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Supporting Information

Pd/Cu-Catalyzed Aerobic Oxidative Aromatic C-H Bond Activation/*N*-Dealkylative Carbonylation towards the Synthesis of Phenanthridinones

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1. General

All reactions were carried out in oven-dried Schlenk tube under a mixed oxygen and carbon monoxide atmosphere with a balloon. Toluene and DMA were dried by molecular sieve. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. GC yields were recorded with a SHIMADZU GC-2014 gas chromatograph instrument with a FID detector and biphenyl was added as an internal standard. ^{1}H and ^{13}C NMR data were recorded with Bruker Advanced II (400 MHz) spectrometers with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. All chemical shifts are reported relative to tetramethylsilane and d-solvent peaks (77.00 ppm, chloroform; 39.600 ppm, d^6-DMSO), respectively. High resolution massspectra (HRMS) were measured with a Waters Micromass GCT instrument and accurate masses were reported for the molecular ion ($[M]^+$) or $[M+H]^+$.

2. Preparation of biphenyl-2-amines

General Procedure: The boronic acid (12 mmol) and the appropriate aniline bromide (6 mmol) were dissolved in a mixture of EtOH/water (10 mL: 3.5 mL). K_2CO_3 (18 mmol) and tetrakis (triphenylphosphine) palladium catalyst (2 mol%) were added to the reaction mixture that was stirred at 90 °C for 24 h. The solvent was removed under reduced pressure and the residue obtained was taken up in dichloromethane and extracted (three times). The organic phase was dried over Na_2SO_4, filtered, and dried in vacuo. Purification by column chromatography on silica gel is conducted.

3. Preparation of *N, N*-disubstituted biphenyl-2-amines

Preparation of *N, N*-disubstituted biphenyl-2-amines employed the procedure of Zimmt [1]. General Procedure: A mixture of fresh biphenyl-2-amines(10.0 mmol), iodoalkane (42.0 mmol), and K_2CO_3(15.0 mmol) in DMF (13 mL) was refluxed at 65 °C for 25 h. Then we increase the temperature to 120 °C for 3 h. The suspension was filtered, and the resulting solid was washed with CH_2Cl_2. The filtered solution was extracted with water, and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. Purification by column chromatography on silica gel is conducted.

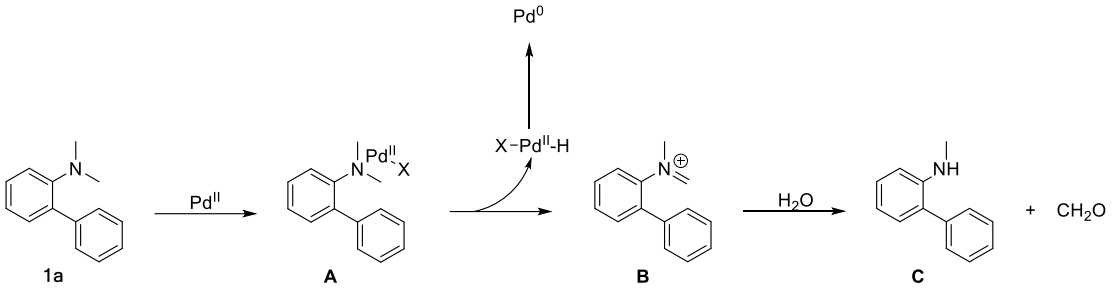
4. Phenanthridinones via Pd/Cu-catalyzed aerobic oxidative aromatic C-H bond activation/N-dealkylative carbonylation

General Procedure: In an oven-dried Schlenk tube equipped with a stir-bar, $PdCl_2$ (3.6 mg, 10 mol%), $Cu(OAc)_2•H_2O$ (12.0 mg, 30 mol%) were combined. A balloon filled with CO and O_2 (the ratio is 2:1) was connected to the Schlenk tube via the side tube and purged for 3 times. Then DMA (0.2 mL) and toluene(1.0 mL) were added to the tube via a syringe. At last, tertiary biphenyl-2-amines

(0.2 mmol), AcOH (4.8 mg, 40 mol%) was added to the tube. The Schlenk tube was heated at 110 ^{o}C for 24 hours and then cooled to room temperature. After the balloon gas was released carefully, the reaction was quenched by water and extracted with CH_2Cl_2 three times. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated in vacuum. The desired products were obtained in the corresponding yields after purification by flash chromatography on silica gel with hexane, ethyl acetate.

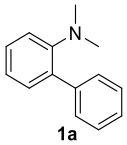
5. Proposed mechanism for Pd-catalyzed C-N bond activation

We have proposed the probable mechanism: firstly: **1a** coordinates to Pd(II) to form intermediate **A**, followed by β-H elimination to access imine cation **B**. The imine cation run hydrolysis to give secondary amine **C**.



6. Analytical Data of Substrates and Products

***N, N*-dimethylbiphenyl-2-amine**

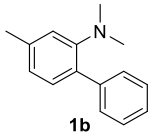


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.30-7.25 (m, 2H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.04 – 6.99 (m, 2H), 2.53 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 141.9, 134.1, 131.7, 128.6, 128.3, 128.0, 126.4, 121.4, 117.5, 43.3.

HRMS (ESI) calcd for $C_{14}H_{15}N$ $[M]^{+}$: 197.1204; Found: 197.1205.

***N, N*, 4-trimethyl-[1, 1'-biphenyl]-2-amine**

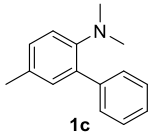


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 2.51 (s, 6H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.90, 141.86, 137.60, 131.52, 131.22, 128.56, 128.16, 126.17, 122.13, 118.21, 43.24, 21.35.

HRMS (ESI) calcd for $C_{15}H_{17}N$ $[M+H]^+$: 212.1434; Found: 212.1434.

***N, N,* 5-trimethyl-[1, 1'-biphenyl]-2-amine**



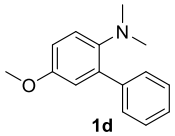
1c

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.28-7.25 (m, 1H), 7.07 (d, *J* = 10.8 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 1H), 2.50 (s, 6H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.82, 141.81, 134.27, 132.31, 130.82, 128.65, 128.44, 128.16, 126.37, 117.59, 43.51, 20.50.

HRMS (ESI) calcd for $C_{15}H_{17}N$ $[M+H]^+$: 212.1434; Found: 212.1434.

5-methoxy-*N, N*-dimethyl-[1, 1'-biphenyl]-2-amine



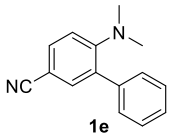
1d

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.25-7.23 (m, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 6.83-6.77 (m, 2H), 3.68 (s, 3H), 2.43 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.74, 144.80, 141.23, 136.08, 128.66, 128.03, 126.51, 118.89, 117.01, 112.61, 55.16, 43.84.

HRMS (ESI) calcd for $C_{15}H_{17}NO$ $[M+H]^+$: 228.1183; Found: 228.1183.

6-(dimethylamino)-[1, 1'-biphenyl]-3-carbonitrile



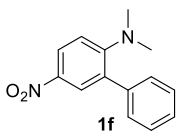
1e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.39 (m, 6H), 7.34-7.31 (m, 1 H), 6.95 (d, *J* = 7.6 Hz, 1H), 2.63 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.14, 140.34, 135.54, 132.17, 131.86, 128.59, 127.91, 127.15, 119.78, 116.73, 101.92, 42.46.

HRMS (ESI) calcd for $C_{15}H_{14}N_2$ $[M+H]^+$: 223.1230; Found: 223.1229.

***N, N*-dimethyl-5-nitro-[1, 1'-biphenyl]-2-amine**



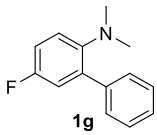
1f

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.07 (m, 2H), 7.48-7.41 (m, 4H), 7.36-7.33 (m, 1H), 6.92 (d, *J* = 8.8 Hz, 1H), 2.71 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.79, 140.43, 139.37, 130.38, 128.62, 128.10, 127.95, 127.23, 123.97, 115.38, 42.61.

HRMS (ESI) calcd for $C_{14}H_{14}N_2O_2$ $[M+H]^+$: 243.1128; Found: 243.1128.

5-fluoro-*N, N*-dimethyl-[1, 1'-biphenyl]-2-amine



1g

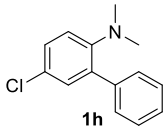
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.2 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 6.96-6.92 (m, 3H), 2.47 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.15 (d, *J* = 262.5 Hz), 147.49 (d, *J* = 2.5 Hz), 140.54 (d, *J* = 1.7 Hz), 136.18 (d, *J* = 8.0 Hz), 128.55, 128.31, 126.95, 118.92 (d, *J* = 8.8 Hz), 117.96 (d, *J* = 24.6 Hz), 113.91 (d, *J* = 23.4 Hz), 43.70.

^{19}F NMR (377 MHz, $CDCl_3$) δ -123.05

HRMS (ESI) calcd for $C_{14}H_{14}NF$ $[M+H]^+$: 216.1183; Found: 216.1183.

4-chloro-*N, N*-dimethyl-[1, 1'-biphenyl]-2-amine



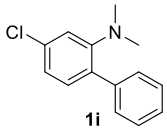
1h

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.21-7.19 (m, 2H), 6.93 (d, *J* = 8.0 Hz, 1H). 2.51 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.77, 140.57, 135.43, 131.22, 128.38, 127.55, 126.94, 126.26, 118.76, 43.23.

HRMS (ESI) calcd for $C_{14}H_{14}NCl$ $[M+H]^+$: 232.0888; Found: 232.0887.

5-chloro-*N, N*-dimethyl-[1, 1'-biphenyl]-2-amine



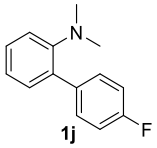
1i

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 9.2 Hz, 2H), 2.51 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.16, 140.92, 133.45, 132.60, 132.04, 128.39, 128.36, 126.71, 120.98, 117.71, 43.00.

HRMS (ESI) calcd for $C_{14}H_{14}NCl$ $[M+H]^+$: 232.0888; Found: 232.0887.

4'-fluoro-*N, N*-dimethylbiphenyl-2-amine



1j

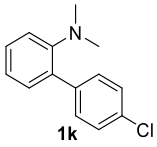
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.53 (m, 2H), 7.29-7.24 (m, 1H), 7.18 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.09-6.99 (m, 4H), 2.52 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 160.5, 151.3, 137.7 (d, *J* = 3.0 Hz), 133.2, 131.5, 130.2 (d, *J* = 7.1 Hz), 128.2, 119.7 (d, *J* = 391.9 Hz), 115.1 (d, *J* = 21.2 Hz), 43.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.3.

HRMS (ESI) calcd for $C_{14}H_{14}FN$ $[M]^+$: 215.1110; Found: 215.1111.

4'-chloro-*N, N*-dimethylbiphenyl-2-amine

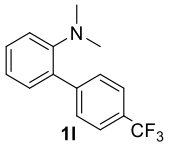


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.51 (m, 2H), 7.37-7.33 (m, 2H), 7.29-725 (m, 1H), 7.18 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.04-6.99 (m, 2H), 2.53 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 140.3, 132.9, 132.3, 131.4, 129.9, 128.5, 128.4, 121.6, 117.7, 43.4.

HRMS (ESI) calcd for $C_{14}H_{14}ClN$ $[M]^+$: 231.0815; Found: 231.0808.

***N, N*-dimethyl-4'-(trifluoromethyl)biphenyl-2-amine**



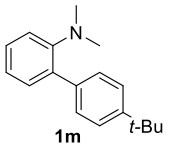
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.32-7.28 (m, 1H), 7.20 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.07-7.01 (m, 2H), 2.53 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.3, 145.6, 132.6, 131.5, 128.9, 128.8, 128.5 (q, *J* = 32.3 Hz), 125.2 (q, *J* = 3.8 Hz), 124.4 (q, *J* = 272.7 Hz), 121.7, 117.9, 43.4.

^{19}F NMR (377 MHz, $CDCl_3$) δ -62.3.

HRMS (ESI) calcd for $C_{15}H_{14}F_3N$ $[M]^+$: 265.1078; Found: 265.1075.

4'-tert-butyl-*N, N*-dimethylbiphenyl-2-amine

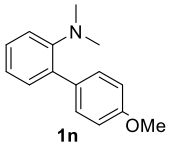


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.4 (d, *J* = 8.4 Hz, 2H), 7.26-7.21 (m, 2H), 7.02-6.97 (m, 2H), 2.53 (s, 6H), 1.35 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.3, 149.2, 138.9, 134.1, 131.7, 128.1, 127.8, 125.1, 121.4, 117.4, 43.4, 34.5, 31.4.

HRMS (ESI) calcd for $C_{18}H_{23}N$ $[M]^+$: 253.1830; Found: 253.1823.

4'-methoxy- *N, N*-dimethylbiphenyl-2-amine

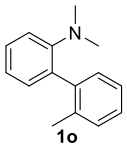


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.50 (m, 2H), 7.27-7.22 (m, 1H), 7.20 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.03-6.98 (m, 2H), 6.96-6.92 (m, 2H), 3.85 (s, 3H), 2.54 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 151.2, 134.3, 133.8, 131.5, 129.6, 127.6, 121.5, 117.5, 113.6, 55.2, 43.30.

HRMS (ESI) calcd for $C_{15}H_{17}NO$ $[M]^+$: 227.1310; Found: 227.1308.

***N, N*, 2'-trimethylbiphenyl-2-amine**



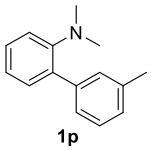
1o

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.27 (m, 1H), 7.25-7.21 (m, 4H), 7.09 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), .6.99 (td, *J* = 7.2, 1.2 Hz, 1H), 2.51 (s, 6H), 2.15 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 141.7, 136.2, 134.5, 131.7, 130.0, 129.9, 127.9, 126.7, 125.6, 121.0, 117.4, 43.1, 20.0.

HRMS (ESI) calcd for $C_{15}H_{17}N$ $[M]^+$: 211.1361; Found: 211.1362.

***N, N*, 3'-trimethylbiphenyl-2-amine**



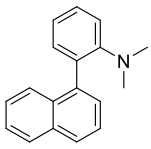
1p

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.36 (m, 2H), 7.29-7.19 (m, 3H), 7.10 (d, *J* = 7.2 Hz, 1H), 7.02-6.97 (m, 2H), 2.54 (s, 6H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1, 141.9, 137.7, 134.1, 131.7, 129.2, 128.1, 127.9, 127.1, 125.7, 121.2, 117.4, 43.3, 21.5.

HRMS (ESI) calcd for $C_{15}H_{17}N$ $[M]^+$: 211.1361; Found: 211.1358.

***N, N*-dimethyl-2-(naphthalen-1-yl)aniline**



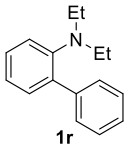
1q

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.54-7.43 (m, 3H), 7.39-7.34 (m, 2H), 7.21 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.03 (td, *J* = 7.6, 0.8 Hz, 1H), 2.42 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 139.9, 133.7, 132.8, 132.4, 131.5, 128.3, 128.0, 127.1, 127.1, 126.6, 125.6, 125.5, 125.5, 120.7, 117.53, 43.1.

HRMS (ESI) calcd for $C_{18}H_{17}N$ $[M]^+$: 247.1361; Found: 247.1358.

***N, N*-diethylbiphenyl-2-amine**



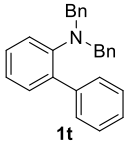
1r

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.54 (m, 2H), 7.38-.35 (m, 2H), 7.29-7.21 (m, 3H), 7.08 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.03 (td, *J* = 7.6, 1.2 Hz, 1H), 2.87 (q, *J* = 7.1 Hz, 4H), 0.89 (t, *J* = 7.0 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.7, 141.8, 136.8, 131.4, 129.0, 128.0, 127.5, 126.3, 122.1, 121.1, 46.0, 11.9.

HRMS (ESI) calcd for $C_{16}H_{19}N$ $[M]^+$: 225.1517; Found:. 225.1511

***N, N*-dibenzyl-[1, 1'-biphenyl]-2-amine**



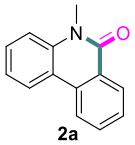
1t

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.51 (t, *J* = 7.6, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.34-7.23 (m, 8H), 7.16-7.04 (m, 5H), 7.05 (d, *J* = 8.0 Hz, 1H), 3.97(s, 4H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.88, 141.63, 138.04, 136.48, 131.58, 129.19, 128.88, 128.26, 128.00, 127.84, 126.84, 126.69, 122.70, 121.66, 55.71.

HRMS (ESI) calcd for $C_{26}H_{23}N$ $[M+H]^+$: 350.1909; Found:. 350.1895

5-methylphenanthridin-6(5*H*)-one



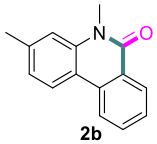
2a

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (dd, *J* = 8.0, 0.8 Hz, 1H), 8.26-8.23 (m, 2H), 7.76-7.72 (m, 1H), 7.59-7.51 (m, 2H), 7.40-7.38 (m, 1H), 7.33-7.29 (m, 1H), 3.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6, 137.9, 133.4, 132.3, 129.5, 128.8, 127.9, 125.5, 123.1, 122.4, 121.5, 119.2, 115.0, 29.9.

HRMS (ESI) calcd for $C_{14}H_{11}NO$ $[M]^+$: 209.0841; Found: 209.0847.

3, 5-dimethylphenanthridin-6(5*H*)-one



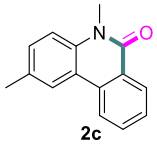
2b

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.0 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.19 (s, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 3.79 (s, 3H), 2.5 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.75, 139.84, 137.92, 133.59, 132.27, 128.78, 127.39, 125.07, 123.57, 123.03, 121.32, 116.77, 115.36, 29.89, 21.91.

HRMS (ESI) calcd for $C_{15}H_{13}NO$ $[M+H]^+$: 224.1070 ; Found: 224.1068

2, 5-dimethylphenanthridin-6(5*H*)-one



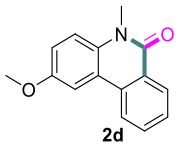
2c

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.0 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.97 (s, 1 H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.22 (d, *J* = 8.8 Hz, 1H), 3.73 (s, 3 H), 2.44 (s, 3 H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.33, 135.73, 133.31, 132.09, 131.71, 130.38, 128.73, 127.63, 125.49, 123.18, 121.42, 118.90, 114.78, 29.81, 20.88.

HRMS (ESI) calcd for $C_{15}H_{13}NO$ $[M+H]^+$: 244.1070 ; Found: 244.1069

2-methoxy-5-methylphenanthridin-6(5*H*)-one



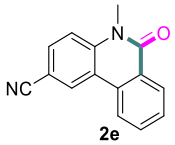
2d

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.74-7.67 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.10 (dd, *J* = 9.2 Hz, 2.8 Hz, 1H), 3.91 (s, 3H), 3.76 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.02, 154.95, 133.05, 132.22, 132.12, 128.88, 127.96, 125.75, 121.54, 120.04, 116.35, 116.07, 106.92, 77.32, 77.00, 76.68, 55.63, 29.96.

HRMS (ESI) calcd for $C_{15}H_{13}NO$ $[M+H]^+$: 240.1017; Found: 240.1017

2-cyano-5-methylphenanthridin-6(5*H*)-one



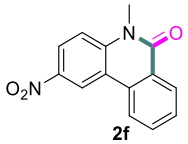
2e

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 7.2 Hz, 2H), 8.26 (d, *J* = 8.0 Hz, 1H), 7.88-7.81 (m, 2H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 8.8 Hz, 1H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.42, 140.85, 133.16, 132.31, 131.84, 129.30, 129.12, 127.79, 125.67, 121.66, 119.86, 118.76, 115.85, 105.93, 30.25.

HRMS (ESI) calcd for $C_{15}H_{10}N_2O$ $[M+H]^+$: 235.0866 ; Found: 235.0865

5-methyl-2-nitrophenanthridin-6(5*H*)-one



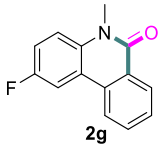
2f

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (d, *J* = 2.4 Hz, 1H), 8.55 (d, *J* = 8.0 Hz, 1H), 8.40 (dd, *J* = 9.2 Hz, 2.8 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 7.86 (t, *J* = 8.8 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 9.2 Hz, 1H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.49, 142.56, 142.34, 133.29, 132.20, 129.47, 129.16, 125.63, 124.33, 122.03, 119.48, 119.35, 115.55, 30.56.

HRMS (ESI) calcd for $C_{14}H_{10}N_2O_3$ $[M+H]^+$: 255.0764 ; Found: 255.0763

2-fluoro-5-methylphenanthridin-6(5*H*)-one



2g

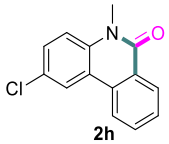
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.89 (dd, *J* = 10.0 Hz, 2.4 Hz, 1H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.37-7.33 (m, 1H), 7.27-7.23 (m, 1H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.16, 159.60, 157.20, 134.39, 132.47, 128.97, 128.59, 125.74, 121.74, 120.60, 120.53, 116.82, 116.59, 116.50, 116.42, 109.28, 109.05, 30.17.

^{19}F NMR (377 MHz, $CDCl_3$) δ

HRMS (ESI) calcd for $C_{14}H_{10}FNO$ $[M+H]^+$: 228.0819 ; Found: 228.0817

2-chloro-5-methylphenanthridin-6(5*H*)-one



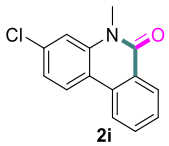
2h

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.0 Hz, 1H), 8.08-8.08 (m, 2H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.42 (dd, *J* = 8.8 Hz, 2.2 Hz, 1H), 7.25 (d, *J* = 8.8 Hz, 1H), 3.72 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.09, 136.35, 132.48, 132.14, 129.19, 128.84, 128.52, 128.02, 125.54, 122.79, 121.53, 120.40, 116.27, 30.00.

HRMS (ESI) calcd for $C_{14}H_{10}ClNO$ $[M+H]^+$: 244.05121; Found: 244.0524

3-chloro-5-methylphenanthridin-6(5*H*)-one



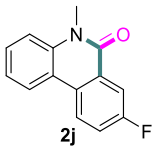
2i

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 8.11-8.07 (m, 2H), 7.71 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.32 (s, 1H), 7.22 (d, *J* = 8.8 Hz, 1H), 3.72 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.40, 138.80, 135.27, 132.71, 132.55, 128.90, 128.15, 125.20, 124.30, 122.52, 121.46, 117.68, 114.99, 30.01.

HRMS (ESI) calcd for $C_{14}H_{10}ClNO$ $[M+H]^+$: 244.0524 ; Found: 244.0524

8-fluoro-5-methylphenanthridin-6(5*H*)-one



2j

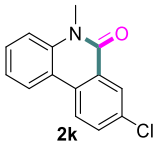
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.8, 5.0 Hz, 1H), 8.18-8.15 (m, 2H), 7.56-7.51 (m, 1H), 7.48-7.43 (m, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.34-7.30 (m, 1H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2 (d, *J* = 249.5 Hz), 160.60 (d, *J* = 3.0 Hz), 137.4, 129.9 (d, *J* = 3.0 Hz), 129.4, 127.3 (d, *J* = 8.1 Hz), 124.1 (d, *J* = 8.1 Hz), 123.0, 122.7, 120.7 (d, *J* = 23.2 Hz), 118.6, 115.1, 114.2 (d, *J* = 23.2 Hz), 30.1.

^{19}F NMR (377 MHz, $CDCl_3$) δ -112.2.

HRMS (ESI) calcd for $C_{14}H_{10}FNO$ $[M]^+$: 227.0746; Found: 227.0747.

8-chloro-5-methylphenanthridin-6(5*H*)-one



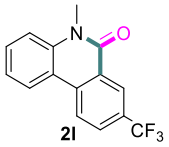
2k

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.4 (d, *J* = 2.0 Hz, 1H), 8.15-8.11 (m, 2H), 7.64 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.56-7.52 (m, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.32-7.28 (m, 1H), 3.76 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 137.7, 134.0, 132.6, 131.8, 129.8, 128.3, 126.6, 123.3, 123.1, 122.6, 118.4, 115.1, 30.0.

HRMS (ESI) calcd for $C_{14}H_{10}ClNO$ $[M]^+$: 243.0451; Found: 243.0454.

5-methyl-8-(trifluoromethyl)phenanthridin-6(5*H*)-one



2l

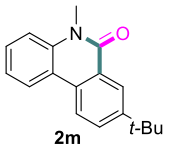
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 8.26 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.93 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.63-7.59 (m, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.37-7.33 (m, 1H), 3.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7, 138.5, 136.2, 130.8, 129.8 (q, *J* = 33.3 Hz), 128.46 (q, *J* = 3.4 Hz), 126.5 (q, *J* = 4.0 Hz), 125.5, 123.8 (q, *J* = 272.7 Hz), 123.7, 122.8, 122.5, 118.1, 115.3, 30.1.

^{19}F NMR (377 MHz, $CDCl_3$) δ -62.5.

HRMS (ESI) calcd for $C_{15}H_{10}F_3NO$ $[M]^+$: 227.0714; Found: 227.0712.

8-tert-butyl-5-methylphenanthridin-6(5*H*)-one



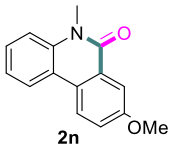
2m

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 2.0 Hz, 1H), 8.24 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.20 (d, *J* = 8.8 Hz, 1H), 7.81 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.53-7.49 (m, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.32–7.38 (m, 1H), 3.81 (s, 3H), 1.43 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 151.2, 137.7, 131.0, 130.2, 129.0, 125.1, 124.9, 123.0, 122.4, 121.5, 119.3, 114.9, 35.0, 31.2, 29.9.

HRMS (ESI) calcd for $C_{18}H_{19}NO$ $[M]^+$: 265.1467; Found: 265.1471.

8-methoxy-5-methylphenanthridin-6(5*H*)-one



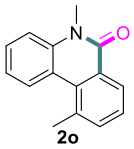
2n

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.11 (m, 2H), 7.92 (d, *J* = 2.8 Hz, 1H), 7.48-7.44 (m, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.31-7.25 (m, 2H), 3.94 (s, 3H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 159.4, 136.8, 128.3, 126.9, 126.7, 123.3, 122.5, 122.4, 122.1, 119.2, 114.9, 109.0, 55.6, 30.0.

HRMS (ESI) calcd for $C_{15}H_{13}NO_2$ $[M]^+$: 239.0946; Found: 239.0942.

5, 10-dimethylphenanthridin-6(5*H*)-one



2o

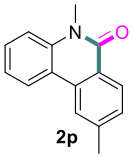
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 1H),

7.54-7.50 (m, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.45-7.42 (m, 1H), 7.31-7.27 (m, 1H), 3.78 (s, 3H), 2.93 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 138.2, 136.8, 134.3, 132.9, 128.6, 127.8, 127.2, 127.2, 121.5, 120.7, 114.7, 30.3, 26.0.

HRMS (ESI) calcd for $C_{15}H_{13}NO$ $[M]^+$: 223.0997; Found: 223.0996.

5, 9-dimethylphenanthridin-6(5*H*)-one



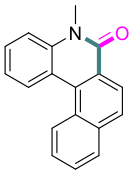
2p

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.0 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.96 (s, 1H), 7.50-7.46 (m, 1H), 7.36-7.31 (m, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 3.74 (s, 3H), 2.52 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5, 142.7, 137.9, 133.3, 129.2, 129.2, 128.7, 123.1, 123.0, 122.1, 121.5, 119.0, 114.9, 29.7, 22.0.

HRMS (ESI) calcd for $C_{15}H_{13}NO$ $[M]^+$: 223.0997; Found: 223.0999.

5-methylbenzo[k]phenanthridin-6(5*H*)-one



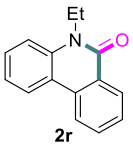
2q

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82-8.80 (m, 1H), 8.56 (d, *J* = 8.4 Hz, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 7.98-7.95 (m, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.66-7.59 (m, 2H), 7.58-7.53 (m, 1H), 7.48-7.46 (m, 1H), 7.34-7.30 (m, 1H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7, 138.3, 136.1, 132.6, 129.0, 128.8, 128.7, 128.4, 128.4, 127.7, 127.6, 126.6, 124.4, 123.8, 121.8, 119.4, 114.7, 30.3.

HRMS (ESI) calcd for $C_{18}H_{13}NO$ $[M]^+$: 259.0997; Found: 259.0993.

5-ethylphenanthridin-6(5*H*)-one



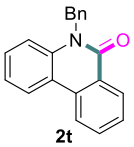
2r

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.29-8.24 (m, 2H), 7.76-7.72 (m, 1H), 7.60-7.51 (m, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.32-7.28 (m, 1H), 4.46 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0, 136.8, 133.5, 132.3, 129.5, 128.7, 127.8, 125.5, 123.4, 122.2, 121.5, 119.4, 114.9, 37.6, 12.7.

HRMS (ESI) calcd for $C_{15}H_{13}NO$ $[M]^+$: 223.0997; Found: 223.0998.

5-benzylphenanthridin-6(5H)-one



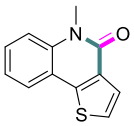
2t

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.34 (t, *J* = 8.0 Hz, 2H), 7.86-7.8 (m, 1H), 7.68- 7.64 (m, 1H), 7.45-7.25 (m, 8H), 5.71 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.88, 137.29, 136.53, 133.80, 132.68, 129.53, 129.14, 128.77, 128.02, 127.15, 126.47, 125.37, 123.25, 122.54, 121.66, 119.48, 116.00, 46.45.

HRMS (ESI) calcd for $C_{20}H_{12}NO$ $[M+H]^+$: 286.1232; Found: 286.1230.

5-methylthieno[3,2-c]quinolin-4(5H)-one

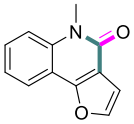


2u 35%

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 2.0 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.67-7.65 (m, 2H), 7.42- 7.38 (m, 1H), 7.11 (d, *J* = 2.0 Hz, 1H), 3.71 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.54, 154.50, 145.79, 137.97, 130.21, 122.81, 120.84, 116.12, 114.98, 112.33, 108.32, 29.45.

5-methylfuro[3,2-c]quinolin-4(5H)-one

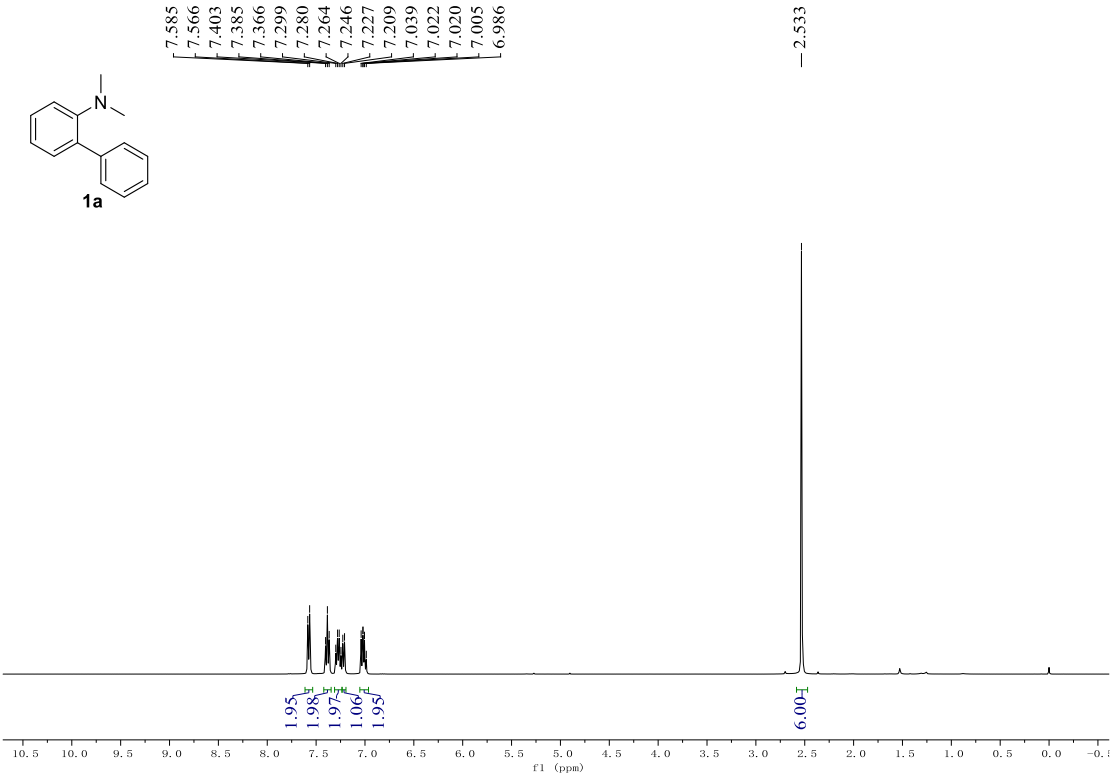


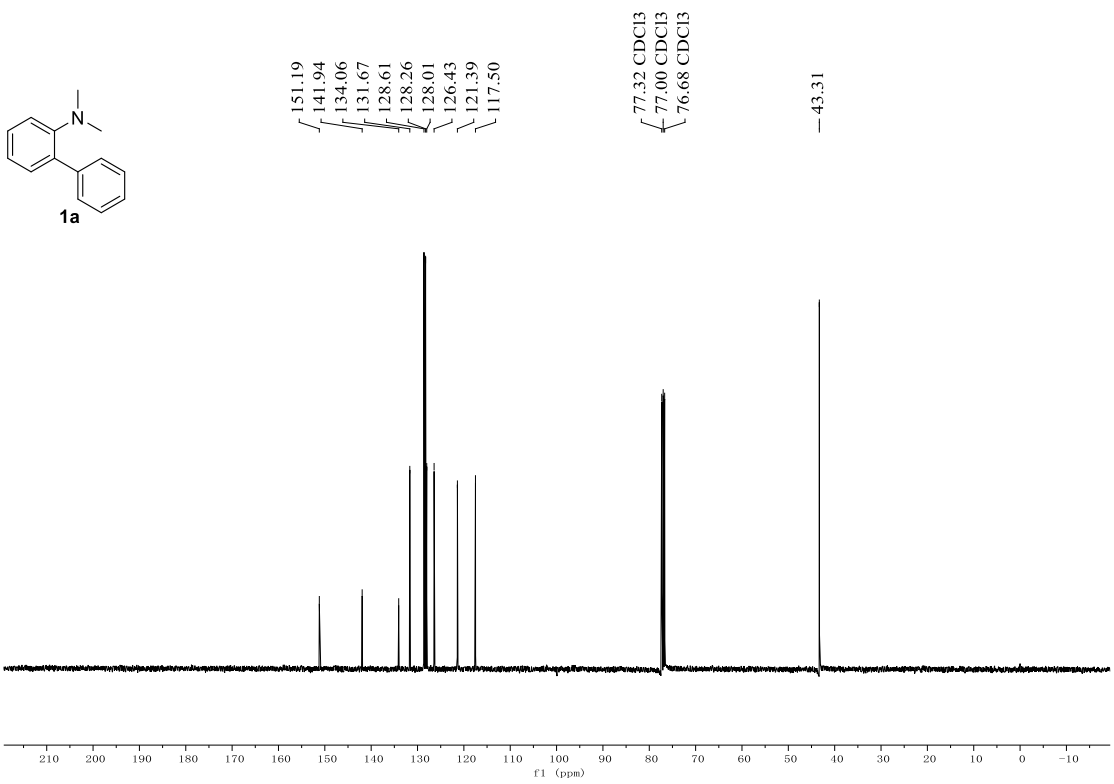
2v 47%

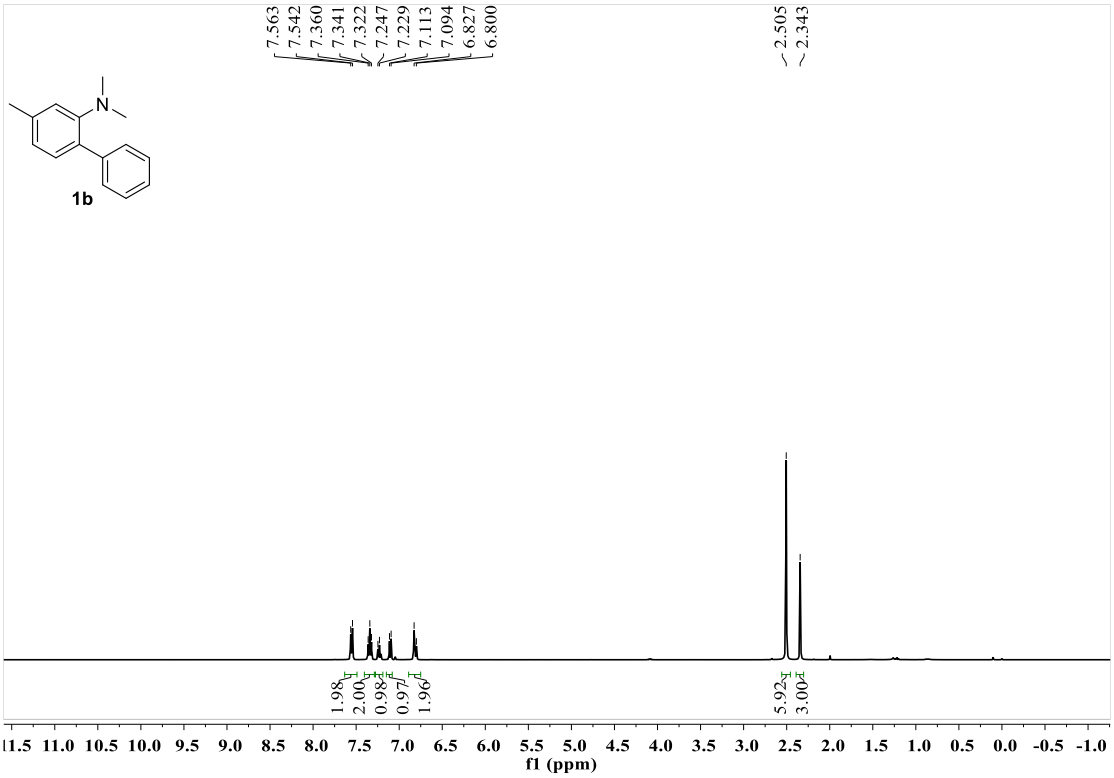
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.73 (d, *J* = 5.6 Hz, 1H), 7.57-7.51 (m, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.37 (d, *J* = 5.2 Hz, 1H), 7.30- 7.26 (m, 1H), 3.80 (s, 3H).

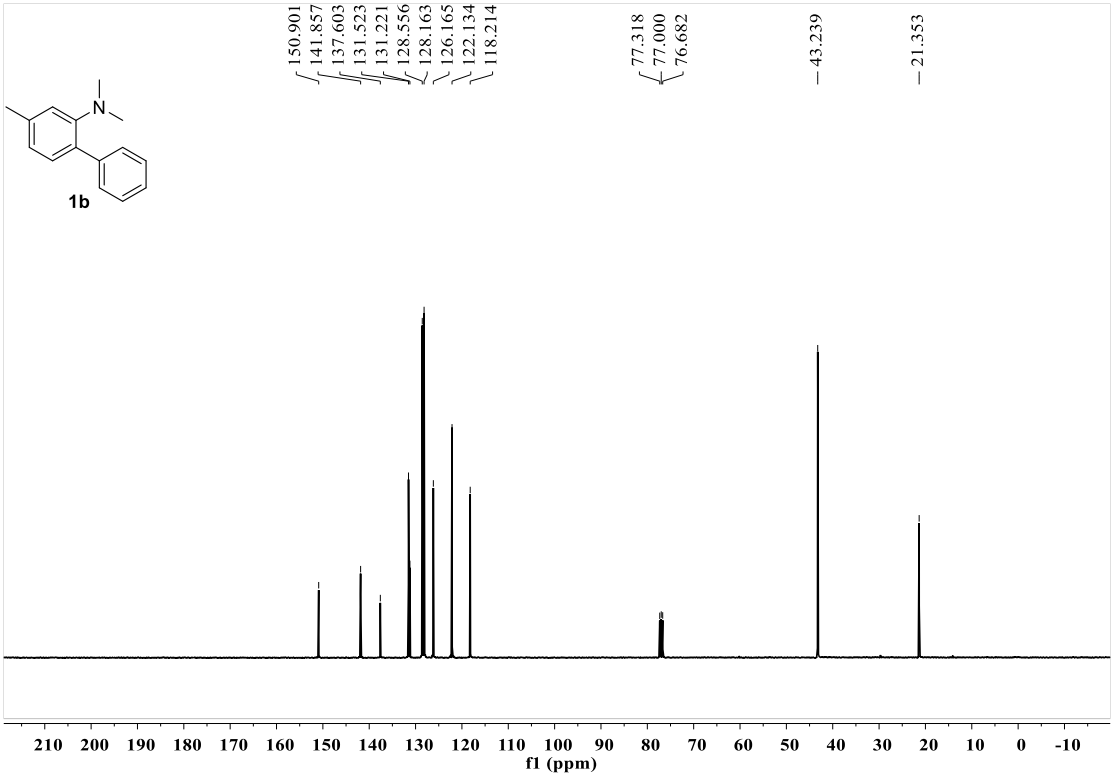
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.78, 145.30, 137.47, 130.79, 129.33, 126.52, 124.77, 124.23, 122.46, 118.05, 115.20, 29.48.

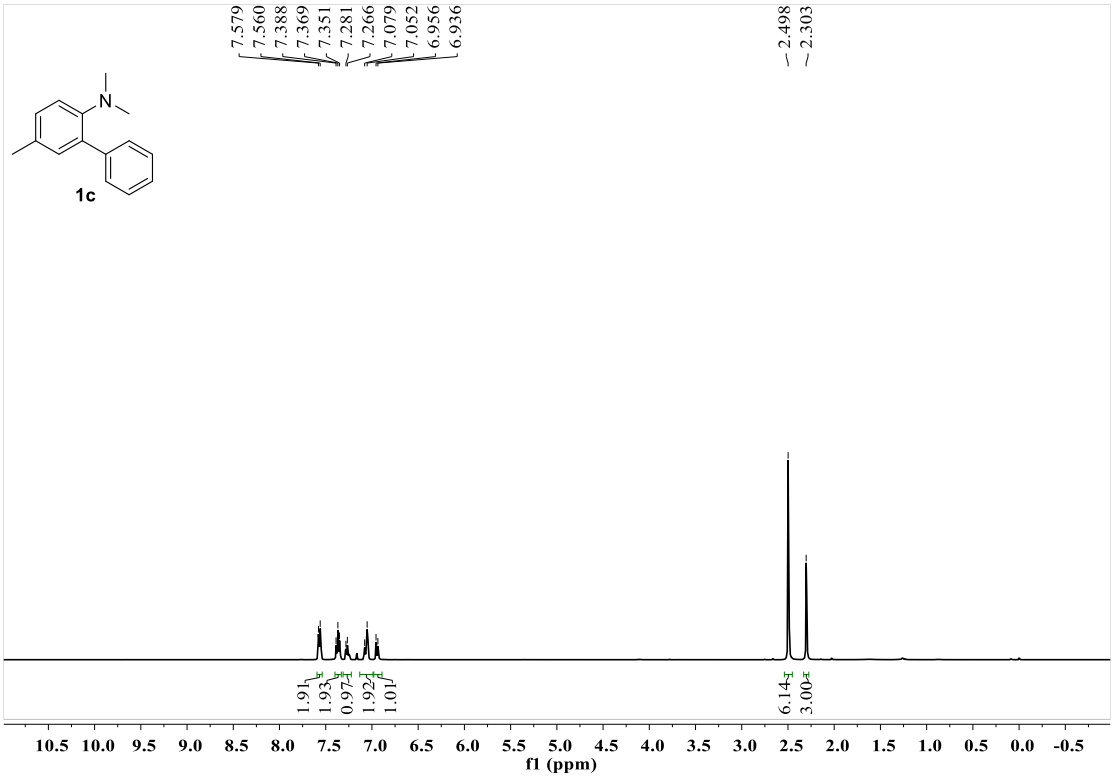
7. NMR Spectra of Substrates and Products

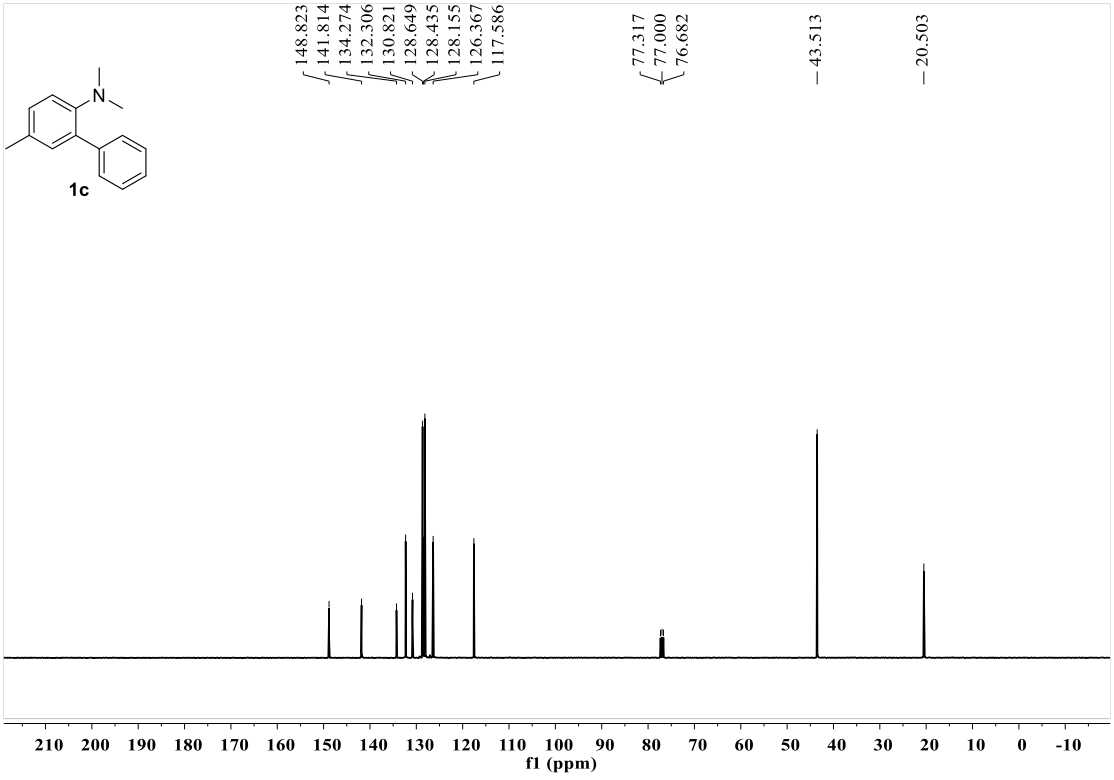


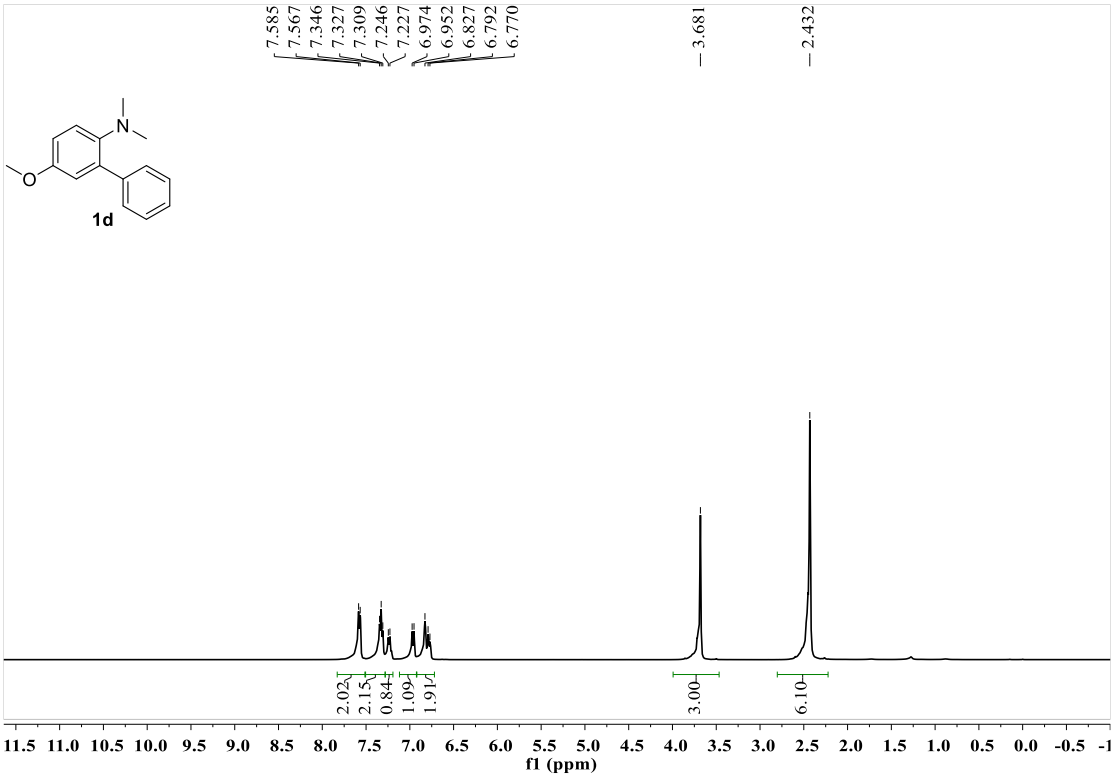


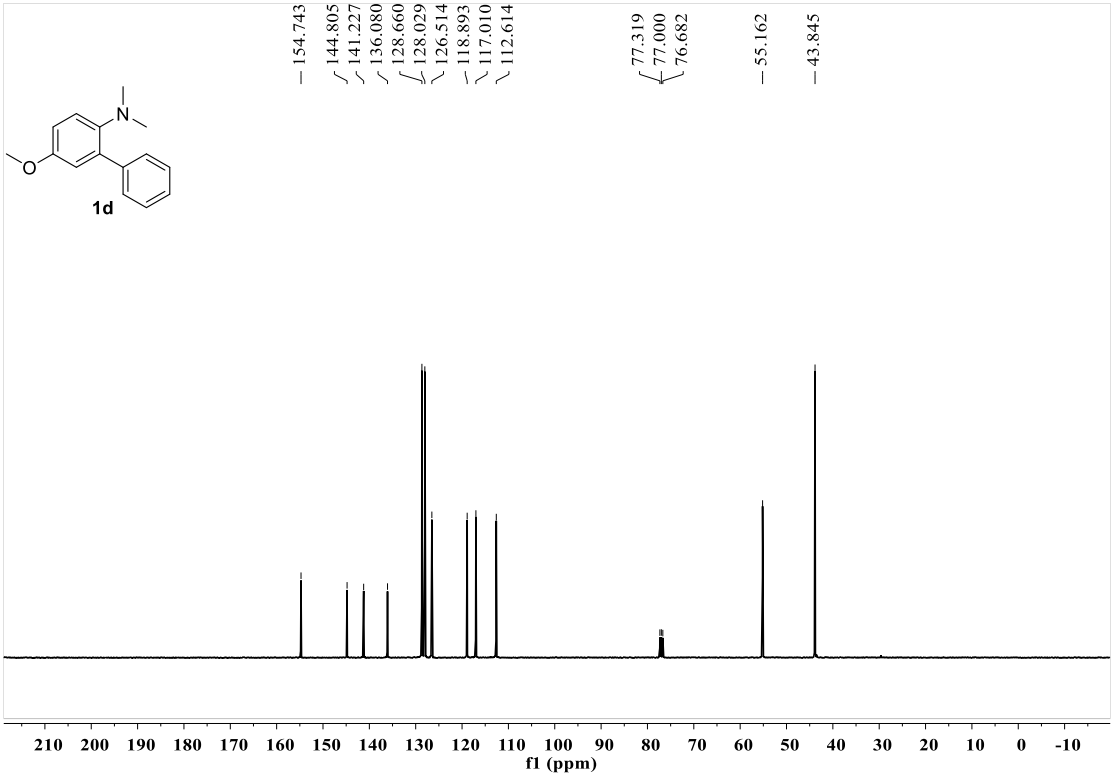

7.563
7.542
7.360
7.341
7.322
7.247
7.229
7.113
7.094
6.827
6.800
2.505
2.343
1.98
2.00
0.98
0.97
1.96
5.92
3.00
1b
f1 (ppm)

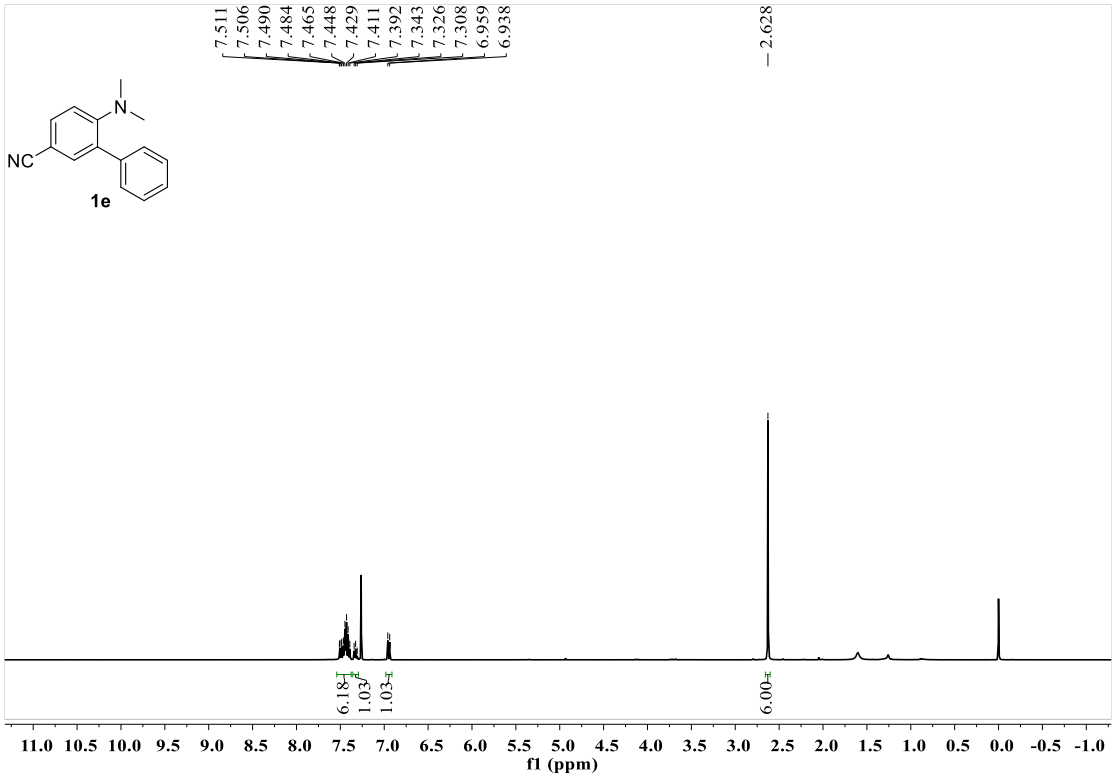

150.901
141.857
137.603
131.523
131.221
128.556
128.163
126.165
122.134
118.214
77.318
77.000
76.682
43.239
21.353
1b
f1 (ppm)

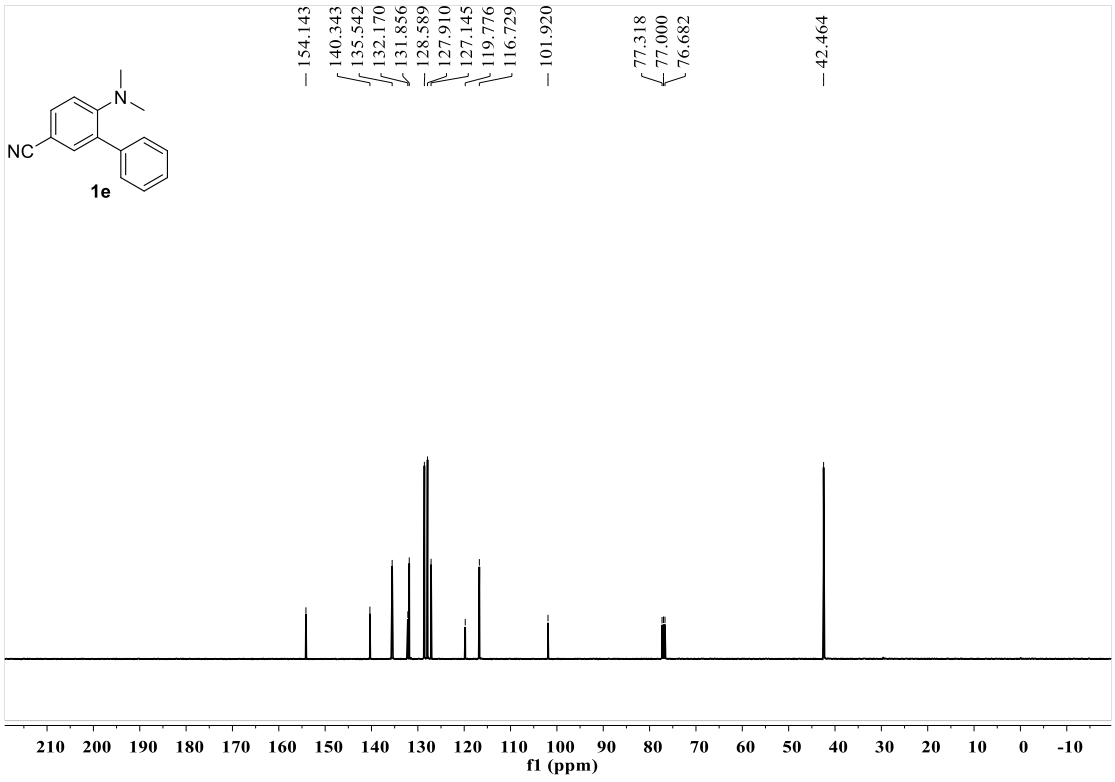

7.579
7.560
7.388
7.369
7.351
7.281
7.266
7.079
7.052
6.956
6.936
2.498
2.303
1c
1.91
1.93
0.97
1.92
1.01
6.14
3.00
f1 (ppm)

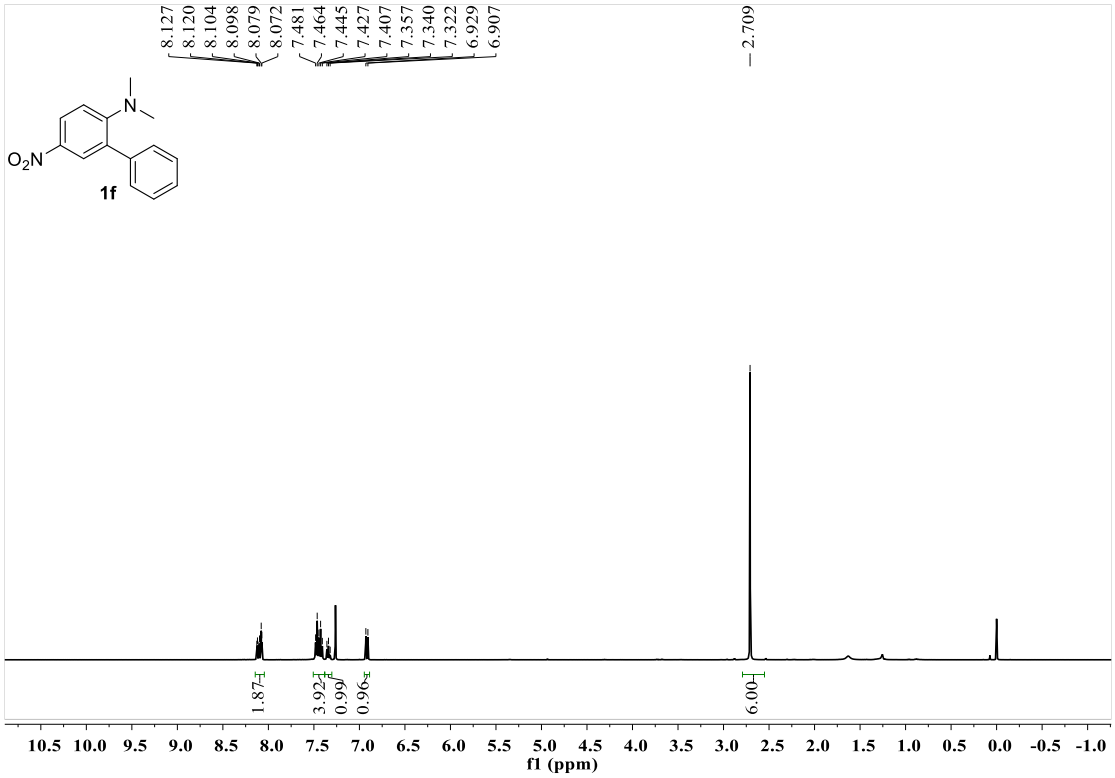

148.823
141.814
134.274
132.306
130.821
128.649
128.435
128.155
126.367
117.586
77.317
77.000
76.682
43.513
20.503
1c
f1 (ppm)

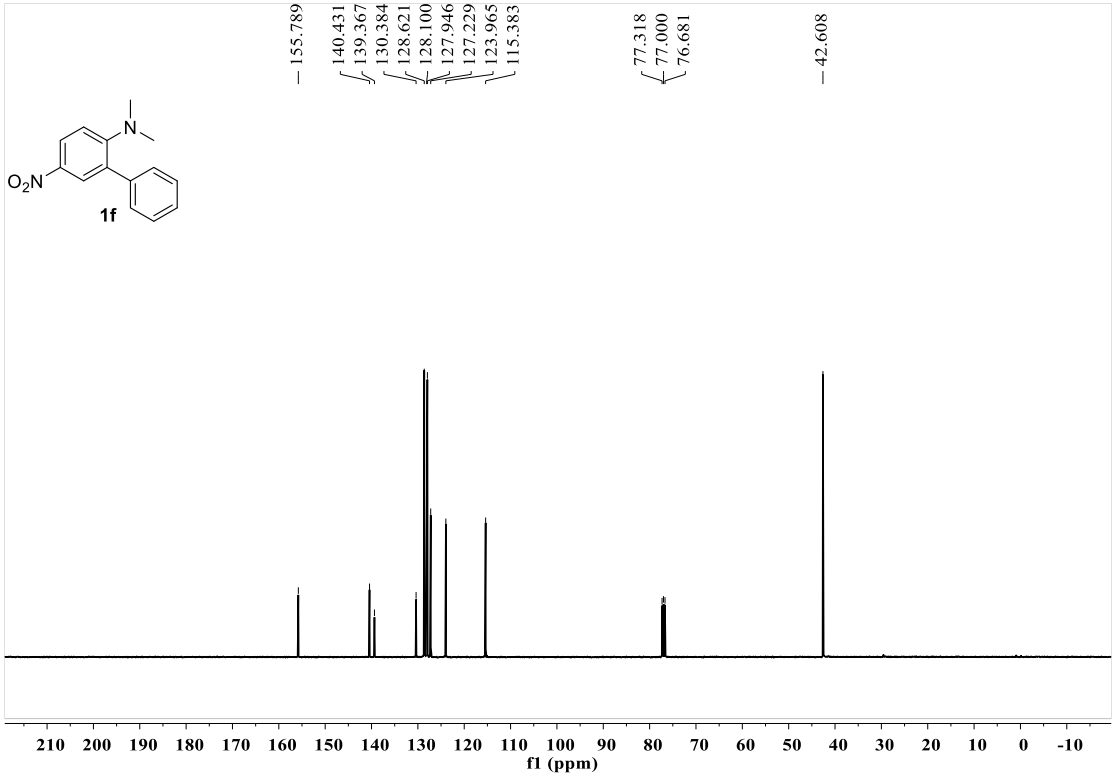

7.585
7.567
7.346
7.327
7.309
7.246
7.227
6.974
6.952
6.827
6.792
6.770
3.681
2.432
1d
2.02
2.15
0.84
1.09
1.91
3.00
6.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

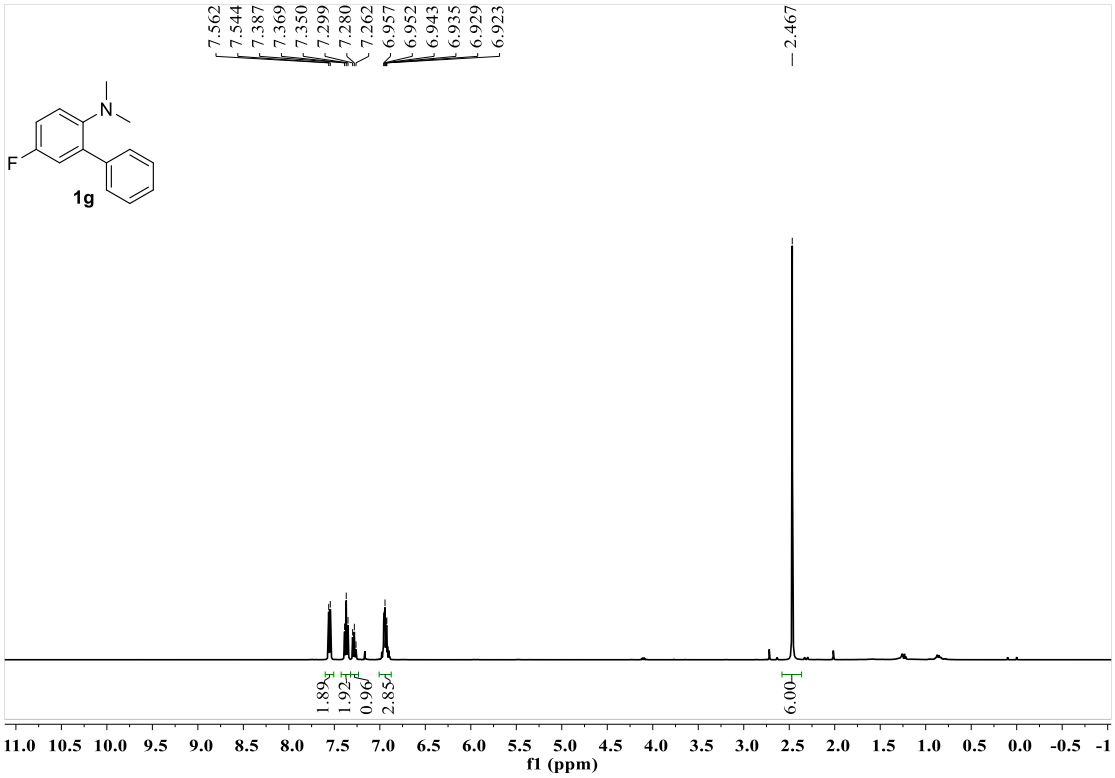

154.743
144.805
141.227
136.080
128.660
128.029
126.514
118.893
117.010
112.614
77.319
77.000
76.682
55.162
43.845
1d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

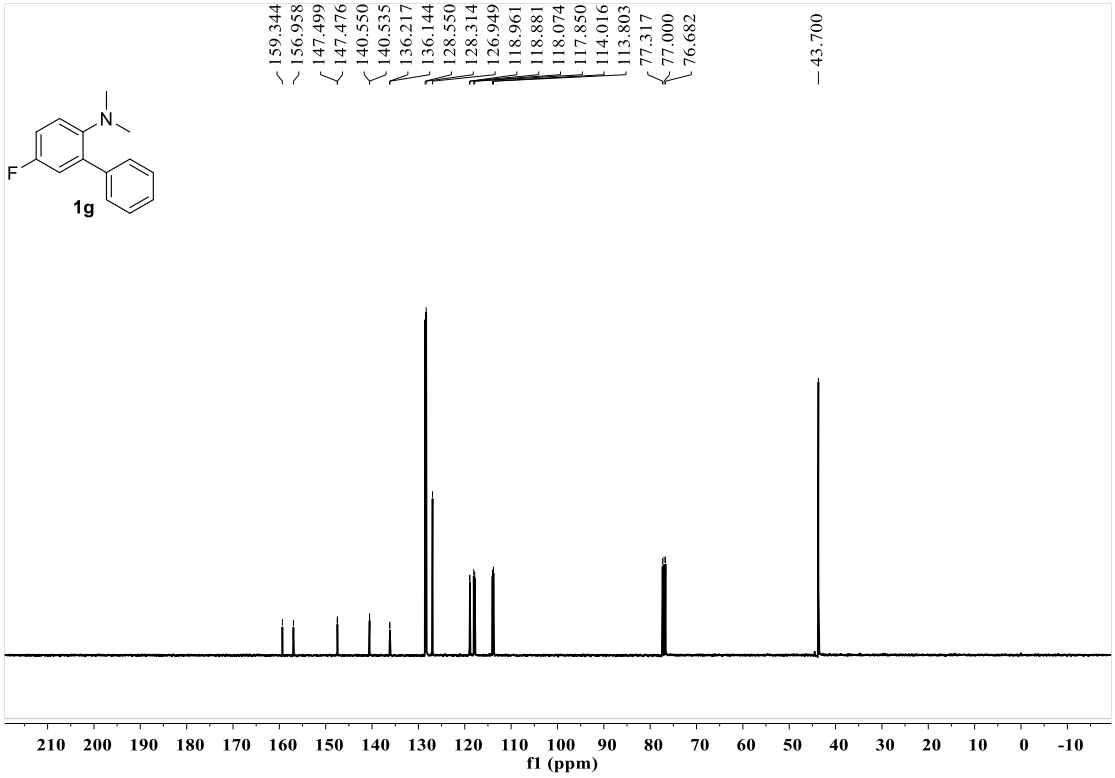

7.511
7.506
7.490
7.484
7.465
7.448
7.429
7.411
7.392
7.343
7.326
7.308
6.959
6.938
2.628
NC
N
1e
6.18
1.03
1.03
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


154.143
140.343
135.542
132.170
131.856
128.589
127.910
127.145
119.776
116.729
101.920
77.318
77.000
76.682
42.464
NC
N
1e
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)


8.127
8.120
8.104
8.098
8.079
8.072
7.481
7.464
7.445
7.427
7.407
7.357
7.340
7.322
6.929
6.907
2.709
1.87
3.92
0.99
0.96
6.00
O2N
N
1f
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


155.789
140.431
139.367
130.384
128.621
128.100
127.946
127.229
123.965
115.383
77.318
77.000
76.681
42.608
O2N
N
1f
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)


7.562
7.544
7.387
7.369
7.350
7.299
7.280
7.262
6.957
6.952
6.943
6.935
6.929
6.923
2.467
1.89
1.92
0.96
2.85
6.00
1g
f1 (ppm)


159.344
156.958
147.499
147.476
140.550
140.535
136.217
136.144
128.550
128.314
126.949
118.961
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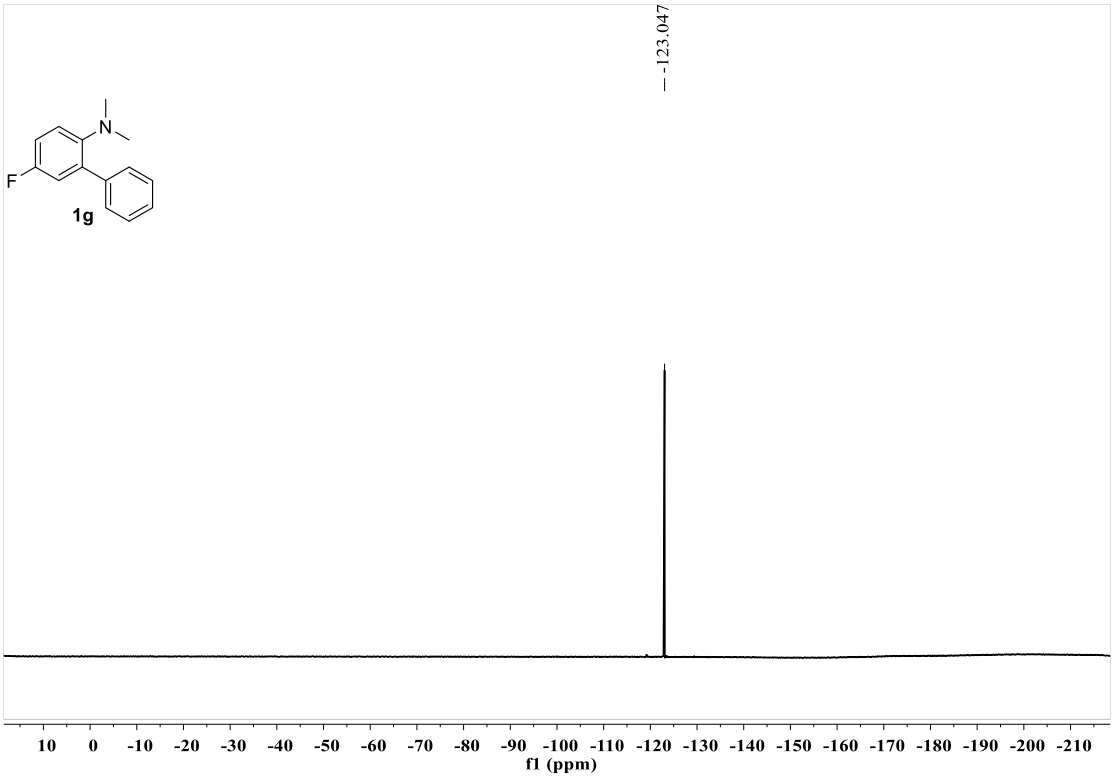
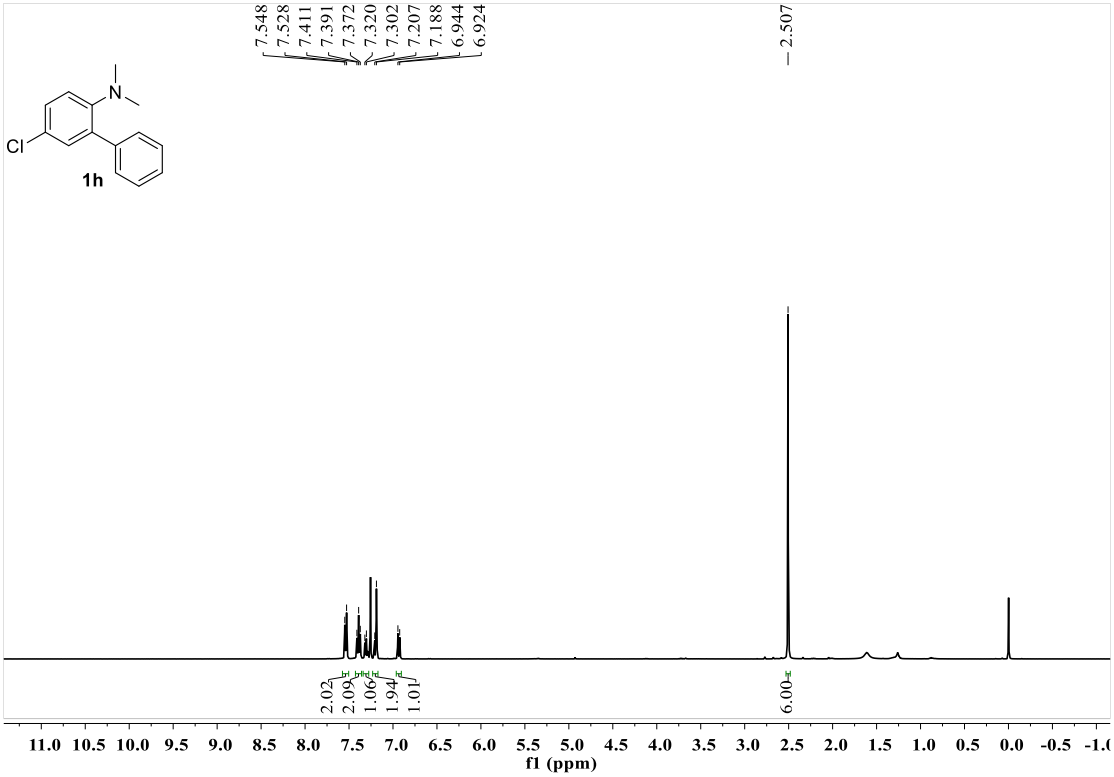
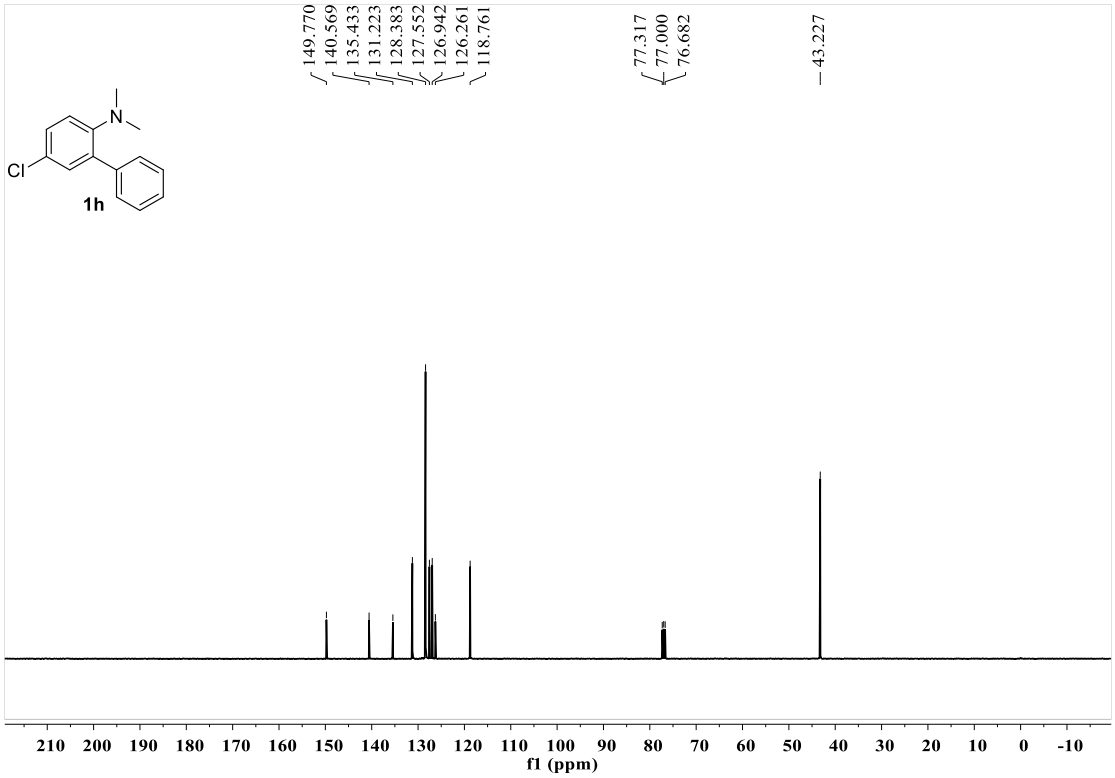
118.074
117.850
114.016
113.803
77.317
77.000
76.682
43.700
1g
f1 (ppm)


-123.047
F
1g
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)


7.548
7.528
7.411
7.391
7.372
7.320
7.302
7.207
7.188
6.944
6.924
2.507
Cl
1h
2.02
2.09
1.06
1.94
1.01
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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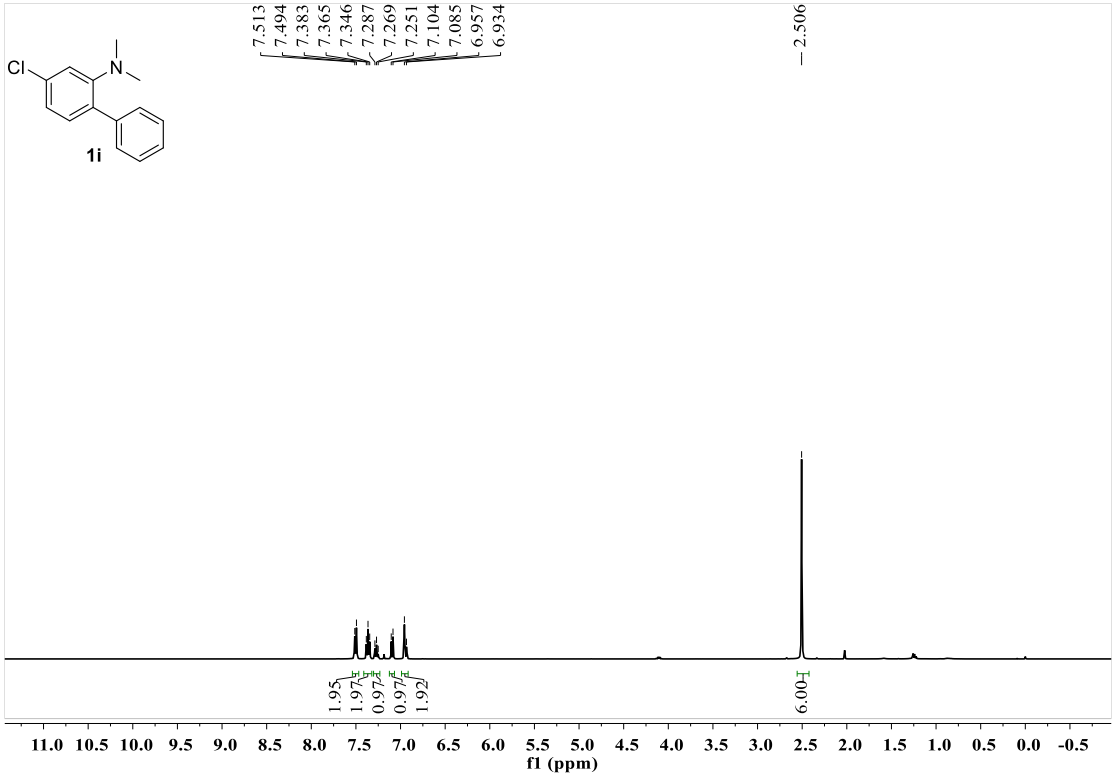
127.552
126.942
126.261
118.761
77.317
77.000
76.682
43.227
Cl
N
1h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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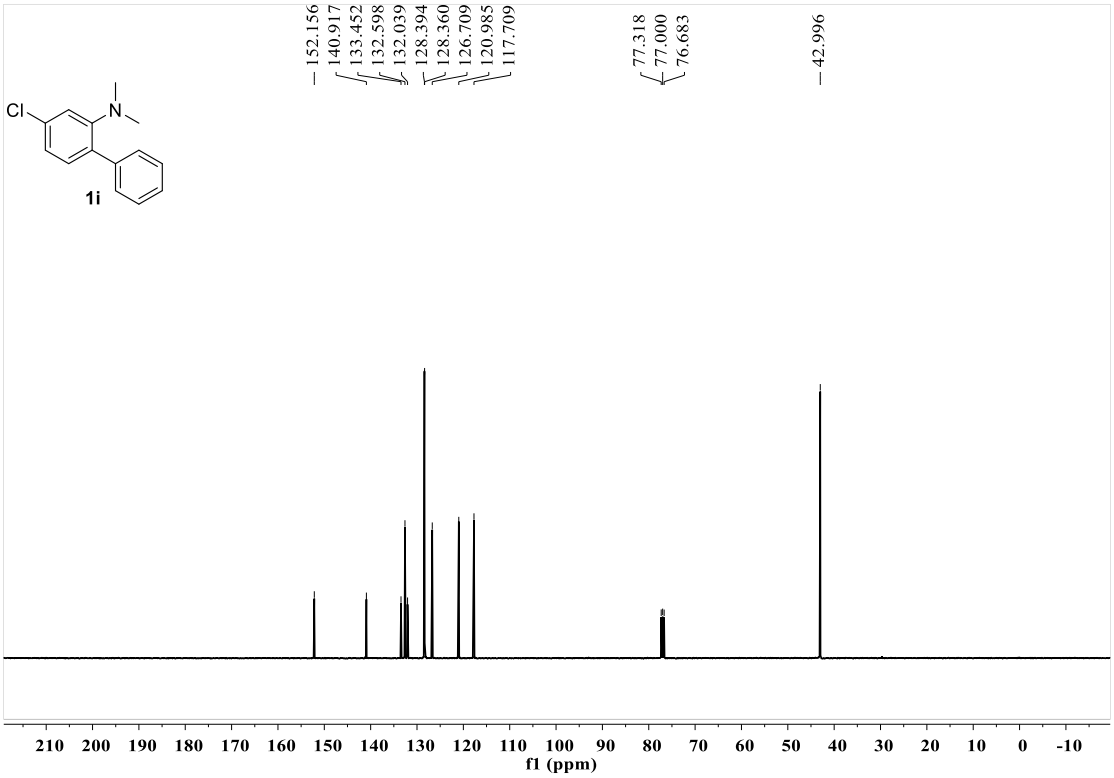
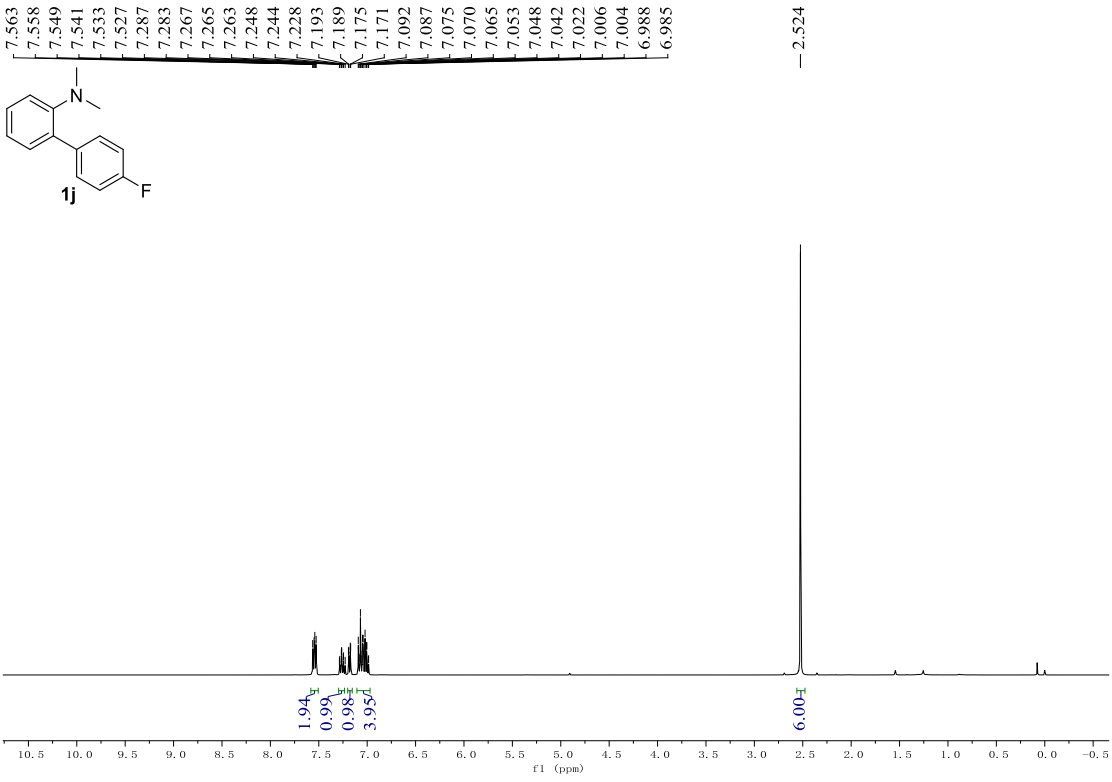
7.287
7.269
7.251
7.104
7.085
6.957
6.934
2.506
Cl
N
1i
1.95
1.97
0.97
0.97
1.92
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


152.156
140.917
133.452
132.598
132.039
128.394
128.360
126.709
120.985
117.709
77.318
77.000
76.683
42.996
Cl
N
1i
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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7.283
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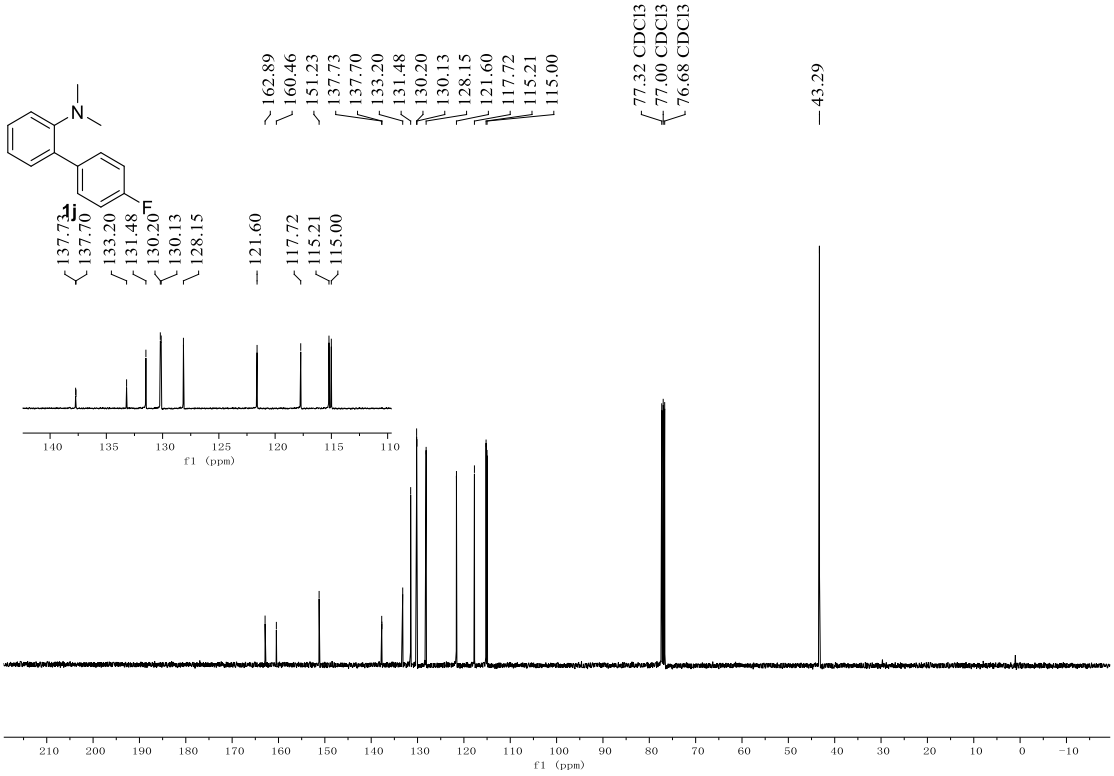
7.265
7.263
7.248
7.244
7.228
7.193
7.189
7.175
7.171
7.092
7.087
7.075
7.070
7.065
7.053
7.048
7.042
7.022
7.006
7.004
6.988
6.985
2.524
N
F
1j
1.94
0.99
0.98
3.95
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


1j
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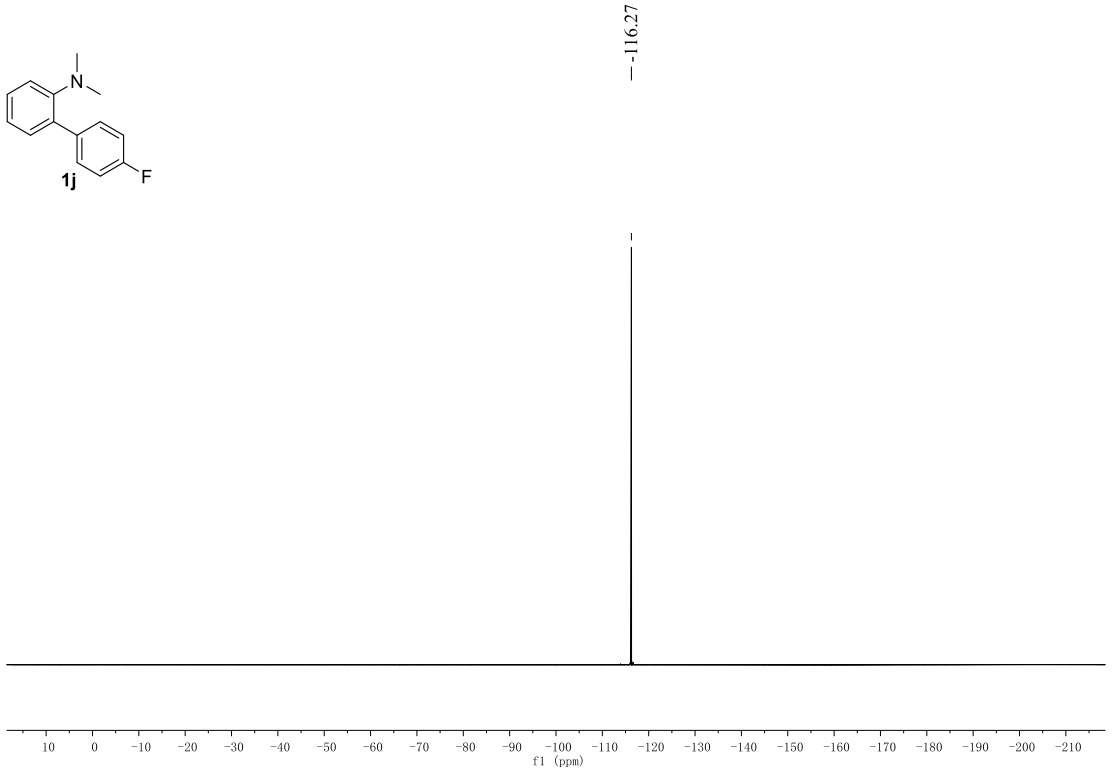
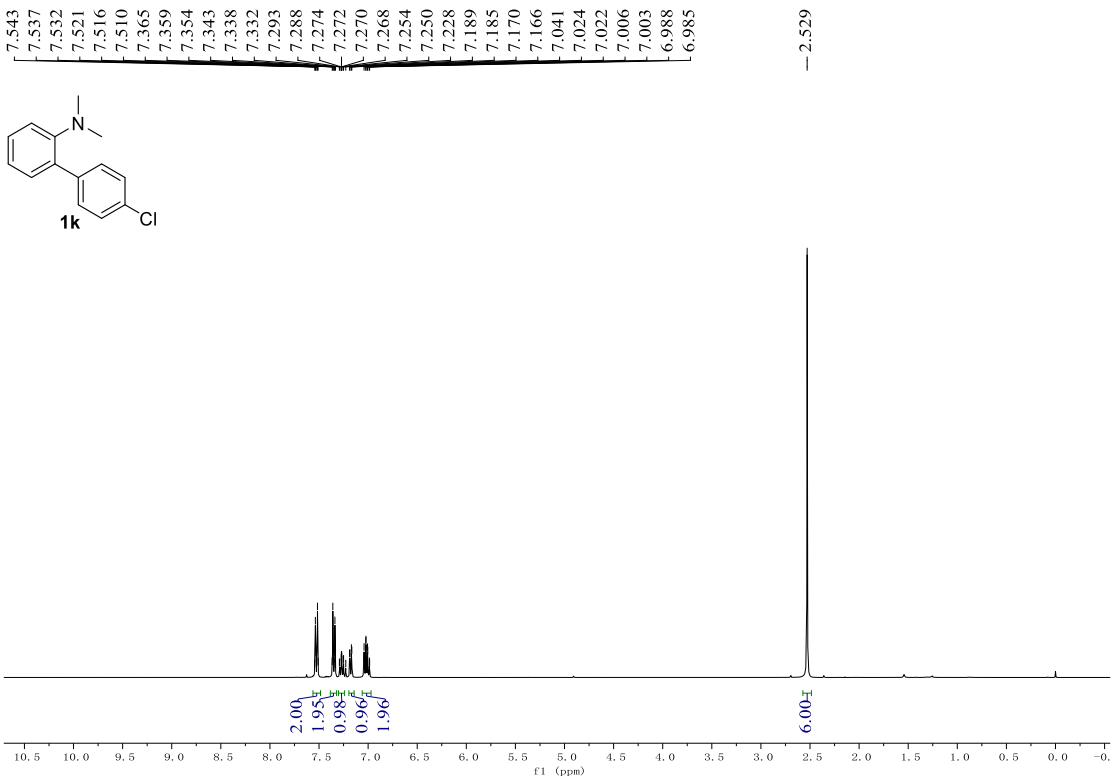
160.46
151.23
137.73
137.70
133.20
131.48
130.20
130.13
128.15
121.60
117.72
115.21
115.00
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
43.29
f1 (ppm)


1j
-116.27
f1 (ppm)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7.359
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7.293
7.288
7.274
7.272
7.270
7.268
7.254
7.250
7.228
7.189
7.185
7.170
7.166
7.041
7.024
7.022
7.006
7.003
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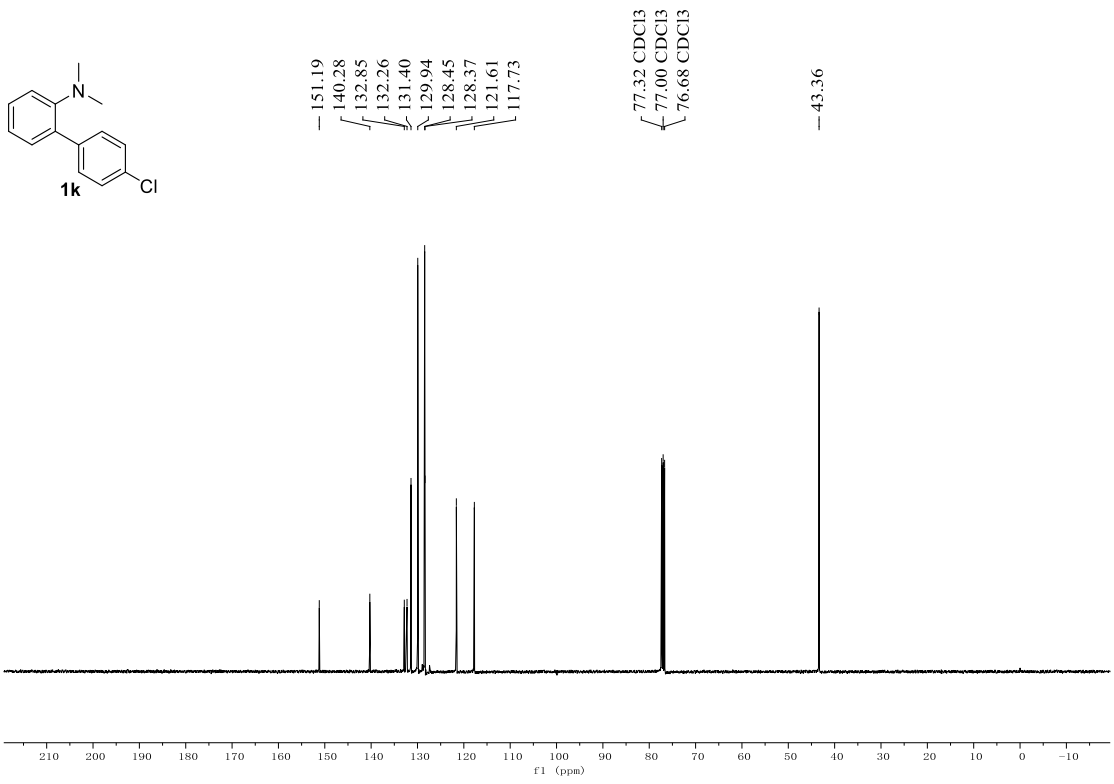
6.985
2.529
1k
Cl
2.00
1.95
0.98
0.96
1.96
6.00
f1 (ppm)


151.19
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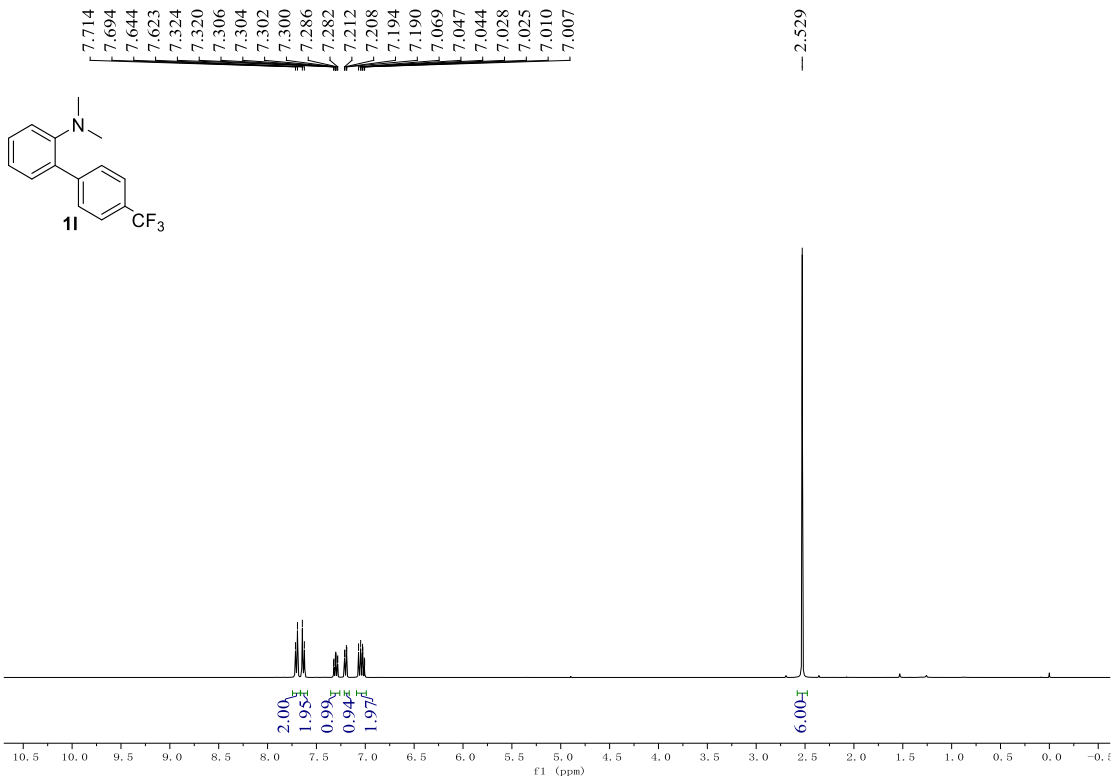
131.40
129.94
128.45
128.37
121.61
117.73
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
43.36
1k
Cl
f1 (ppm)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7.304
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7.300
7.286
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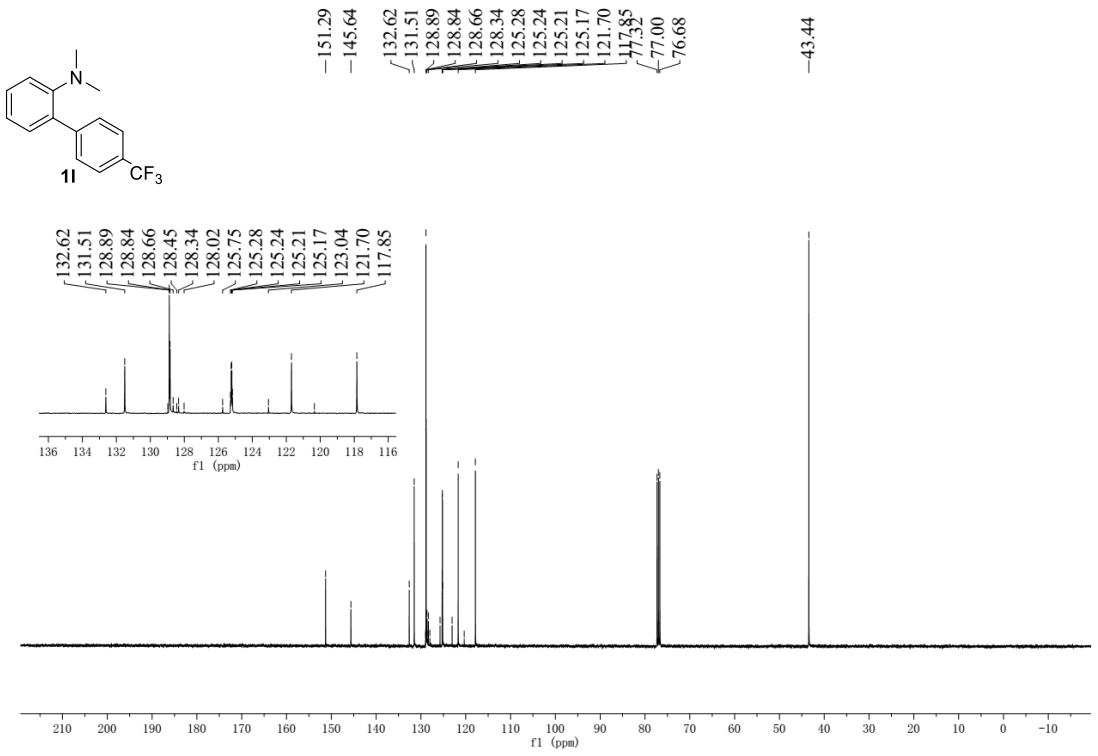
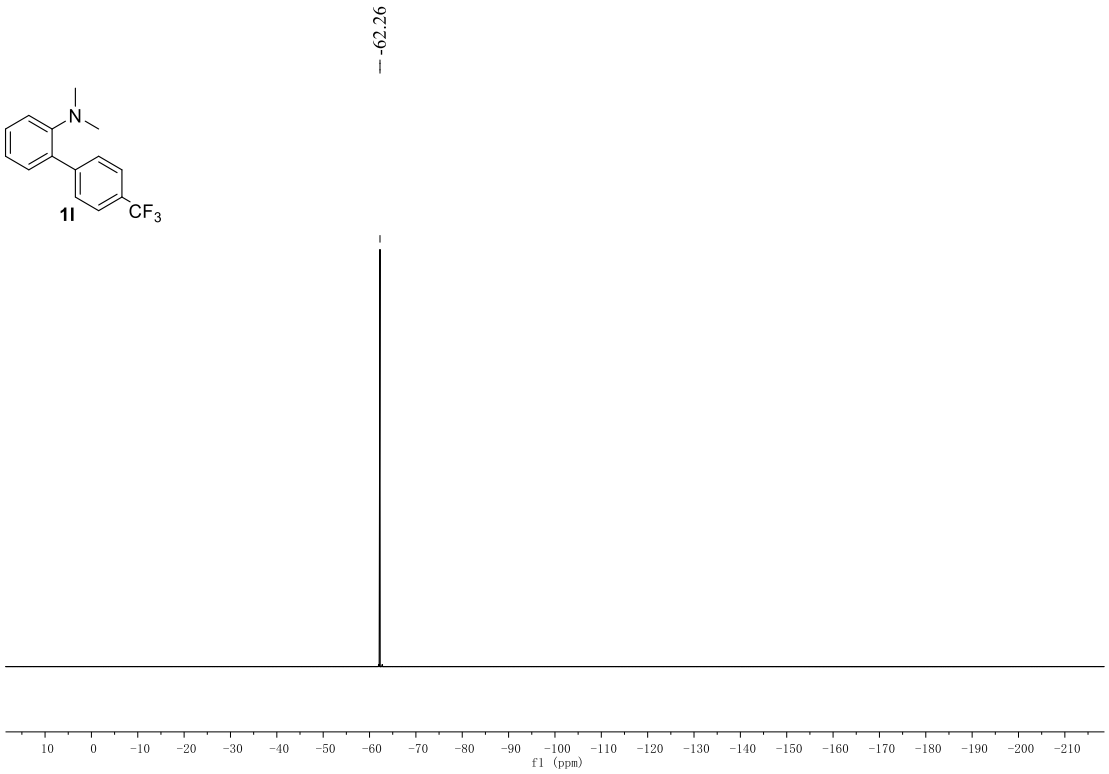
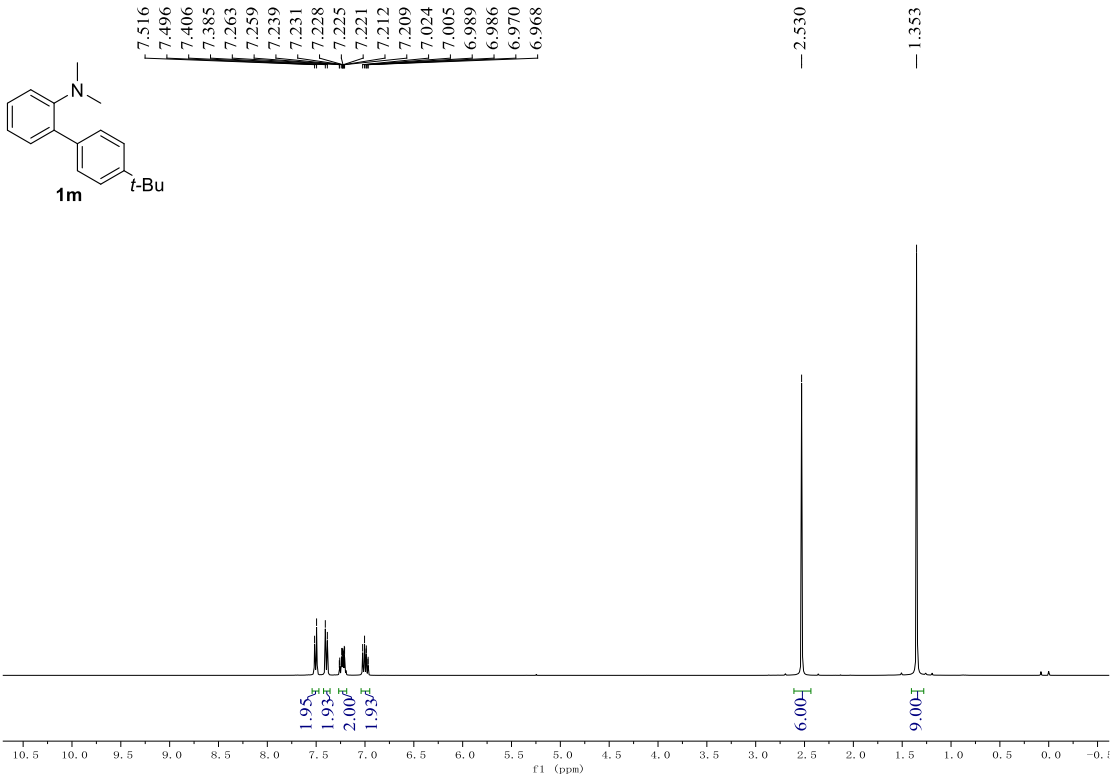
7.190
7.069
7.047
7.044
7.028
7.025
7.010
7.007
2.529
1l
CF3
2.00
1.95
0.99
0.94
1.97
6.00
f1 (ppm)


151.29
145.64
132.62
131.51
128.89
128.84
128.66
128.34
125.28
125.24
125.21
125.17
121.70
117.85
77.32
77.00
76.68
43.44
1l
CF3
132.62
131.51
128.89
128.84
128.66
128.45
128.34
128.02
125.75
125.28
125.24
125.21
125.17
123.04
121.70
117.85
f1 (ppm)
f1 (ppm)


-62.26
1l
CF3
f1 (ppm)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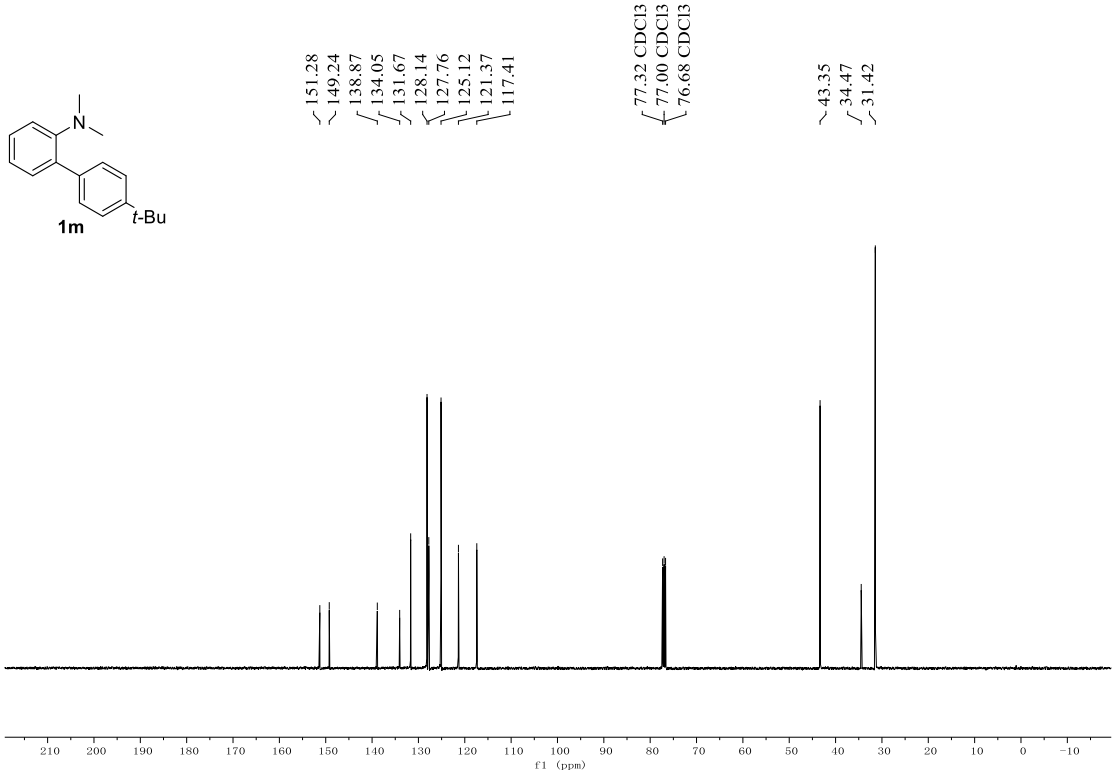
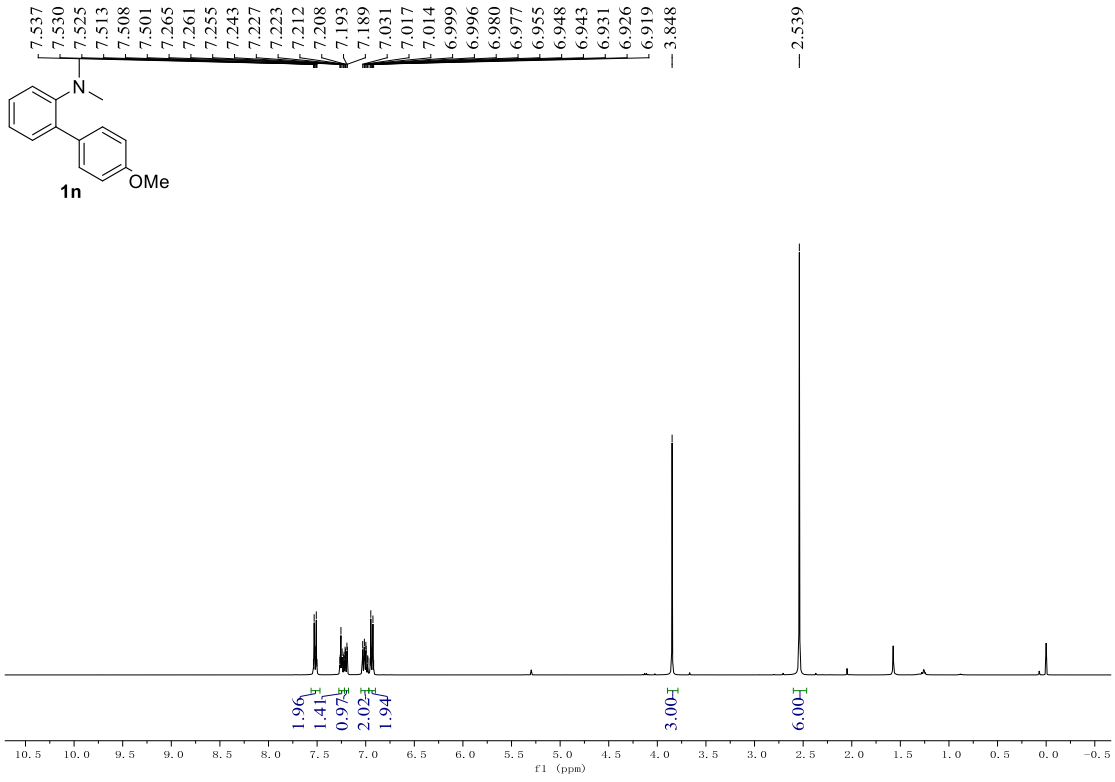
7.496
7.406
7.385
7.263
7.259
7.239
7.231
7.228
7.225
7.221
7.212
7.209
7.024
7.005
6.989
6.986
6.970
6.968
2.530
1.353
1m
t-Bu
1.95
1.93
2.00
1.93
6.00
9.00
f1 (ppm)


151.28
149.24
138.87
134.05
131.67
128.14
127.76
125.12
121.37
117.41
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
43.35
34.47
31.42
N
t-Bu
1m
f1 (ppm)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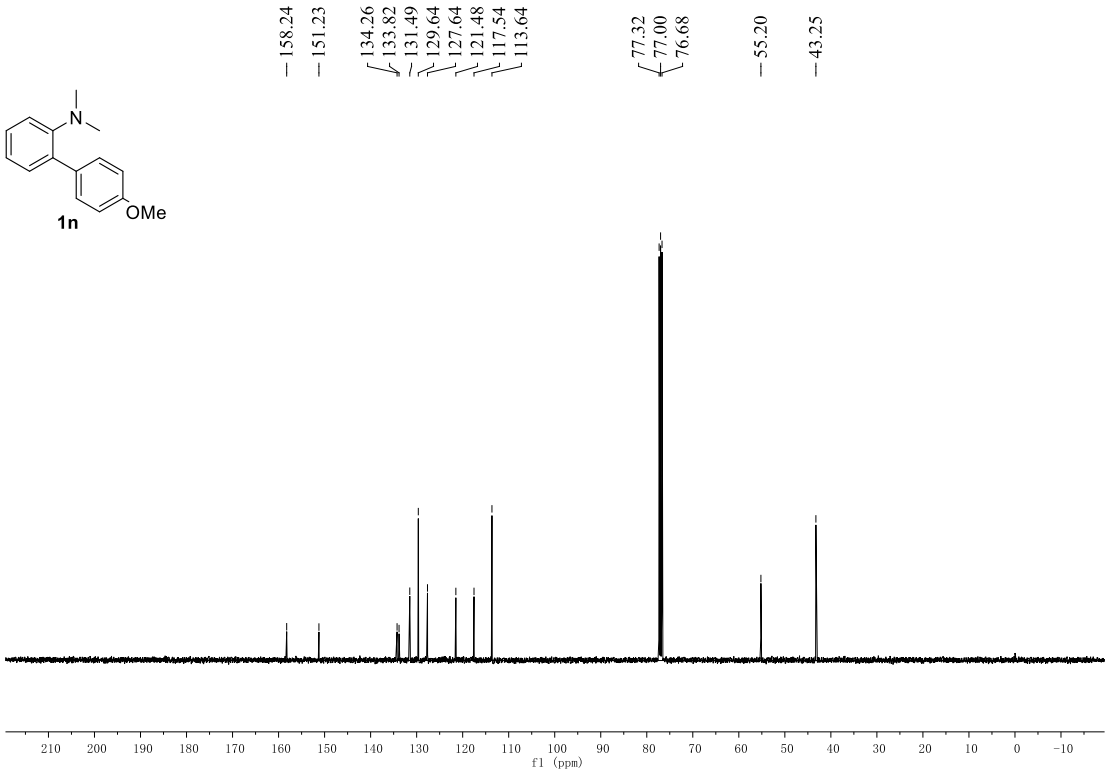
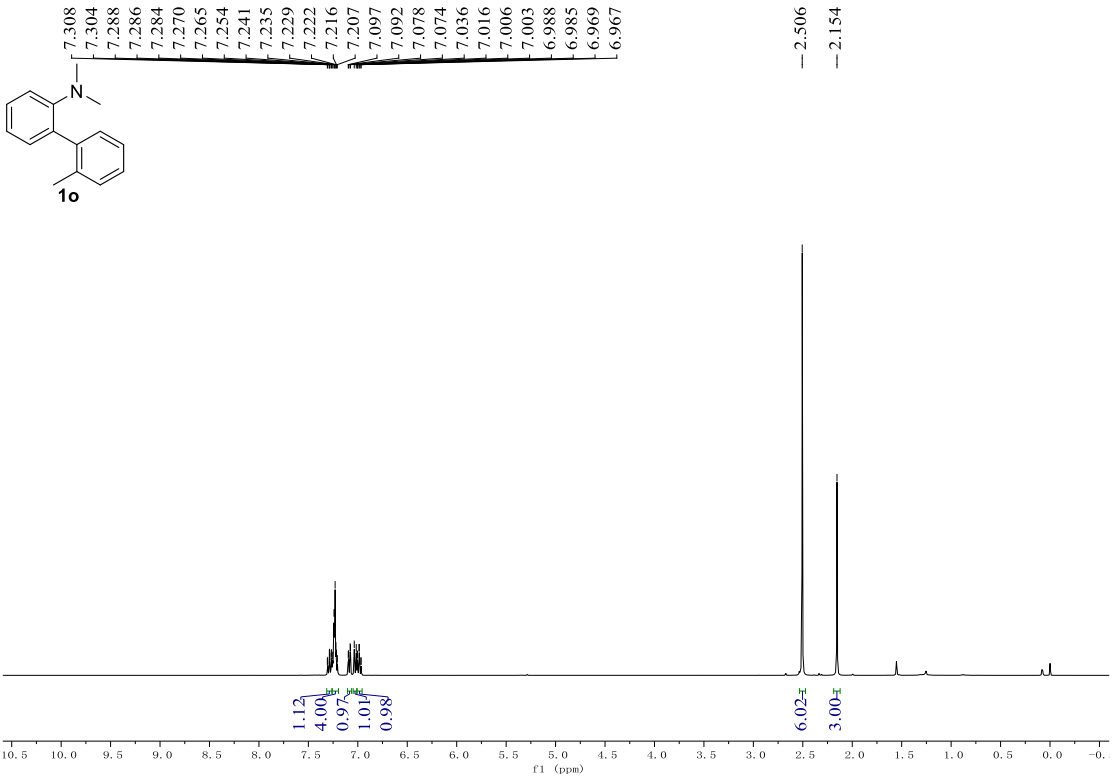
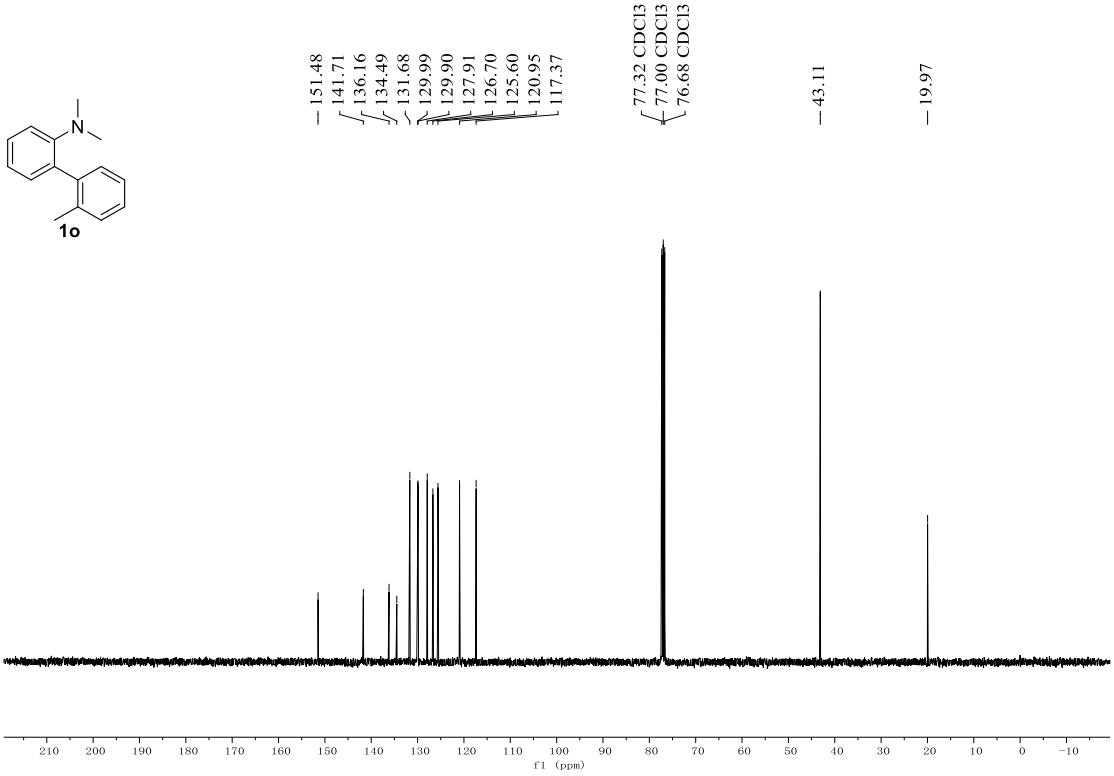
7.530
7.525
7.513
7.508
7.501
7.265
7.261
7.255
7.243
7.227
7.223
7.212
7.208
7.193
7.189
7.031
7.017
7.014
6.999
6.996
6.980
6.977
6.955
6.948
6.943
6.931
6.926
6.919
3.848
2.539
N
OMe
1n
1.96
1.41
0.97
2.02
1.94
3.00
6.00
f1 (ppm)


158.24
151.23
134.26
133.82
131.49
129.64
127.64
121.48
117.54
113.64
77.32
77.00
76.68
55.20
43.25
N
OMe
1n
f1 (ppm)


7.308
7.304
7.288
7.286
7.284
7.270
7.265
7.254
7.241
7.235
7.229
7.222
7.216
7.207
7.097
7.092
7.078
7.074
7.036
7.016
7.006
7.003
6.988
6.985
6.969
6.967
2.506
2.154
N
1o
1.12
4.00
0.97
1.01
0.98
6.02
3.00
f1 (ppm)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141.71
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134.49
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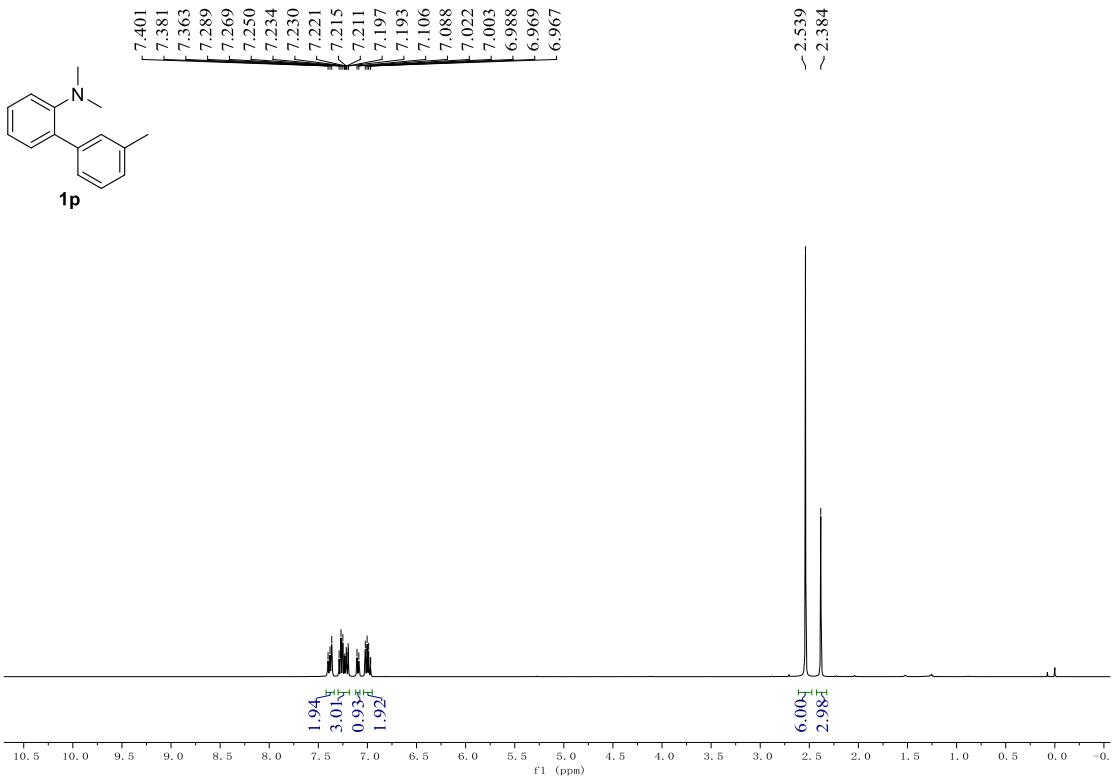
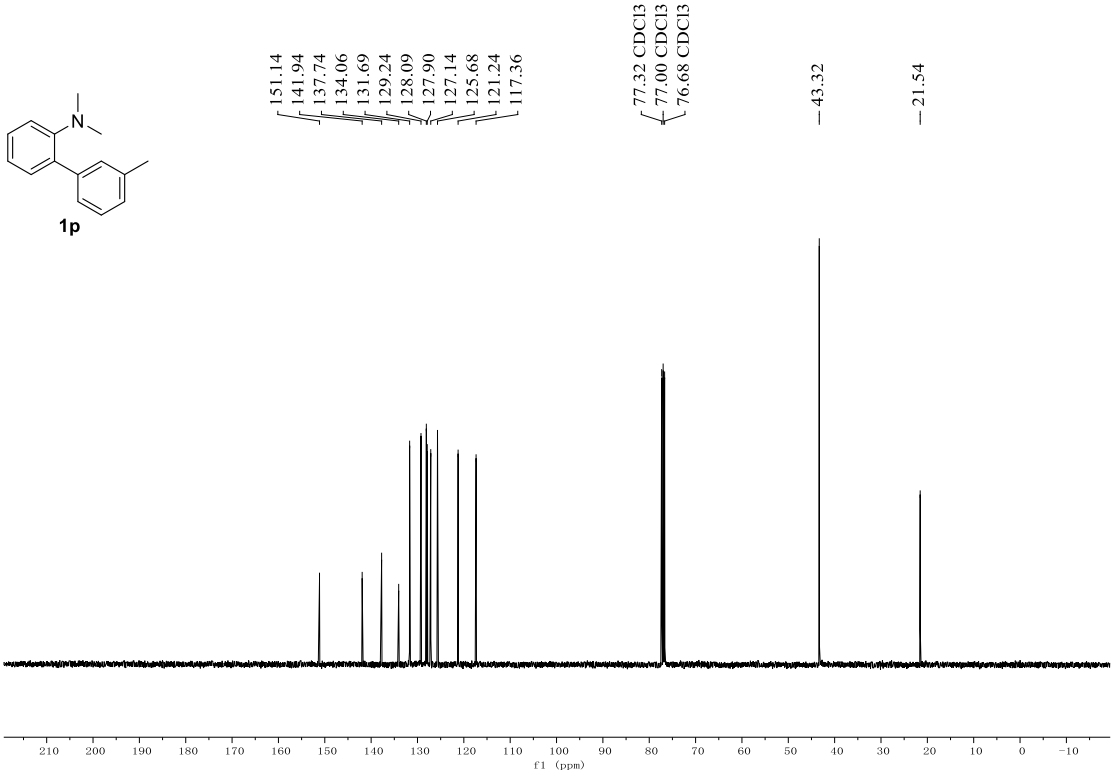
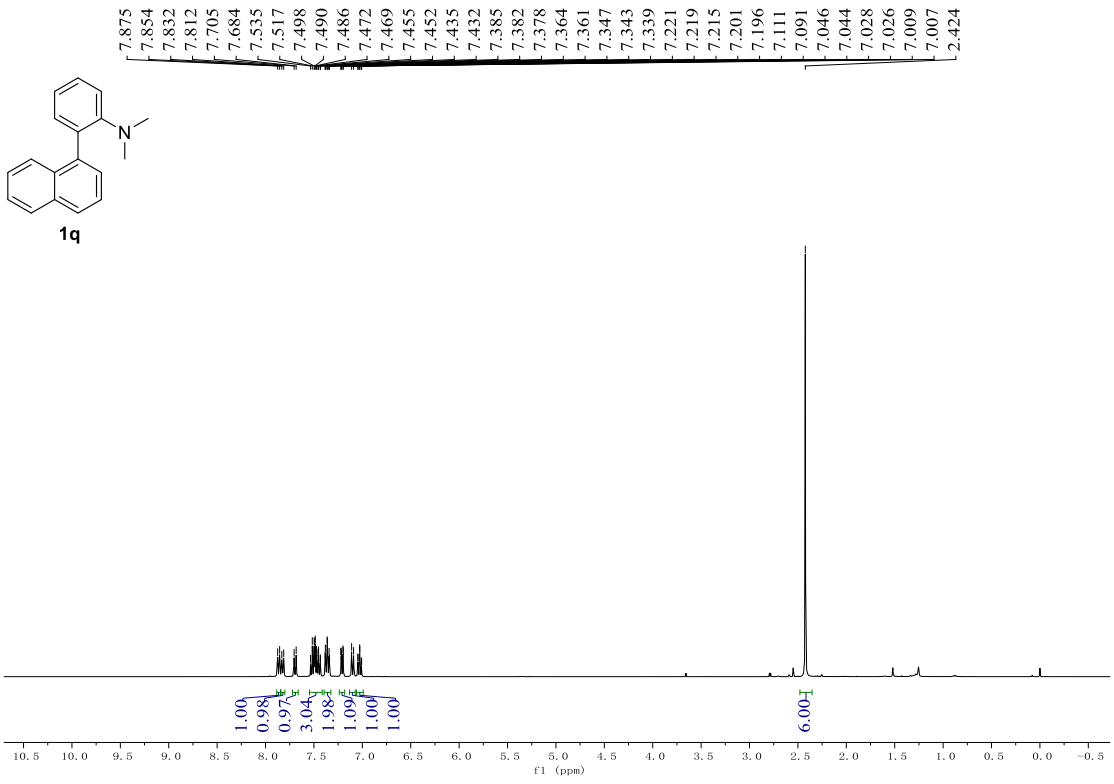
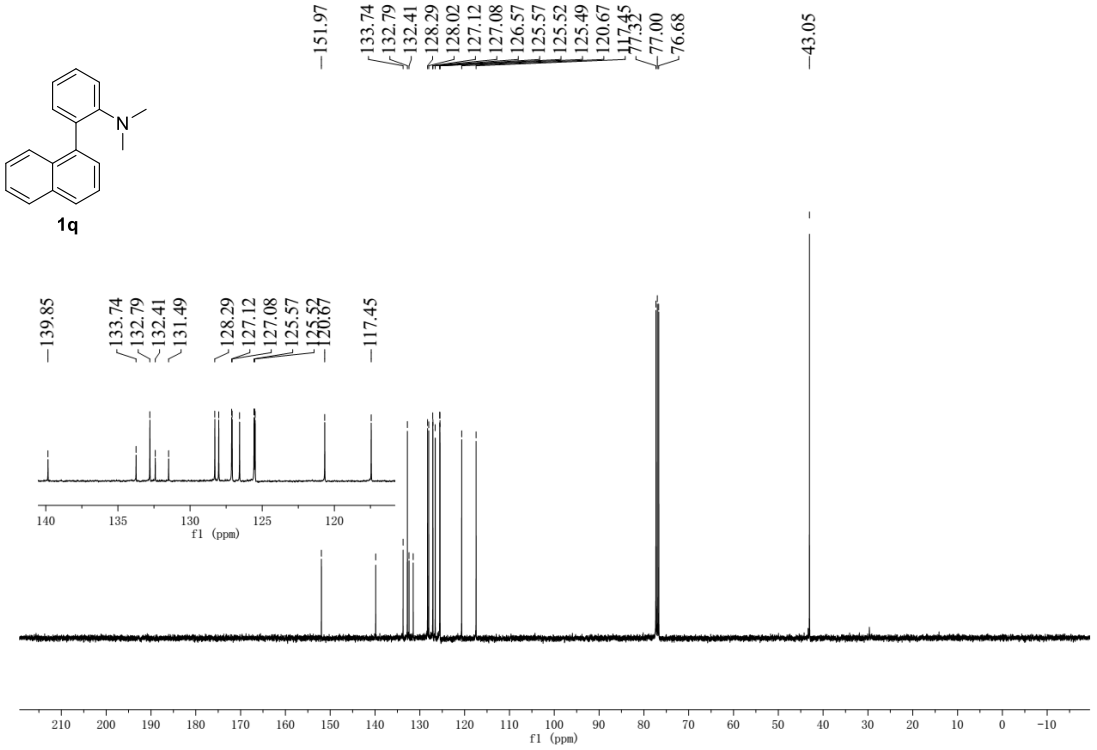
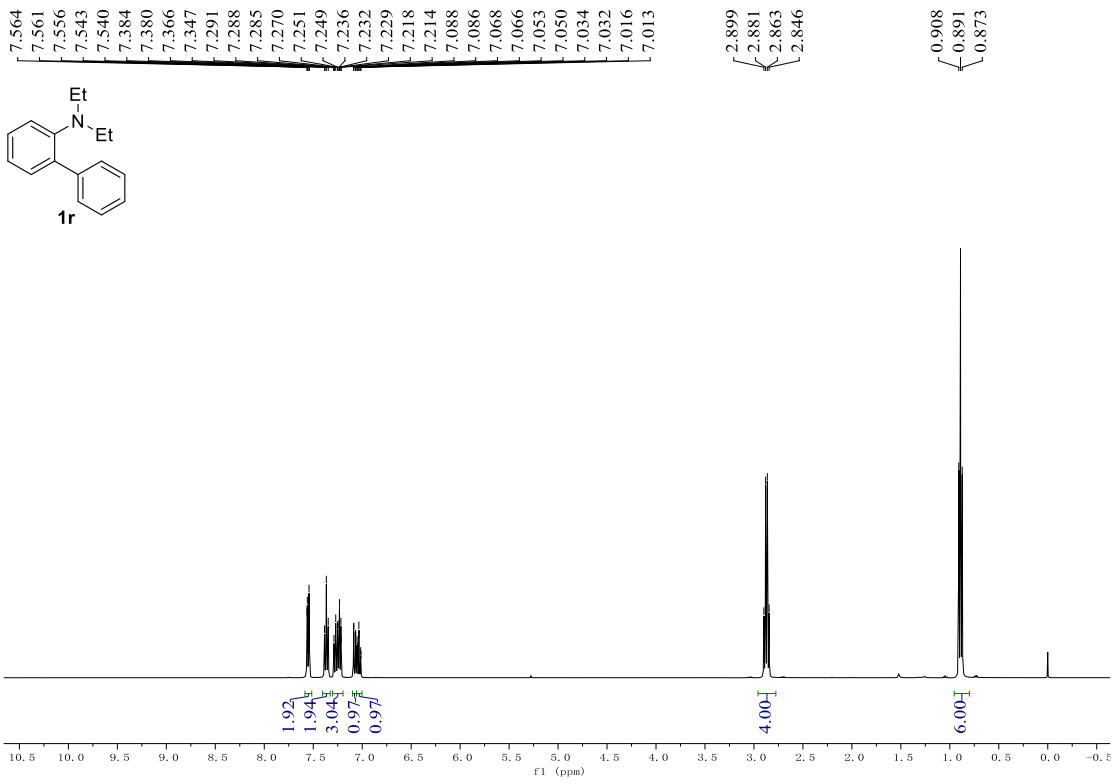
129.90
127.91
126.70
125.60
120.95
117.37
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
43.11
19.97
1o
f1 (ppm)


7.401
7.381
7.363
7.289
7.269
7.250
7.234
7.230
7.221
7.215
7.211
7.197
7.193
7.106
7.088
7.022
7.003
6.988
6.969
6.967
2.539
2.384
1p
1.94
3.01
0.93
1.92
6.00
2.98
f1 (ppm)


151.14
141.94
137.74
134.06
131.69
129.24
128.09
127.90
127.14
125.68
121.24
117.36
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
43.32
21.54
1p
f1 (ppm)


7.875
7.854
7.832
7.812
7.705
7.684
7.535
7.517
7.498
7.490
7.486
7.472
7.469
7.455
7.452
7.435
7.432
7.385
7.382
7.378
7.364
7.361
7.347
7.343
7.339
7.221
7.219
7.215
7.201
7.196
7.111
7.091
7.046
7.044
7.028
7.026
7.009
7.007
2.424
1q
1.00
0.98
0.97
3.04
1.98
1.09
1.00
1.00
6.00
f1 (ppm)


151.97
133.74
132.79
132.41
128.29
128.02
127.12
127.08
126.57
125.57
125.52
125.49
120.67
117.45
77.32
77.00
76.68
43.05
N
1q
139.85
133.74
132.79
132.41
131.49
128.29
127.12
127.08
125.57
125.52
120.67
117.45
140
135
130
125
120
f1 (ppm)
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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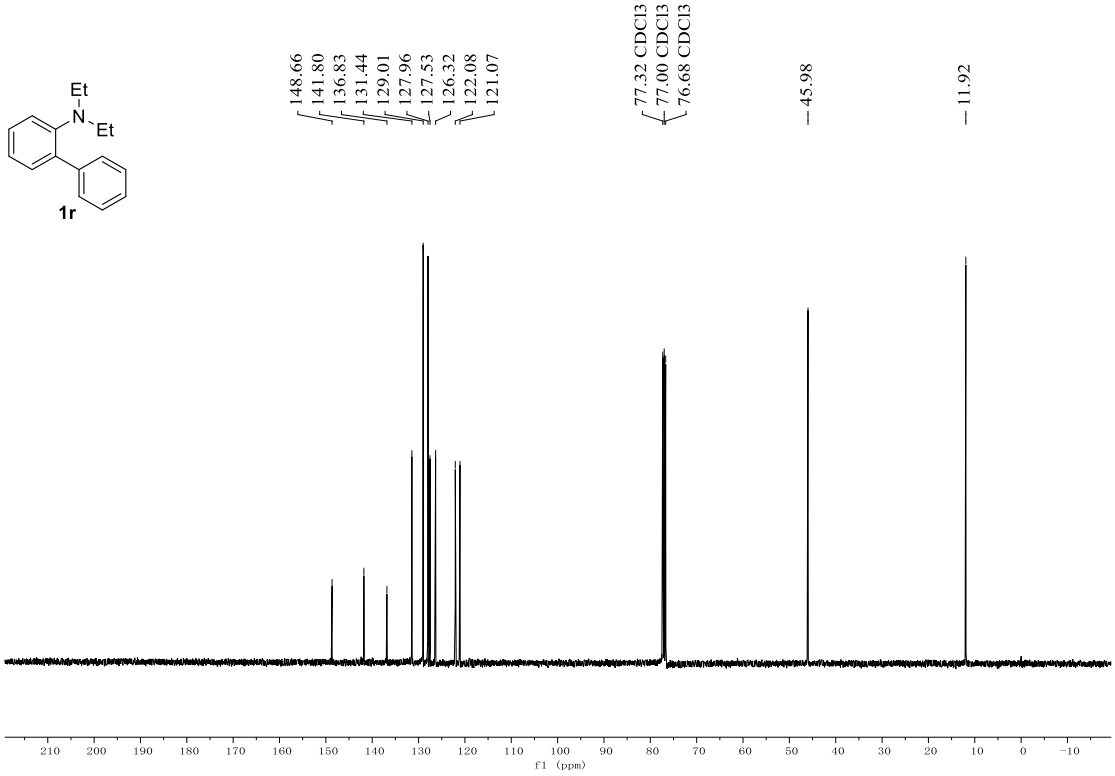
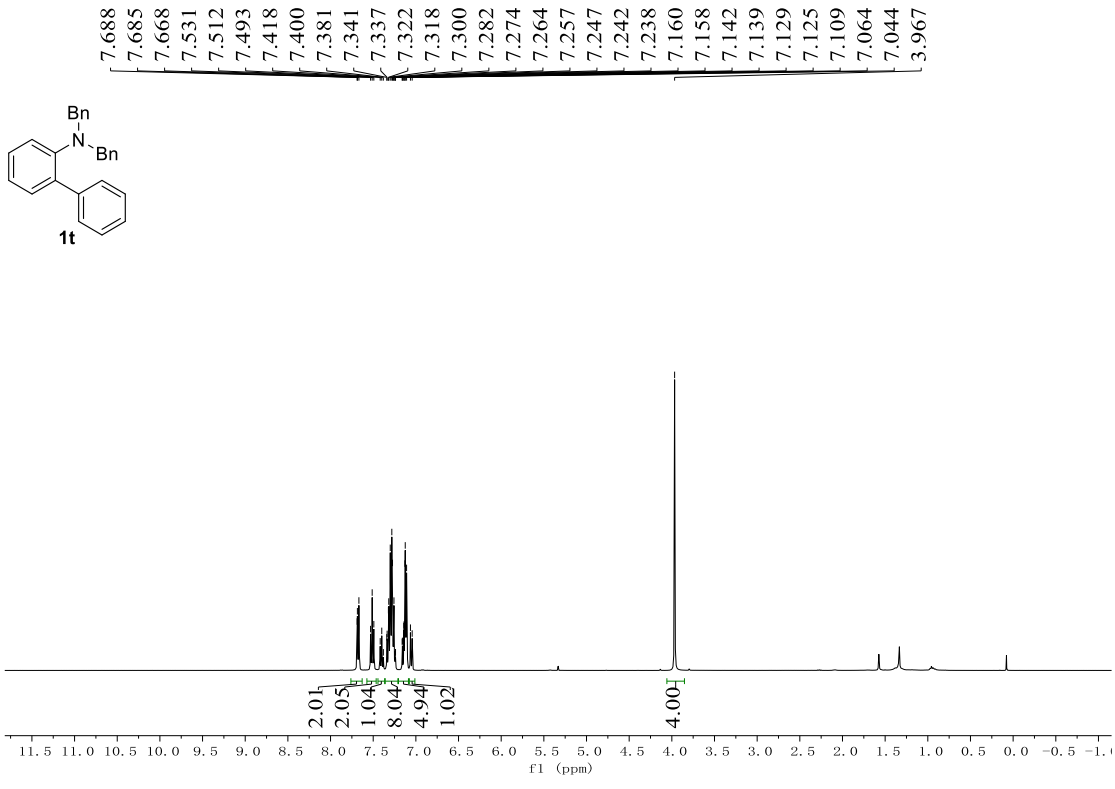
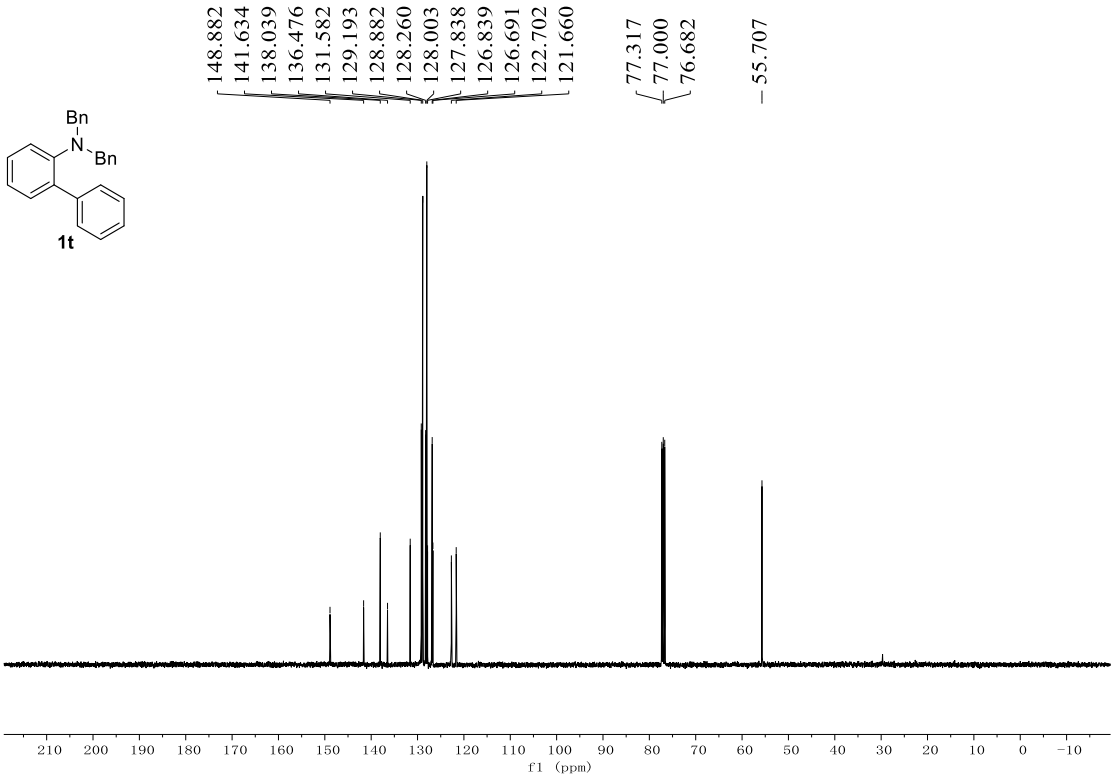
7.561
7.556
7.543
7.540
7.384
7.380
7.366
7.347
7.291
7.288
7.285
7.270
7.251
7.249
7.236
7.232
7.229
7.218
7.214
7.088
7.086
7.068
7.066
7.053
7.050
7.034
7.032
7.016
7.013
2.899
2.881
2.863
2.846
0.908
0.891
0.873
Et
N
Et
1r
1.92
1.94
3.04
0.97
0.97
4.00
6.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Et
N
Et
1r
148.66
141.80
136.83
131.44
129.01
127.96
127.53
126.32
122.08
121.07
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
45.98
11.92
f1 (ppm)


7.688
7.685
7.668
7.531
7.512
7.493
7.418
7.400
7.381
7.341
7.337
7.322
7.318
7.300
7.282
7.274
7.264
7.257
7.247
7.242
7.238
7.160
7.158
7.142
7.139
7.129
7.125
7.109
7.064
7.044
3.967
Bn
N
Bn
1t
2.01
2.05
1.04
8.04
4.94
1.02
4.00
f1 (ppm)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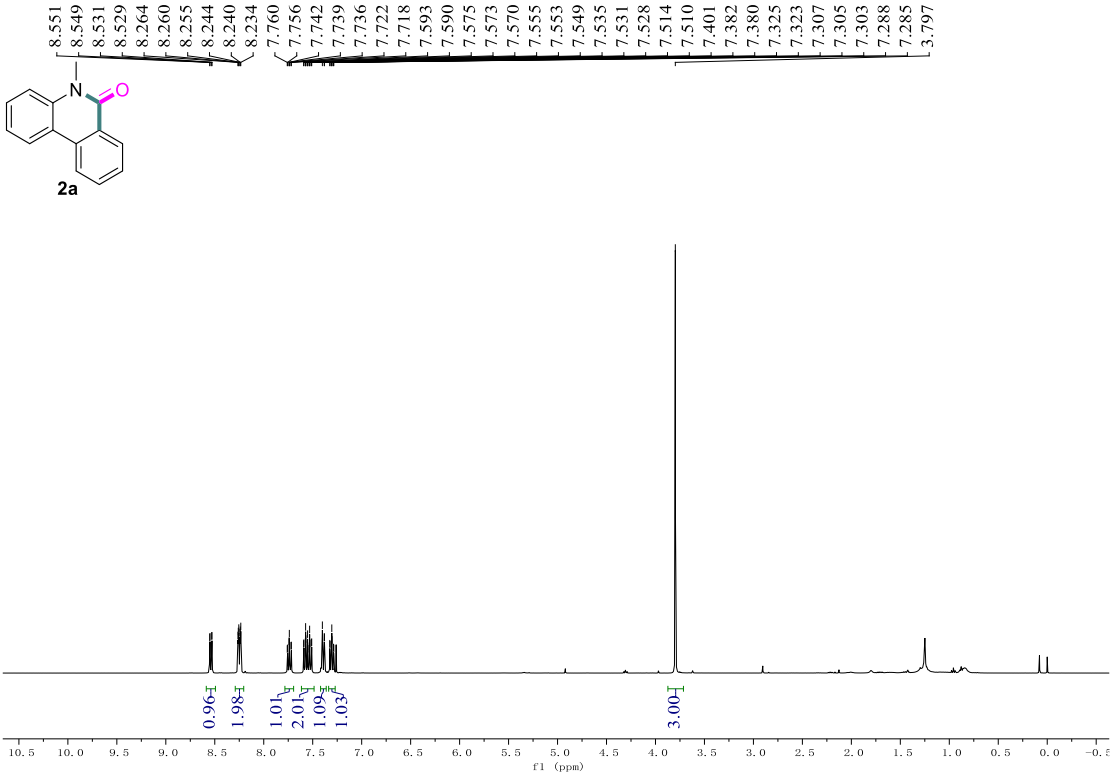
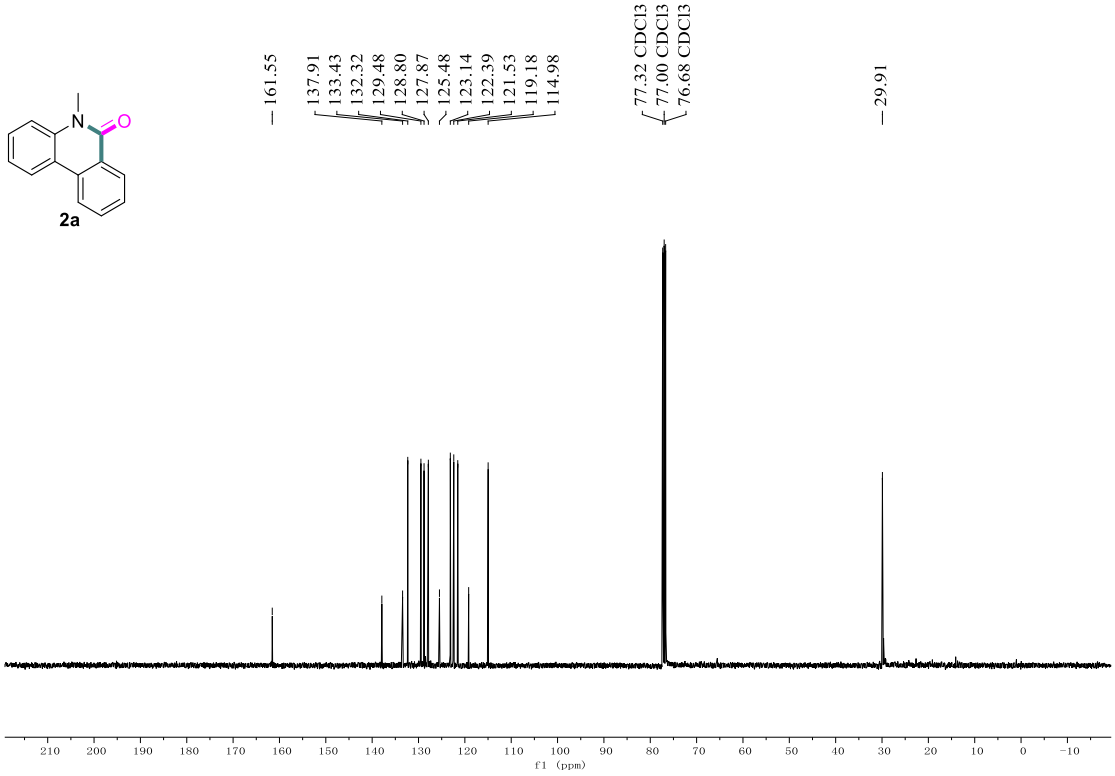
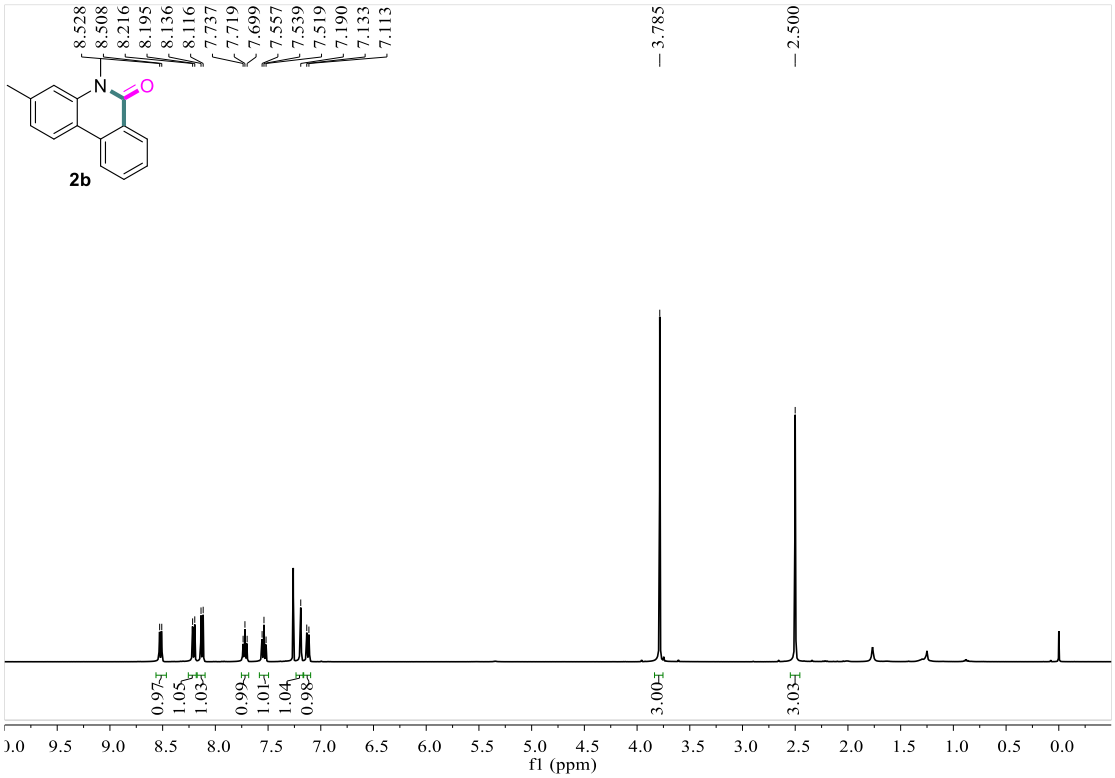
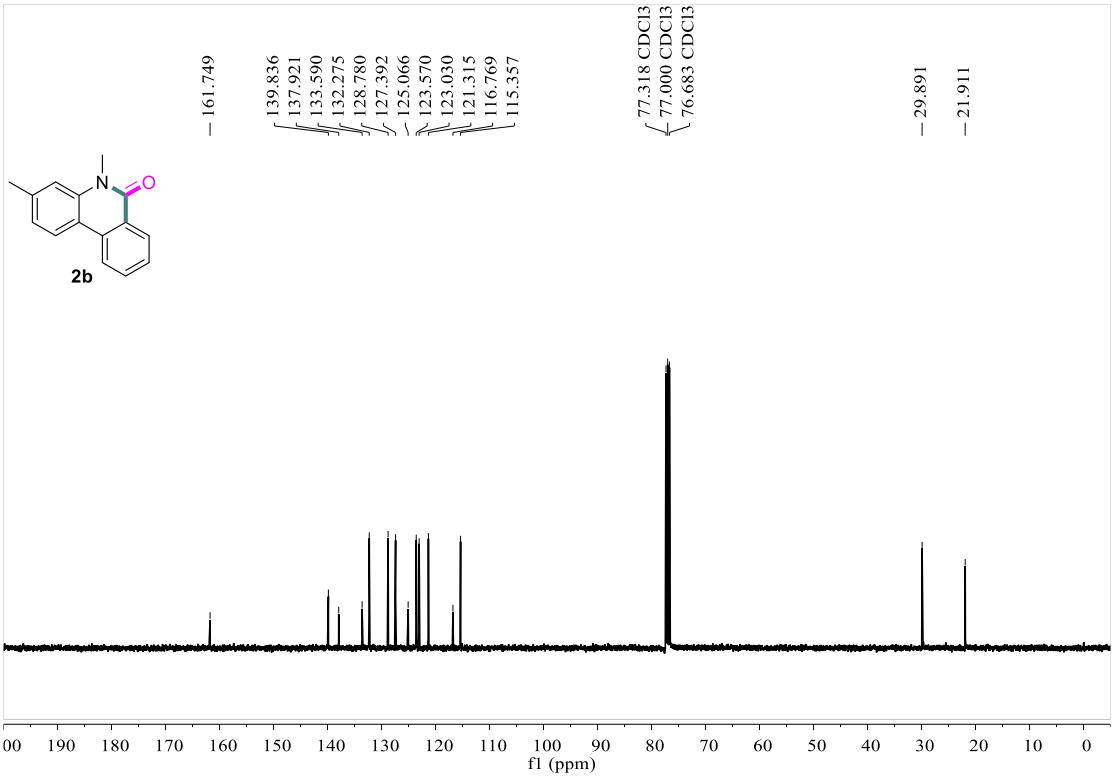
141.634
138.039
136.476
131.582
129.193
128.882
128.260
128.003
127.838
126.839
126.691
122.702
121.660
77.317
77.000
76.682
55.707
Bn
N
Bn
1t
f1 (ppm)


8.551
8.549
8.531
8.529
8.264
8.260
8.255
8.244
8.240
8.234
7.760
7.756
7.742
7.739
7.736
7.722
7.718
7.593
7.590
7.575
7.573
7.570
7.555
7.553
7.549
7.535
7.531
7.528
7.514
7.510
7.401
7.382
7.380
7.325
7.323
7.307
7.305
7.303
7.288
7.285
3.797
N
O
2a
0.96
1.98
1.01
2.01
1.09
1.03
3.00
f1 (ppm)


2a
161.55
137.91
133.43
132.32
129.48
128.80
127.87
125.48
123.14
122.39
121.53
119.18
114.98
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
29.91
f1 (ppm)


2b
8.528
8.508
8.216
8.195
8.136
8.116
7.737
7.719
7.699
7.557
7.539
7.519
7.190
7.133
7.113
3.785
2.500
0.97
1.05
1.03
0.99
1.01
1.04
0.98
3.00
3.03
f1 (ppm)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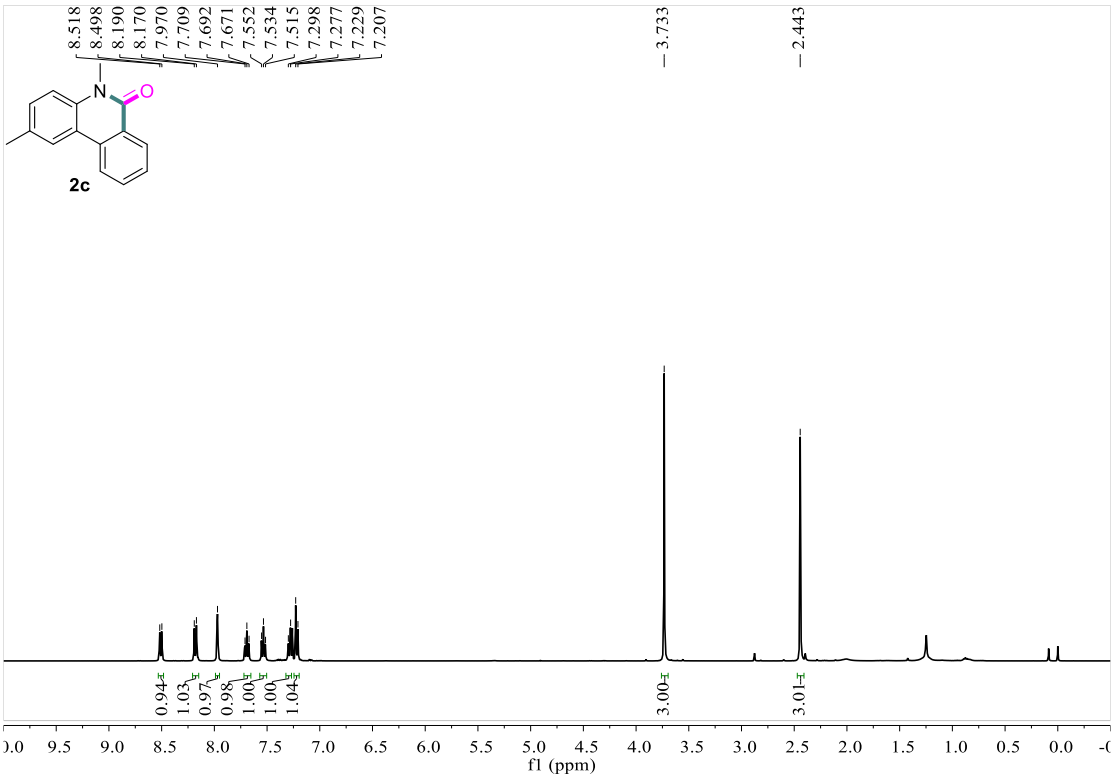
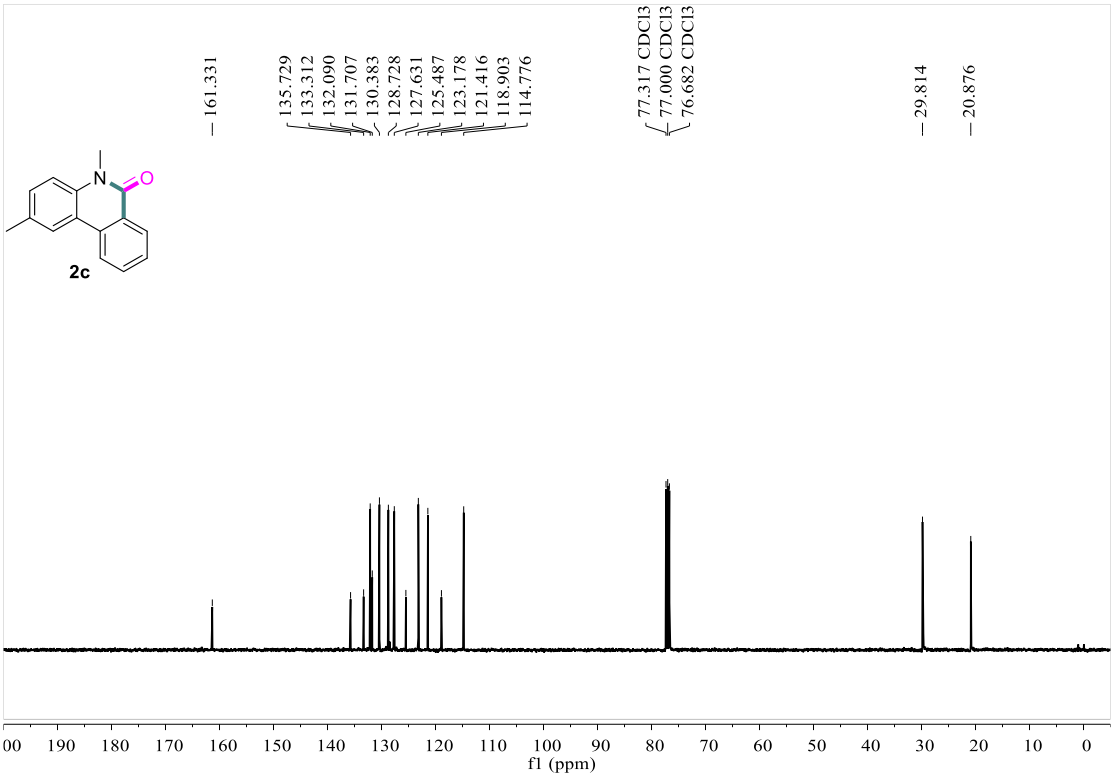
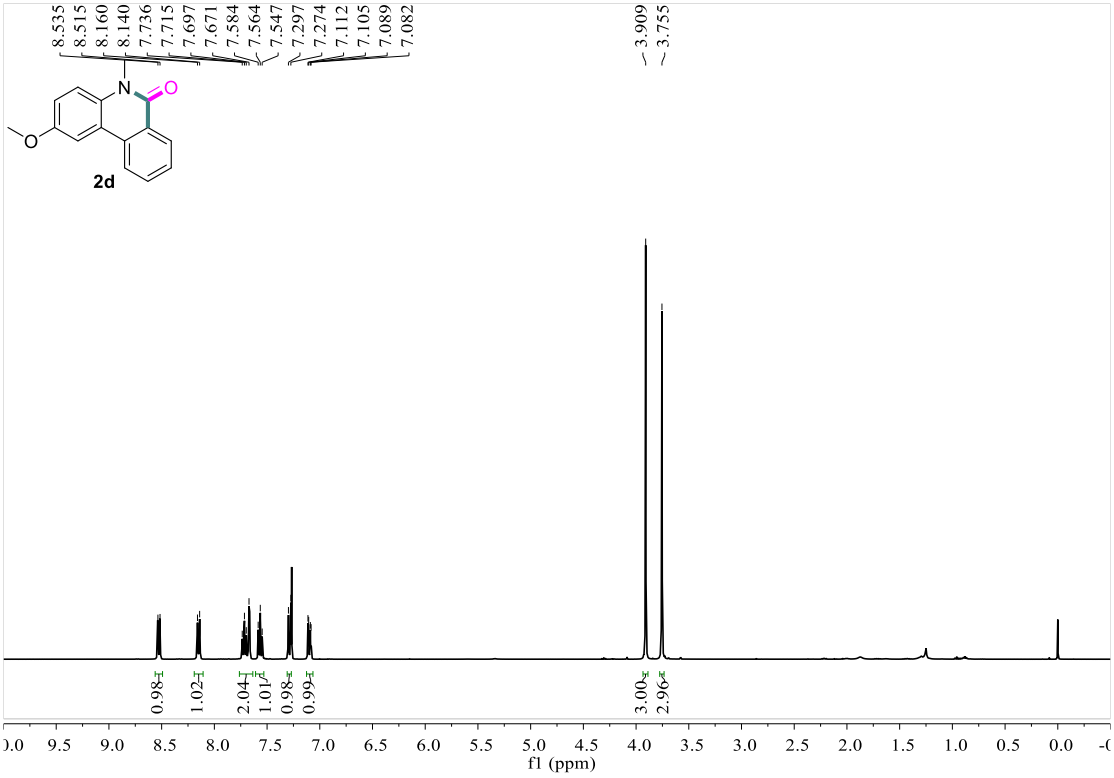
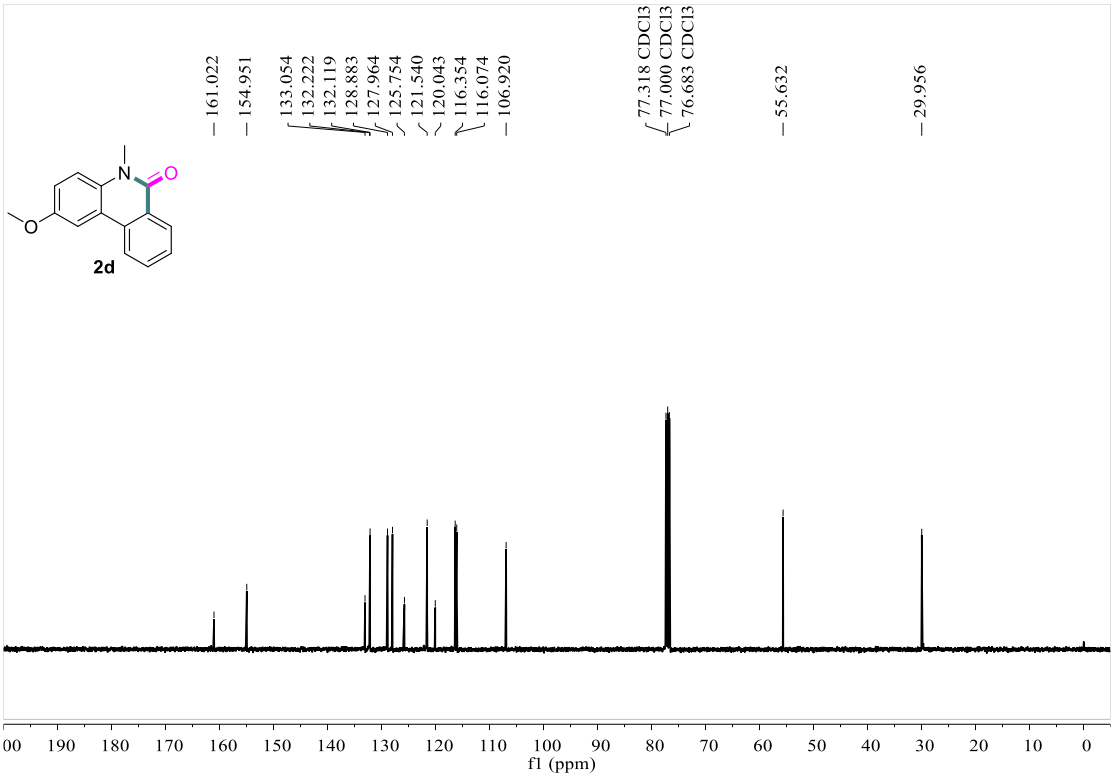
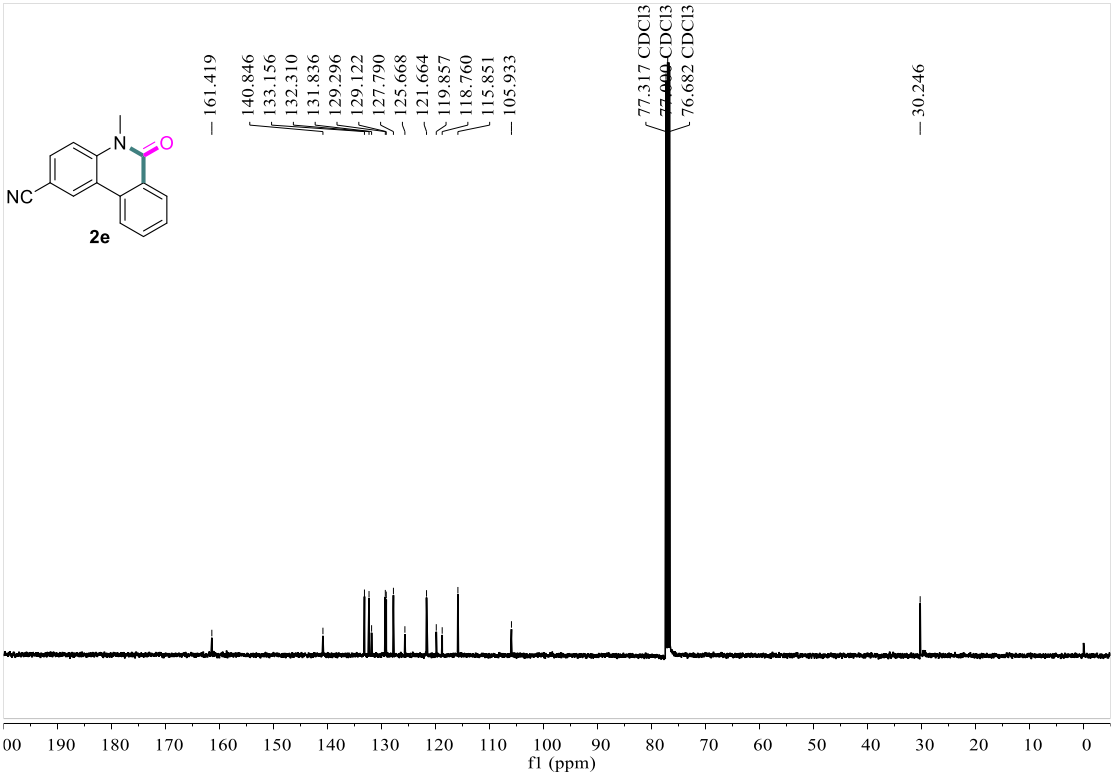
139.836
137.921
133.590
132.275
128.780
127.392
125.066
123.570
123.030
121.315
116.769
115.357
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
29.891
21.911
2b
f1 (ppm)


8.518
8.498
8.190
8.170
7.970
7.709
7.692
7.671
7.552
7.534
7.515
7.298
7.277
7.229
7.207
3.733
2.443
0.94
1.03
0.97
0.98
1.00
1.00
1.04
3.00
3.01
2c
f1 (ppm)


161.331
135.729
133.312
132.090
131.707
130.383
128.728
127.631
125.487
123.178
121.416
118.903
114.776
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
29.814
20.876
2c
f1 (ppm)


8.535
8.515
8.160
8.140
7.736
7.715
7.697
7.671
7.584
7.564
7.547
7.297
7.274
7.112
7.105
7.089
7.082
3.909
3.755
2d
0.98
1.02
2.04
1.01
0.98
0.99
3.00
2.96
f1 (ppm)


161.022
154.951
133.054
132.222
132.119
128.883
127.964
125.754
121.540
120.043
116.354
116.074
106.920
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
55.632
29.956
O
N
O
2d
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


161.419
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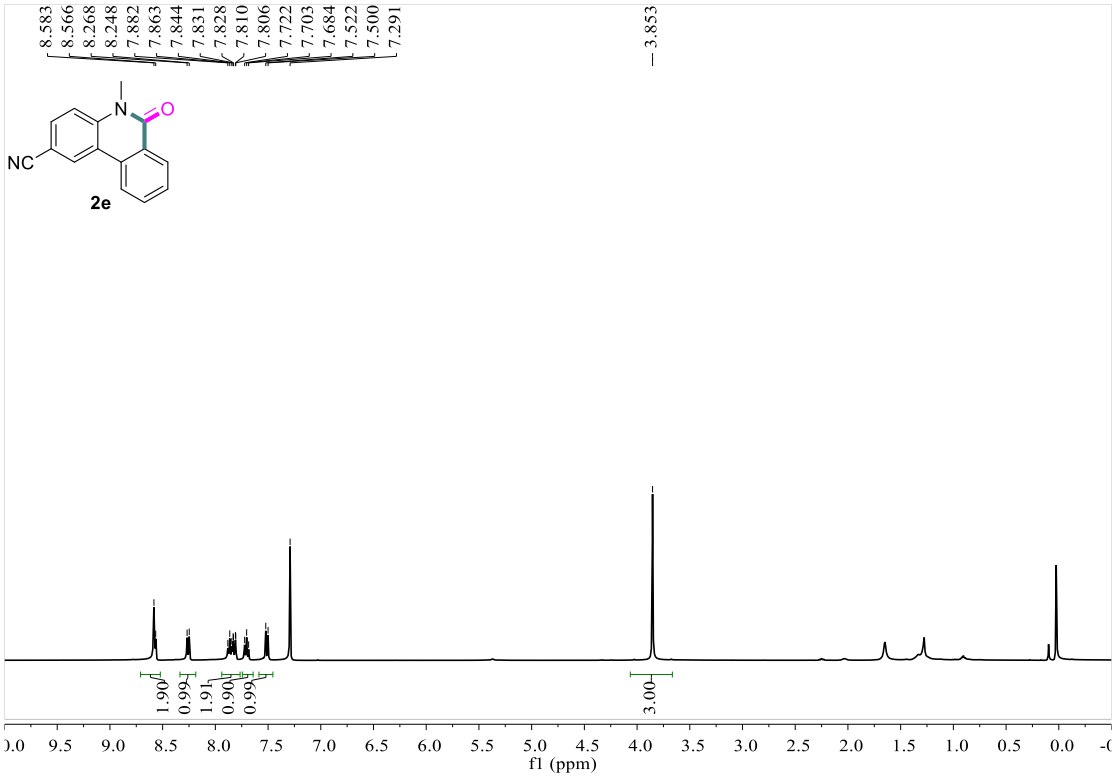
133.156
132.310
131.836
129.296
129.122
127.790
125.668
121.664
119.857
118.760
115.851
105.933
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
30.246
NC
O
N
2e
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.583
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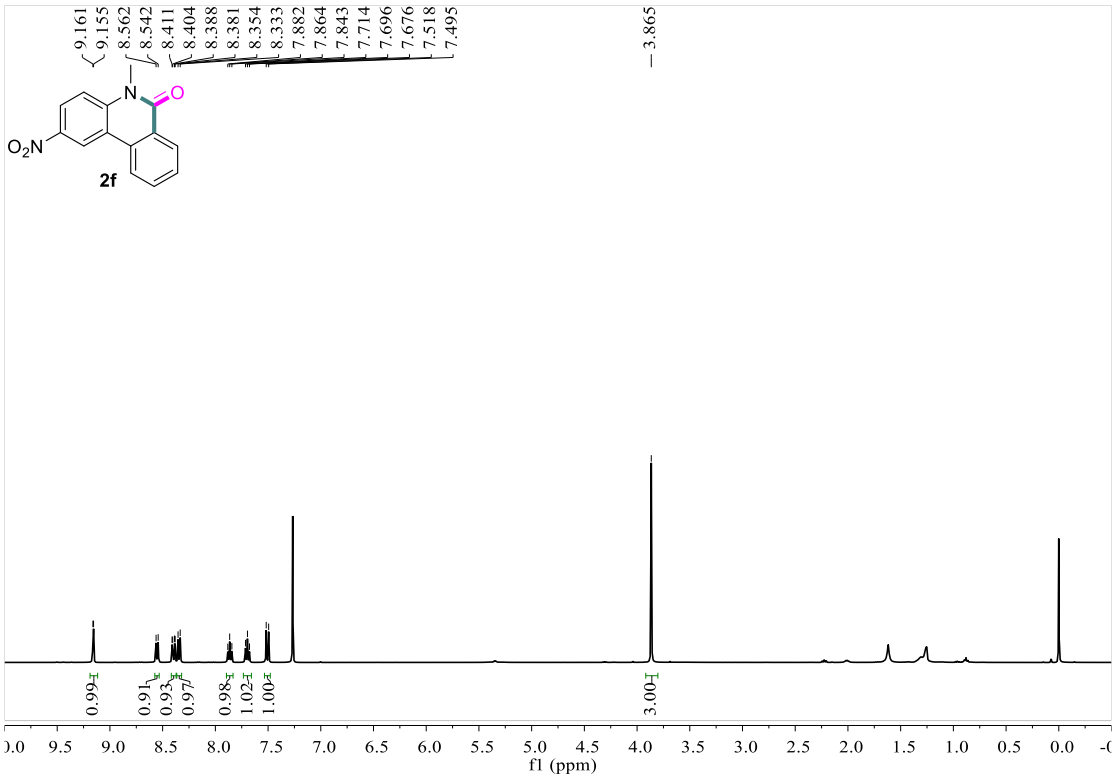
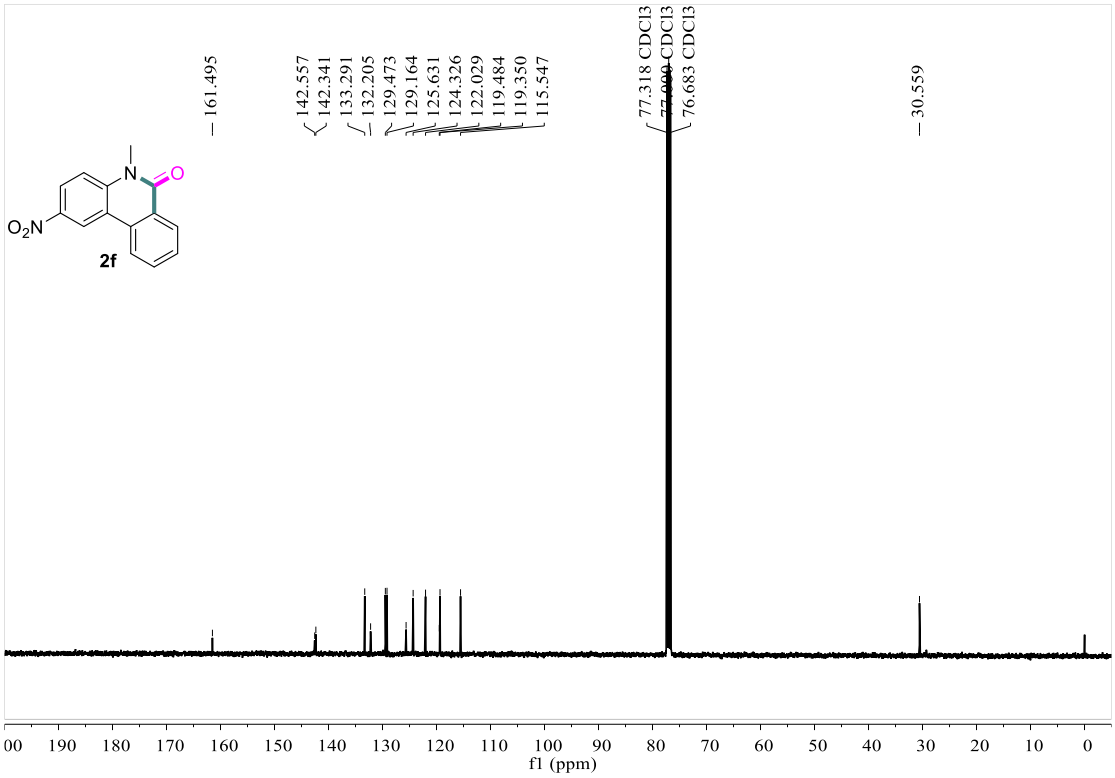
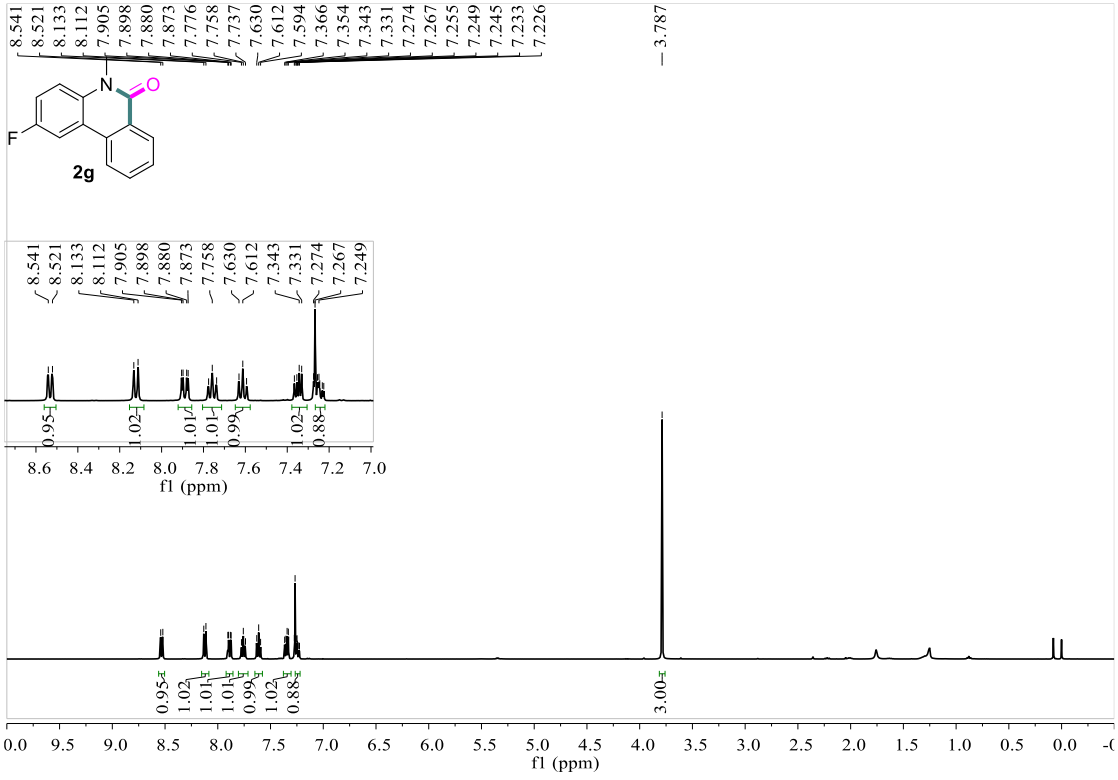
8.268
8.248
7.882
7.863
7.844
7.831
7.828
7.810
7.806
7.722
7.703
7.684
7.522
7.500
7.291
3.853
NC
N
O
2e
1.90
0.99
1.91
0.90
0.99
3.00
f1 (ppm)


9.161
9.155
8.562
8.542
8.411
8.404
8.388
8.381
8.354
8.333
7.882
7.864
7.843
7.714
7.696
7.676
7.518
7.495
3.865
O2N
N
O
2f
0.99
0.91
0.93
0.97
0.98
1.02
1.00
3.00
f1 (ppm)


161.495
142.557
142.341
133.291
132.205
129.473
129.164
125.631
124.326
122.029
119.484
119.350
115.547
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
30.559
O2N
2f
f1 (ppm)


8.541
8.521
8.133
8.112
7.905
7.898
7.880
7.873
7.776
7.758
7.737
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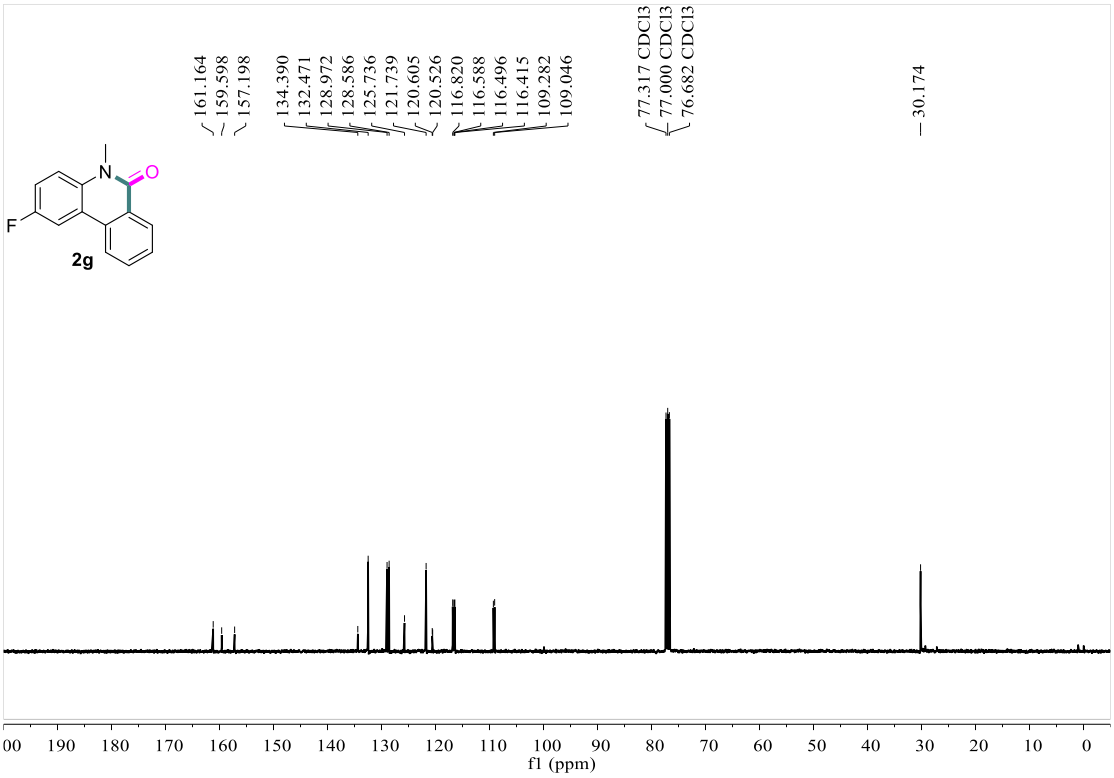
7.612
7.594
7.366
7.354
7.343
7.331
7.274
7.267
7.255
7.249
7.245
7.233
7.226
3.787
F
2g
0.95
1.02
1.01
1.01
0.99
1.02
0.88
3.00
f1 (ppm)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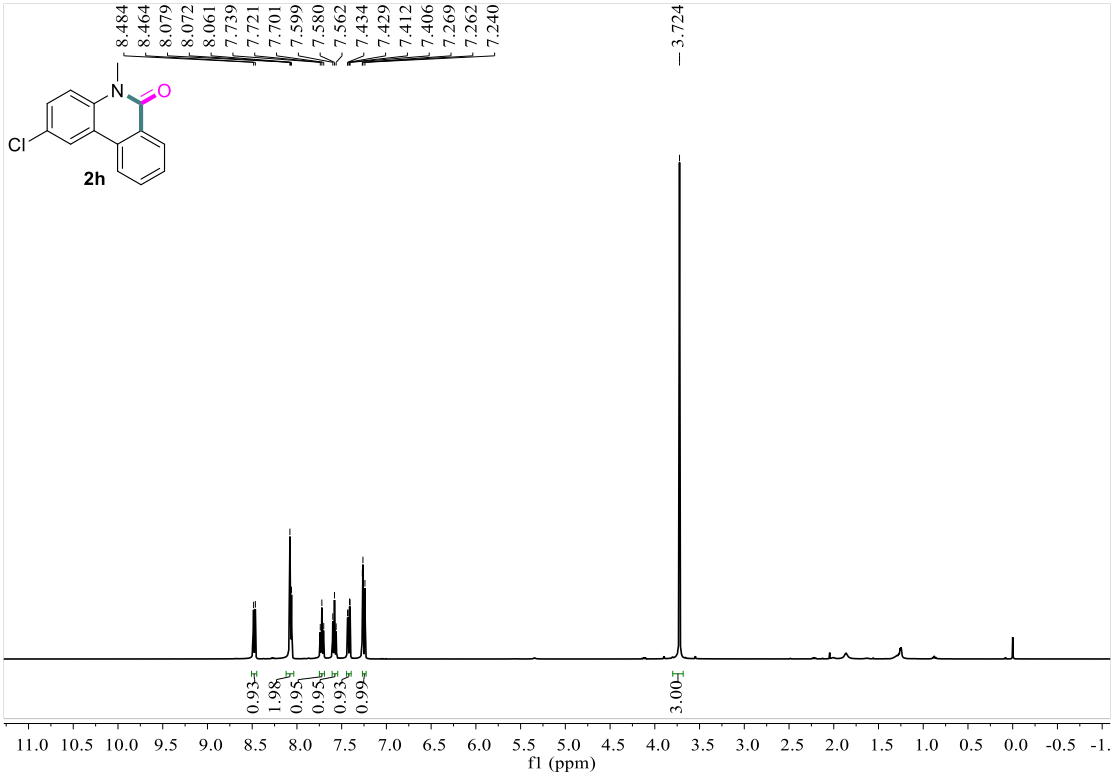
157.198
134.390
132.471
128.972
128.586
125.736
121.739
120.605
120.526
116.820
116.588
116.496
116.415
109.282
109.046
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
30.174
F
N
O
2g
f1 (ppm)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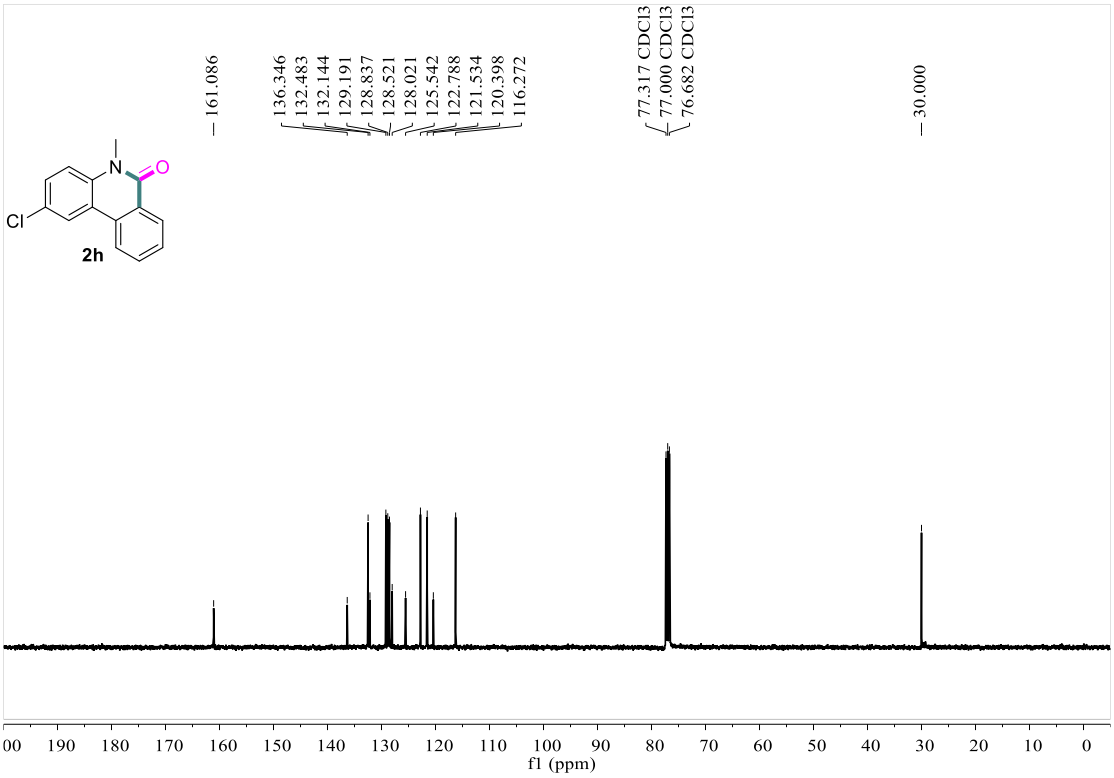
8.464
8.079
8.072
8.061
7.739
7.721
7.701
7.599
7.580
7.562
7.434
7.429
7.412
7.406
7.269
7.262
7.240
3.724
Cl
N
O
2h
0.93
1.98
0.95
0.95
0.93
0.99
3.00
f1 (ppm)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136.346
132.483
132.144
129.191
128.837
128.521
128.021
125.542
122.788
121.534
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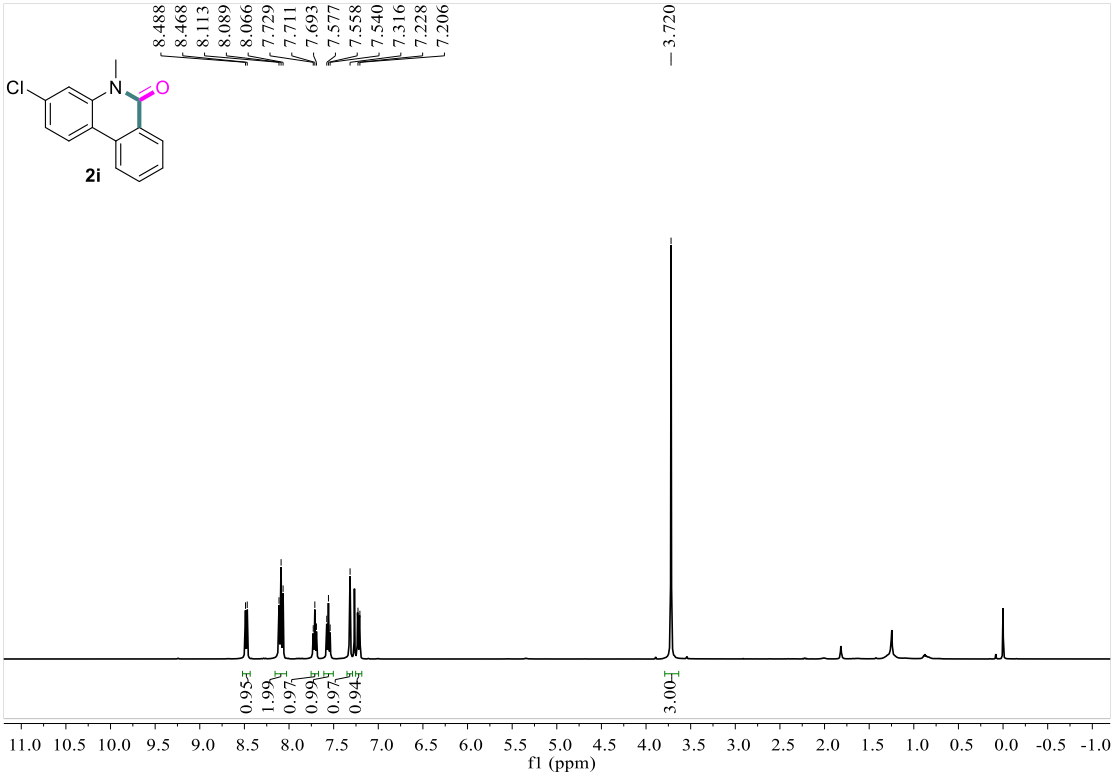
116.272
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
30.000
Cl
N
O
2h
f1 (ppm)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7.729
7.711
7.693
7.577
7.558
7.540
7.316
7.228
7.206
3.720
Cl
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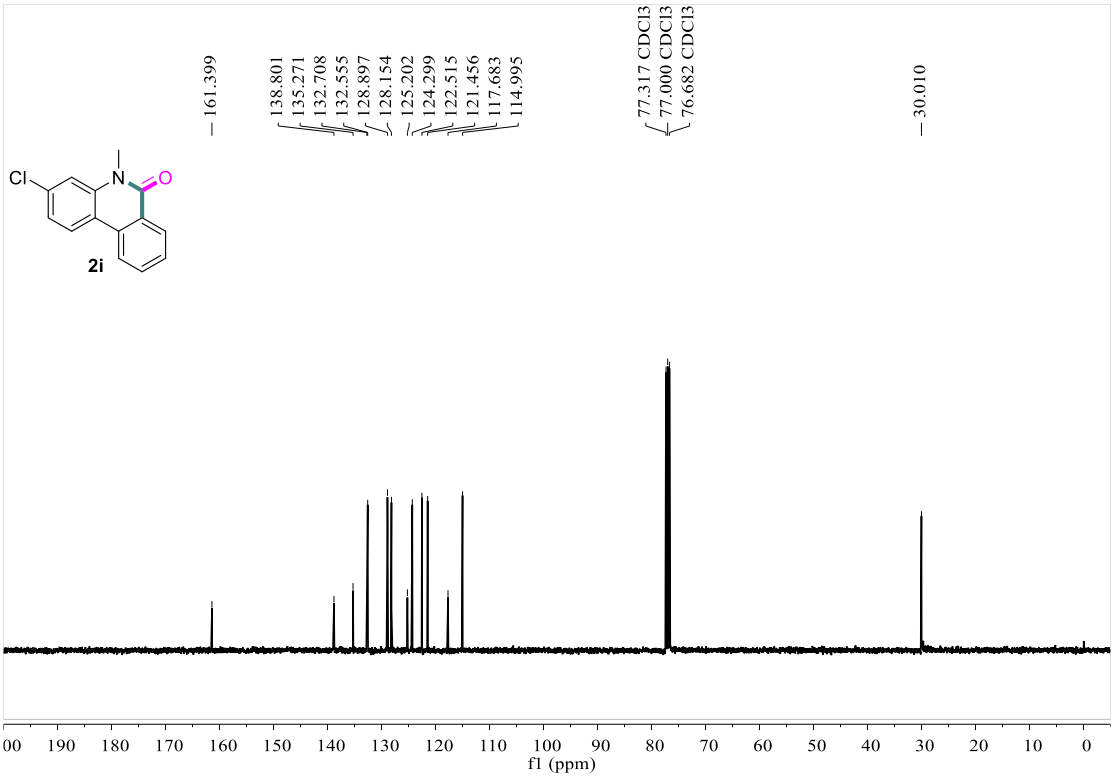
O
2i
0.95
1.99
0.97
0.99
0.97
0.94
3.00
f1 (ppm)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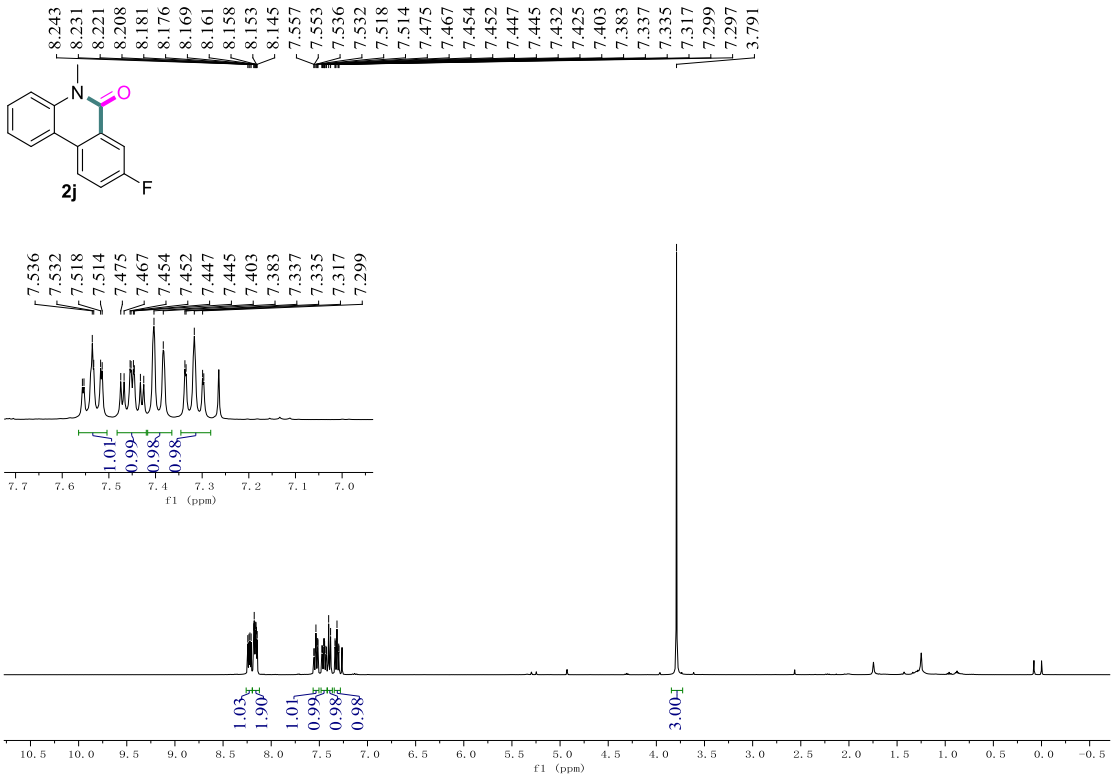
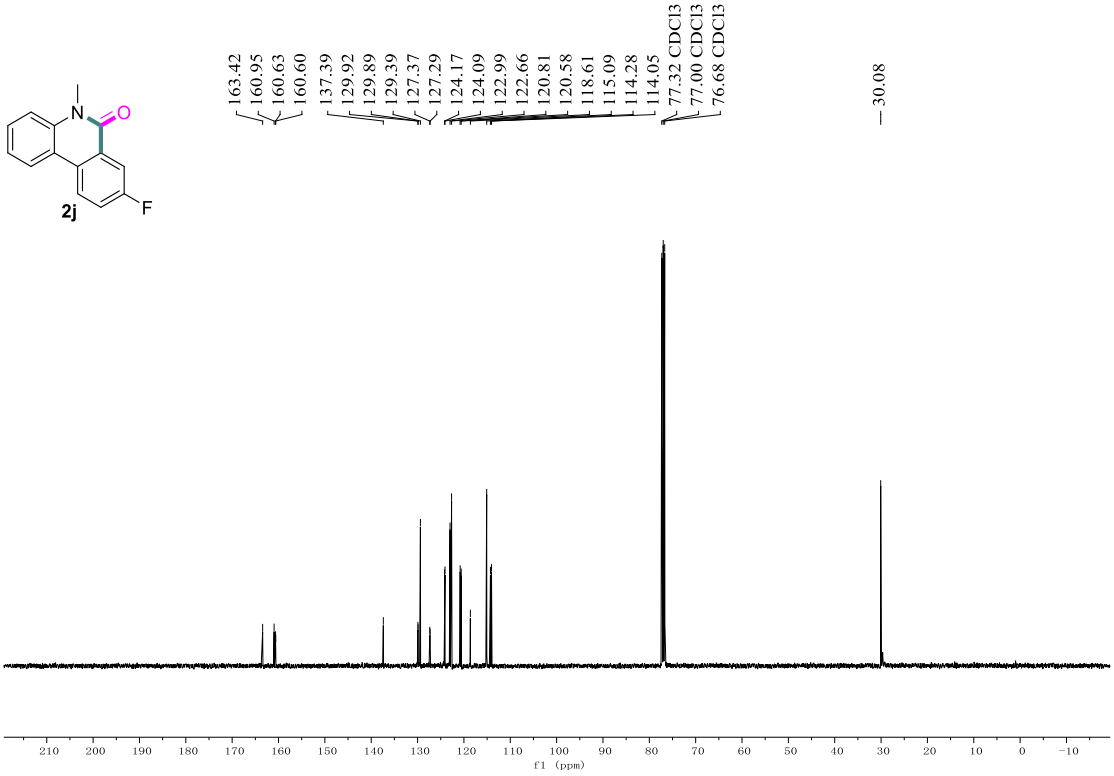
138.801
135.271
132.708
132.555
128.897
128.154
125.202
124.299
122.515
121.456
117.683
114.995
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
30.010
Cl
N
O
2i
f1 (ppm)


8.243
8.231
8.221
8.208
8.181
8.176
8.169
8.161
8.158
8.153
8.145
7.557
7.553
7.536
7.532
7.518
7.514
7.475
7.467
7.454
7.452
7.447
7.445
7.432
7.425
7.403
7.383
7.337
7.335
7.317
7.299
7.297
3.791
N
O
F
2j
1.03
1.90
1.01
0.99
0.98
0.98
3.00
f1 (ppm)


2j
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160.95
160.63
160.60
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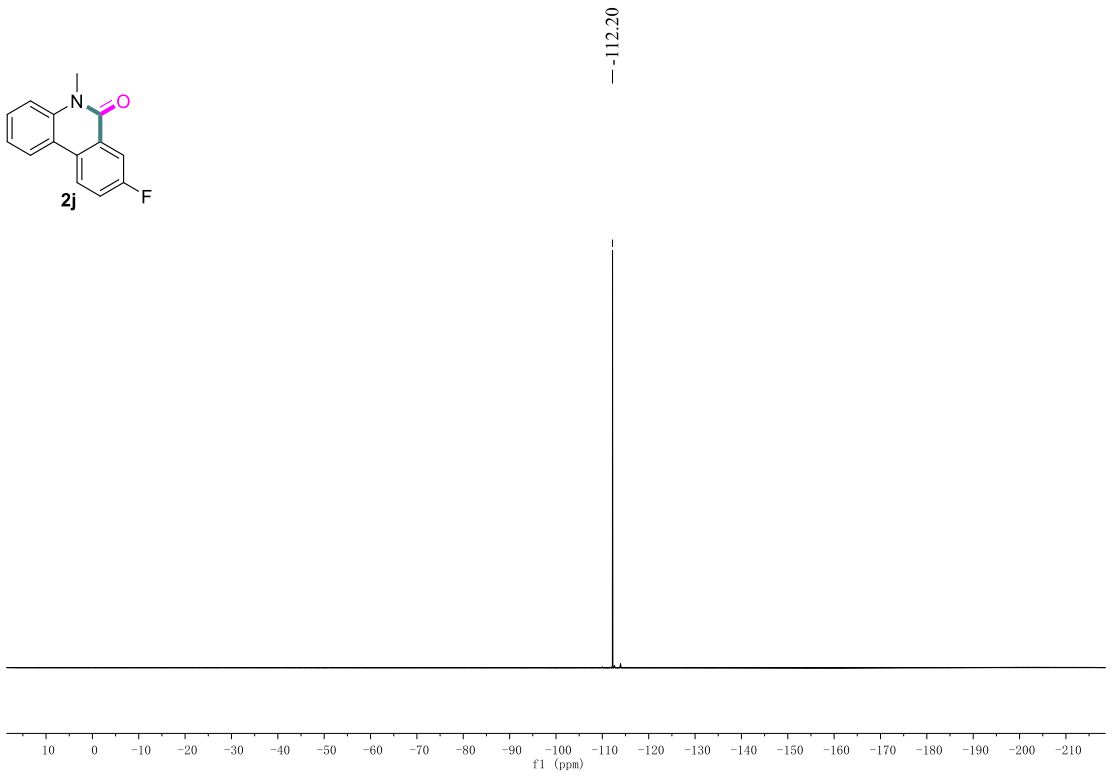
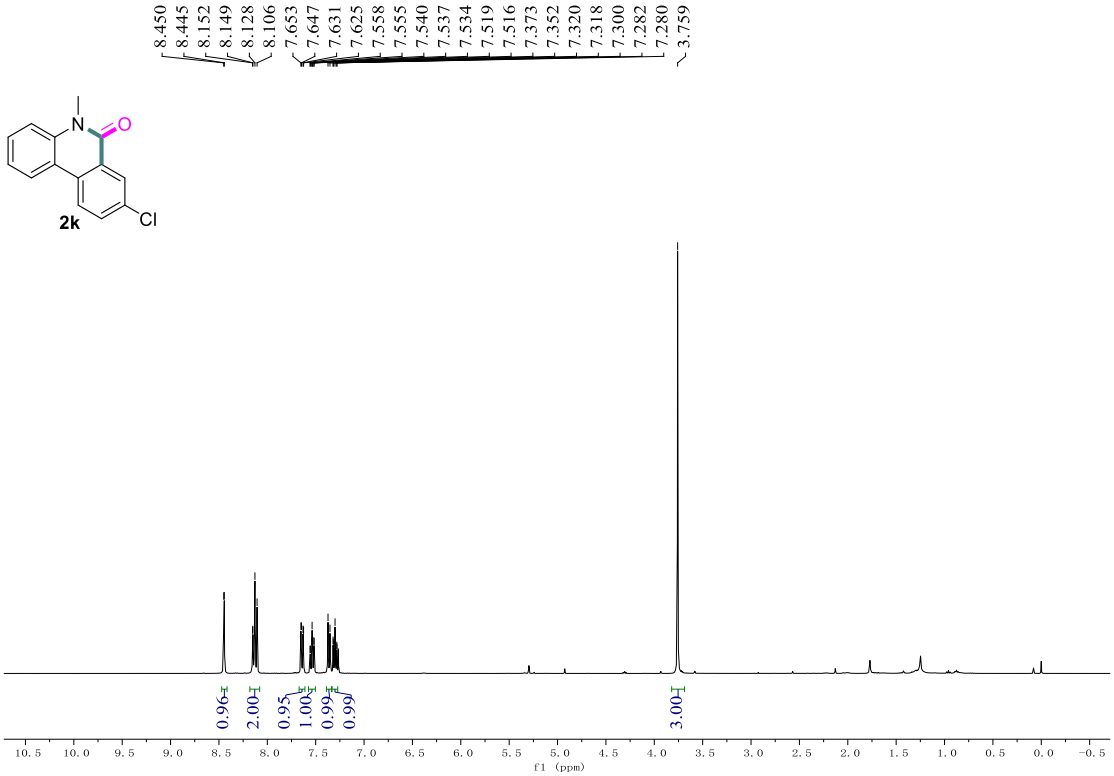
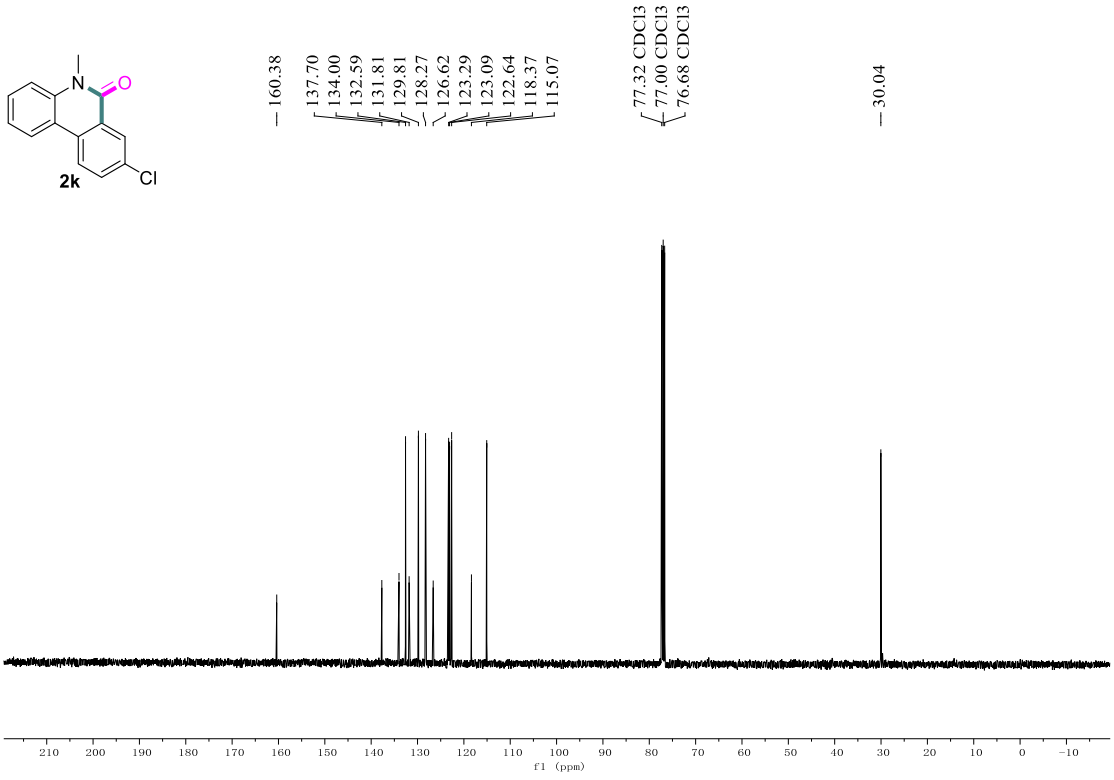
129.92
129.89
129.39
127.37
127.29
124.17
124.09
122.99
122.66
120.81
120.58
118.61
115.09
114.28
114.05
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
30.08
f1 (ppm)


2j
-112.20
f1 (ppm)


8.450
8.445
8.152
8.149
8.128
8.106
7.653
7.647
7.631
7.625
7.558
7.555
7.540
7.537
7.534
7.519
7.516
7.373
7.352
7.320
7.318
7.300
7.282
7.280
3.759
N
O
Cl
2k
0.96
2.00
0.95
1.00
0.99
0.99
3.00
f1 (ppm)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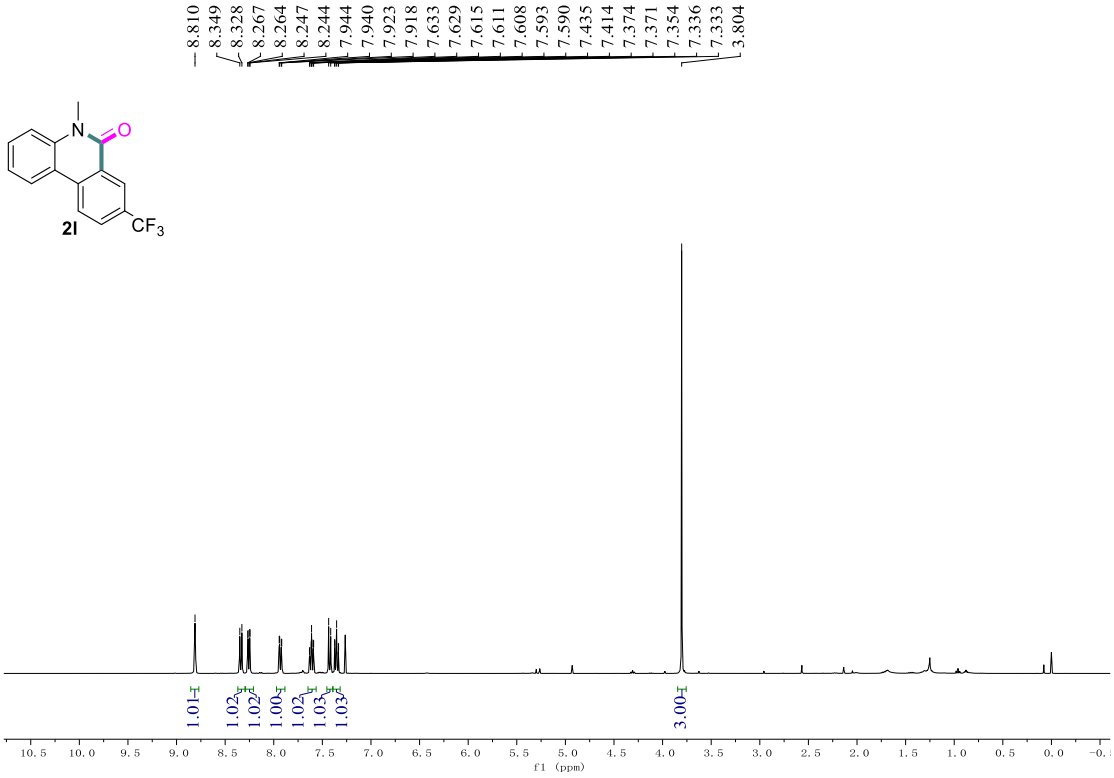
137.70
134.00
132.59
131.81
129.81
128.27
126.62
123.29
123.09
122.64
118.37
115.07
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
30.04
N
O
Cl
2k
f1 (ppm)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8.349
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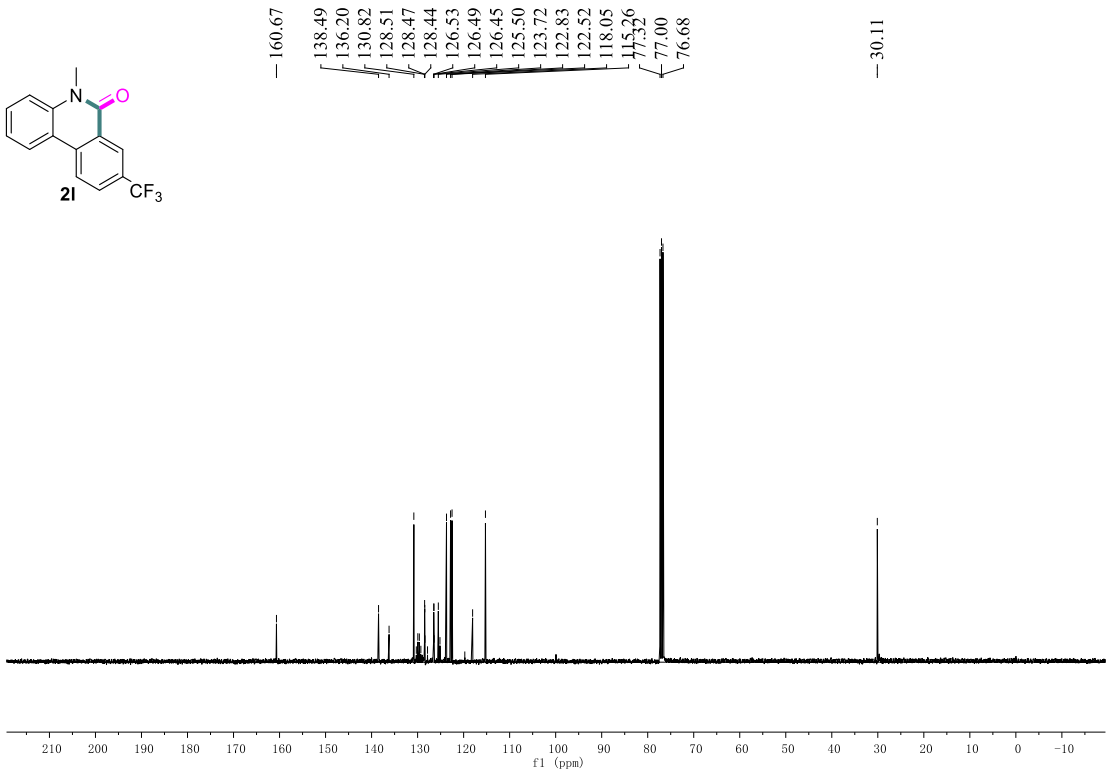
8.267
8.264
8.247
8.244
7.944
7.940
7.923
7.918
7.633
7.629
7.615
7.611
7.608
7.593
7.590
7.435
7.414
7.374
7.371
7.354
7.336
7.333
3.804
2l
CF3
1.01
1.02
1.02
1.00
1.02
1.03
1.03
3.00
f1 (ppm)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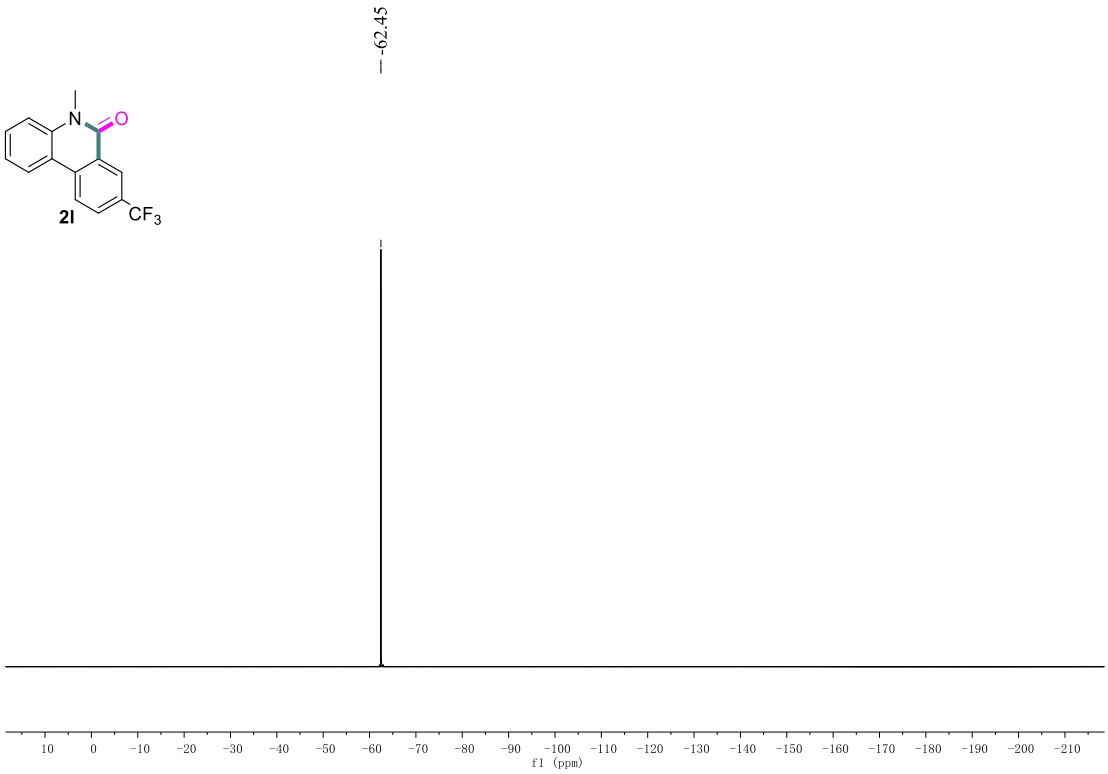
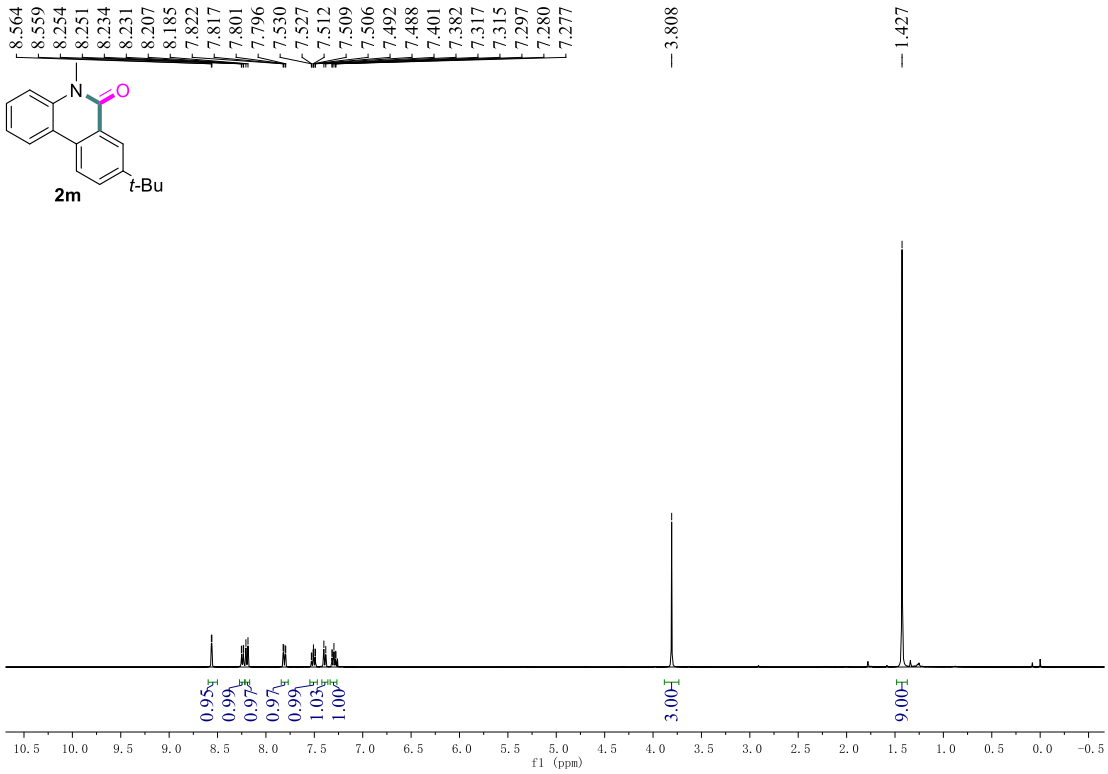
138.49
136.20
130.82
128.51
128.47
128.44
126.53
126.49
126.45
125.50
123.72
122.83
122.52
118.05
115.26
77.32
77.00
76.68
30.11
2l
CF3
f1 (ppm)


-62.45
2l
CF3
f1 (ppm)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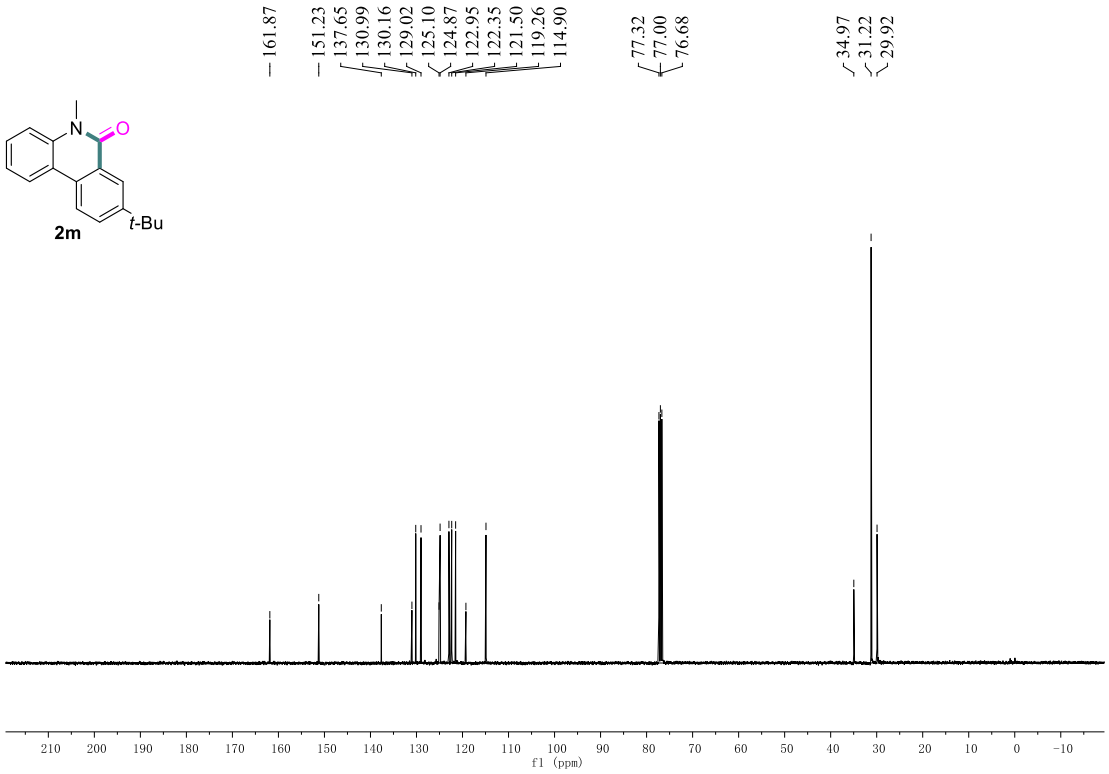
8.251
8.234
8.231
8.207
8.185
7.822
7.817
7.801
7.796
7.530
7.527
7.512
7.509
7.506
7.492
7.488
7.401
7.382
7.317
7.315
7.297
7.280
7.277
3.808
1.427
2m
t-Bu
0.95
0.99
0.97
0.97
0.99
1.03
1.00
3.00
9.00
f1 (ppm)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130.99
130.16
129.02
125.10
124.87
122.95
122.35
121.50
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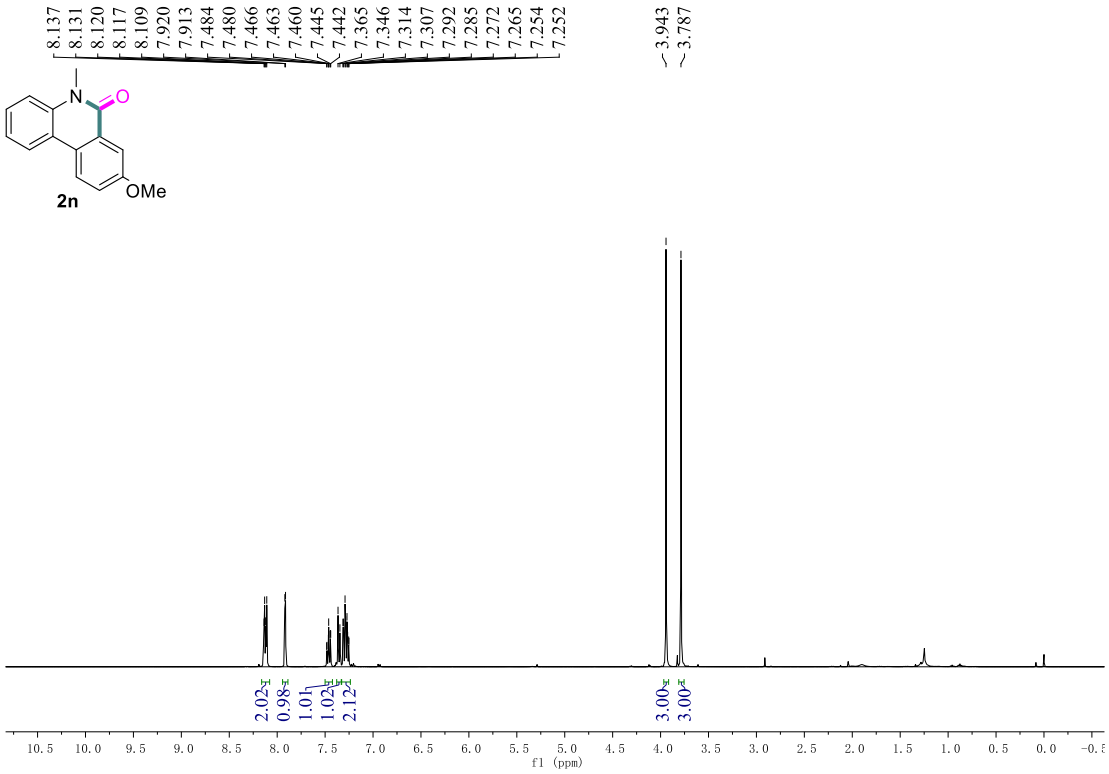
77.00
76.68
34.97
31.22
29.92
N
O
t-Bu
2m
f1 (ppm)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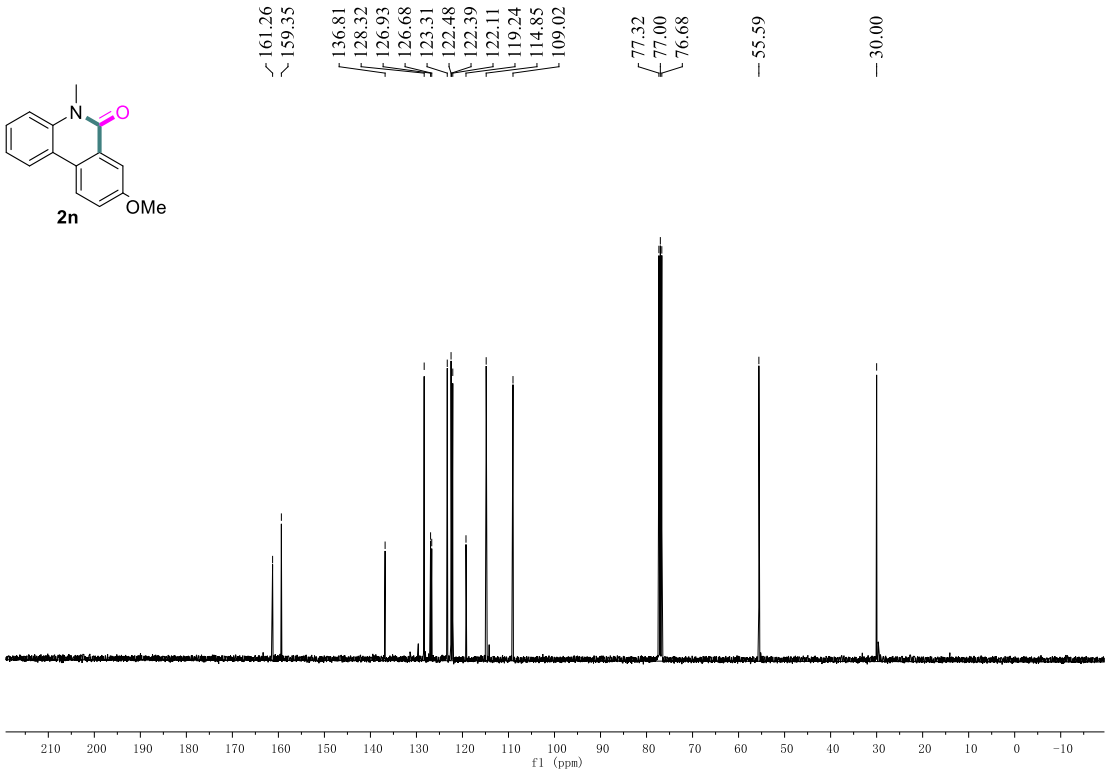
8.131
8.120
8.117
8.109
7.920
7.913
7.484
7.480
7.466
7.463
7.460
7.445
7.442
7.365
7.346
7.314
7.307
7.292
7.285
7.272
7.265
7.254
7.252
3.943
3.787
N
O
OMe
2n
2.02
0.98
1.01
1.02
2.12
3.00
3.00
f1 (ppm)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126.68
123.31
122.48
122.39
122.11
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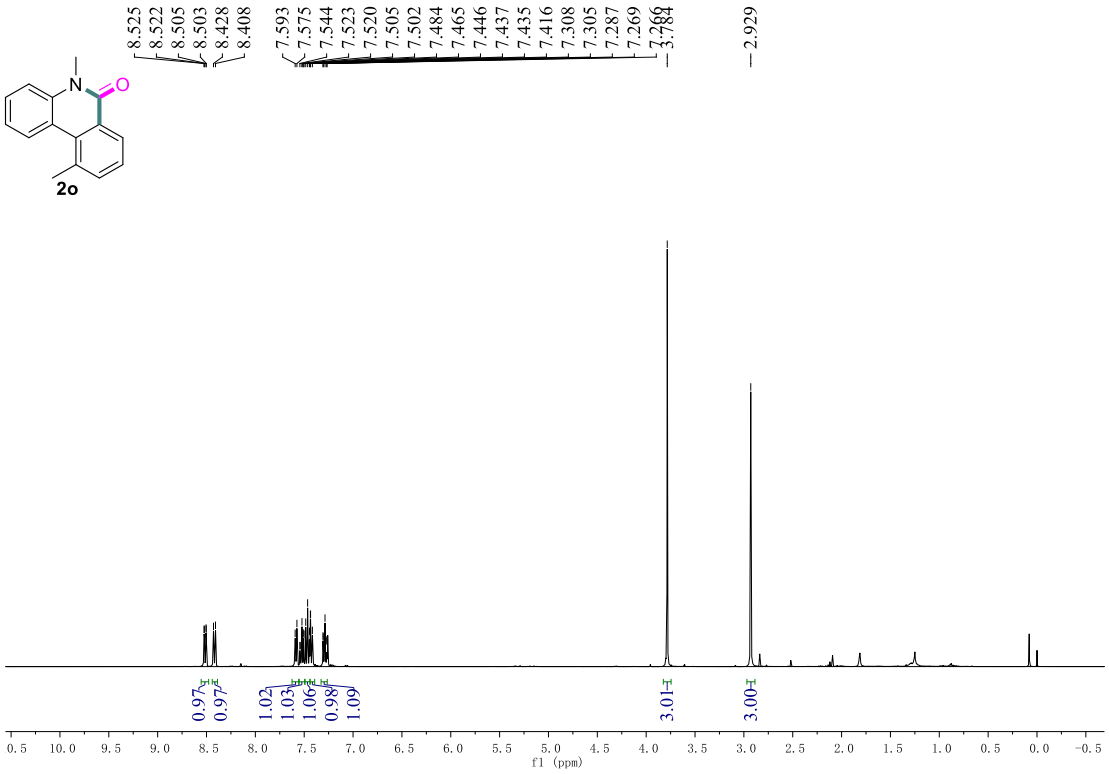
109.02
77.32
77.00
76.68
55.59
30.00
N
O
OMe
2n
f1 (ppm)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8.505
8.503
8.428
8.408
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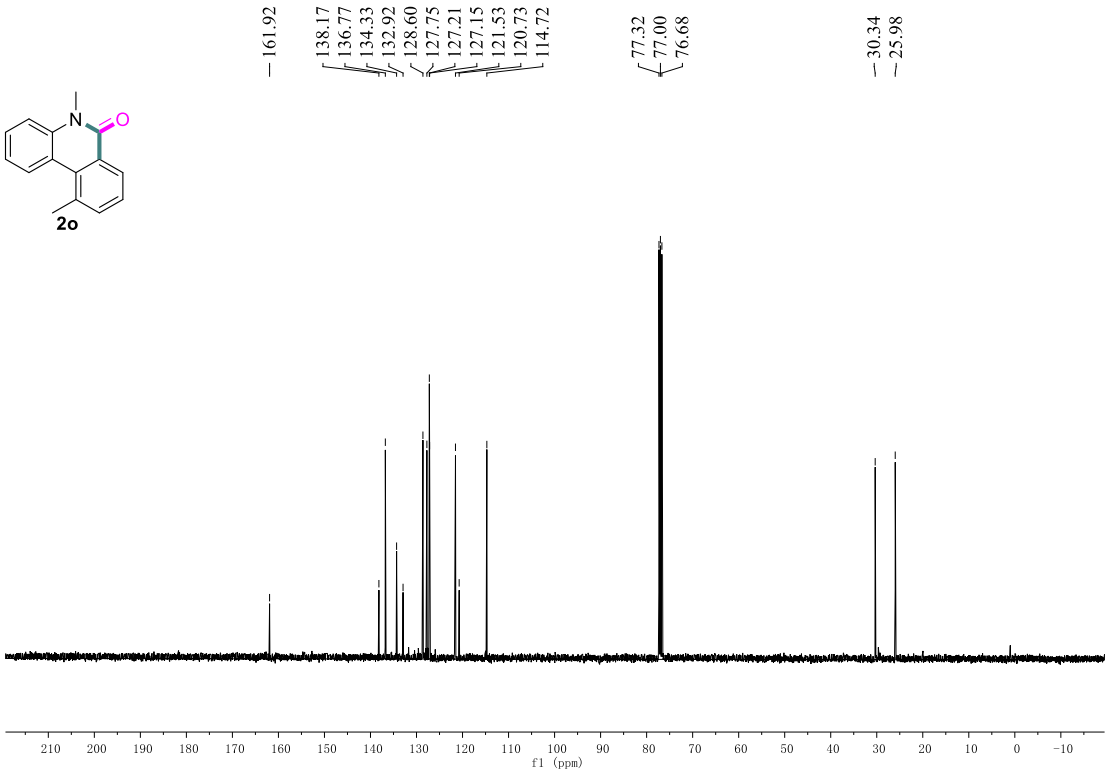
7.575
7.544
7.523
7.520
7.505
7.502
7.484
7.465
7.446
7.437
7.435
7.416
7.308
7.305
7.287
7.269
7.266
3.784
2.929
N
O
2o
0.97
0.97
1.02
1.03
1.06
0.98
1.09
3.01
3.00
f1 (ppm)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120.73
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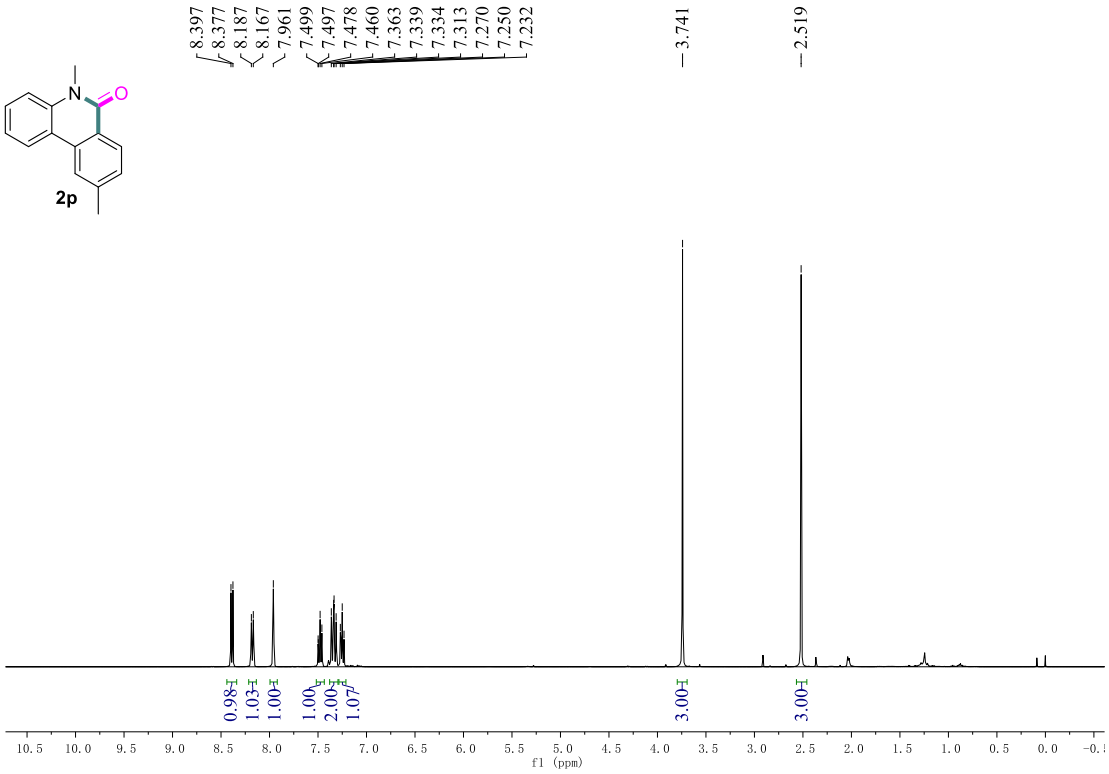
76.68
30.34
25.98
2o
f1 (ppm)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7.478
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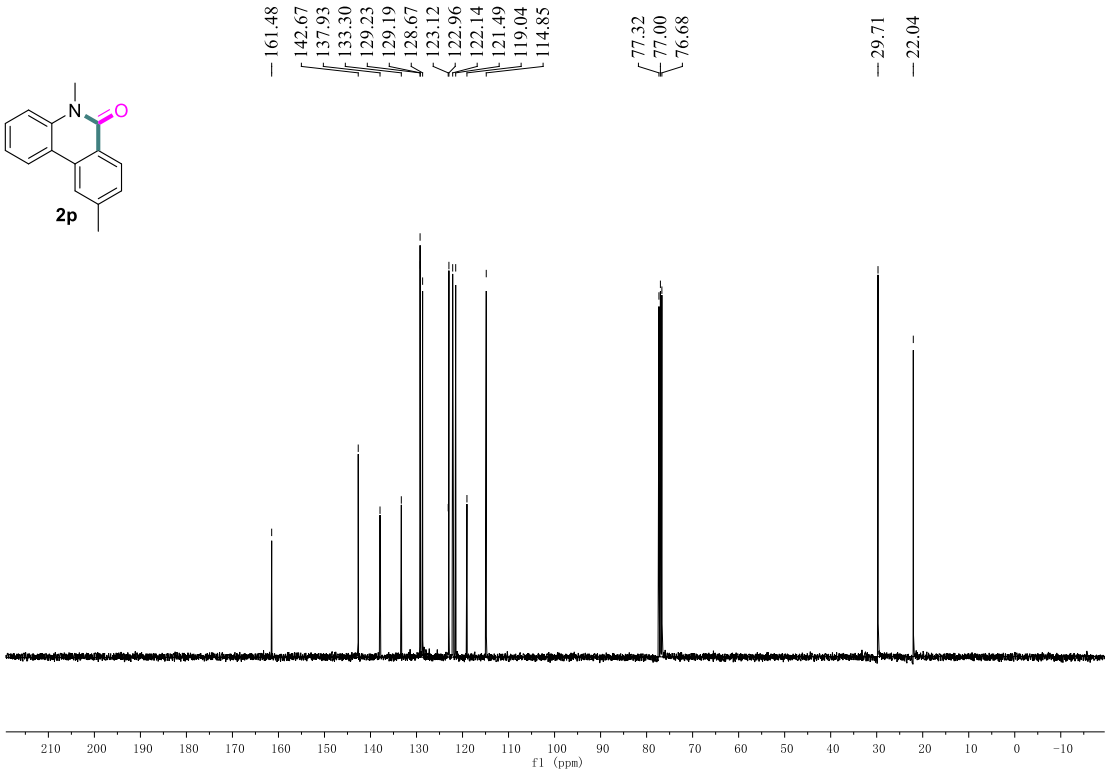
7.334
7.313
7.270
7.250
7.232
3.741
2.519
2p
0.98
1.03
1.00
1.00
2.00
1.07
3.00
3.00
f1 (ppm)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129.23
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128.67
123.12
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121.49
119.04
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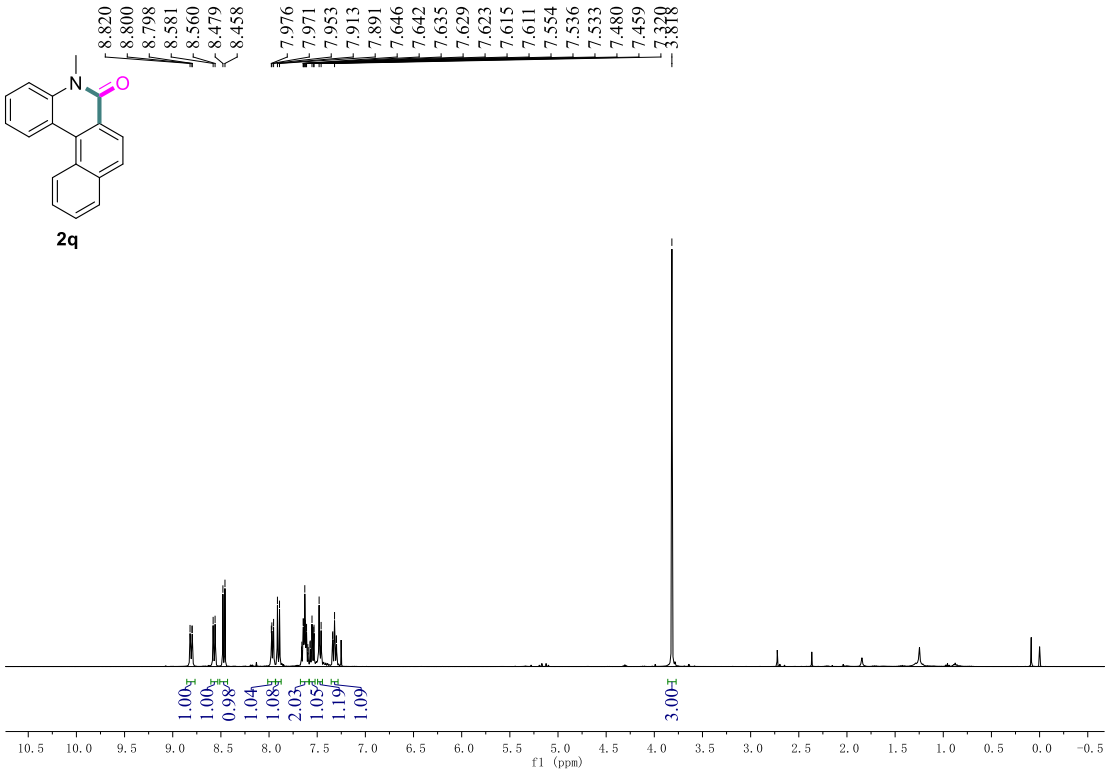
76.68
29.71
22.04
2p
f1 (ppm)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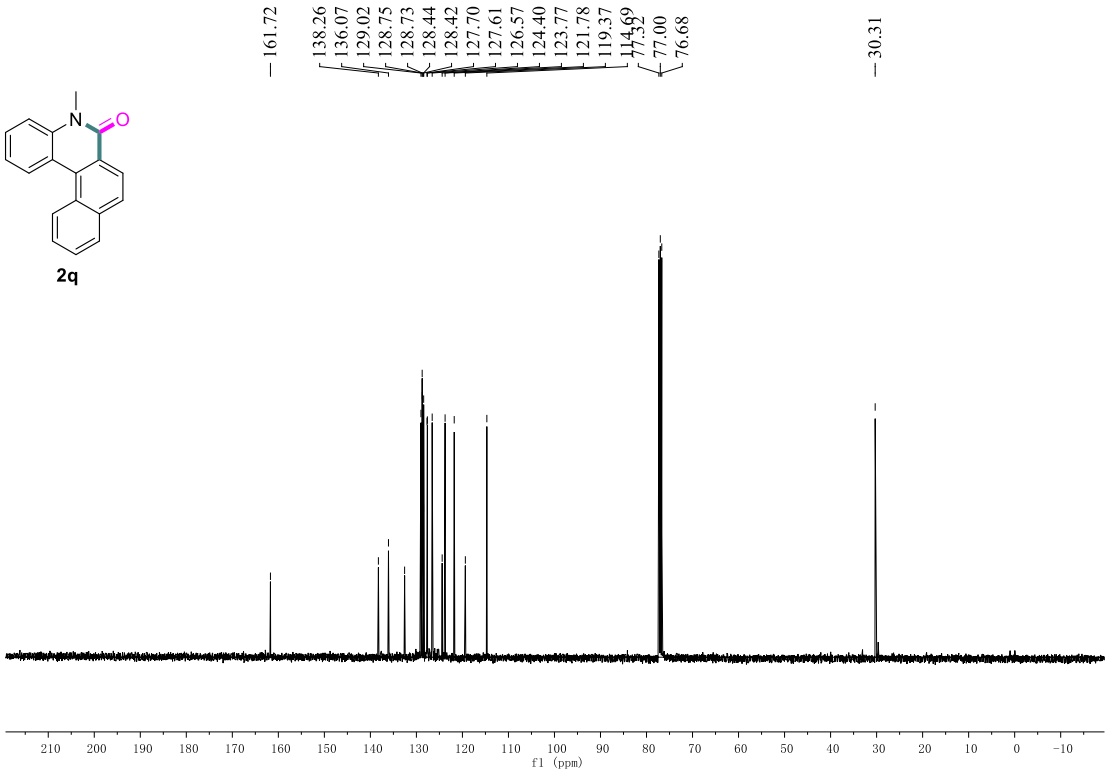
7.646
7.642
7.635
7.629
7.623
7.615
7.611
7.554
7.536
7.533
7.480
7.459
3.818
2q
1.00
1.00
0.98
1.04
1.08
2.03
1.05
1.19
1.09
3.00
f1 (ppm)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128.42
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121.78
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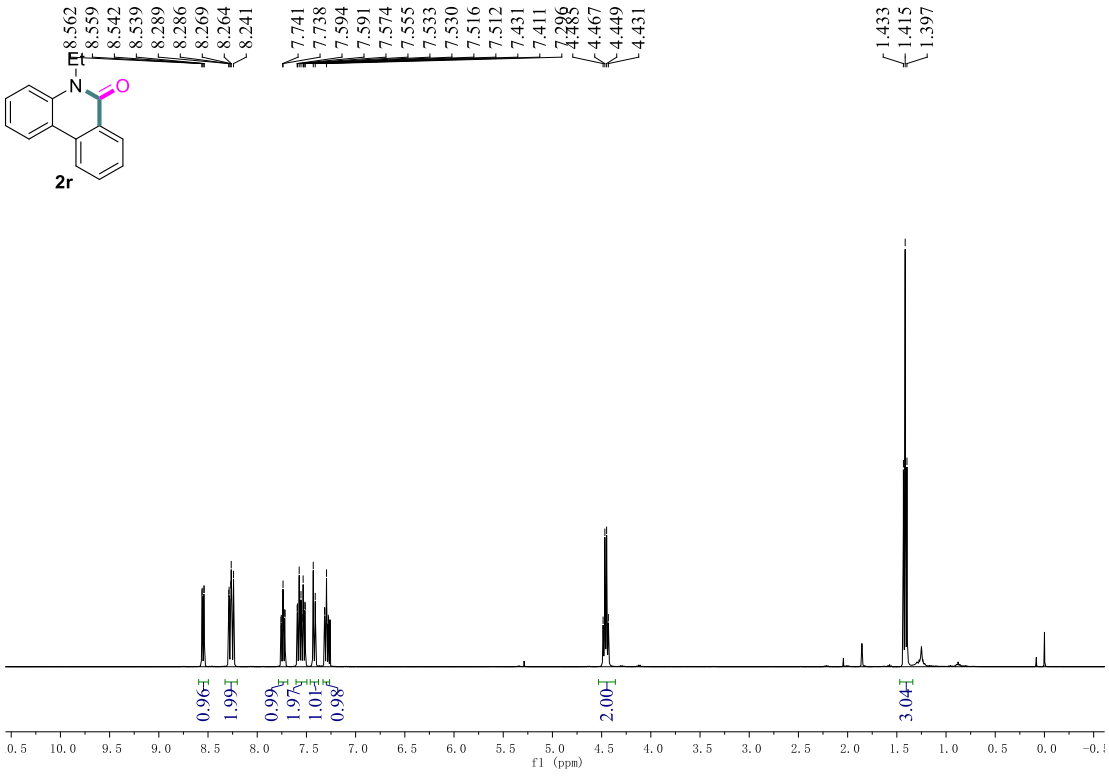
77.32
77.00
76.68
30.31
2q
f1 (ppm)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8.264
8.241
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7.594
7.591
7.574
7.555
7.533
7.530
7.516
7.512
7.431
7.411
4.467
4.449
4.431
1.433
1.415
1.397
Et
2r
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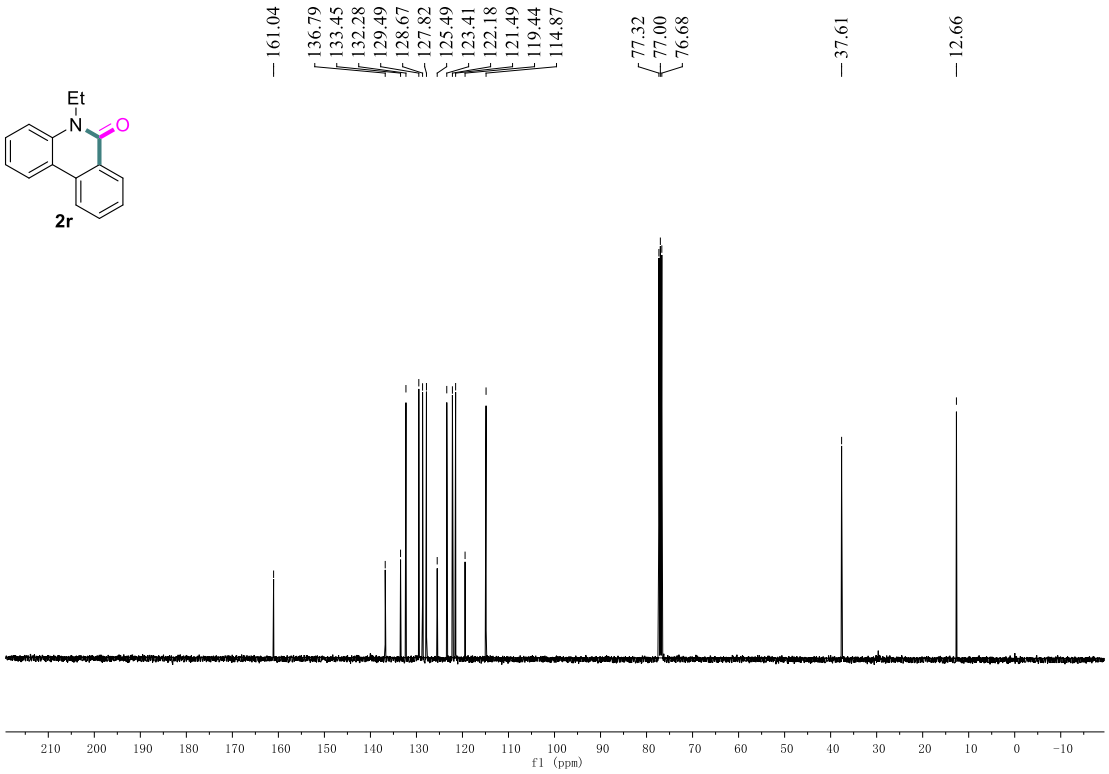
0.99
1.97
1.01
0.98
2.00
3.04
f1 (ppm)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123.41
122.18
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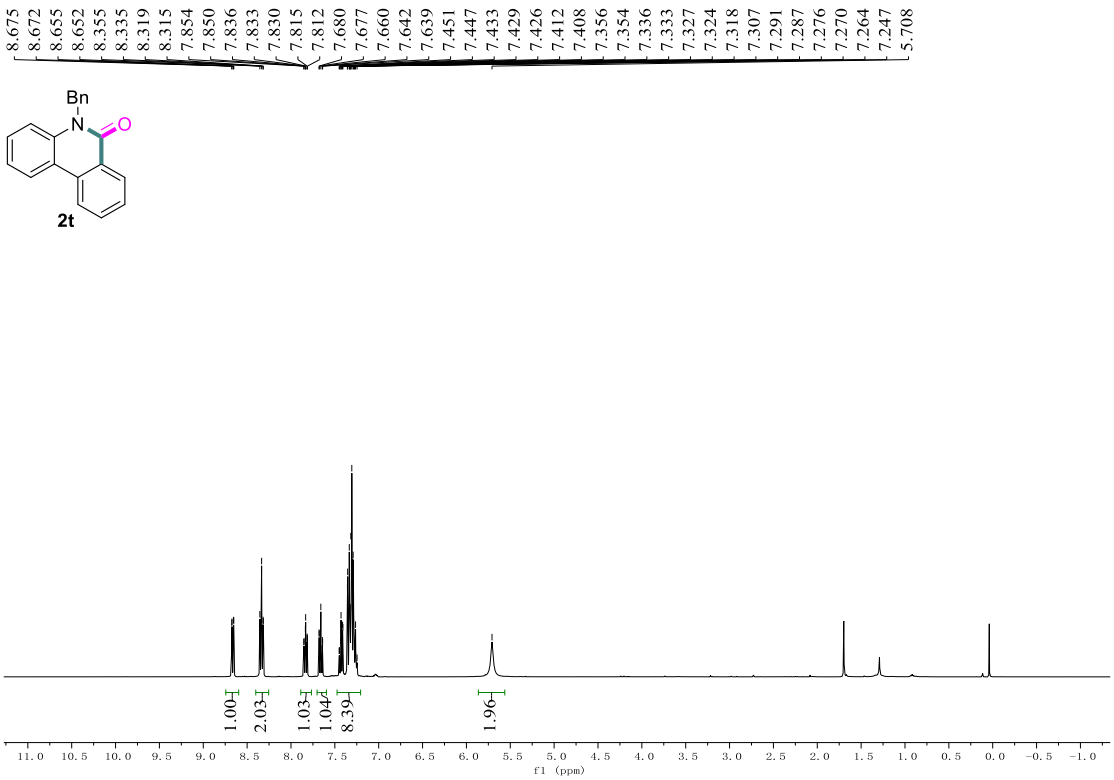
76.68
37.61
12.66
Et
N
O
2r
f1 (ppm)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7.815
7.812
7.680
7.677
7.660
7.642
7.639
7.451
7.447
7.433
7.429
7.426
7.412
7.408
7.356
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7.336
7.333
7.327
7.324
7.318
7.307
7.291
7.287
7.276
7.270
7.264
7.247
5.708
Bn
N
O
2t
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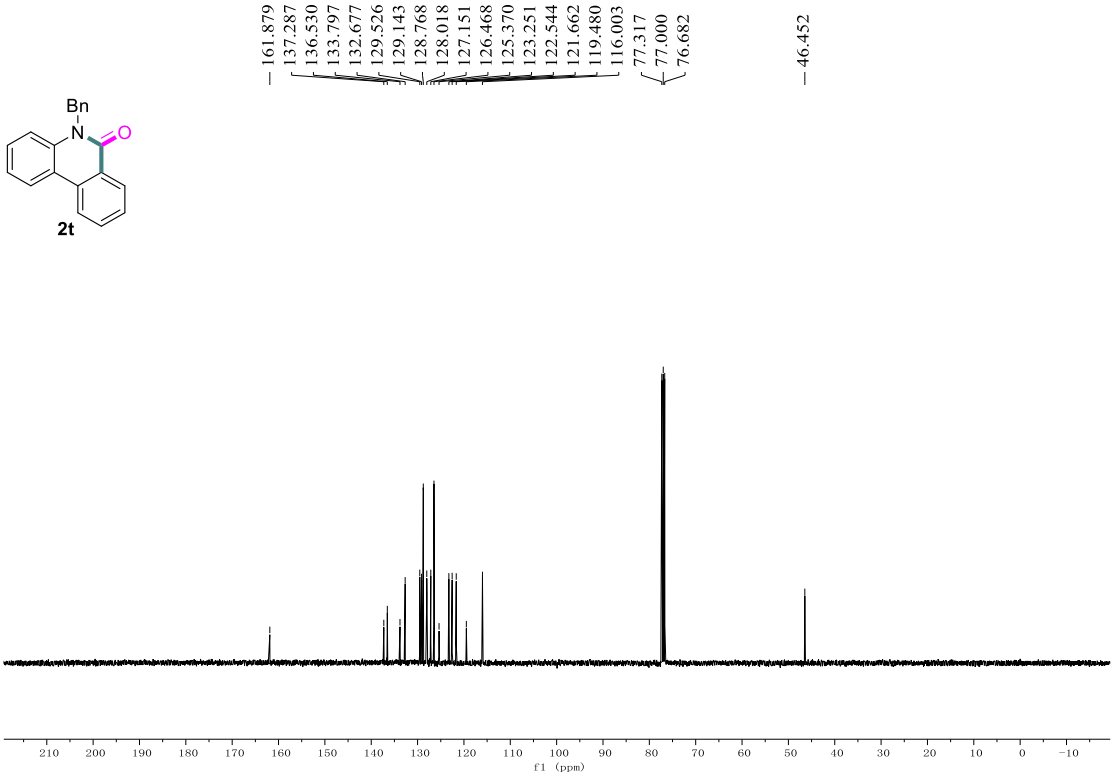
2.03
1.03
1.04
8.39
1.96
f1 (ppm)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126.468
125.370
123.251
122.544
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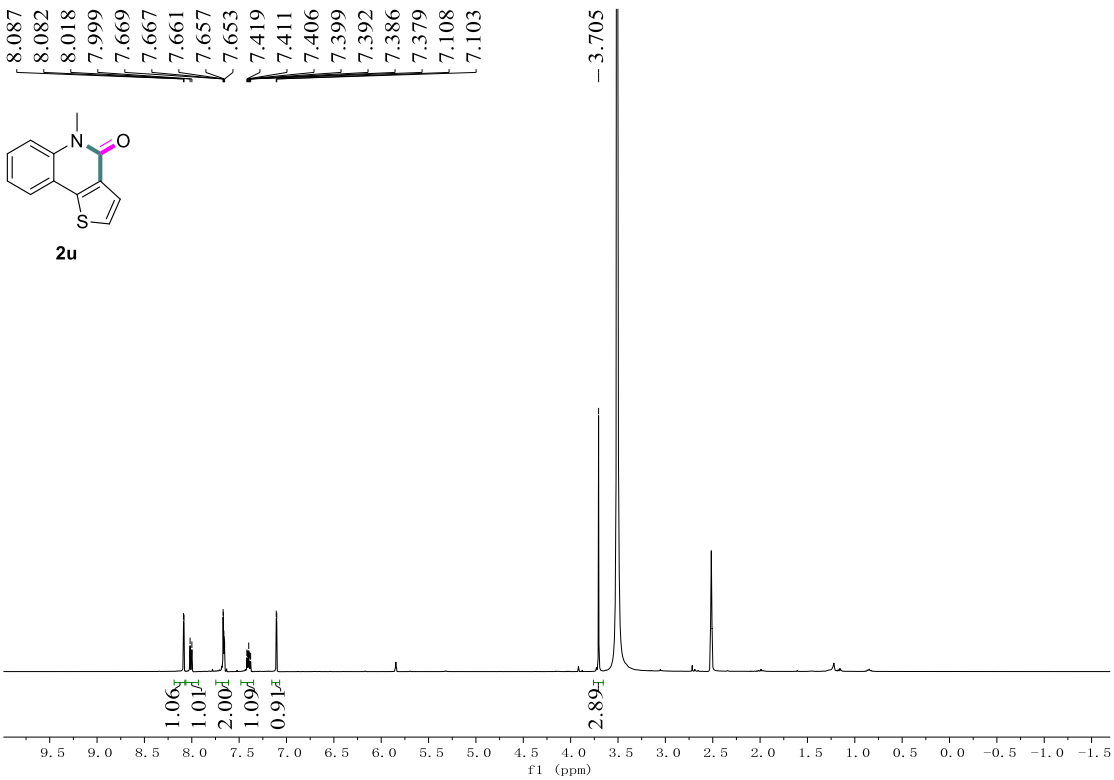
119.480
116.003
77.317
77.000
76.682
46.452
Bn
N
O
2t
f1 (ppm)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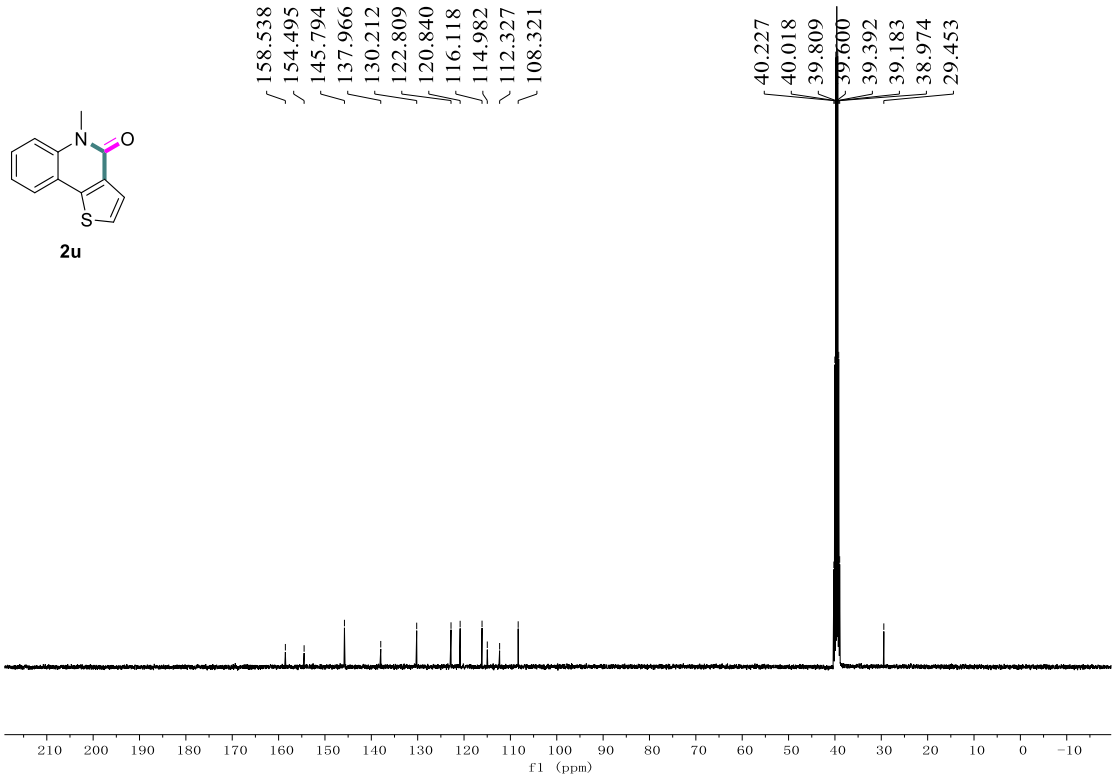
7.411
7.406
7.399
7.392
7.386
7.379
7.108
7.103
3.705
N
O
S
2u
1.06
1.01
2.00
1.09
0.91
2.89
f1 (ppm)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39.809
39.600
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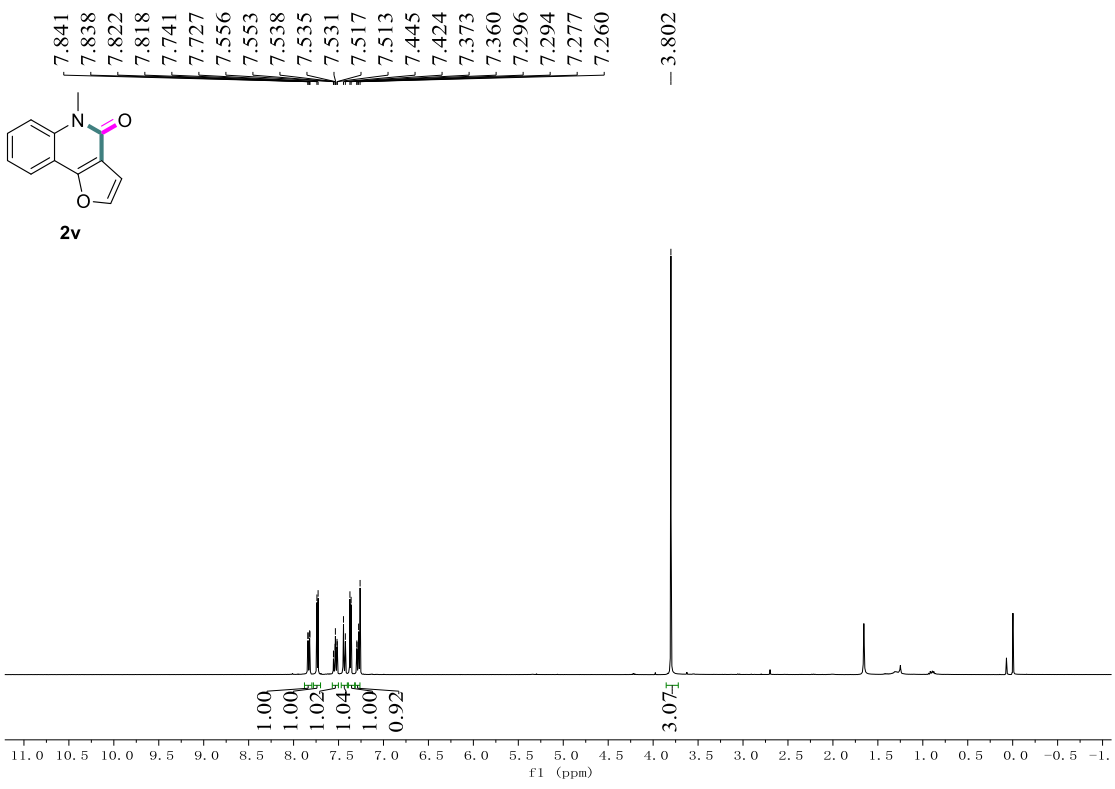
39.183
38.974
29.453
f1 (ppm)

2u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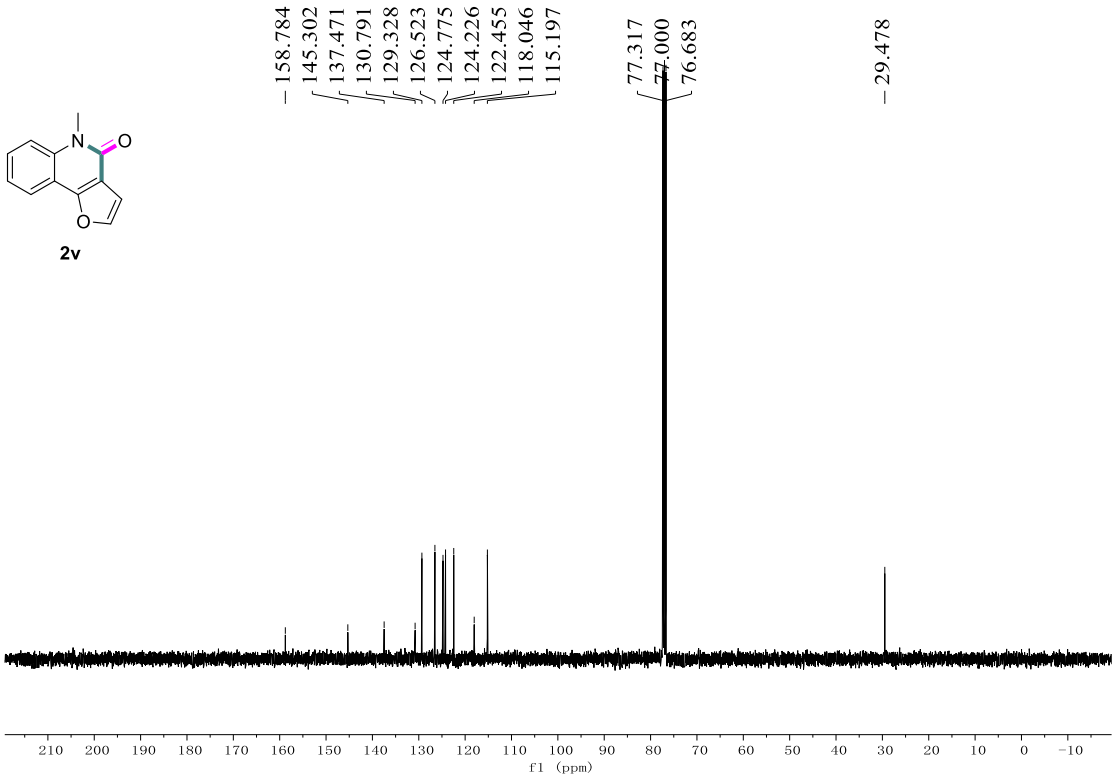
7.513
7.445
7.424
7.373
7.360
7.296
7.294
7.277
7.260
3.802
1.00
1.00
1.02
1.04
1.00
0.92
3.07
f1 (ppm)

2v



8. Reference

[1] Krishna Kumar, Ronald Tepper, Yang Zeng, and Matthew Zimmt, *J. Org. Chem*. **1996**, *60*, 4051-4066