.299
7.280
7.253
6.965
6.945
3.852
OMe
S
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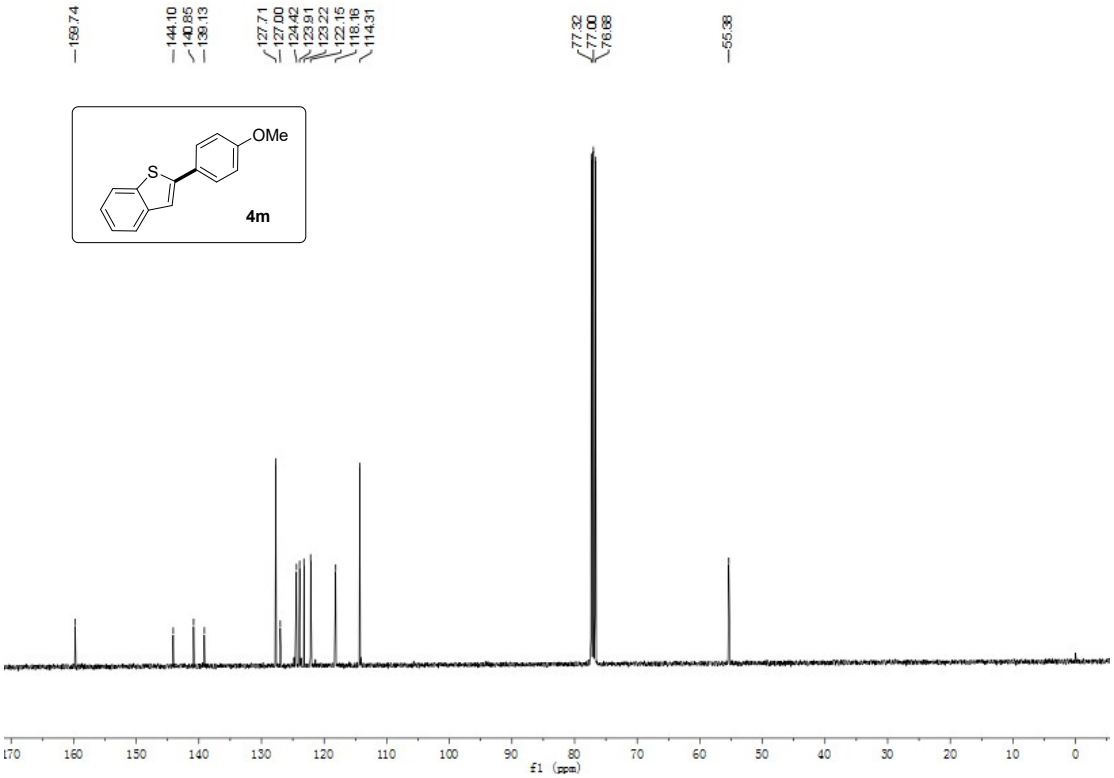
1.00
1.03
2.02
1.00
2.00
2.02
3.01
f1 (ppm)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139.13
127.71
127.00
124.42
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123.22
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118.16
114.31
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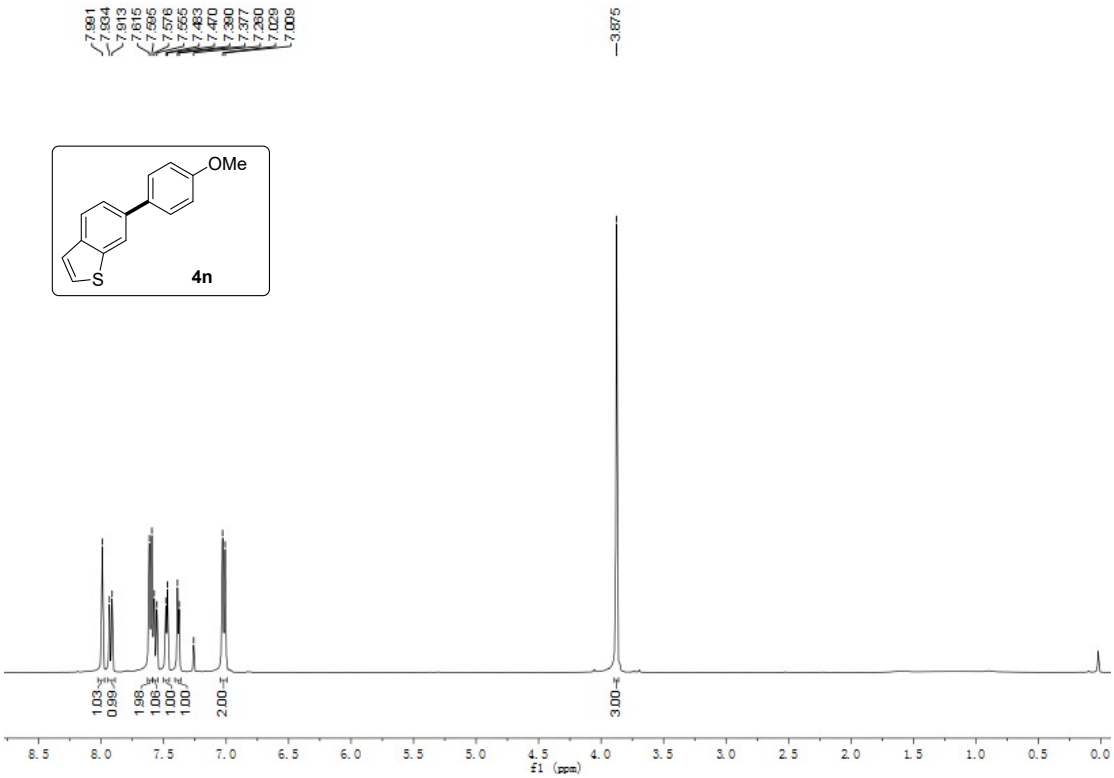
76.68
55.38
OMe
S
4m
f1 (ppm)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7.913
7.615
7.595
7.576
7.565
7.483
7.470
7.390
7.377
7.260
7.029
7.009
3.875
OMe
S
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0.99
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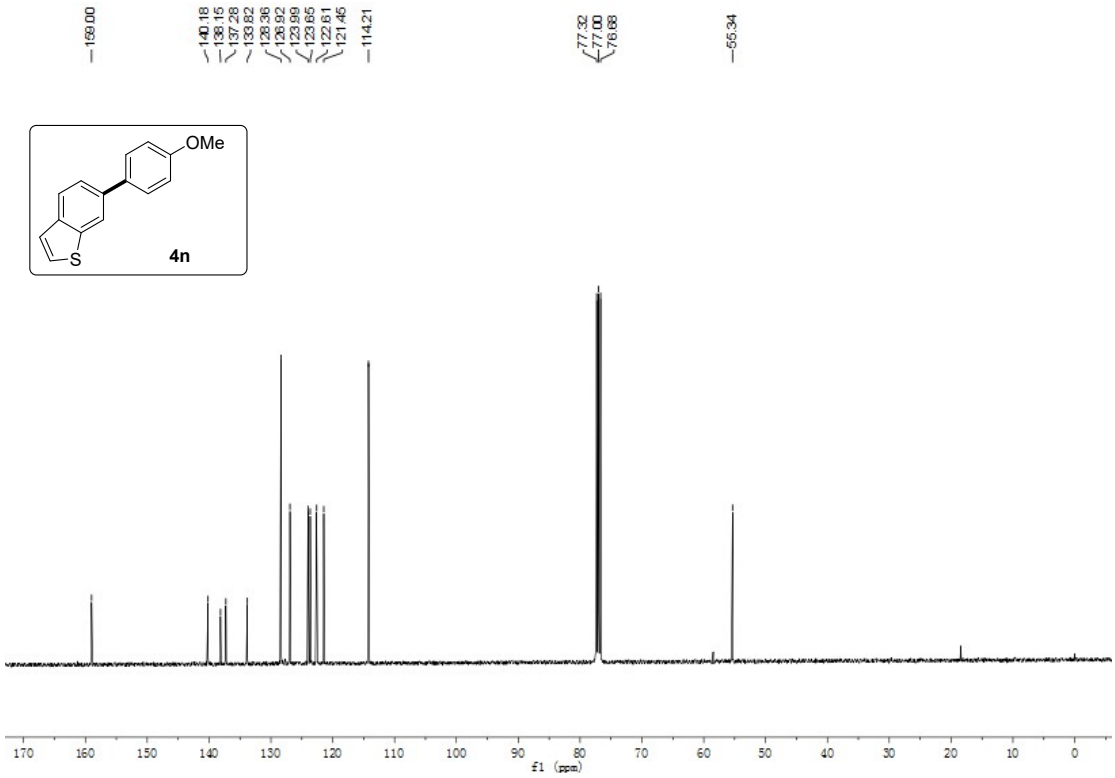
1.06
1.00
1.00
2.00
3.00
f1 (ppm)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137.28
133.82
128.36
126.92
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123.65
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121.45
114.21
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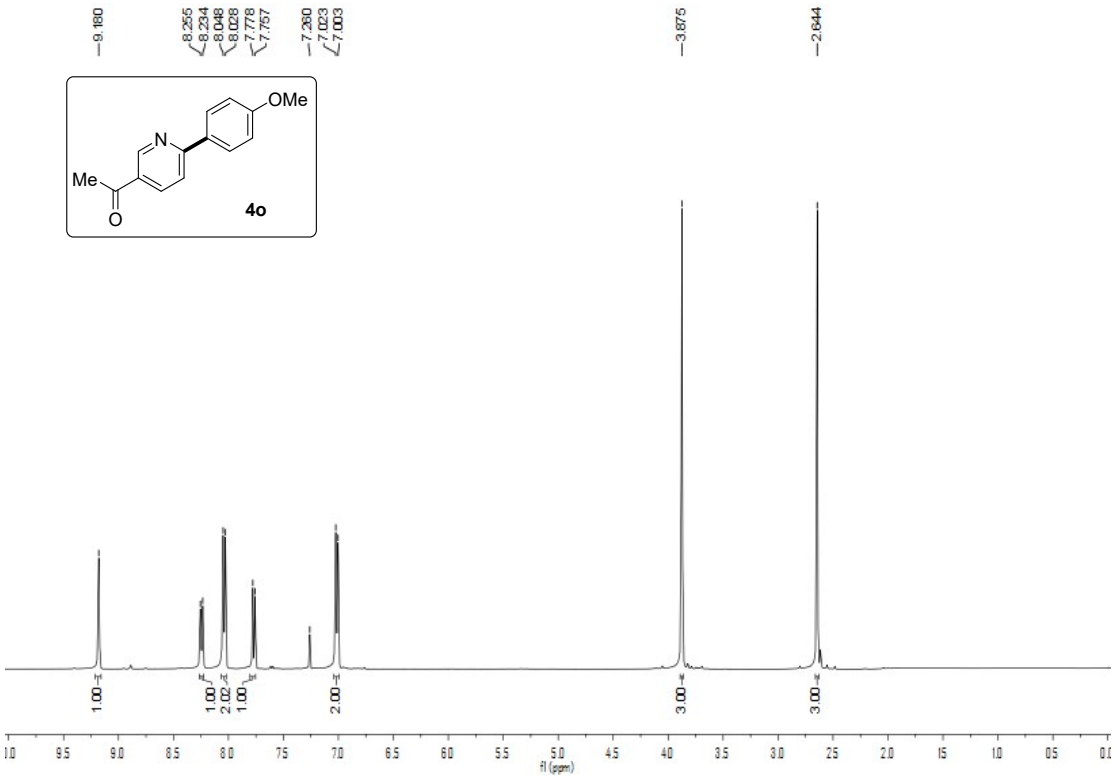
76.68
55.34
OMe
S
4n
f1 (ppm)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8.234
8.048
8.028
7.778
7.757
7.260
7.023
7.003
3.875
2.644
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Me
O
4o
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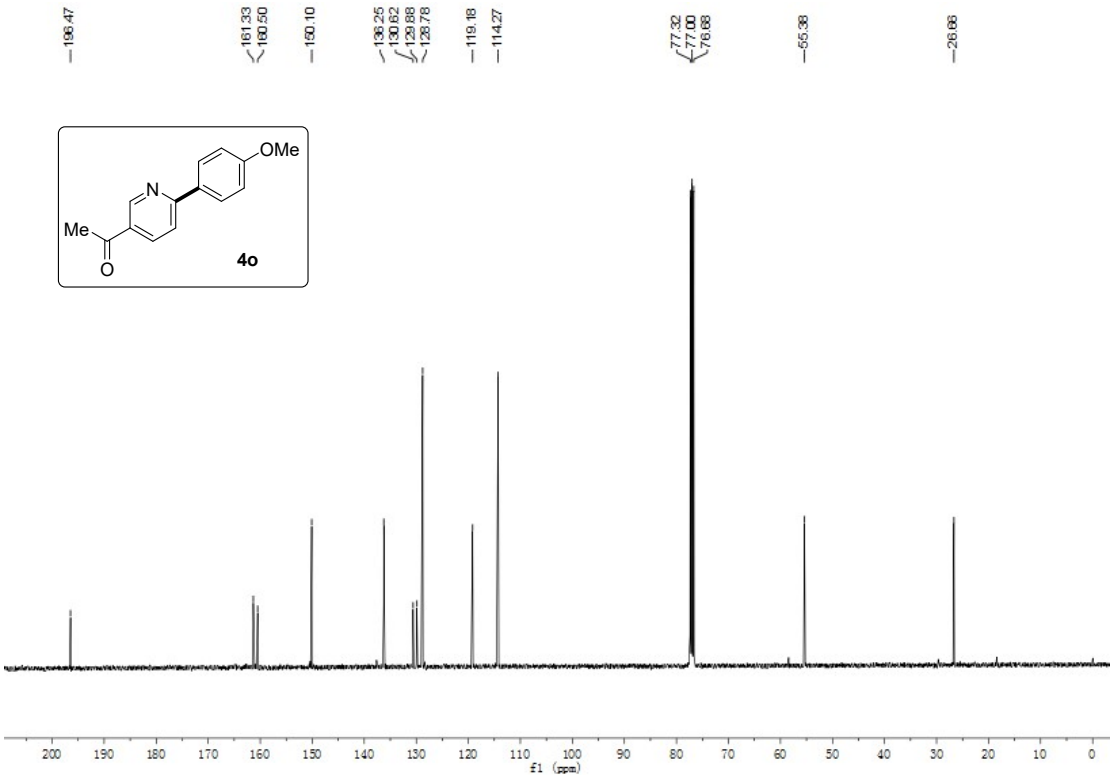
1.00
2.02
1.00
2.00
3.00
3.00
f1 (ppm)


196.47
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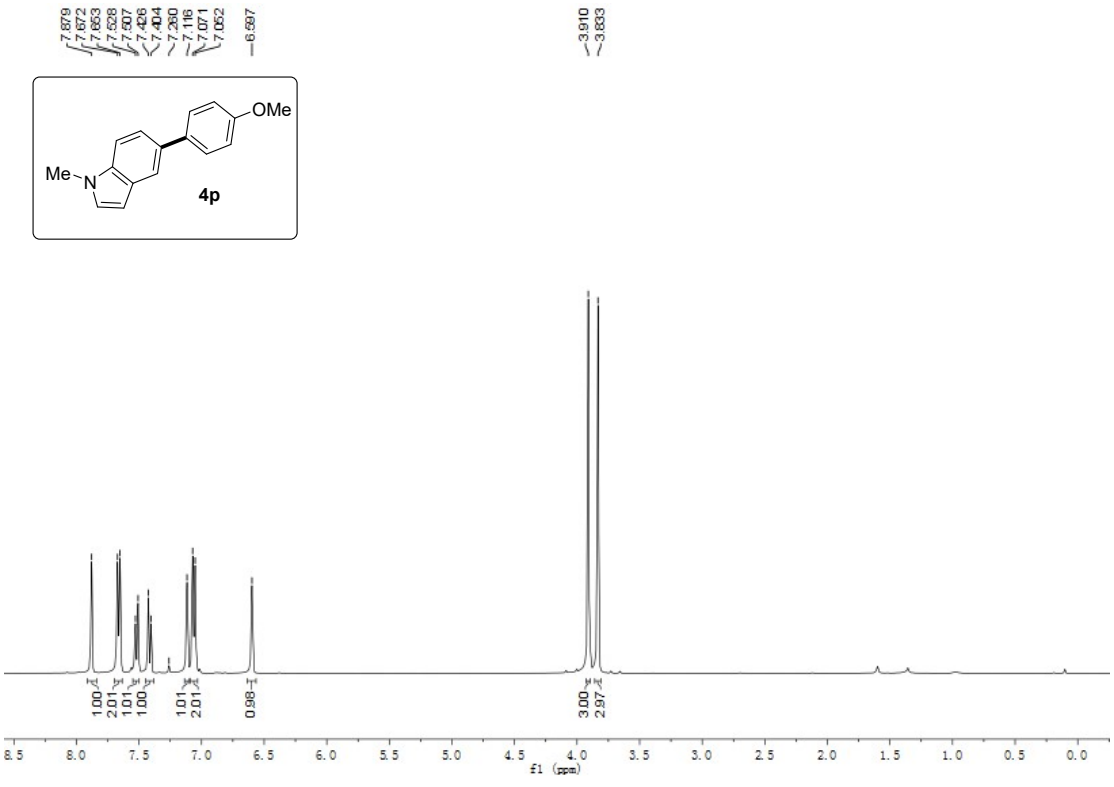
150.10
136.25
130.62
129.88
128.78
119.18
114.27
77.32
77.00
76.68
55.38
26.68
OMe
N
Me
O
4o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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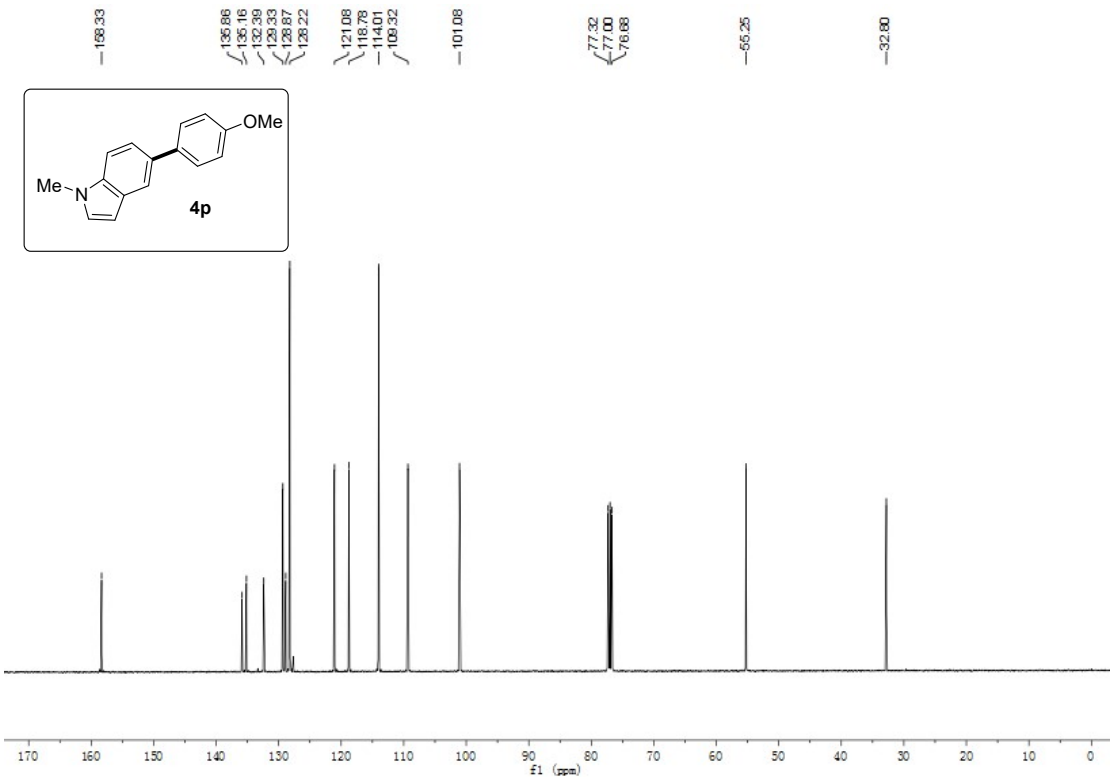
7.653
7.528
7.507
7.426
7.404
7.260
7.116
7.071
7.052
6.597
3.910
3.833
OMe
Me
N
4p
1.00
2.01
1.01
1.00
1.01
2.01
0.98
3.00
2.97
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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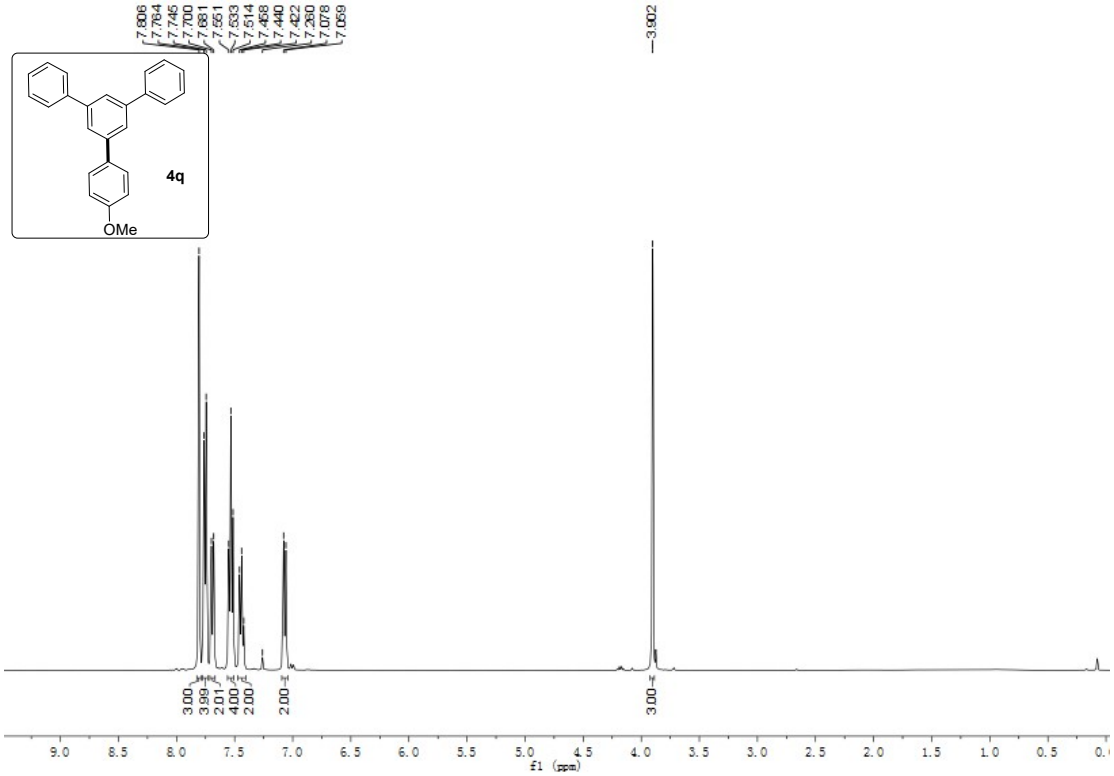
135.16
132.39
129.33
128.87
128.22
121.08
118.78
114.01
109.32
101.08
77.32
77.00
76.68
55.25
32.80
OMe
Me
N
4p
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.681
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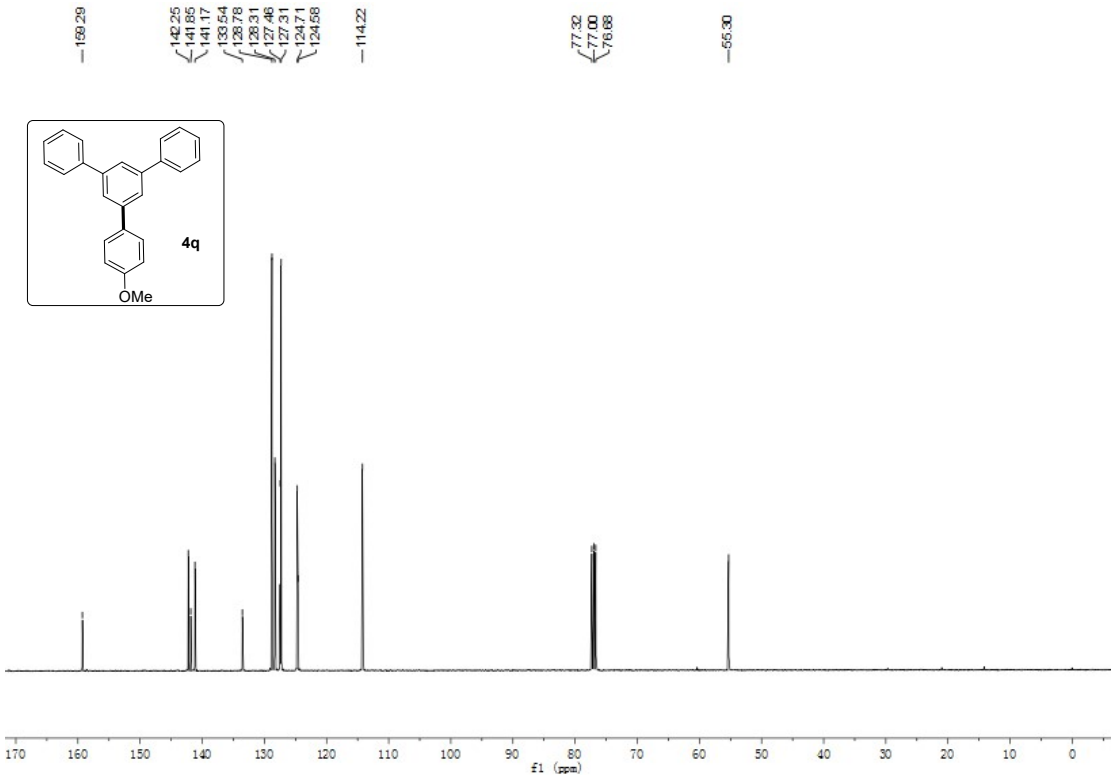
7.533
7.514
7.458
7.440
7.422
7.260
7.078
7.059
3.902
4q
OMe
3.00
3.99
2.01
4.00
2.00
2.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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141.85
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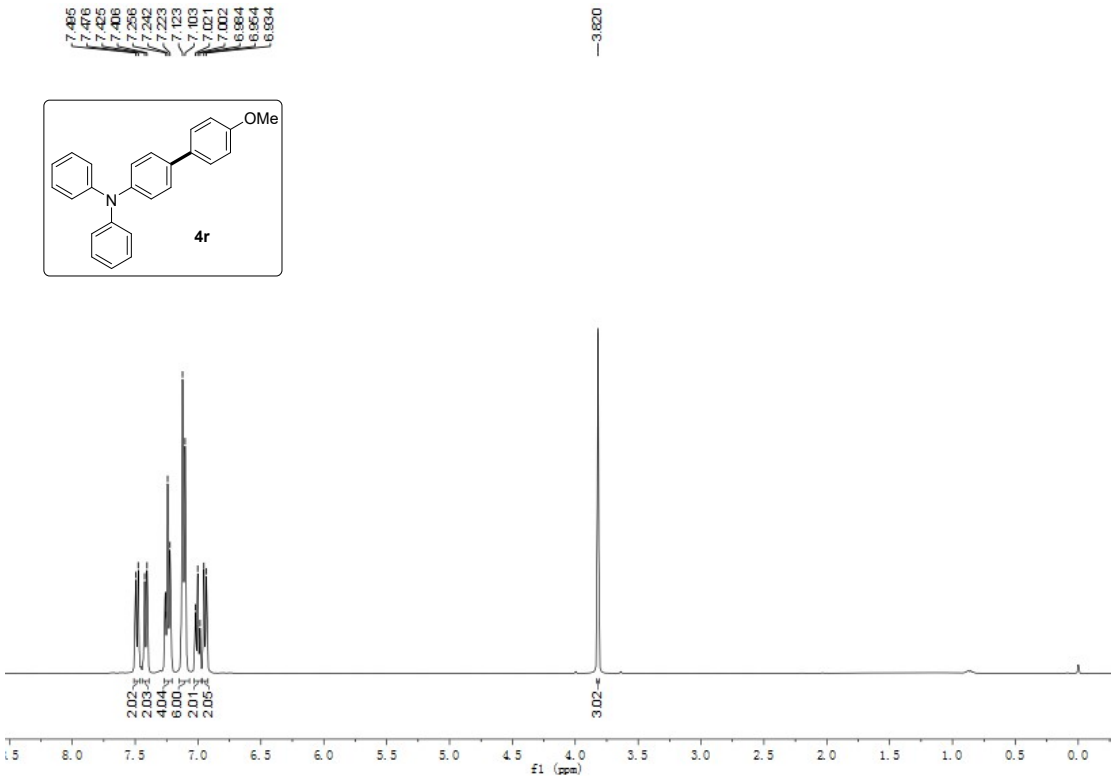
133.54
128.78
128.31
127.46
127.31
124.71
124.58
114.22
77.32
77.00
76.68
55.30
4q
OMe
f1 (ppm)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7.476
7.425
7.406
7.256
7.242
7.223
7.123
7.103
7.021
7.002
6.984
6.964
6.934
3.820
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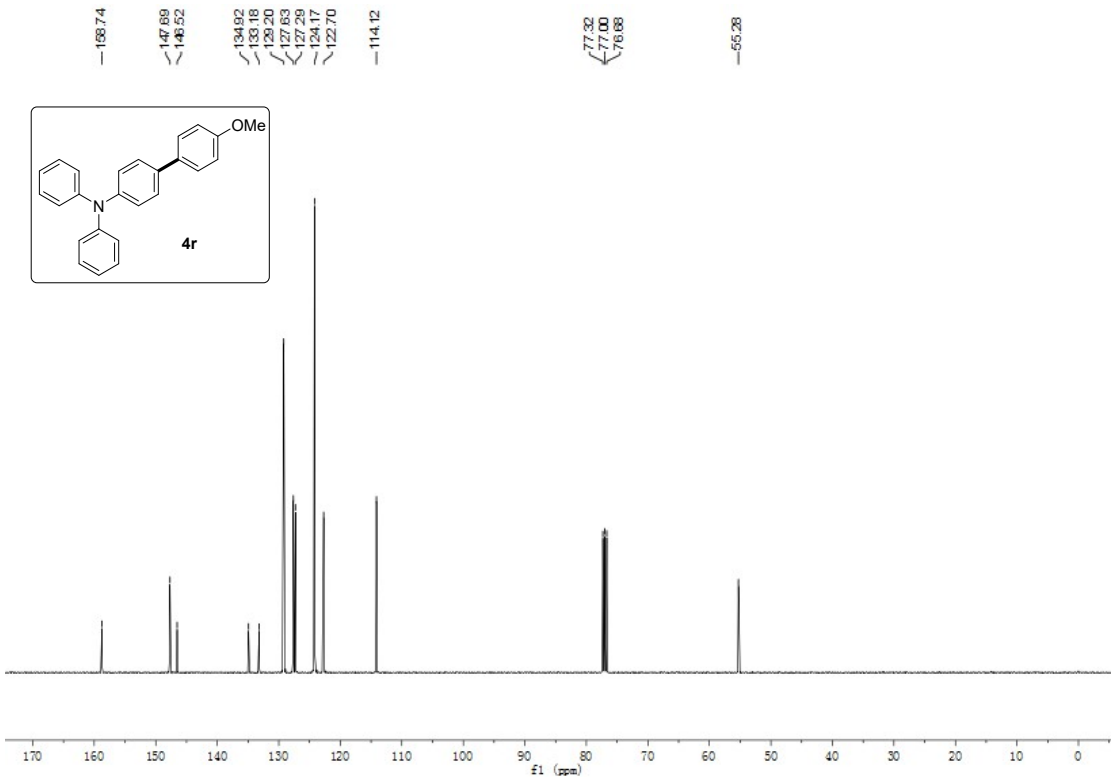
N
4r
2.02
2.03
4.04
6.00
2.01
2.05
3.02
f1 (ppm)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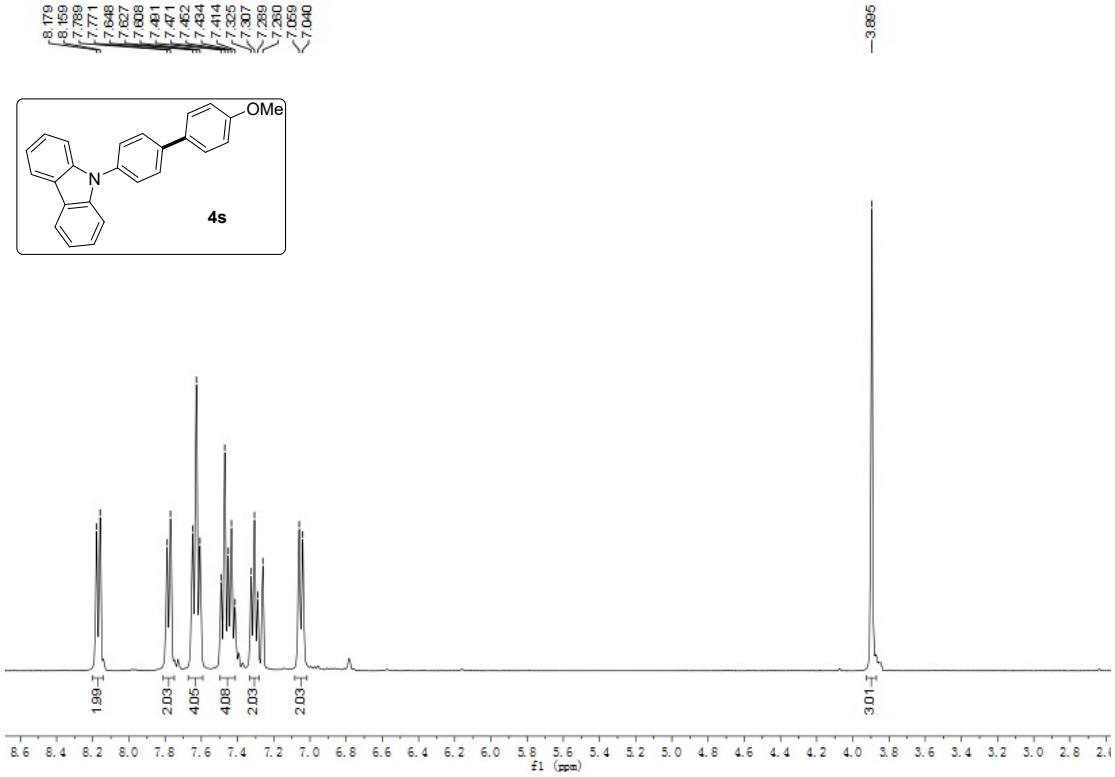
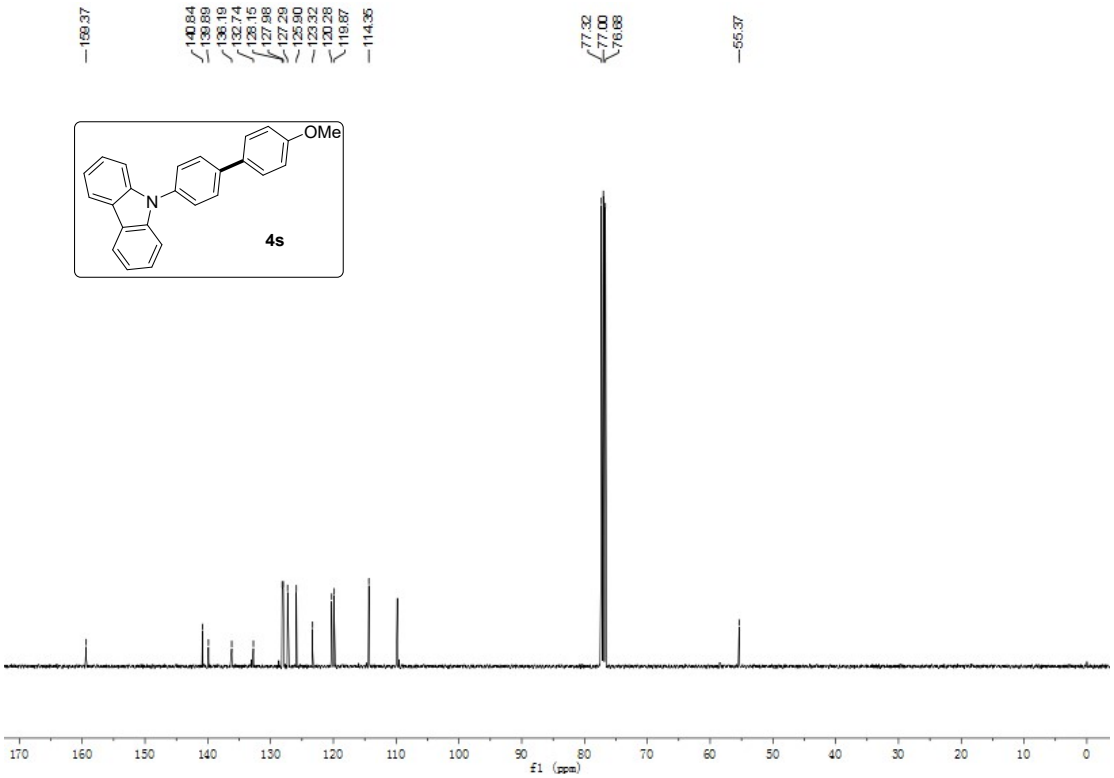
147.89
146.52
134.92
133.18
129.20
127.63
127.29
124.17
122.70
114.12
77.32
77.00
76.68
55.28
OMe
N
4r
f1 (ppm)


8.179
8.159
7.789
7.771
7.648
7.627
7.608
7.491
7.471
7.452
7.434
7.414
7.325
7.307
7.299
7.260
7.059
7.040
3.895
OMe
N
4s
1.99
2.03
4.05
4.08
2.03
2.03
3.01
f1 (ppm)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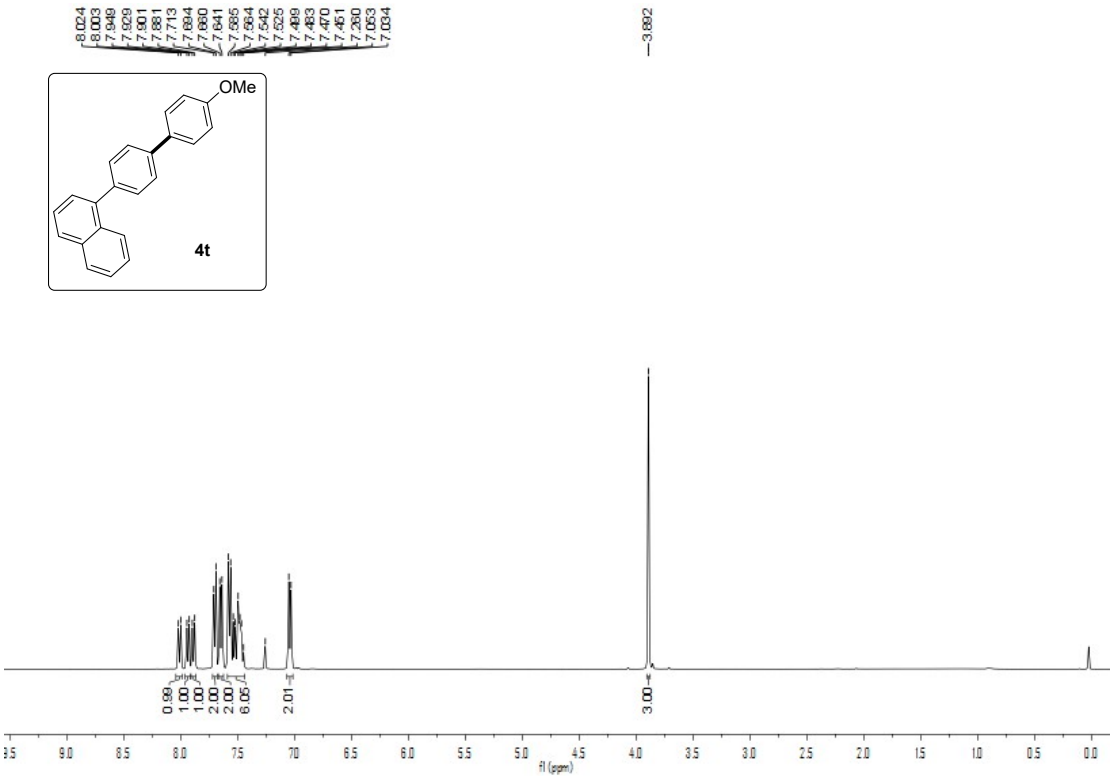
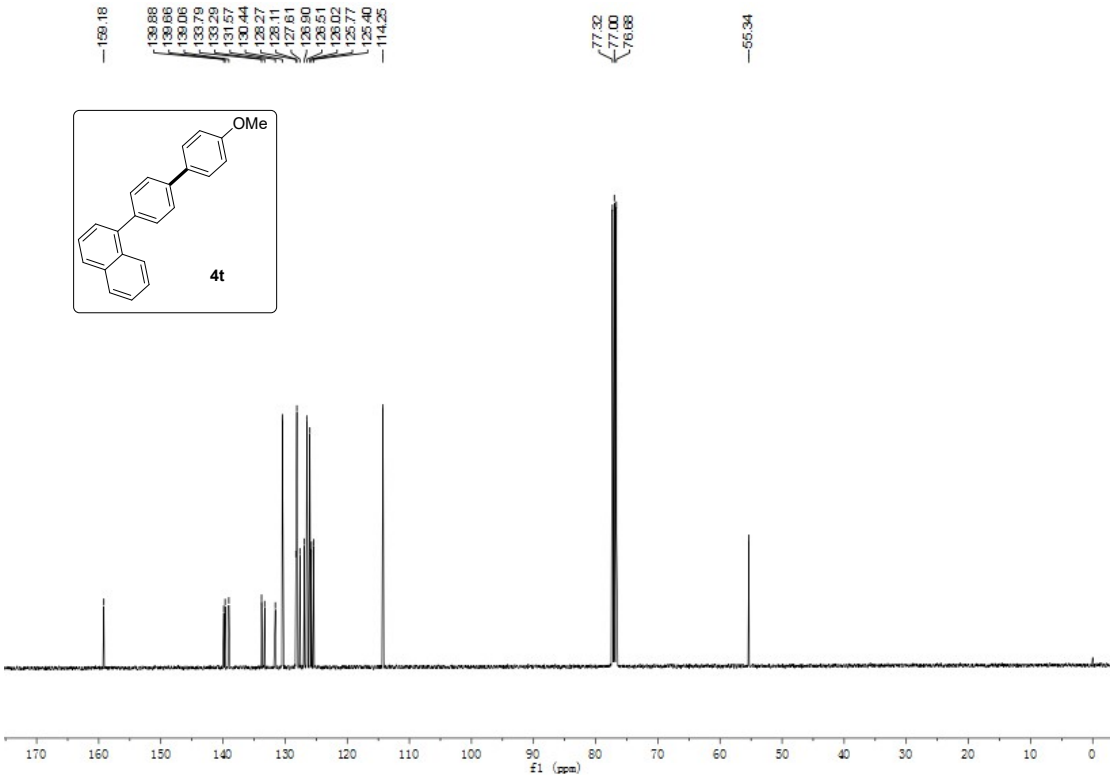
140.84
139.89
136.19
132.74
128.15
127.98
127.29
125.90
123.32
120.28
119.87
114.35
77.32
77.00
76.68
55.37
OMe
N
4s
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.024
8.003
7.949
7.929
7.901
7.881
7.713
7.694
7.660
7.641
7.585
7.564
7.542
7.525
7.499
7.483
7.470
7.451
7.260
7.053
7.034
3.892
OMe
4t
0.99
1.00
1.00
2.00
2.00
6.05
2.01
3.00
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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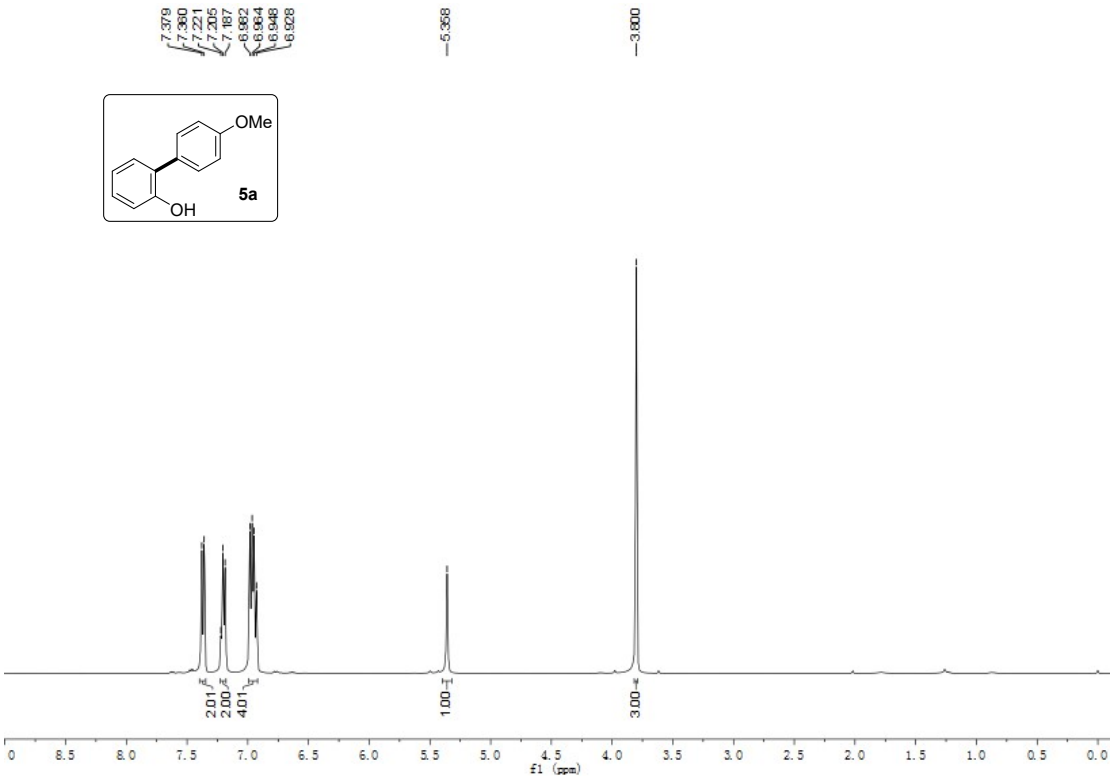
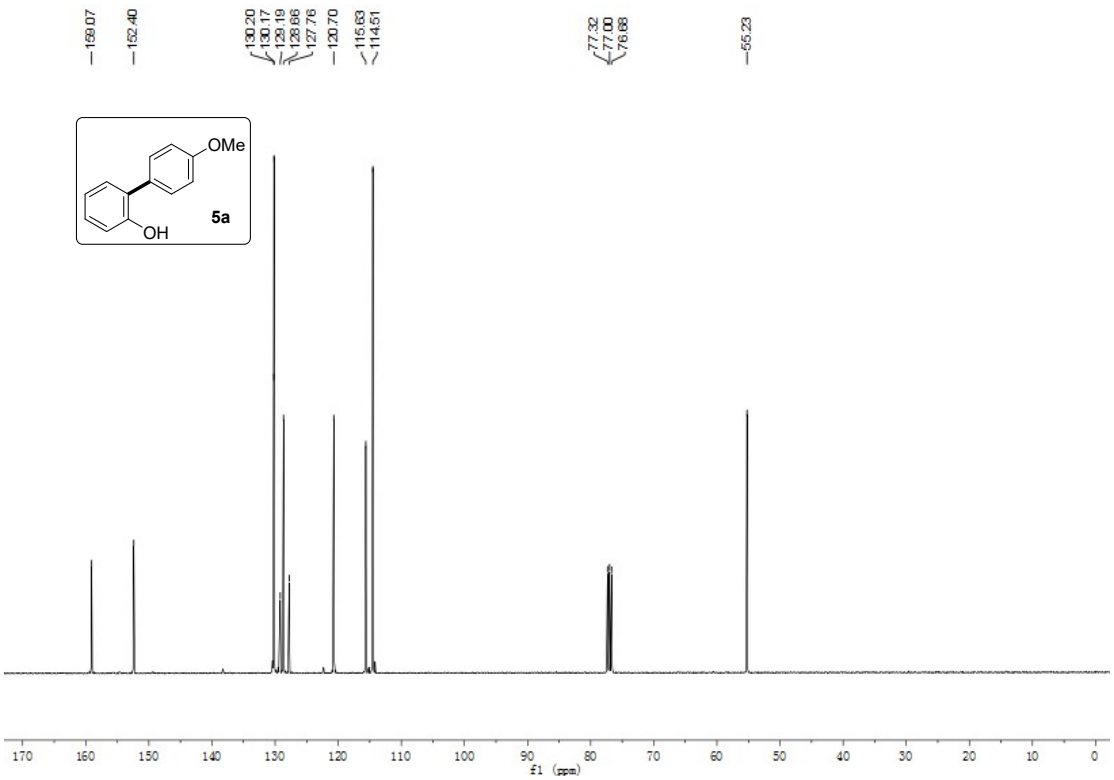
139.88
139.66
139.06
133.79
133.29
131.57
130.44
128.27
128.11
127.61
126.90
126.51
126.02
125.77
125.40
114.25
77.32
77.00
76.68
55.34
OMe
4t
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.379
7.360
7.221
7.205
7.187
6.982
6.964
6.948
6.928
5.368
3.800
OMe
OH
5a
2.01
2.00
4.01
1.00
3.00
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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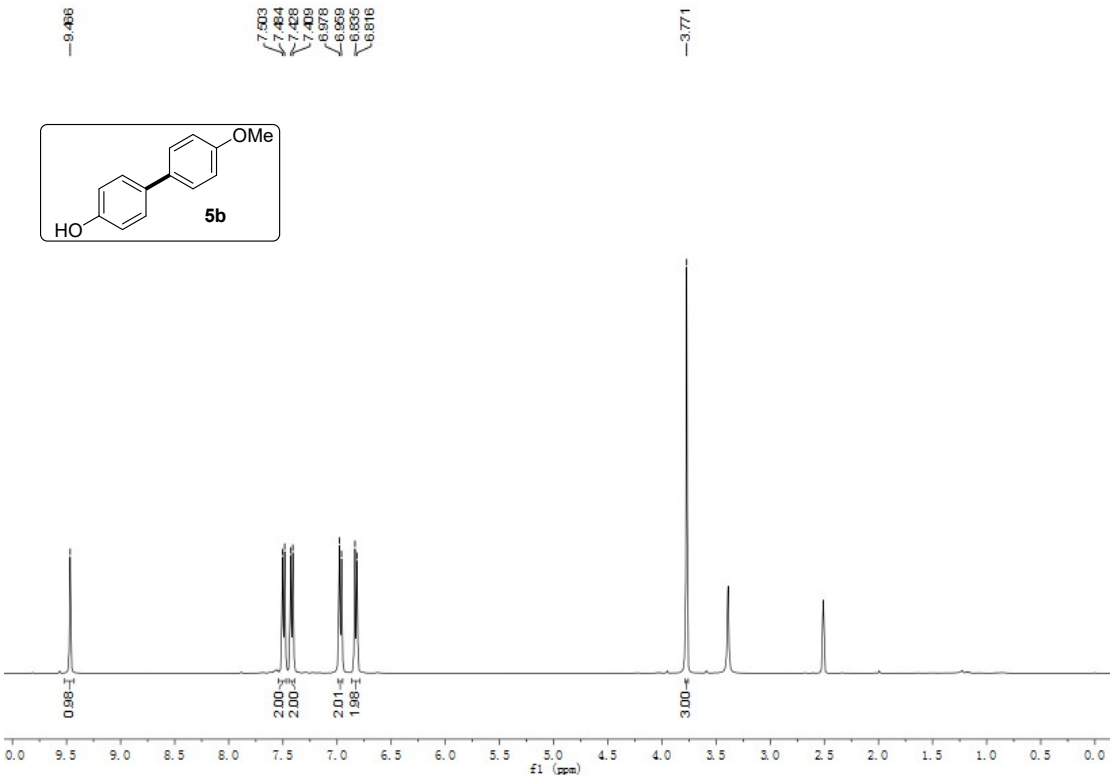
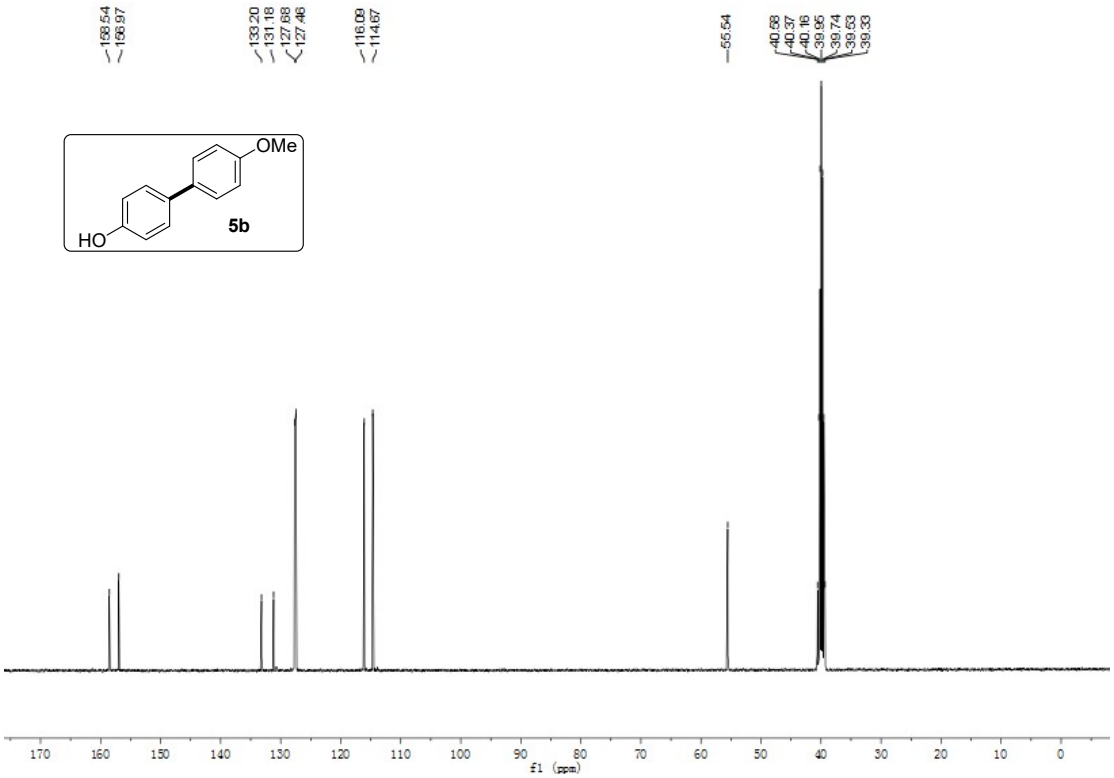
152.40
130.20
130.17
129.19
128.66
127.76
120.70
115.63
114.51
77.32
77.00
76.68
55.23
OMe
OH
5a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.486
7.503
7.484
7.428
7.409
6.978
6.959
6.835
6.816
3.771
OMe
HO
5b
0.98
2.00
2.00
2.01
1.98
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
f1 (ppm)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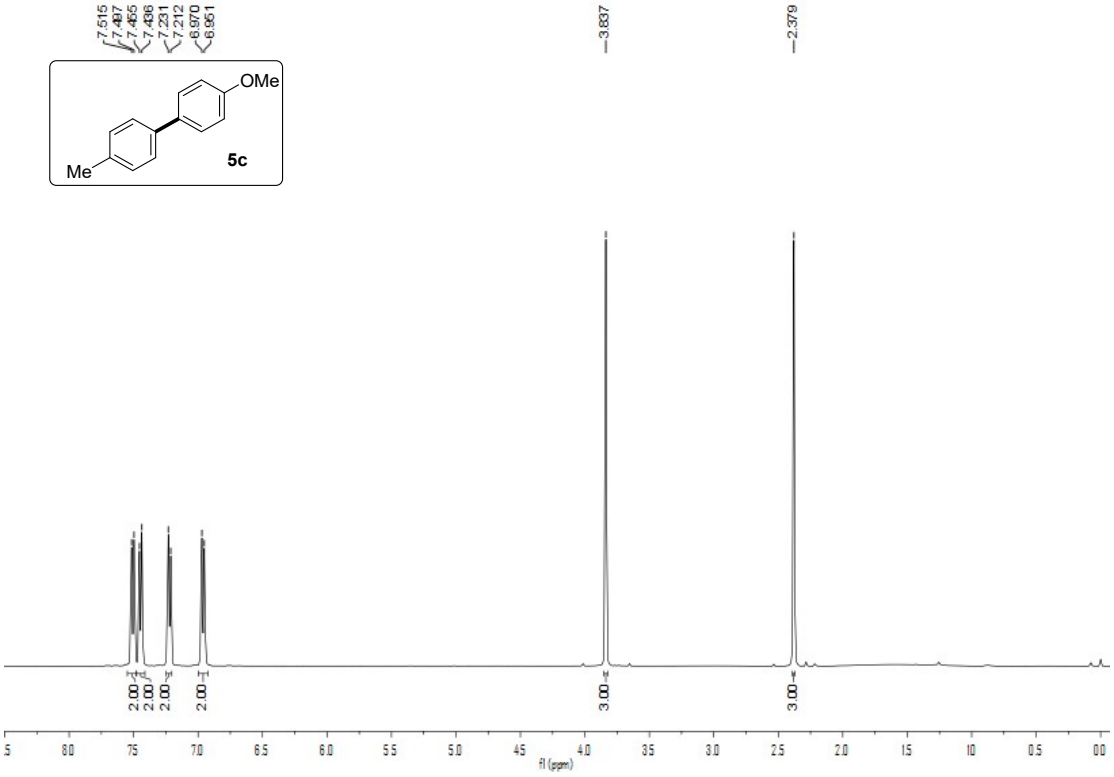
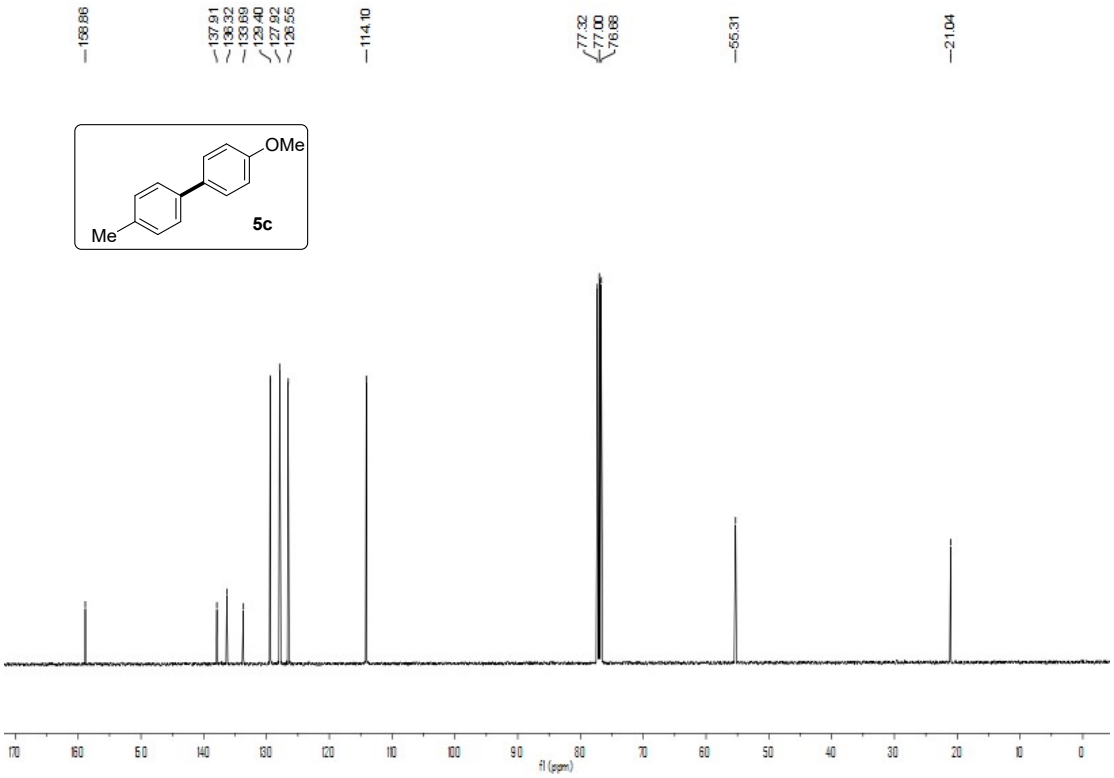
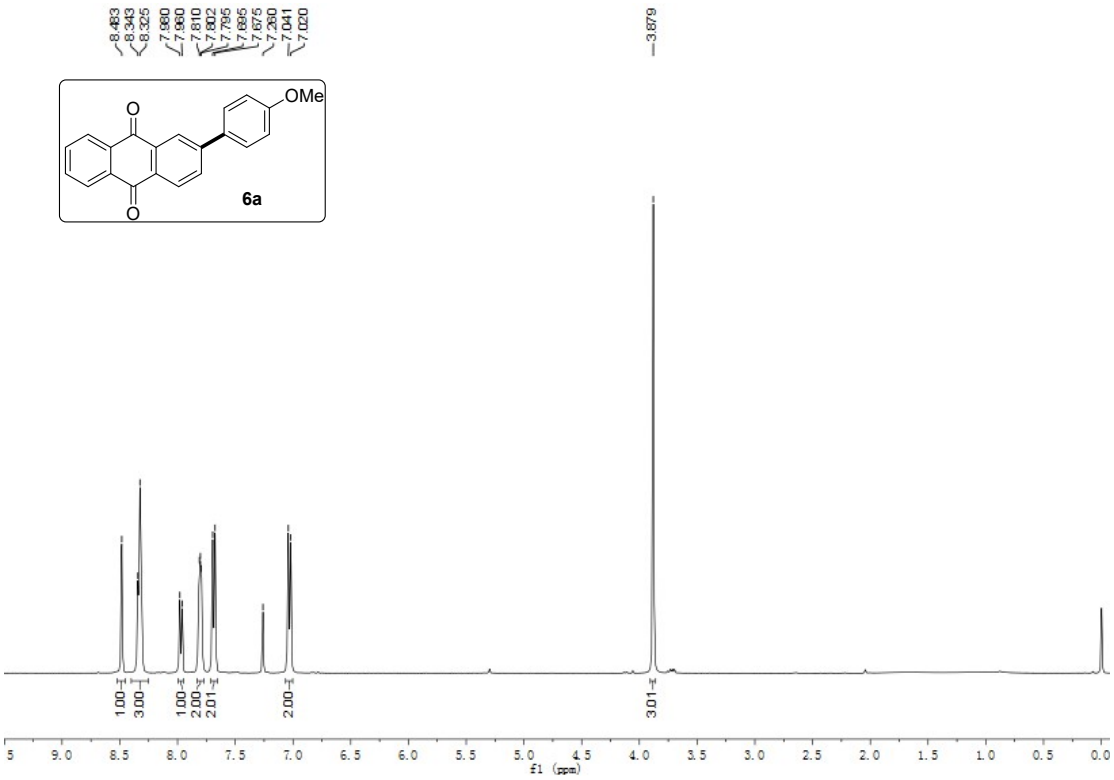
156.97
133.20
131.18
127.68
127.46
116.09
114.67
55.54
40.88
40.37
40.16
39.95
39.74
39.53
39.33
OMe
HO
5b
f1 (ppm)


7.515
7.487
7.465
7.436
7.231
7.212
6.970
6.951
3.837
2.379
OMe
Me
5c
2.00
2.00
2.00
2.00
3.00
3.00
f1 (ppm)


158.86
137.91
136.32
133.69
129.40
127.92
126.55
114.10
77.32
77.00
76.68
55.31
21.04
OMe
Me
5c
f1 (ppm)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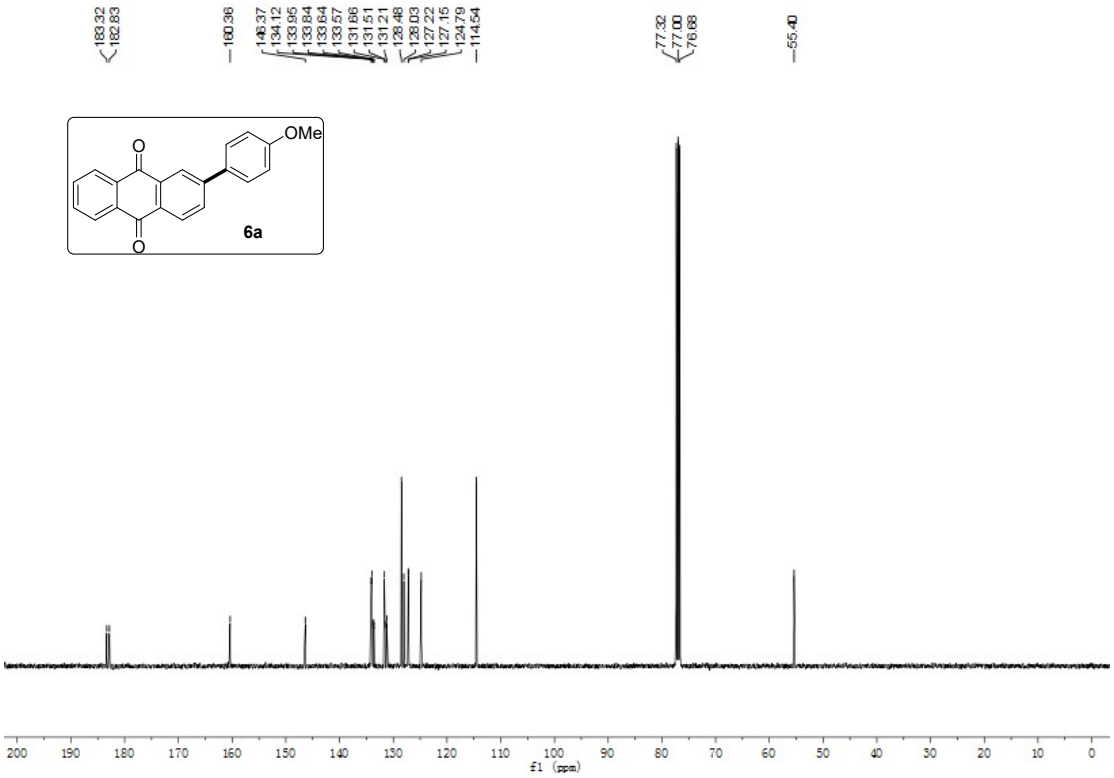
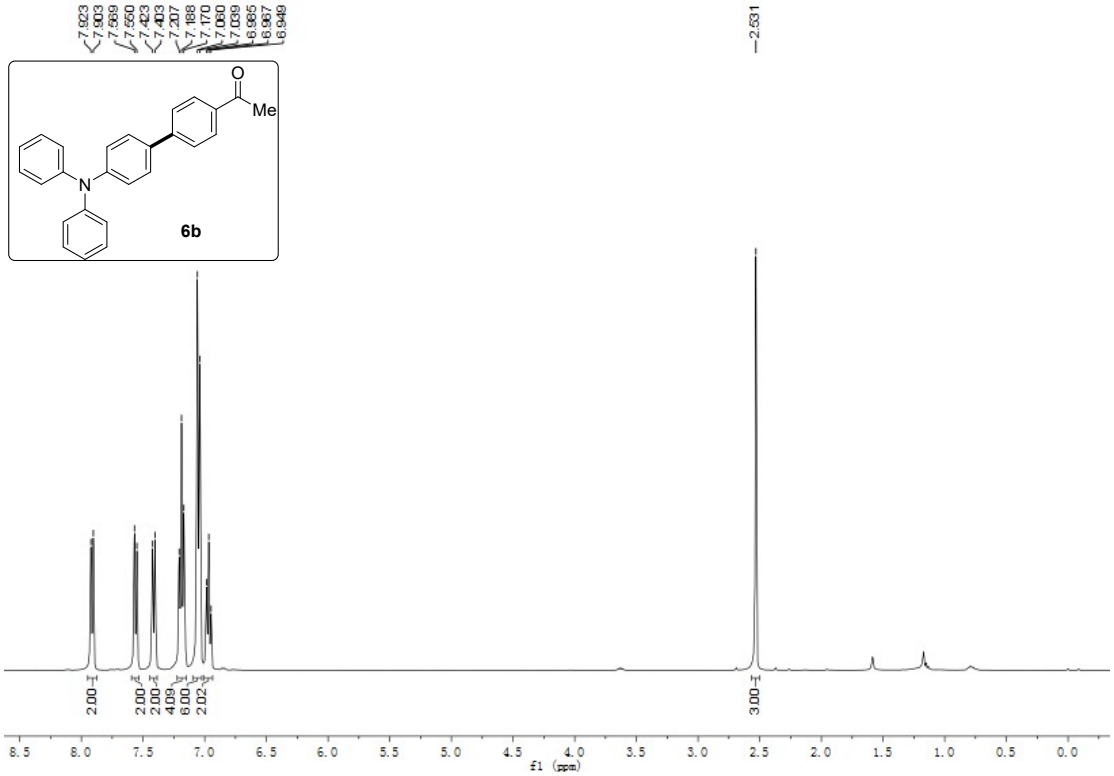
8.343
8.325
7.990
7.960
7.810
7.802
7.795
7.685
7.675
7.260
7.041
7.020
3.879
OMe
O
O
6a
1.00
3.00
1.00
2.00
2.01
2.00
3.01
f1 (ppm)


183.32
182.83
160.36
146.37
134.12
133.95
133.84
133.64
133.57
131.66
131.51
131.21
128.48
128.03
127.22
127.15
124.79
114.54
77.32
77.00
76.68
55.40
OMe
O
O
6a
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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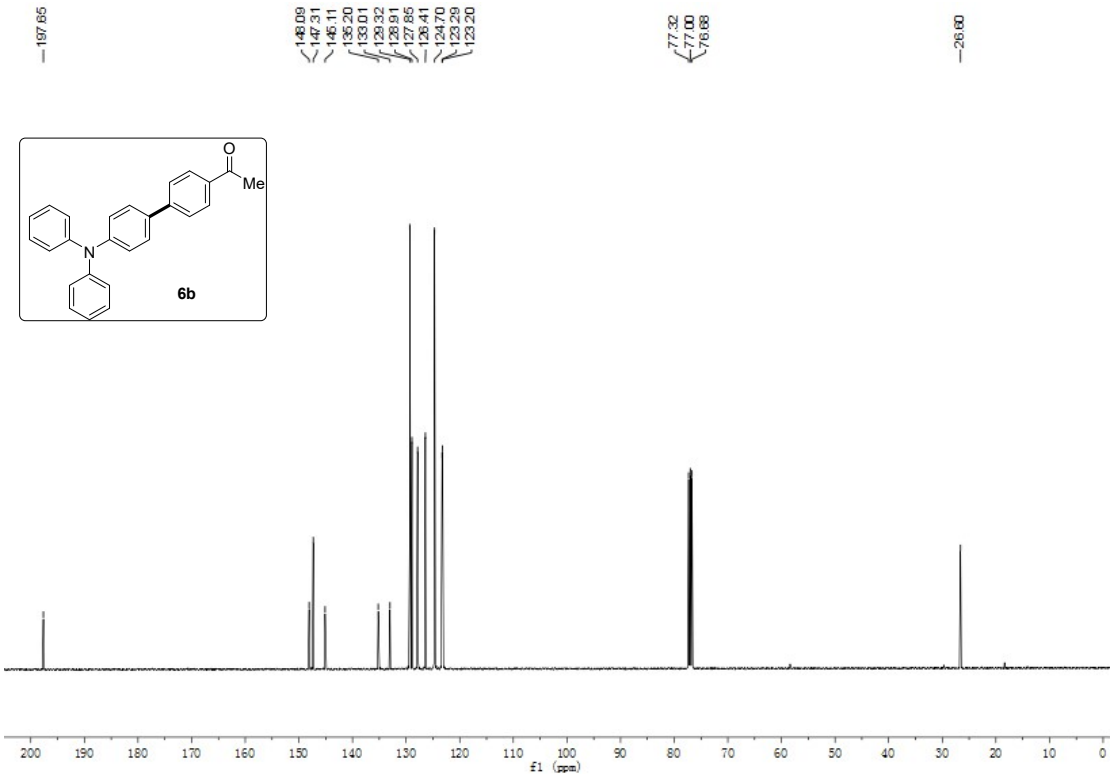
7.188
7.170
7.060
7.039
6.985
6.967
6.949
2.531
O
Me
N
6b
2.00
2.00
2.00
4.09
6.00
2.02
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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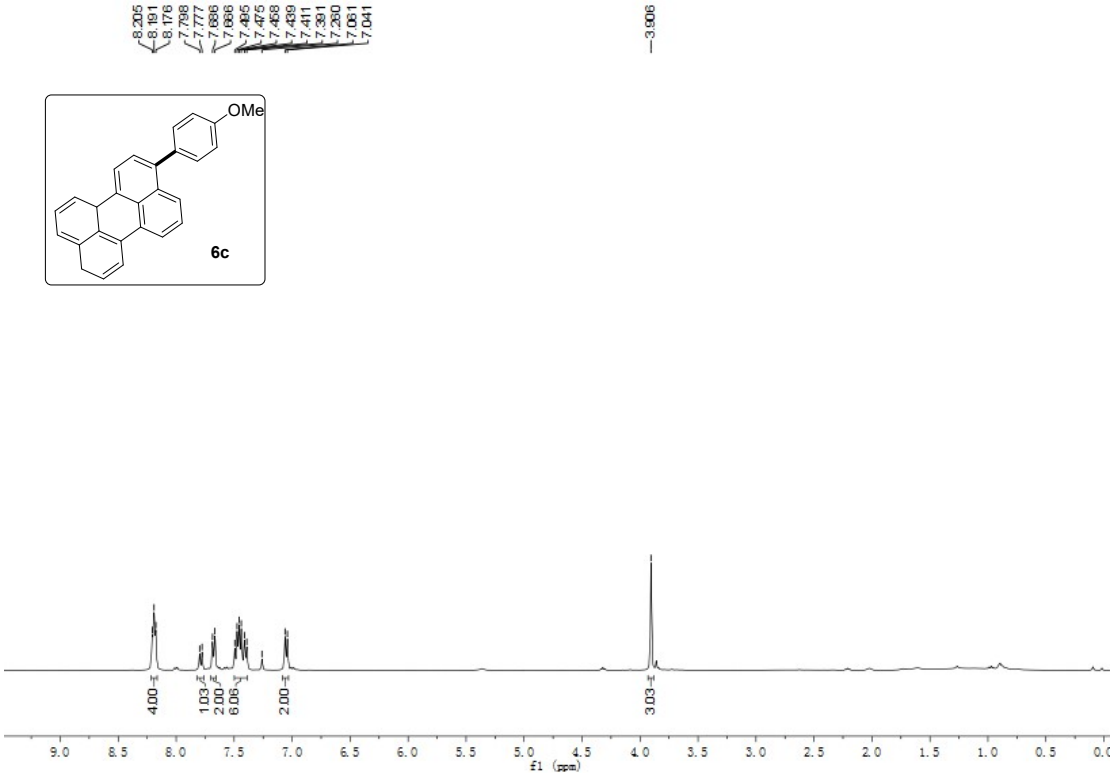
147.31
146.11
135.20
133.01
129.32
128.91
127.85
126.41
124.70
123.29
123.20
77.32
77.00
76.68
26.60
O
Me
N
6b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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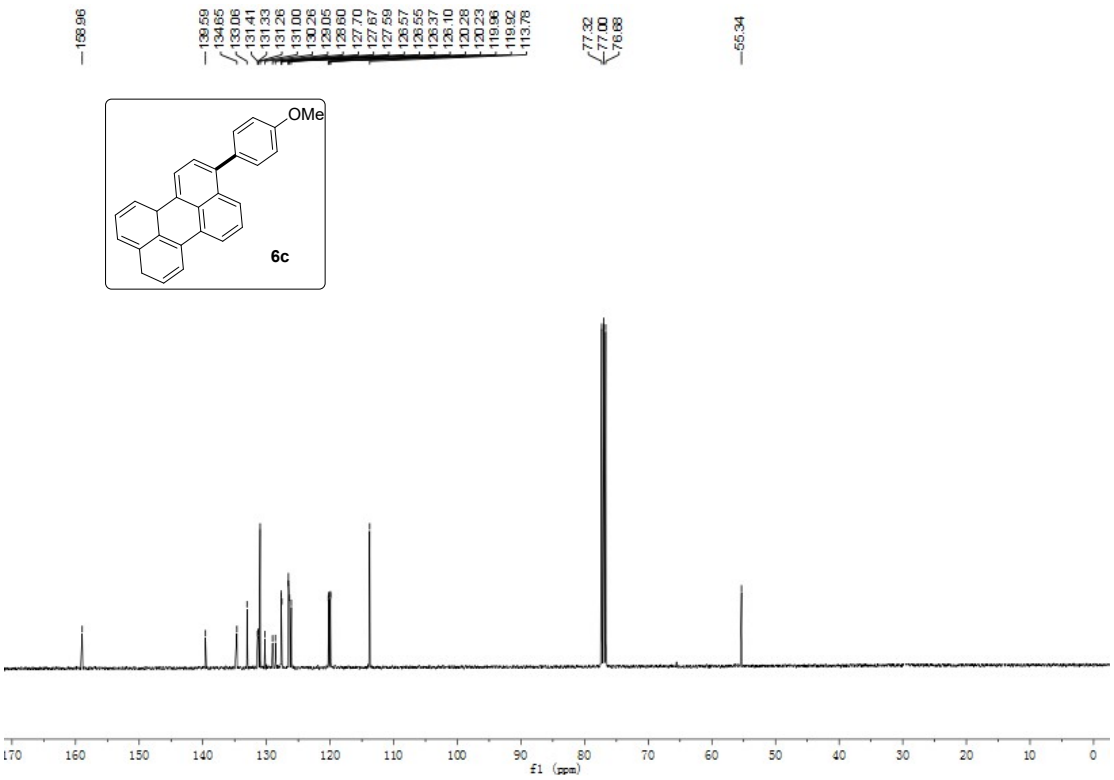
7.475
7.458
7.439
7.411
7.391
7.260
7.061
7.041
3.906
OMe
6c
4.00
1.03
2.00
6.06
2.00
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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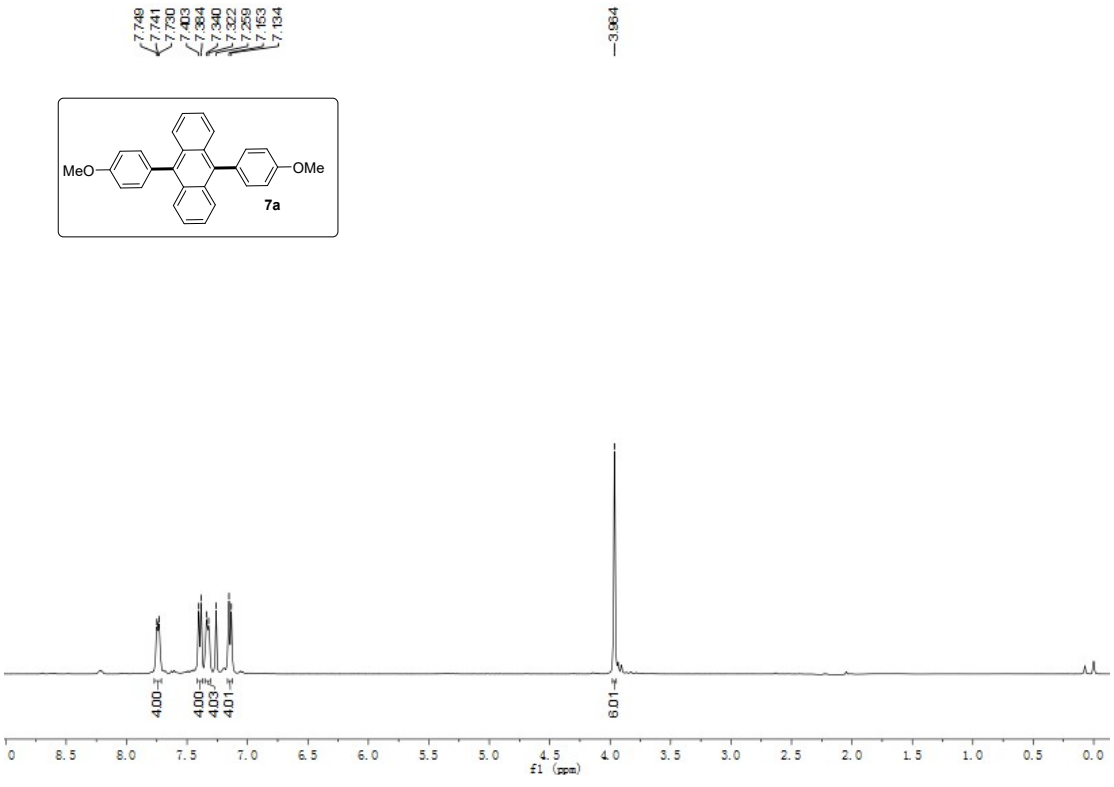
131.33
131.26
131.00
130.26
129.05
128.60
127.70
127.67
127.59
126.57
126.55
126.37
126.10
120.28
120.23
119.96
119.92
113.78
77.32
77.00
76.68
55.34
OMe
6c
f1 (ppm)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7.730
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7.384
7.340
7.322
7.259
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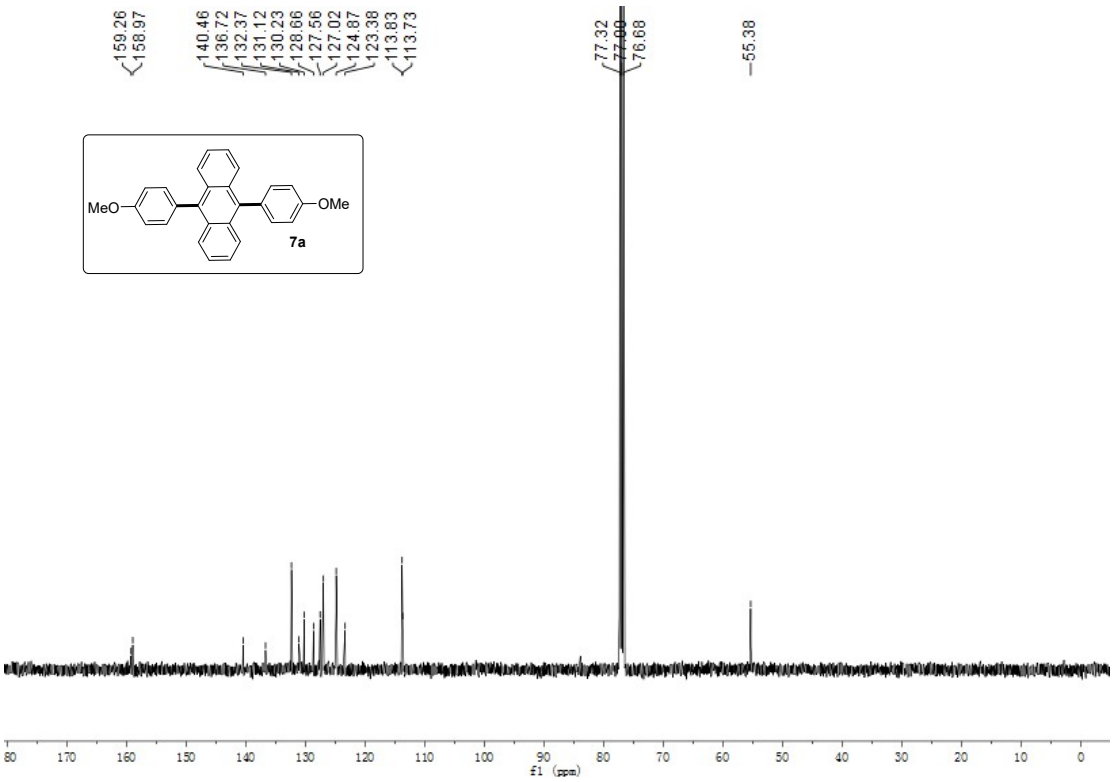
3.964
MeO
OMe
7a
4.00
4.00
4.03
4.01
6.01
f1 (ppm)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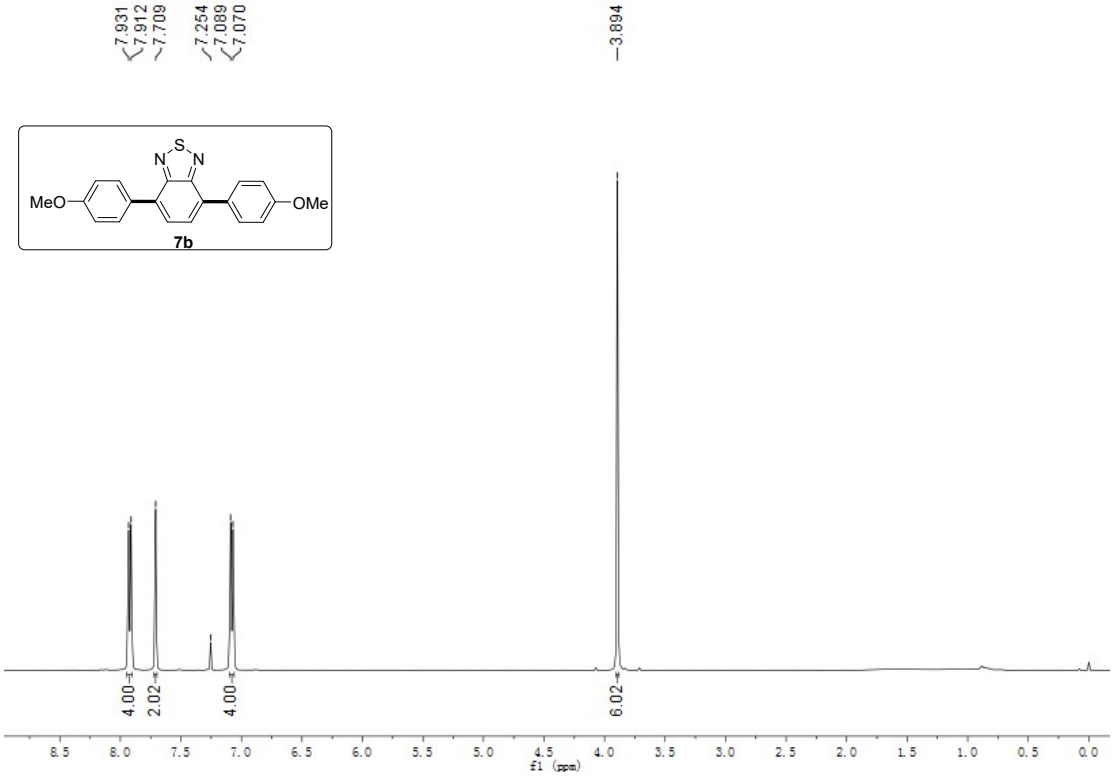
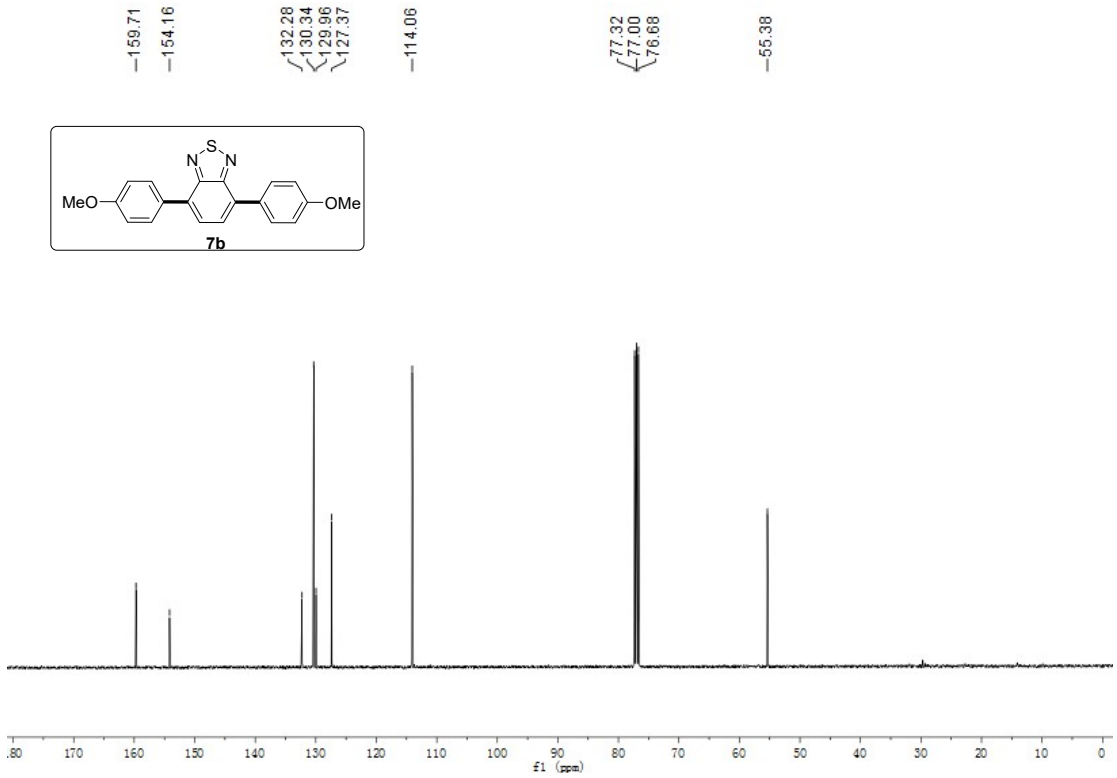
132.37
131.12
130.23
128.66
127.56
127.02
124.87
123.38
113.83
113.73
77.32
77.00
76.68
55.38
MeO
OMe
7a
f1 (ppm)


7.931
7.912
7.709
7.254
7.089
7.070
3.894
N
S
N
MeO
OMe
7b
4.00
2.02
4.00
6.02
f1 (ppm)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154.16
132.28
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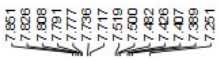
127.37
114.06
77.32
77.00
76.68
55.38
MeO
OMe
7b
f1 (ppm)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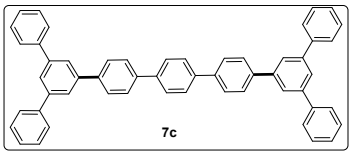
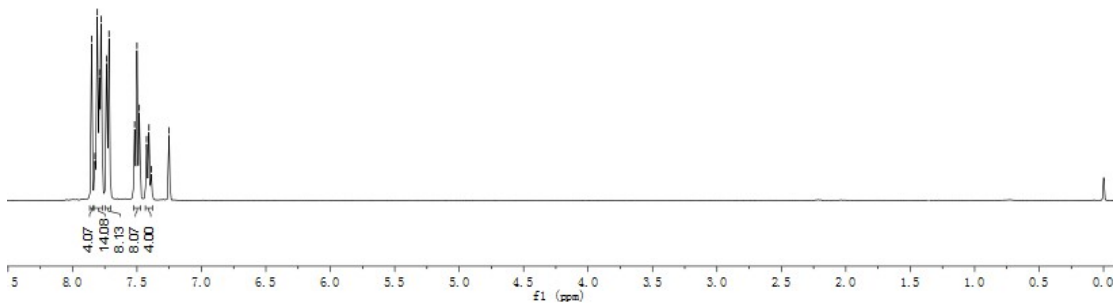
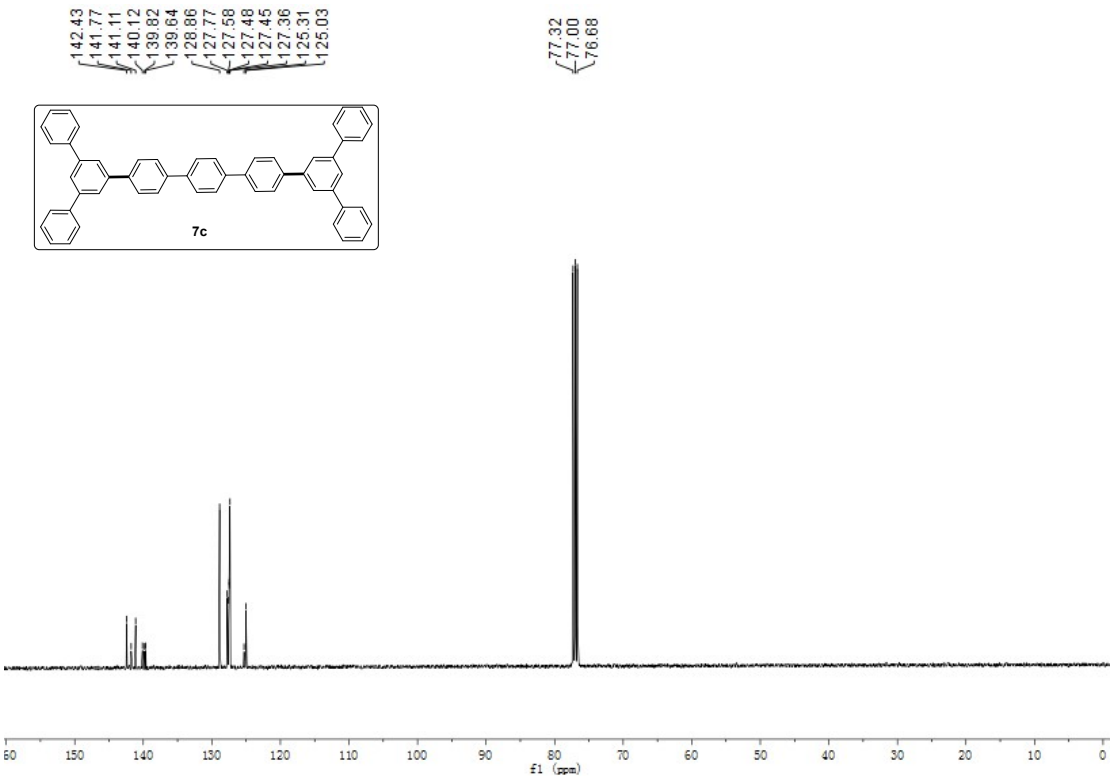
7.482
7.426
7.407
7.389
7.251


7c


4.07
14.08
8.13
8.07
4.00
f1 (ppm)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127.45
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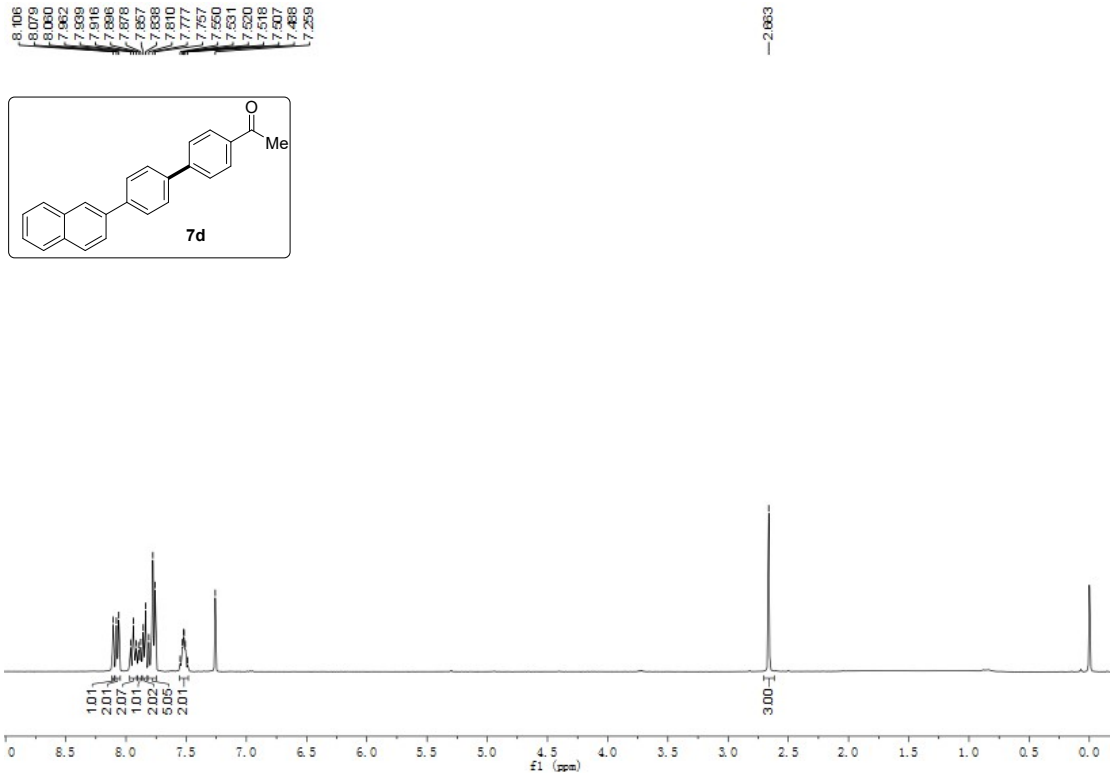
77.32
77.00
76.68
7c
f1 (ppm)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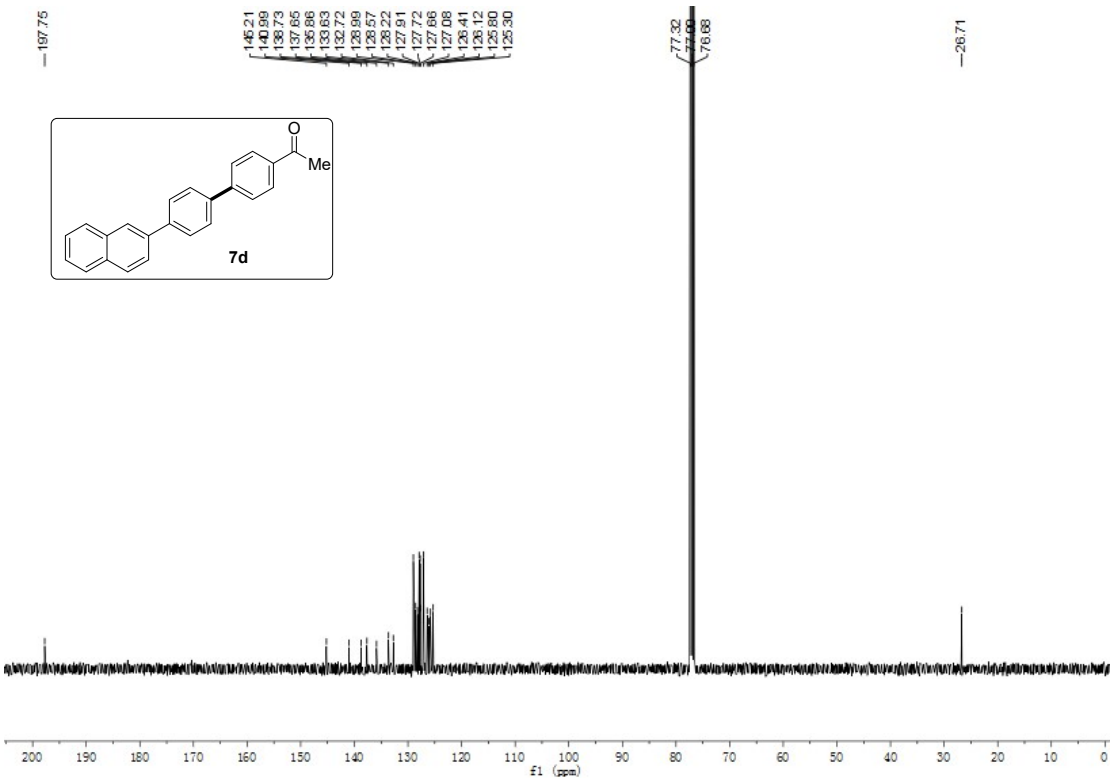
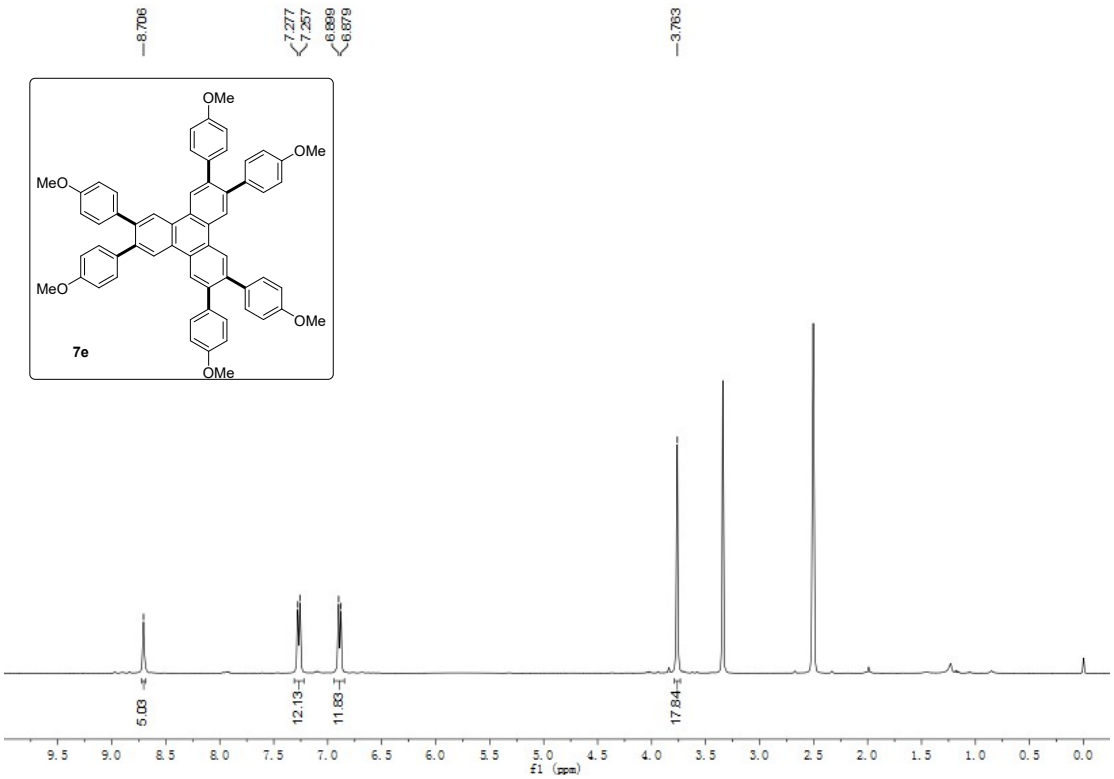
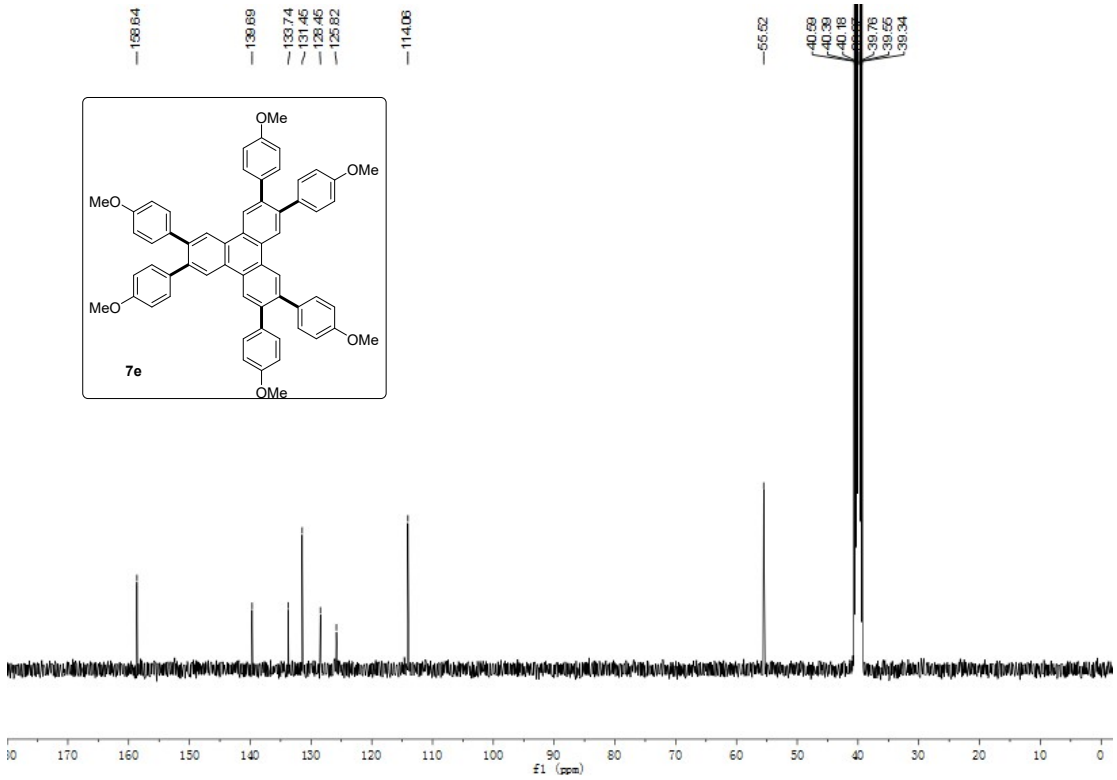
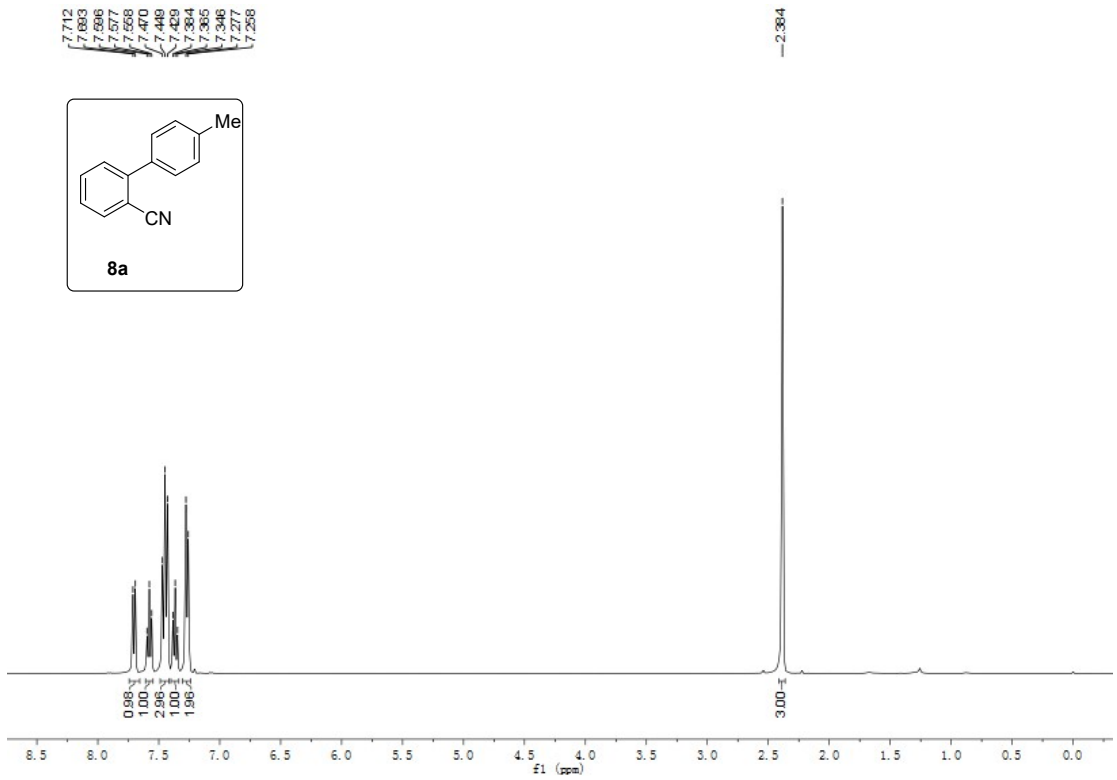
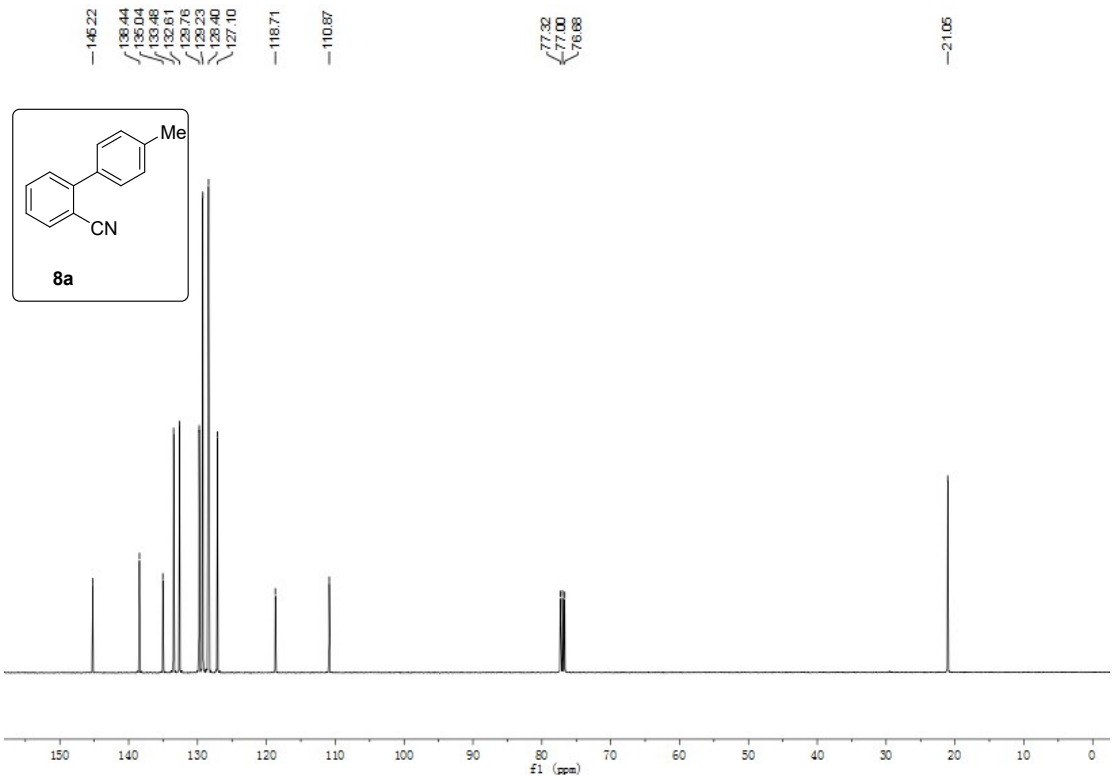
7.757
7.550
7.531
7.520
7.507
7.488
7.259
2.663
O
Me
7d
1.01
2.01
2.07
1.01
2.02
5.05
2.01
3.00
f1 (ppm)


197.75
145.21
140.99
138.73
137.65
135.86
133.63
132.72
128.99
128.57
128.22
127.91
127.72
127.66
127.08
126.41
126.12
125.80
125.30
77.32
77.00
76.68
26.71
O
Me
7d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.706
7.277
7.257
6.899
6.879
3.763
OMe
MeO
7e
5.03
12.13
11.83
17.84
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)


158.64
139.69
133.74
131.45
128.45
125.82
114.06
55.62
40.59
40.39
40.18
39.76
39.55
39.34
OMe
OMe
MeO
MeO
OMe
OMe
7e
f1 (ppm)


7.712
7.693
7.596
7.577
7.558
7.470
7.448
7.429
7.384
7.365
7.346
7.277
7.258
2.384
Me
CN
8a
0.98
1.00
2.96
1.00
1.96
3.00
f1 (ppm)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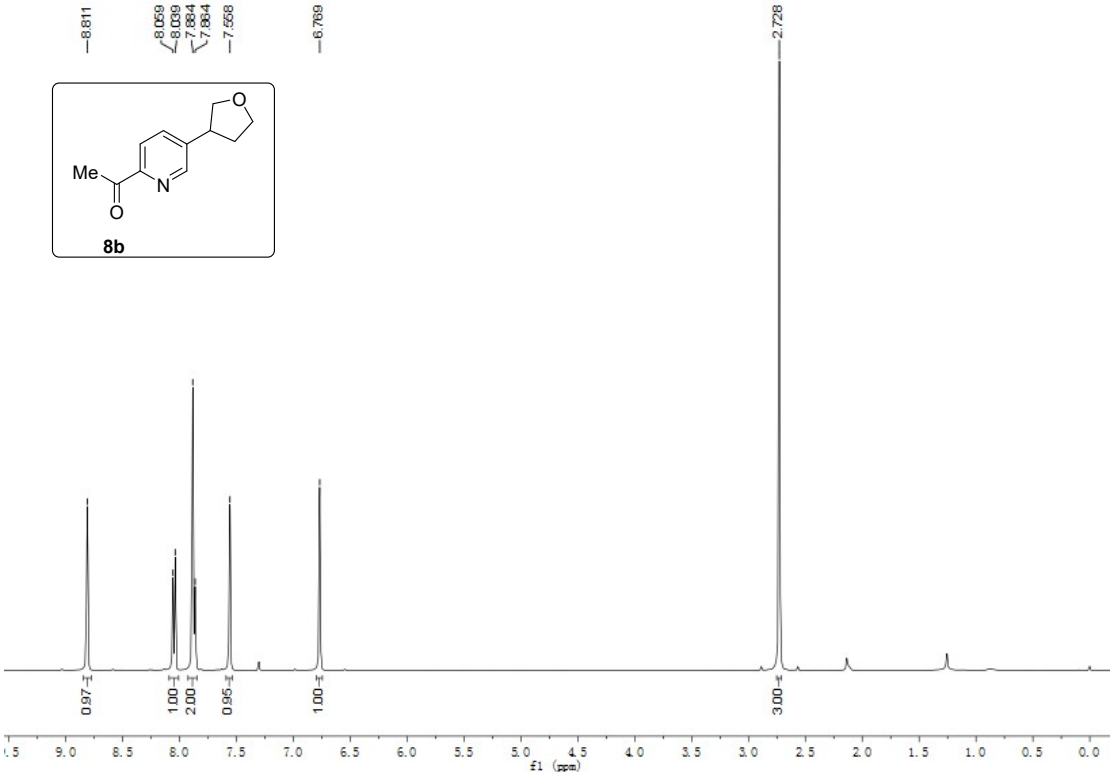
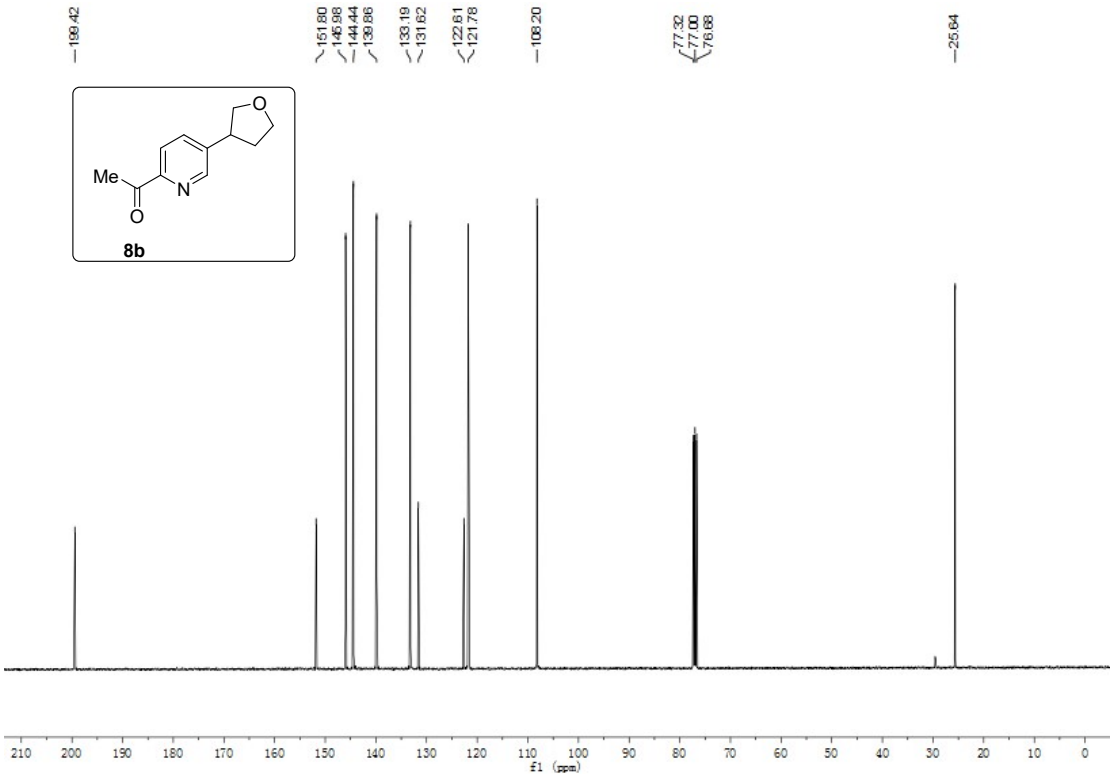
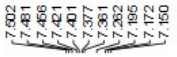
138.44
136.04
133.48
132.61
129.76
129.23
128.40
127.10
118.71
110.87
77.32
77.00
76.68
21.05
Me
CN
8a
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.811
8.059
8.039
7.884
7.864
7.558
6.769
2.728
O
Me
N
O
8b
0.97
1.00
2.00
0.95
1.00
3.00
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)


199.42
151.80
145.98
144.44
139.86
133.19
131.62
122.61
121.78
108.20
77.32
77.00
76.68
25.64
Me
O
N
O
8b
f1 (ppm)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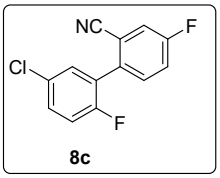
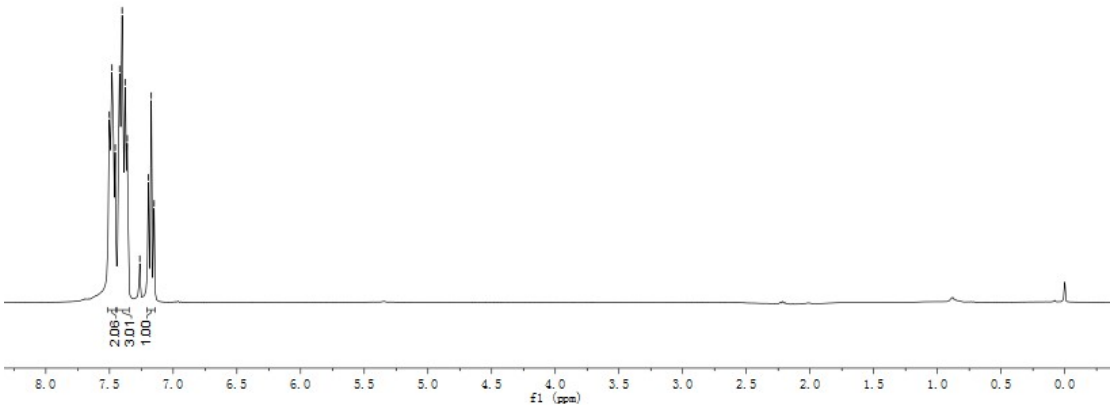
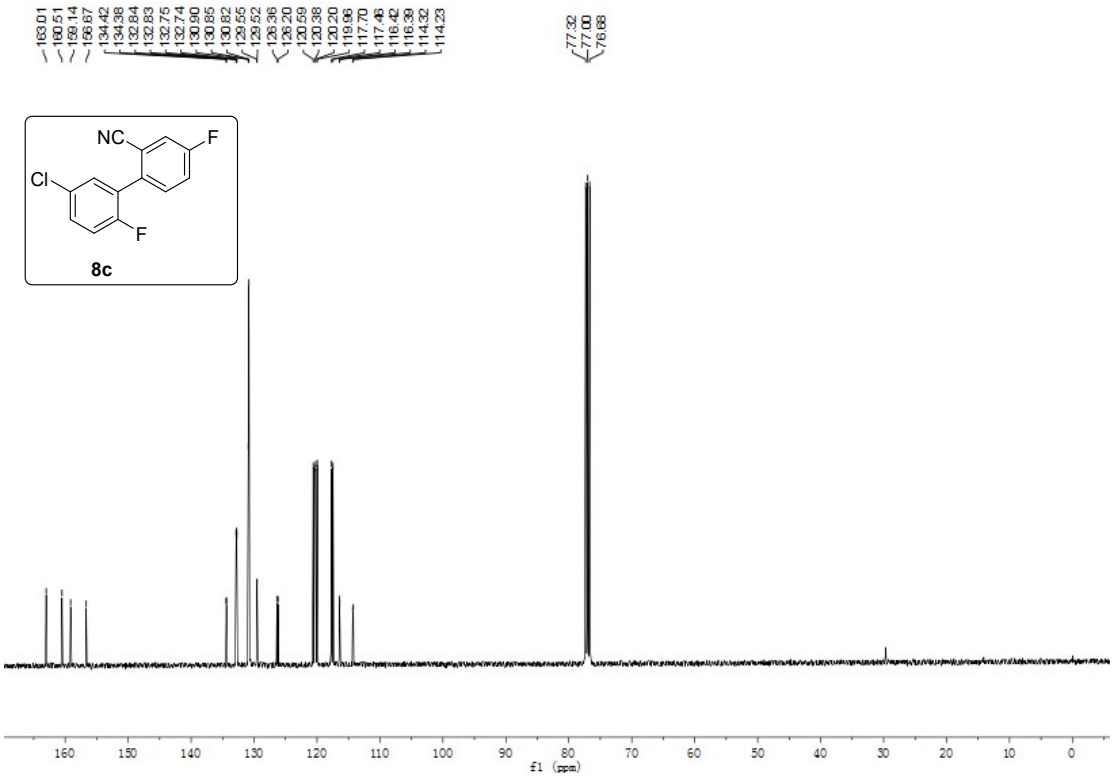
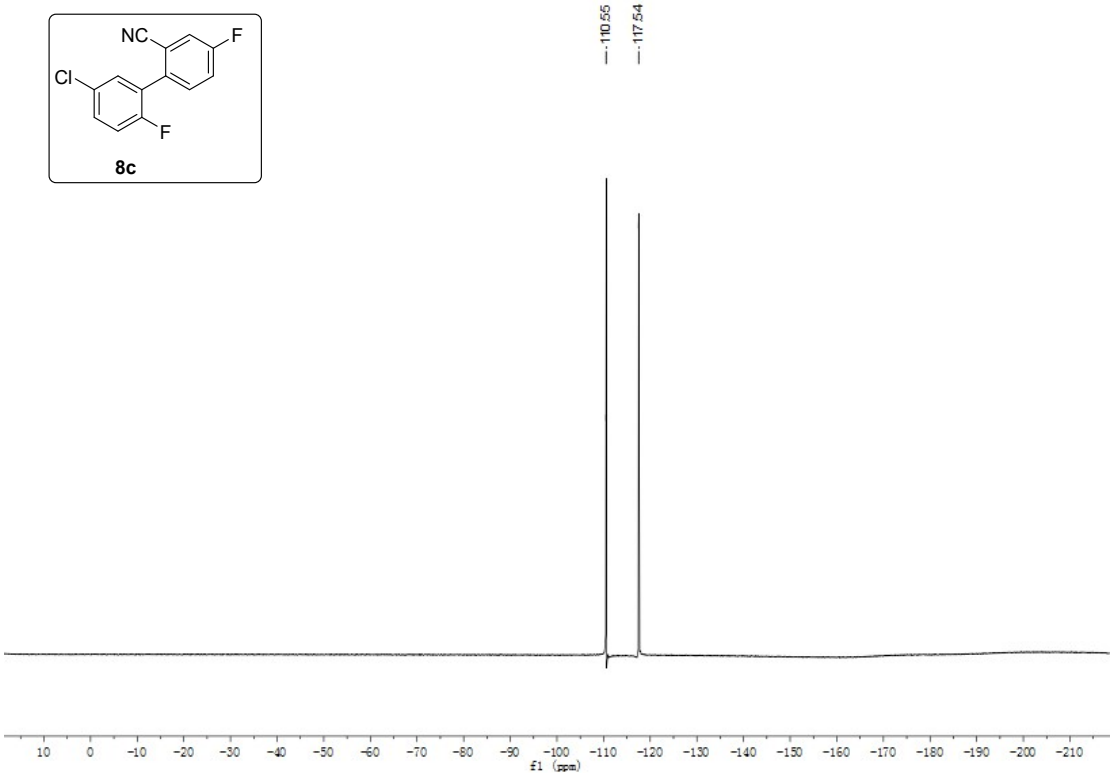
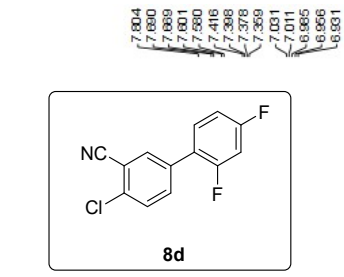
7.481
7.456
7.421
7.401
7.377
7.361
7.262
7.195
7.172
7.150

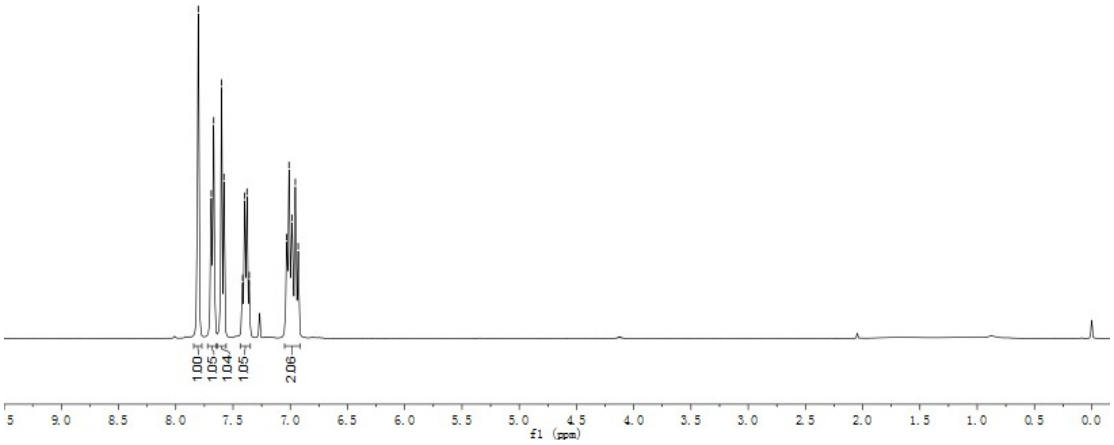

NC
F
Cl
F
8c


2.06
3.01
1.00
f1 (ppm)


163.01
160.51
159.14
156.67
134.42
134.38
132.84
132.83
132.75
132.74
130.90
130.85
130.82
129.55
129.52
126.36
126.20
120.59
120.38
120.20
119.96
117.70
117.48
116.42
116.39
114.32
114.23
77.32
77.00
76.68
NC
F
Cl
F
8c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


NC
F
Cl
F
8c
-110.55
-117.54
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.804
7.890
7.869
7.801
7.390
7.416
7.398
7.378
7.359
7.031
7.011
6.985
6.956
6.931
NC
Cl
F
F
8d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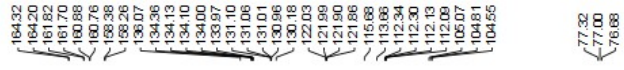
1.05
1.04
1.05
2.06
f1 (ppm)


164.32
164.20
161.82
161.70
160.88
160.76
158.38
158.26
136.07
134.36
134.13
134.10
134.00
133.97
131.10
131.06
131.01
130.96
130.18
122.03
121.99
121.90
121.86
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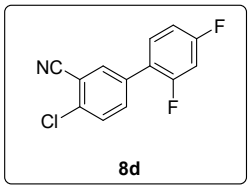
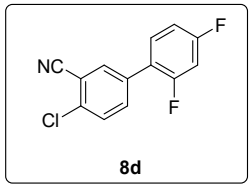
112.34
112.30
112.13
112.09
105.07
104.81
104.55
77.32
77.00
76.68

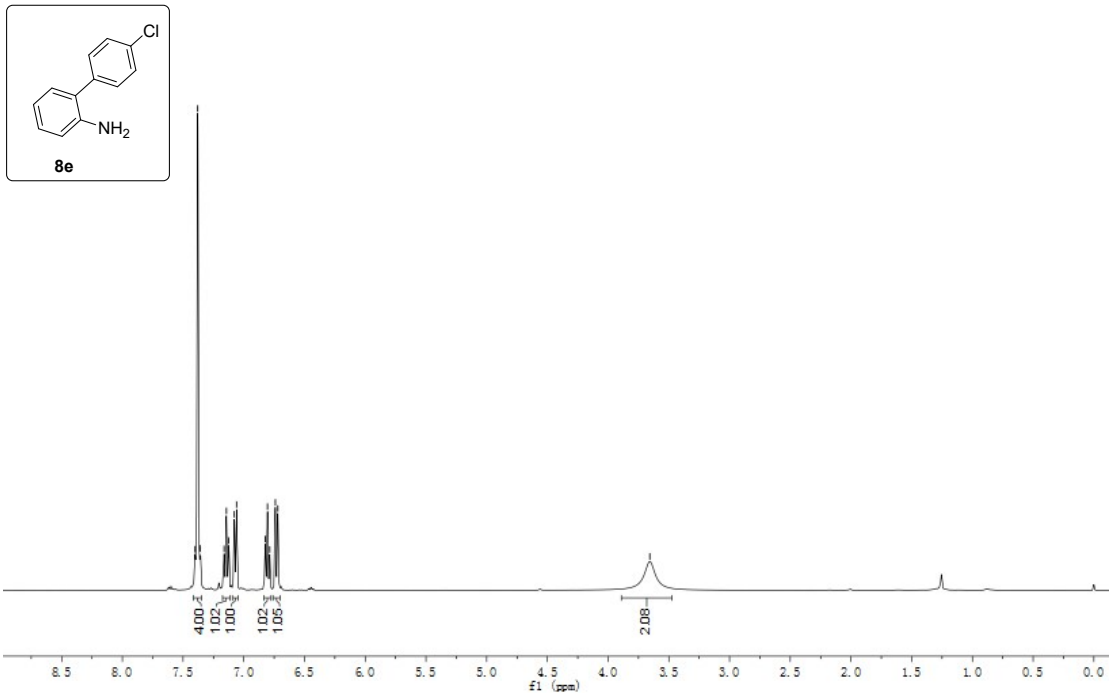

NC
Cl
F
F
8d

f1 (ppm)


NC
Cl
F
F

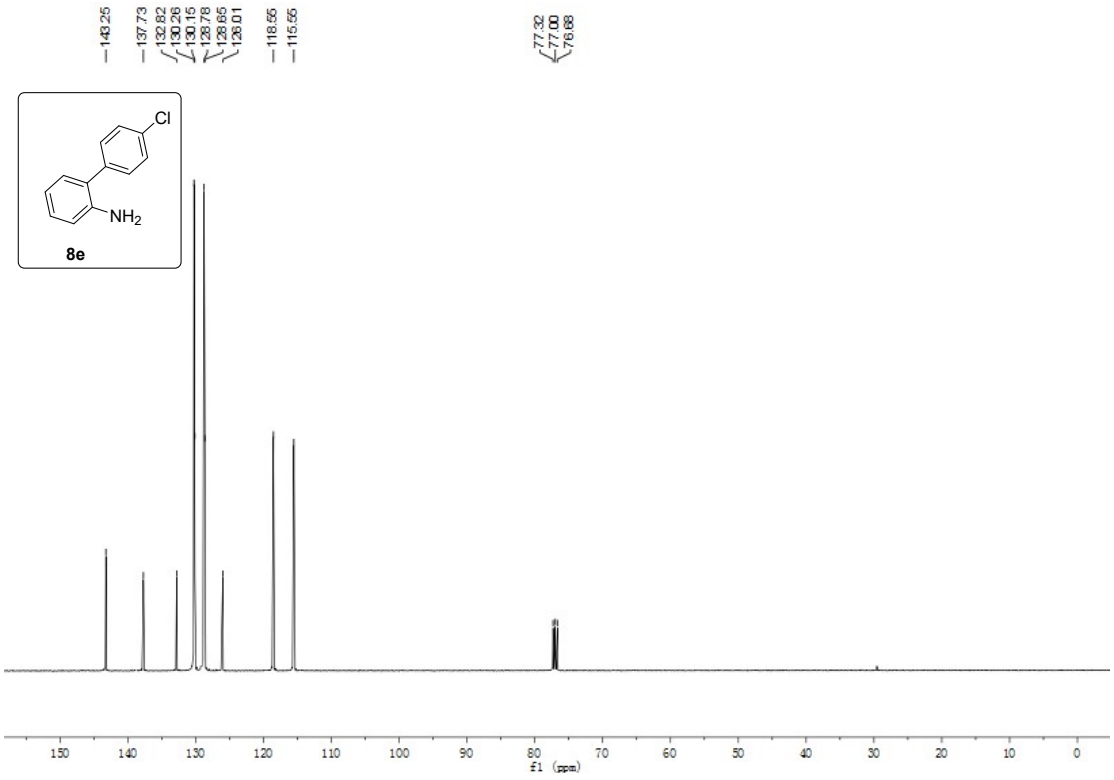
8d

-108.41
-113.19
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.401
7.380
7.358
7.162
7.143
7.124
7.078
7.060
6.824
6.805
6.786
6.740
6.720
3.667
4.00
1.02
1.00
1.02
1.05
2.08
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)

Cl
NH2

8e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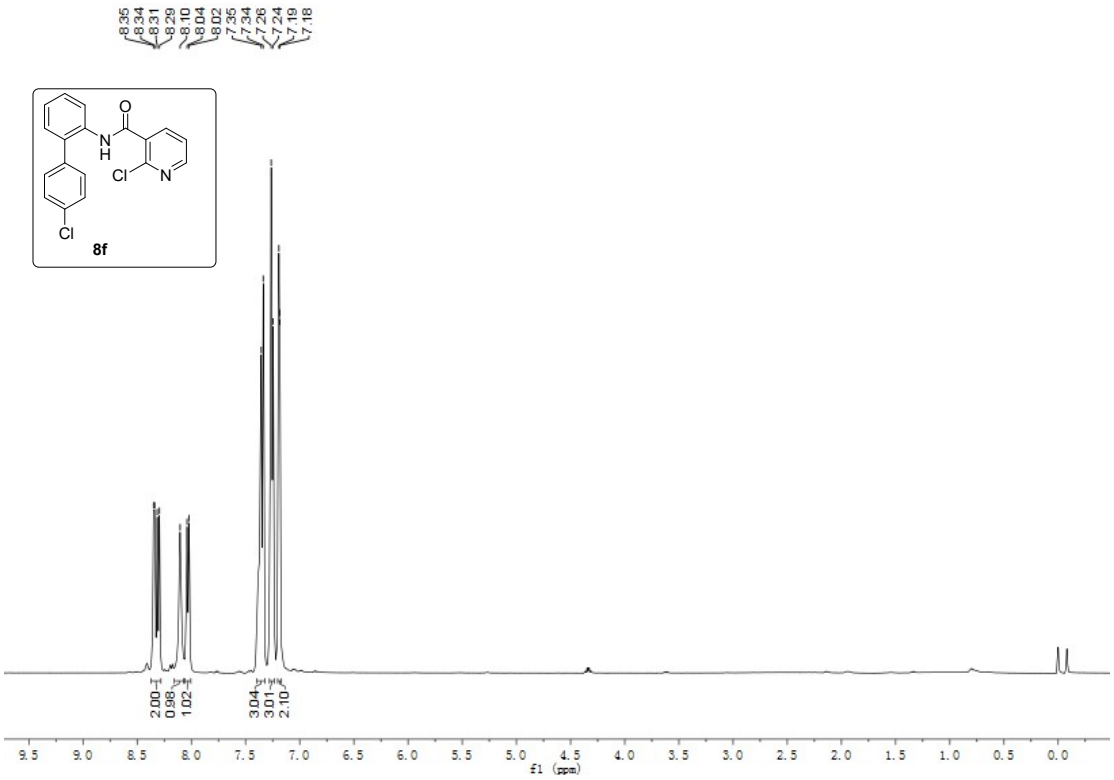
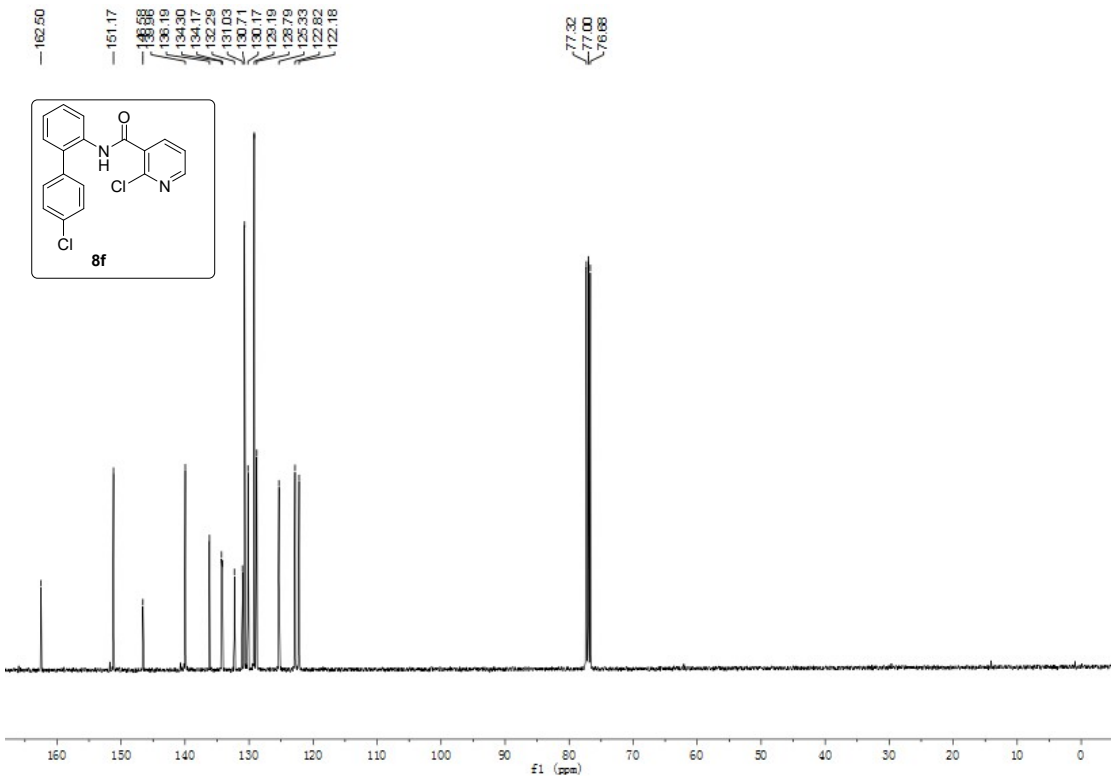
137.73
132.82
130.26
130.15
128.78
128.65
126.01
118.55
115.55
77.32
77.00
76.68
Cl
NH2
8e
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.35
8.34
8.31
8.29
8.10
8.04
8.02
7.35
7.34
7.26
7.24
7.19
7.18
O
N
H
Cl
N
Cl
8f
2.00
0.98
1.02
3.04
3.01
2.10
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)


162.50
151.17
136.19
134.30
134.17
132.29
131.03
130.71
130.17
129.19
128.79
125.33
122.82
122.18
77.32
77.00
76.68
O
N
H
Cl
N
Cl
8f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)