Supporting information for

Synthesis of 2,4-diarylsubstituted-pyridines through Ru-catalyzed four component reaction

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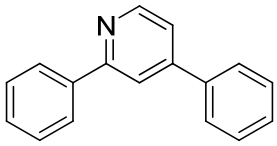
General information:

All experiments were carried out under an atmosphere of oxygen. Flash column chromatography was performed over silica gel 48-75 μm. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to $SiMe_4$ or chloroform signals. MS analyses were performed on an Agilent5975 GC-MS instrument (EI). The new compounds were characterized by ^{1}H NMR, ^{13}C NMR, MS, HRMS. Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Ruthenium salts and acetophenones **1a**, **1b**, **1e**, **1i**, **1j**, **1k**, **1l**, **1n**, **1p** were purchased from Aladdin, **1c**, **1d**, **1f**, **1g**, **1h**, **1m**, **1o**, **1q**, **1r** were purchased from Accela. All of these were used as received without further purification.

General procedure for synthesis of diarylpyridine (2a):

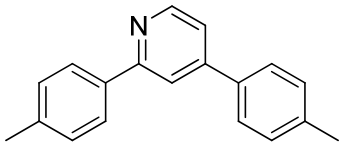
A 20 mL reaction vessel was charged with $RuCl_3{\cdot}3H_2O$ (2.6 mg, 0.01 mmol), acetophenone (**1a**, 48 μ L, 0.4 mmol), NH_4OAc (46.2 mg, 0.6 mmol). The sealed reaction vessel was purged with oxygen three times. DMF (0.5 mL) was added to the sealed reaction vessel by syringe. The resulting solution was stirred at 120 ^{o}C for 24 h. After cooling to room temperature, the volatiles were removed under vacuum and the residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give 36.8 mg **2a** as pale yellow oil; yield 80%.

2,4-Diphenylpyridine(2a)[1]



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.74 (d, J = 5.2 Hz, 1H), 8.05 (d, J = 7.6 Hz, 2H), 7.93 (s, 1H), 7.70 (m, 2H), 7.53–7.42 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.1, 150.1, 149.3, 139.5, 138.6, 138.6, 129.1, 129.0, 128.7, 127.1, 127.0, 120.3, 118.7; MS (EI) m/z (%) 231 (100), 202, 154, 102, 77.

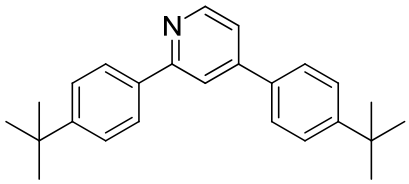
2,4-Diptolylpyridine (2b) [1]



The reaction was conducted with 1-p-tolylethanone (**1b**, 53.7 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2b** as off-white solid; yield 76%; mp 105-107 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 5.2 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.89 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 4.0 Hz, 1H), 7.32-7.30 (m, 4H), 2.43 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) *δ* 158.0, 149.9, 149.0, 139.0, 138.9, 136.7, 135.6, 129.7, 129.4, 126.8, 126.8, 119.7, 118.1, 21.2, 21.1; MS (EI) m/z (%) 259 (100), 244, 115, 91, 77.

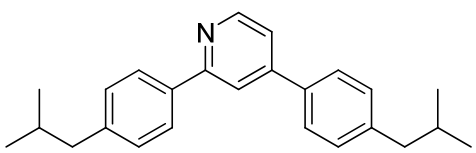
2,4-Bis(4-*tert*-butylphenyl)pyridine (2c)



The reaction was conducted with 1-(4-*tert*-butylphenyl)ethanone (**1c**, 70.5 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2c** as off-white solid; yield 70%; mp 83-86 ℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 5.2 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 2H), 7.91 (s, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.54-7.50 (m, 4H), 7.41 (d, *J* = 5.2 Hz, 1H), 1.38 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) *δ* 158.0, 152.3, 152.1, 149.9, 149.0, 136.8, 135.7, 126.7, 126.0, 125.7, 119.8, 118.3, 34.7, 34.7, 31.3, 31.3; MS (EI) m/z (%) 343, 328 (100), 312, 128, 77; HRMS calcd. for: $C_{25}H_{29}N$ $[M+H]^+$ 344.2373, found 344.2372.

2,4-Bis(4-isobutylphenyl)pyridine (2d)

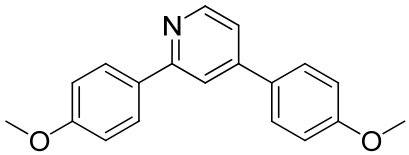


The reaction was conducted with 1-(4-isobutylphenyl)ethanone (**1d**, 70.5 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane =

3:1) to give **2d** as off-white solid; yield 68%; mp 90-93 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (d, J = 5.2 Hz, 1H), 7.95 (d, J = 8.0 Hz, 2H), 7.91 (s, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 4.8 Hz, 1H), 7.29-7.26 (m, 4H), 2.54 (d, J = 6.0 Hz, 4H), 1.95-1.89 (m, 2H), 0.95-0.93 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.1, 149.9, 149.1, 142.9, 142.7, 137.1, 135.9, 129.8, 129.5, 126.8, 126.7, 119.7, 118.2, 45.2, 45.1, 30.2, 30.2, 22.4; MS (EI) m/z (%) 343, 300 (100), 257, 91, 77; HRMS calcd. for: $C_{25}H_{29}N$ $[M+H]^+$ 344.2372, found 344.2372.

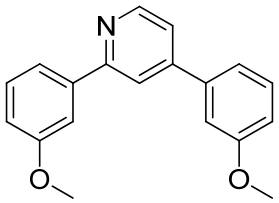
2,4-Bis(4-methoxyphenyl)pyridine (2e) [1]



The reaction was conducted with 1-(4-methoxyphenyl)ethanone (**1e**, 60.1 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2e** as off-white solid; yield 65%; mp 133-135 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.65 (d, J = 4.8 Hz, 1H), 8.01 (d, J = 8.8 Hz, 2H), 7.83 (s, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 4.0 Hz, 1H), 7.04-7.01 (m, 4H), 3.88 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.5, 157.6, 149.9, 148.6, 132.2, 130.9, 129.8, 128.2, 128.1, 119.0, 117.3, 114.5, 114.1, 55.3, 55.3; MS (EI) m/z (%) 291 (100), 276, 204, 145, 77.

2,4-Bis(3-methoxyphenyl)pyridine (2f) [1]

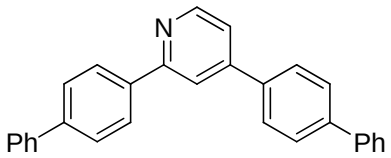


The reaction was conducted with 1-(3-methoxyphenyl)ethanone (**1f**, 60.1 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2f** as orange oil; yield 68%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, J = 4.8 Hz, 1H), 7.90 (s, 1H), 7.63-7.59 (m, 2H), 7.44-7.38 (m, 3H), 7.28 (s, 1H), 7.20 (s, 1H), 7.00-6.98 (m, 2H), 3.91 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.2, 160.1, 157.9, 149.9, 149.2, 140.9, 140.0, 130.1, 129.7,

120.4, 119.5, 119.4, 118.9, 115.1, 114.3, 112.9, 112.2, 55.4, 55.3; MS (EI) m/z (%) 291 (100), 261, 204, 145, 77.

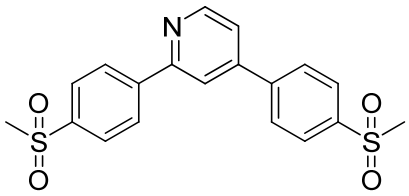
2,4-Di(biphenyl-4-yl)pyridine (2g) [1]



The reaction was conducted with 1-(biphenyl-4-yl)ethanone (**1g**, 78.5 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2g** as a light-yellow solid; yield 48%; mp 176-178 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.78 (d, J = 4.0 Hz, 1H), 8.16 (d, J = 7.2 Hz, 2H), 8.03 (s, 1H), 7.82-7.68 (m, 10H), 7.49-7.38 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.7, 150.2, 148.8, 141.9, 141.8, 140.5, 140.2, 138.3, 137.3, 128.9, 128.8, 127.8, 127.7, 127.5, 127.4, 127.4, 127.1, 120.1, 118.5.

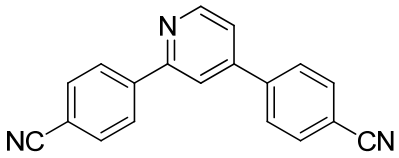
2,4-Bis(4-(methylsulfonyl)phenyl)pyridine (2h)



The reaction was conducted with 1-(4-(methylsulfonyl)phenyl)ethanone (**1h**, 79.3 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 1:1) to give **2h** as a yellow solid; yield 57%; mp 248-249 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.86 (d, J = 4.8 Hz, 1H), 8.28 (d, J = 8.0 Hz, 2H), 8.13-8.08 (m, 4H), 7.99 (s, 1H), 7.89 (d, J = 8.0 Hz, 2H), 7.56 (d, J = 4.8 Hz, 1H), 3.13 (s, 3H), 3.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.3, 150.8, 147.8, 144.1, 143.6, 141.2, 141.0, 128.8, 128.4, 128.2, 128.0, 121.5, 119.4, 44.6, 44.5; HRMS calcd. for: $C_{19}H_{18}O_4NS_2$ $[M+H]^+$ 388.0672, found 388.0667.

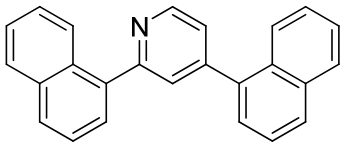
4,4'-(Pyridine-2,4-diyl)dibenzonitrile (2i)



The reaction was conducted with 4-acetylbenzonitrile (**1i**, 58.1 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2i** as pale yellow solid; yield 45%; mp 175-178 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.84 (d, J = 4.2 Hz, 1H), 8.26-8.17 (m, 2H), 7.94 (s, 1H), 7.84-7.80 (m, 6H), 7.52 (d, J = 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.2，150.7, 147.7, 142.9, 138.2, 132.9, 132.5, 132.5, 127.8, 127.5, 127.4, 121.2, 120.2, 118.9, 118.2; MS (EI) m/z (%) 281 (100), 252, 179, 127, 75; HRMS calcd. for: $C_{19}H_{11}N_3$ $[M+H]^+$ 282.1026, found 282.1024.

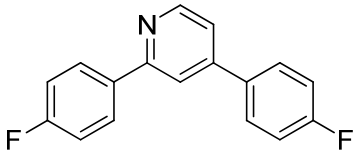
2,4-Di(naphthalen-1-yl)pyridine (2j)



The reaction was conducted with 1-(naphthalen-1-yl)ethanone (**1j**, 68.1 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2j** as a yellow solid; yield 38%; mp 112-114 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.92 (d, J = 4.8 Hz, 1H), 8.26 (d, J = 2.4 Hz, 1H), 8.01-7.92 (m, 5H), 7.77 (s, 1H), 7.70 (d, J = 6.8 Hz, 1H), 7.71-7.51 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) 159.3, 149.5, 149.2, 138.3, 137.4, 134.0, 133.8, 131.2, 130.8, 129.1, 128.9, 128.5, 128.4, 127.7, 127.0, 126.7, 126.6, 126.3, 126.2, 125.9, 125.4, 125.3, 125.2, 123.4; MS (EI) m/z (%) 330 (100), 204, 176, 164, 151; HRMS calcd. for: $C_{25}H_{18}N$ $[M+H]^+$ 332.1434, found 332.1429.

2,4-Bis(4-fluorophenyl)pyridine (2k)

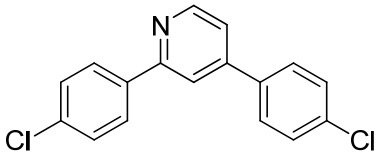


The reaction was conducted with 1-(4-fluorophenyl)ethanone (**1k**, 55.3 mg, 0.4 mmol). The

residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2k** as orange oil; yield 60%; mp 83-85 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.71 (d, J = 4.8 Hz, 1H), 8.05-8.01 (m, 2H), 7.83 (s, 1H), 7.68-7.65 (m, 2H), 7.40 (d, J = 4.8 Hz, 1H), 7.22-7.16 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 163.7 (d, J = 247.2 Hz), 163.5 (d, J = 247.9 Hz), 157.2, 150.2, 148.4, 135.6 (d, J = 3.1 Hz), 134.6 (d, J = 3.4 Hz), 128.9 (d, J = 1.3 Hz), 128.8 (d, J = 1.3 Hz), 120.0, 118.2, 116.2 (d, J = 21.6 Hz), 115.6 (d, J = 21.5 Hz); MS (EI) m/z (%) 267 (100), 238, 172, 120, 75; HRMS calcd. for: $C_{17}H_{11}F_2N$ $[M+H]^+$ 268.0932, found 268.0933.

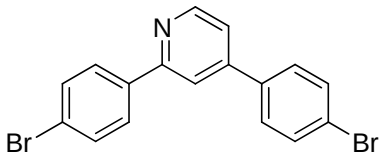
2,4-Bis(4-chlorophenyl)pyridine (2l) [1]



The reaction was conducted with 1-(4-chlorophenyl)ethanone (**1l**, 61.8 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2l** as red-brown solid; yield 65%; mp 103-105 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, J = 4.8 Hz, 1H), 7.99 (d, J = 8.0 Hz, 2H), 7.85 (s, 1H), 7.62 (d, J = 8.4 Hz, 2H), 7.50-7.41 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.9, 150.2, 148.1, 137.6, 136.7, 135.4, 135.3, 129.3, 128.9, 128.3, 128.2, 120.1, 118.1; MS (EI) m/z (%) 299 (100), 264, 202, 114, 75.

2,4-Bis(4-bromophenyl)pyridine (2m) [1]

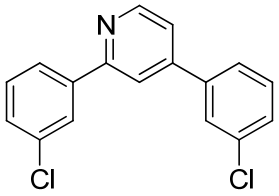


The reaction was conducted with 1-(4-bromophenyl)ethanone (**1m**, 79.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2m** as orange solid; yield 64%; mp 136-138 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.73 (d, J = 5.2 Hz, 1H), 7.93 (d, J = 8.4 Hz, 2H), 8.51 (s, 1H), 7.66-7.62 (m, 4H), 7.55 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 4.8 Hz, 1H); ^{13}C NMR (100 MHz,

$CDCl_3$, ppm) δ 157.0, 150.3, 148.2, 138.1, 137.2, 132.3, 131.9, 128.6, 128.5, 123.6, 123.6, 120.2, 118.1; MS (EI) m/z (%) 389 (100), 310, 228, 114, 75.

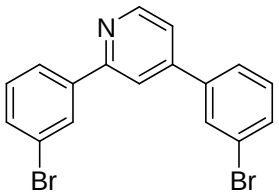
2,4-Bis(3-chlorophenyl)pyridine (2n)



The reaction was conducted with 1-(3-chlorophenyl)ethanone (**1n**, 61.8 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2n** as red-brown solid; yield 66%; mp 95-97 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.75 (d, J = 4.8 Hz, 1H), 8.06 (s, 1H), 7.94-7.92 (dd, J = 3.6 Hz, 2.4Hz, 1H), 7.86 (s, 1H), 7.67 (s, 1H), 7.57-7.55 (dd, J = 2.8 Hz, 4.0 Hz, 1H), 7.45-7.42 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.7, 150.2, 148.0, 140.9, 140.1, 135.1, 134.9, 130.4, 130.0, 129.1, 127.2, 127.2, 125.2, 125.0, 120.6, 118.6, 118.5; MS (EI) m/z (%) 299 (100), 264, 202, 114, 75; HRMS calcd. for: $C_{17}H_{11}Cl_2N$ $[M+H]^+$ 300.0341, found 300.0342.

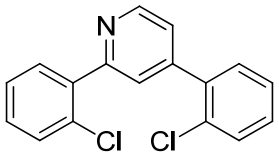
2,4-Bis(3-bromophenyl)pyridine (2o) [1]



The reaction was conducted with 1-(3-chlorophenyl)ethanone (**1o**, 79.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2o** as red-brown solid; yield 66%; mp 89-91 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.76 (d, J = 4.4 Hz, 1H), 8.22 (s, 1H), 7.98 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 10.0 Hz, 2H), 7.62-7.57 (m, 3H), 7.45-7.36 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.8, 150.5, 147.2, 138.8, 138.0, 133.6, 133.7, 131.2, 130.7, 128.9, 128.9, 127.2, 126.2, 126.0, 120.6, 118.1, 109.9; MS (EI) m/z (%) 389 (100), 310, 228, 114, 75.

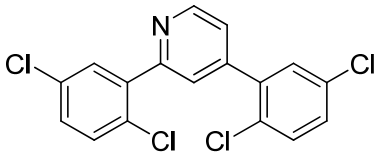
2,4-Bis(2-chlorophenyl)pyridine (2p)



The reaction was conducted with 1-(2-chlorophenyl)ethanone (**1p**, 61.8 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2p** as red-brown oil; yield 38%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.78 (d, J = 4.8 Hz, 1H), 7.76 (s, 1H), 7.68-7.66 (m, 1H), 7.53-7.48 (m, 2H), 7.40-7.33 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.8, 149.34, 146.9, 139.1, 135.4, 132.3, 131.7, 131.0, 130.3, 130.1, 129.8, 129.7, 129.3, 127.2, 127.0, 125.5, 123.0; MS (EI) m/z (%) 299 (100), 264, 202, 114, 75; HRMS calcd. for: $C_{17}H_{11}Cl_2N$ $[M+H]^+$ 300.0341, found 300.0342.

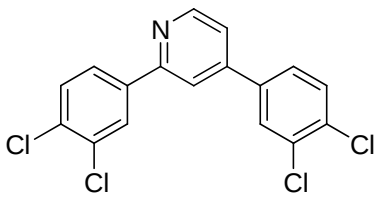
2,4-Bis(2,5-dichlorophenyl)pyridine (2q)



The reaction was conducted with 1-(2,4-dichlorophenyl)ethanone (**1q**, 75.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane = 3:1) to give **2q** as red-brown solid; yield 40%; mp 161-163 ℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.80 (d, J = 4.8 Hz, 1H), 7.73 (s, 1H), 7.681 (d, J = 2.4 Hz, 1H), 7.47-7.32 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.7, 149.7, 146.0, 140.1, 139.0, 133.1, 133.1, 131.6, 131.4, 131.3, 130.7, 130.6, 130.5, 129.9, 129.8, 125.1, 123.1; MS (EI) m/z (%) 299 (100), 264, 202, 114, 75; HRMS calcd. for: $C_{17}H_9Cl_4N$ $[M+H]^+$ 367.9562, found 367.9562.

2,4-Bis(3,4-dichlorophenyl)pyridine (2r)

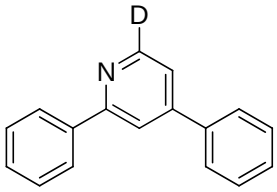


The reaction was conducted with 1-(3-chlorophenyl)ethanone (**1r**, 75.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/dichloromethane =

3:1) to give **2r** as red-brown solid; yield 70%; mp 130-133 ℃.

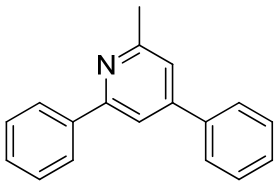
^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.76 (d, J = 4.8 Hz, 1H), 8.184 (s, 1H), 7.896 (d, J = 8.0 Hz, 1H), 7.83 (s, 1H), 7.77 (s, 1H), 7.61-7.51 (m, 3H), 7.44 (d, J = 4.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.6, 150.3, 148.0, 141.2, 140.3, 132.1, 132.1, 130.7, 130.3, 130.1, 130.1, 125.7, 125.5, 123.3, 123.1, 120.7, 118.6; MS (EI) m/z (%) 369, 334 (100), 261, 148, 75; HRMS calcd. for: $C_{17}H_9Cl_4N$ $[M+H]^+$ 367.9562, found 367.9558.

2,4-Diphenyl-6-D-pyridine (2s)



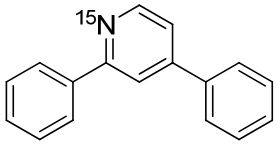
^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05 (d, J = 7.6 Hz, 2H), 7.94 (s, 1H), 7.71 (d, J = 7.2 Hz, 2H), 7.54-7.46 (m, 7H).

2-Methyl-4,6-diphenylpyridine (2t)



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.03 (d, J = 7.6 Hz, 2H), 7.72 (s, 1H), 7.68 (d, J = 7.2 Hz, 2H), 7.52-7.40 (m, 6H), 7.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.8, 157.7, 149.5, 139.8, 138.8, 129.0, 128.8, 128.8, 128.7, 127.1, 127.1, 119.8, 116.1, 24.8; MS (EI) m/z (%) 245 (100), 230, 202, 115, 77.

2,4-Diphenyl-^{15}N-pyridine (2u)

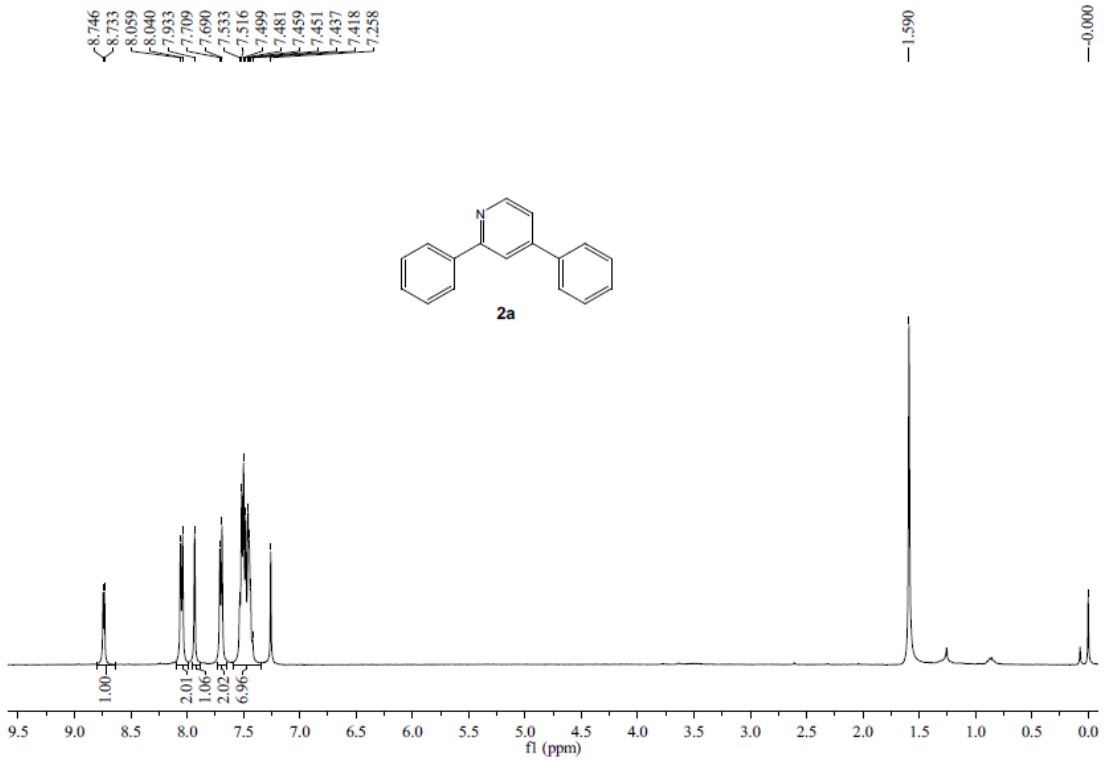


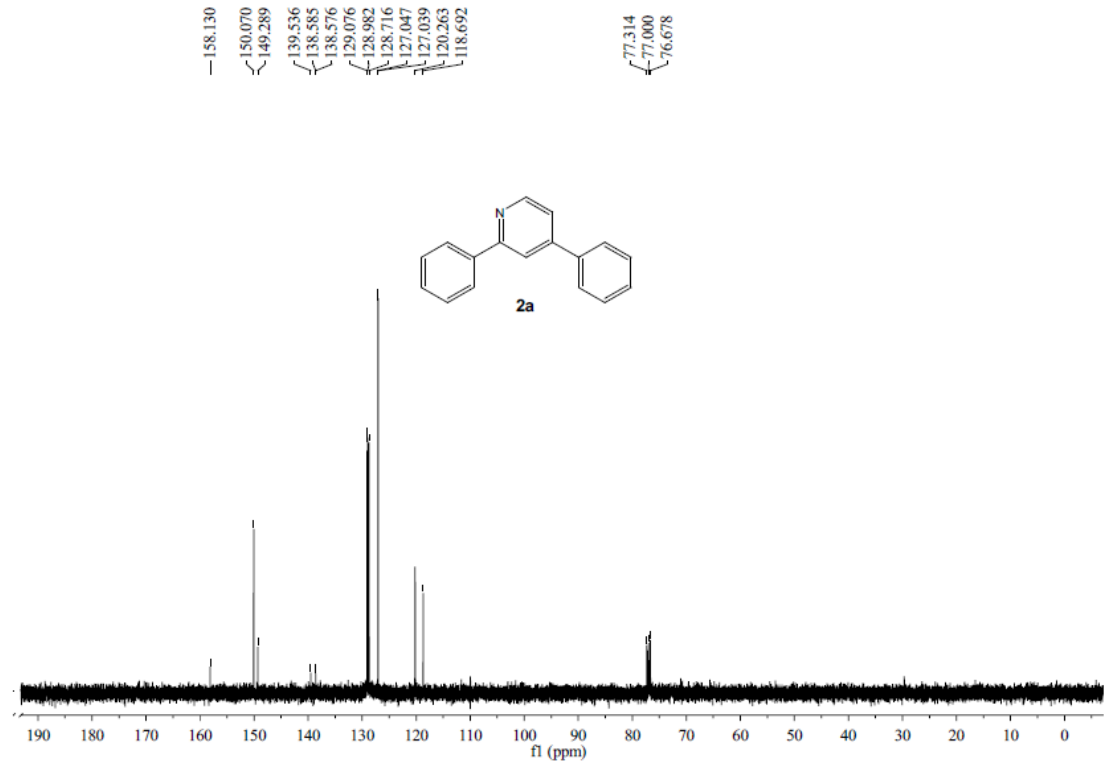
MS (EI) m/z (%) 232 (100), 202, 155, 102, 77.

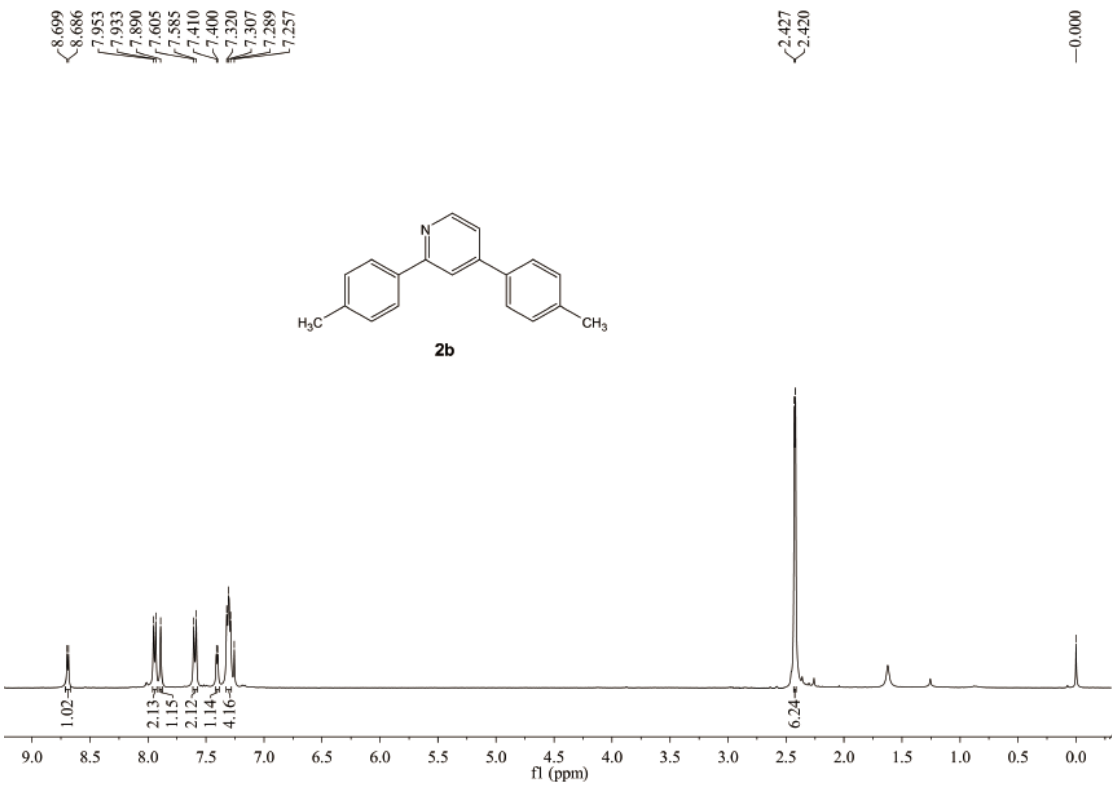
References

[1] Liu, J.; Wang, C.-X.; Wu, L. S.; Liang, F.; Huang, G. S. *Synthesis* **2010**, *24*, 4228.

Copies of ^{1}H and ^{13}C NMR spectra of products



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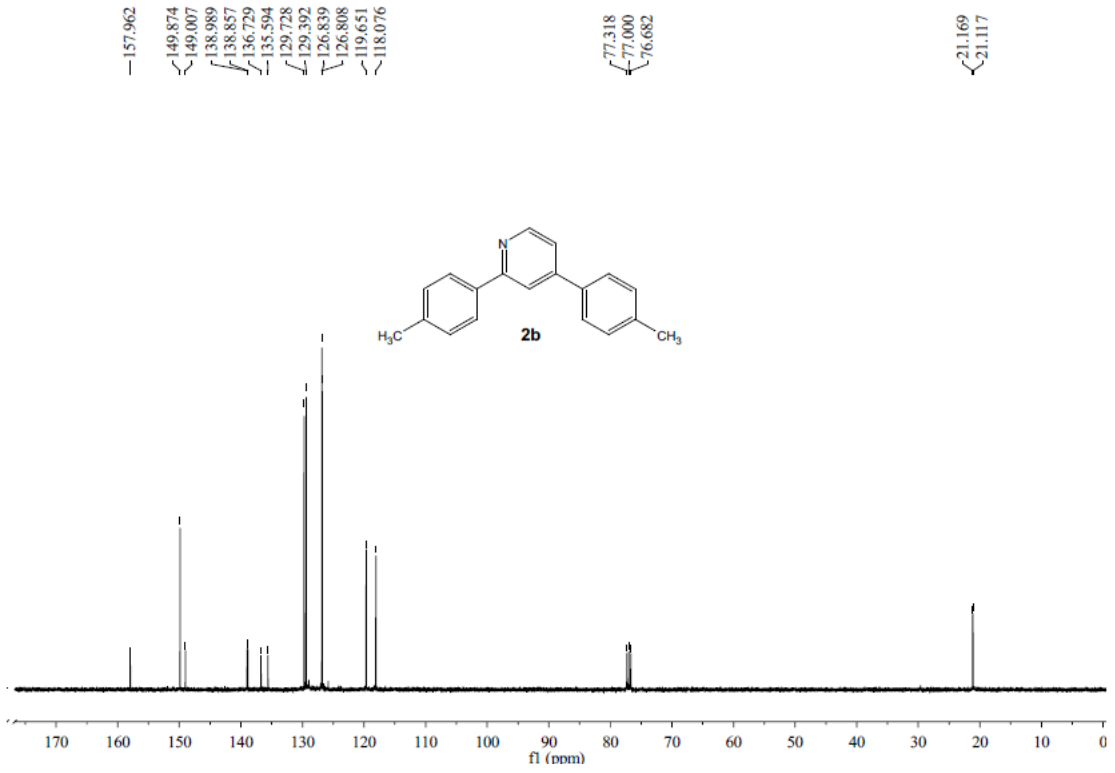
7.953
7.933
7.890
7.605
7.585
7.410
7.400
7.320
7.307
7.289
7.257
2.427
2.420
0.000
2b
1.02
2.13
1.15
2.12
1.14
4.16
6.24
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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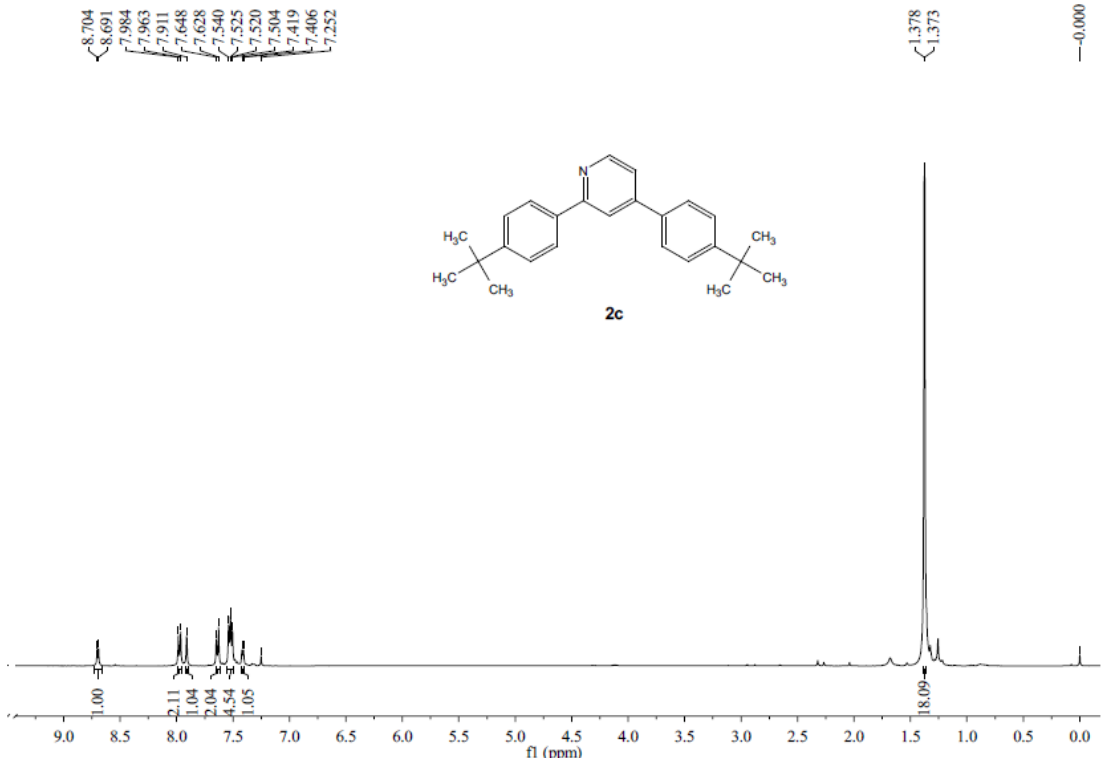
149.874
149.007
138.989
138.857
136.729
135.594
129.728
129.392
126.839
126.808
119.651
118.076
77.318
77.000
76.682
21.169
21.117
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.691
7.984
7.963
7.911
7.648
7.628
7.540
7.525
7.520
7.504
7.419
7.406
7.252
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1.373
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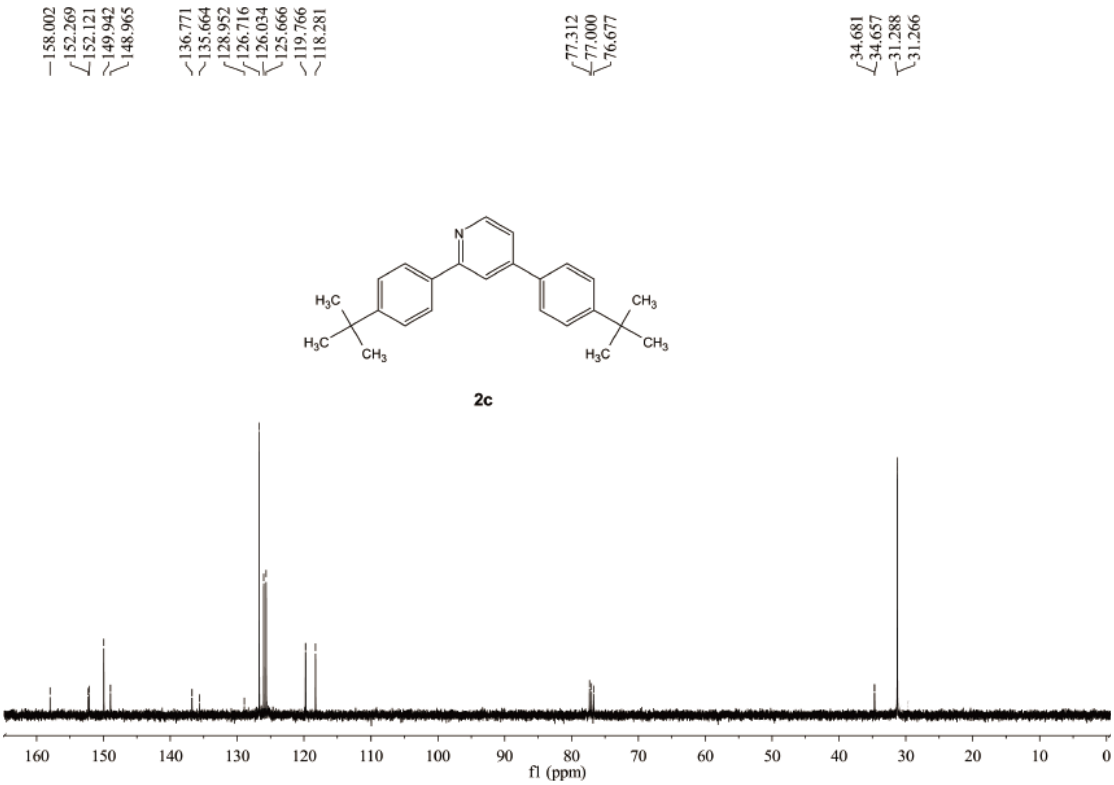
2c
1.00
2.11
1.04
2.04
4.54
1.05
18.09
f1 (ppm)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152.269
152.121
149.942
148.965
136.771
135.664
128.952
126.716
126.034
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119.766
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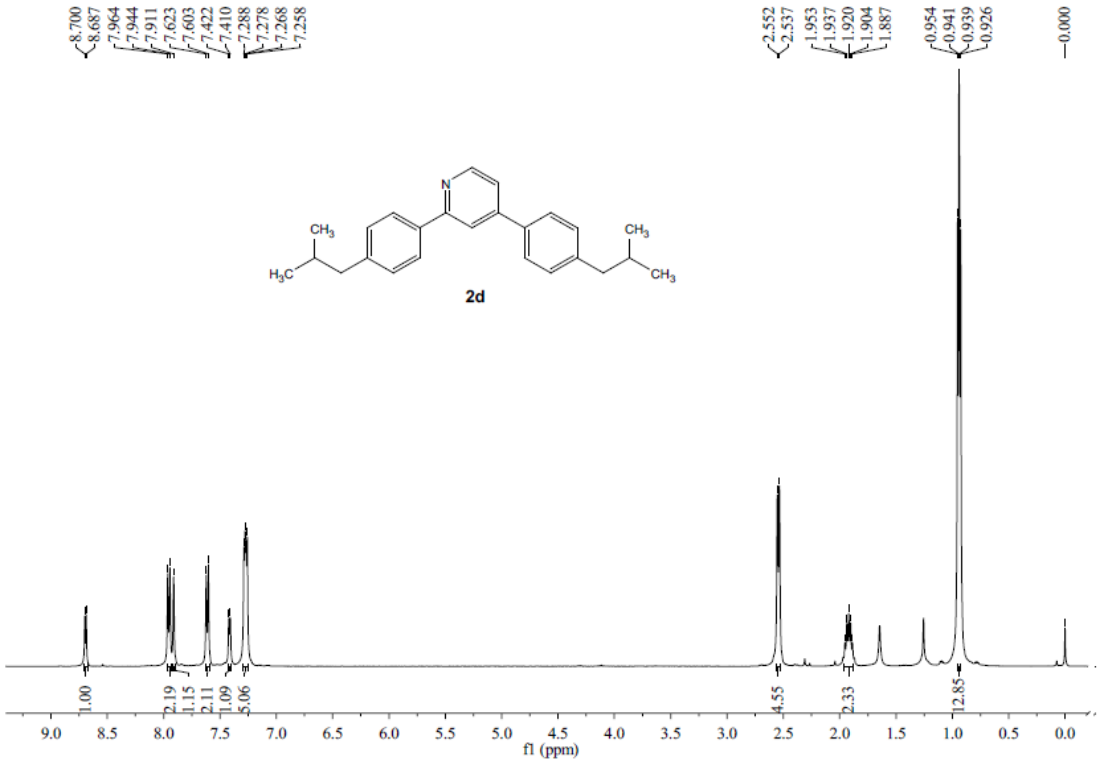
77.312
77.000
76.677
34.681
34.657
31.288
31.266
2c
f1 (ppm)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8.687
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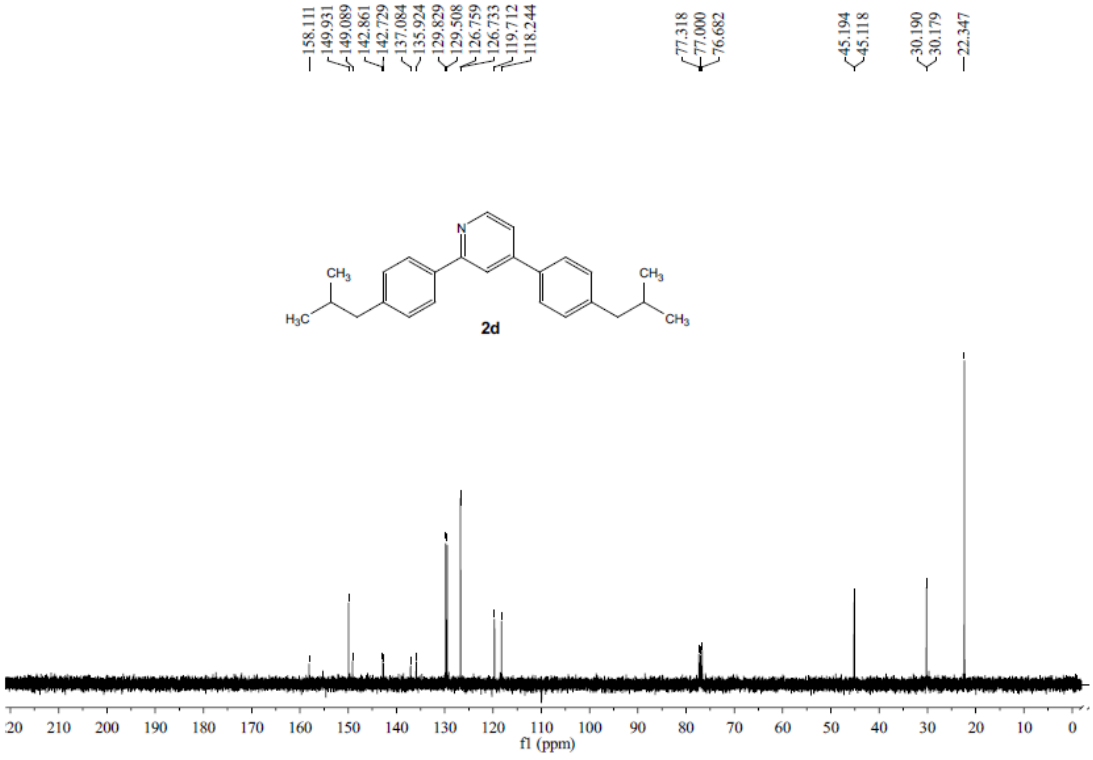
7.944
7.911
7.623
7.603
7.422
7.410
7.288
7.278
7.268
7.258
2.552
2.537
1.953
1.937
1.920
1.904
1.887
0.954
0.941
0.939
0.926
0.000
N
CH3
H3C
CH3
CH3
2d
1.00
2.19
1.15
2.11
1.09
5.06
4.55
2.33
12.85
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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149.089
142.861
142.729
137.084
135.924
129.829
129.508
126.759
126.733
119.712
118.244
77.318
77.000
76.682
45.194
45.118
30.190
30.179
22.347
N
CH3
H3C
CH3
CH3
2d
220
210
200
190
180
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130
120
110
100
90
80
70
60
50
40
30
20
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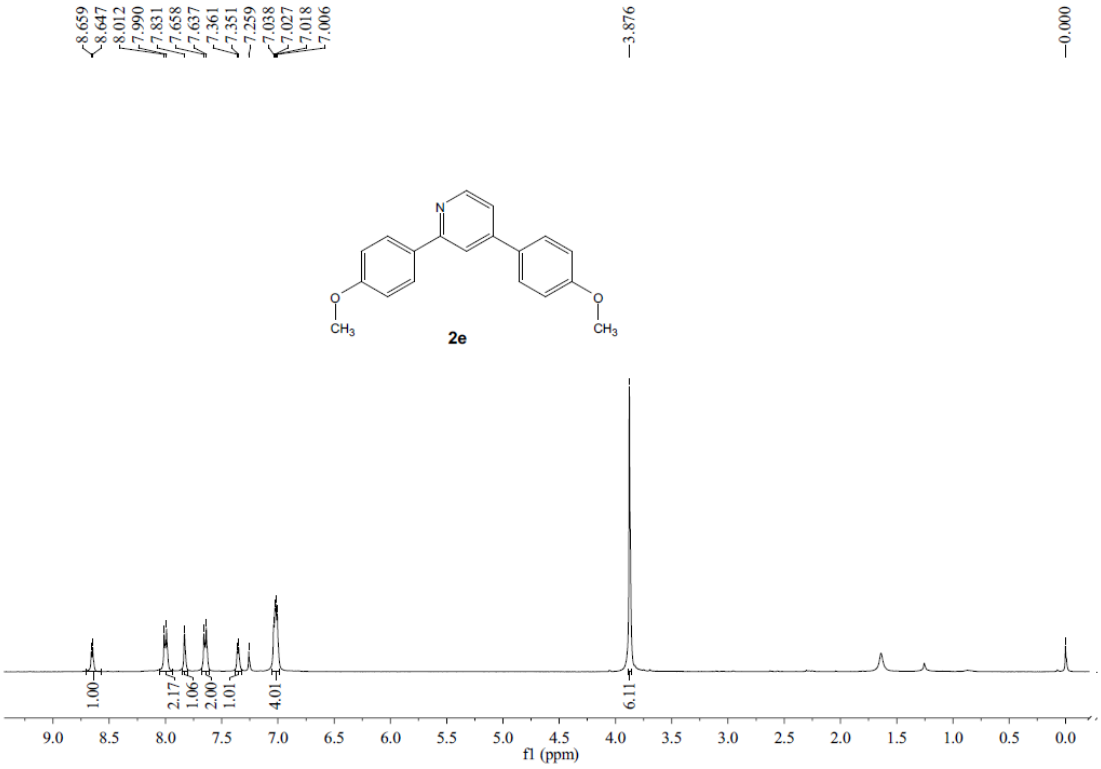
f1 (ppm)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7.831
7.658
7.637
7.361
7.351
7.259
7.038
7.027
7.018
7.006
3.876
0.000
2e
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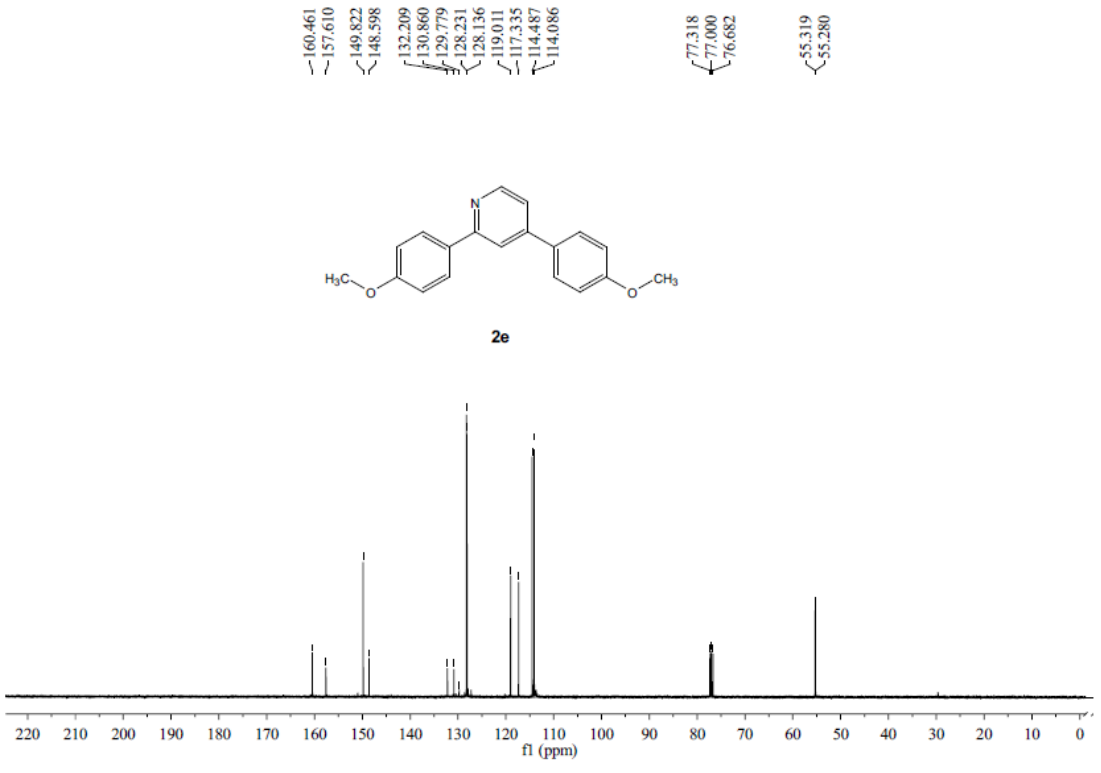
2.17
1.06
2.00
1.01
4.01
6.11
f1 (ppm)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149.822
148.598
132.209
130.860
129.779
128.231
128.136
119.011
117.335
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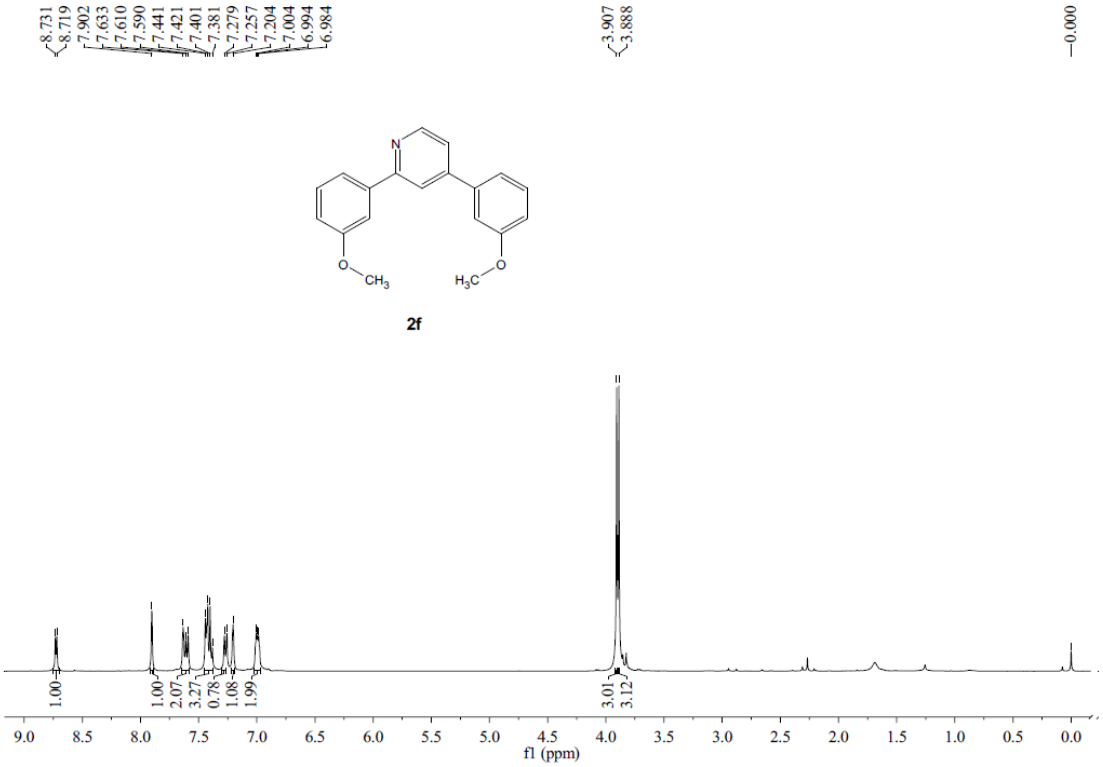
76.682
55.319
55.280
2e
f1 (ppm)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8.719
7.902
7.633
7.610
7.590
7.441
7.421
7.401
7.381
7.279
7.257
7.204
7.004
6.994
6.984
3.907
3.888
0.000
N
O
CH3
H3C
O
2f
1.00
1.00
2.07
3.27
0.78
1.08
1.99
3.01
3.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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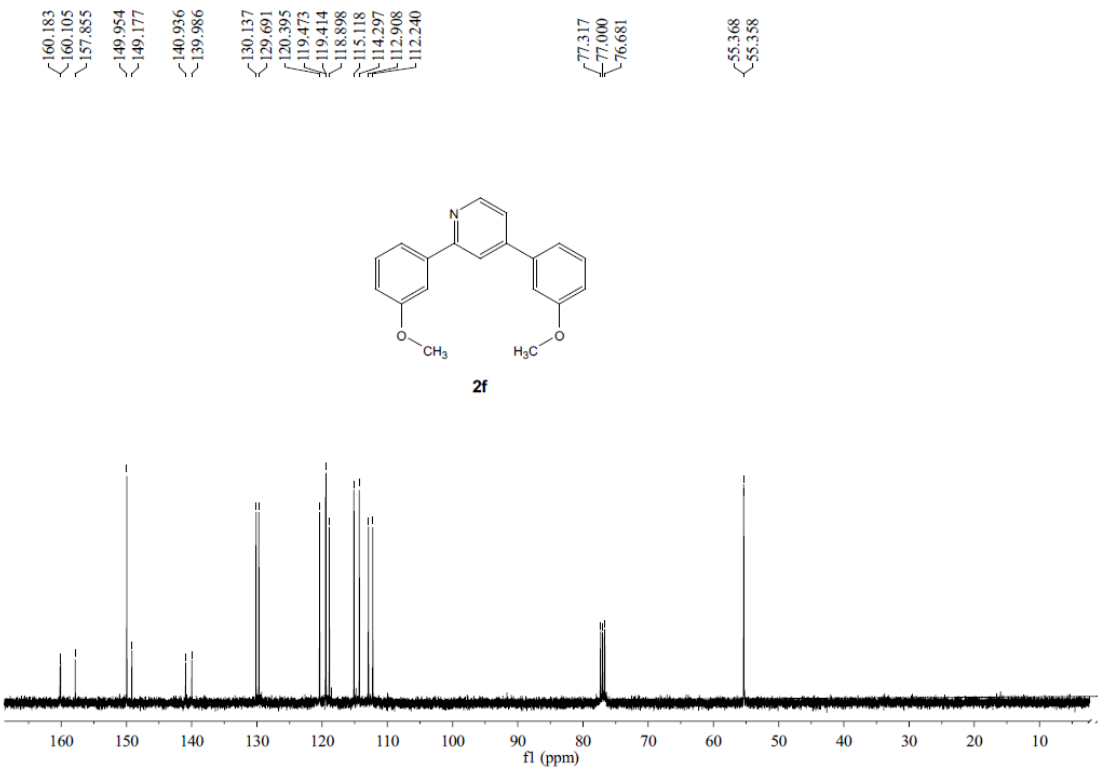
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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157.855
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149.177
140.936
139.986
130.137
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119.414
118.898
115.118
114.297
112.908
112.240
77.317
77.000
76.681
55.368
55.358
N
O
CH3
H3C
O
2f
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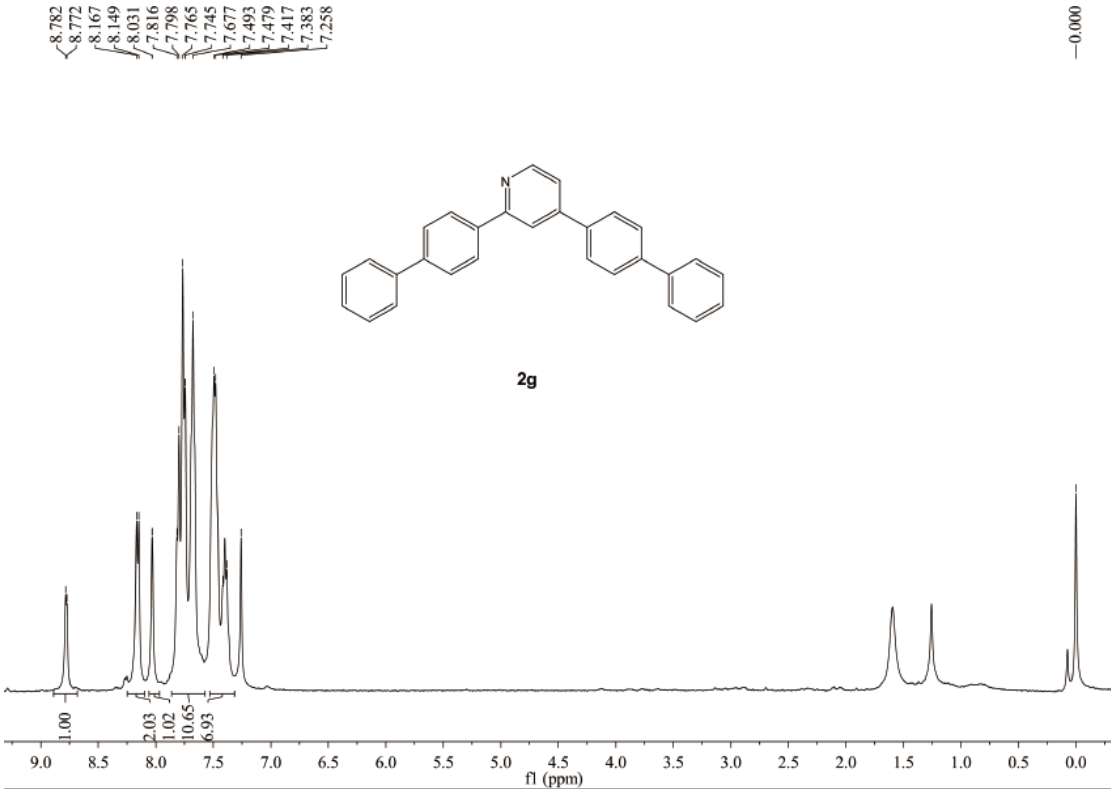
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.765
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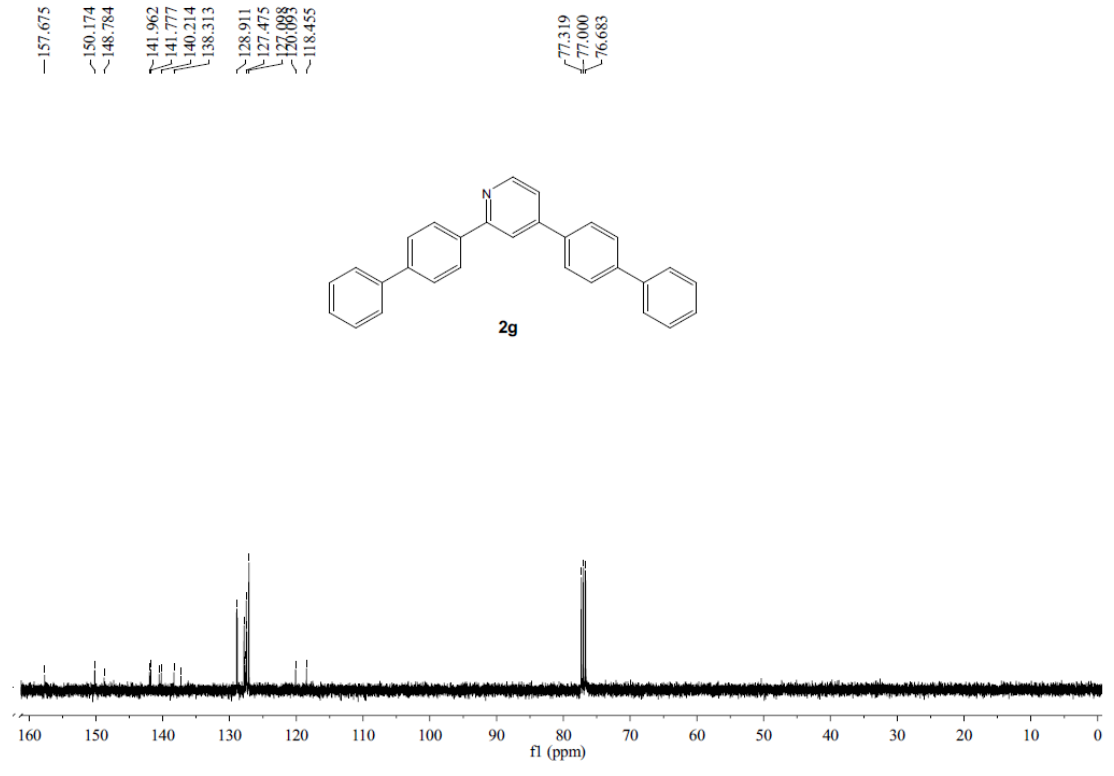
7.677
7.493
7.479
7.417
7.383
7.258
0.000
N
2g
1.00
2.03
1.02
10.65
6.93
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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141.777
140.214
138.313
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77.000
76.683
N
2g
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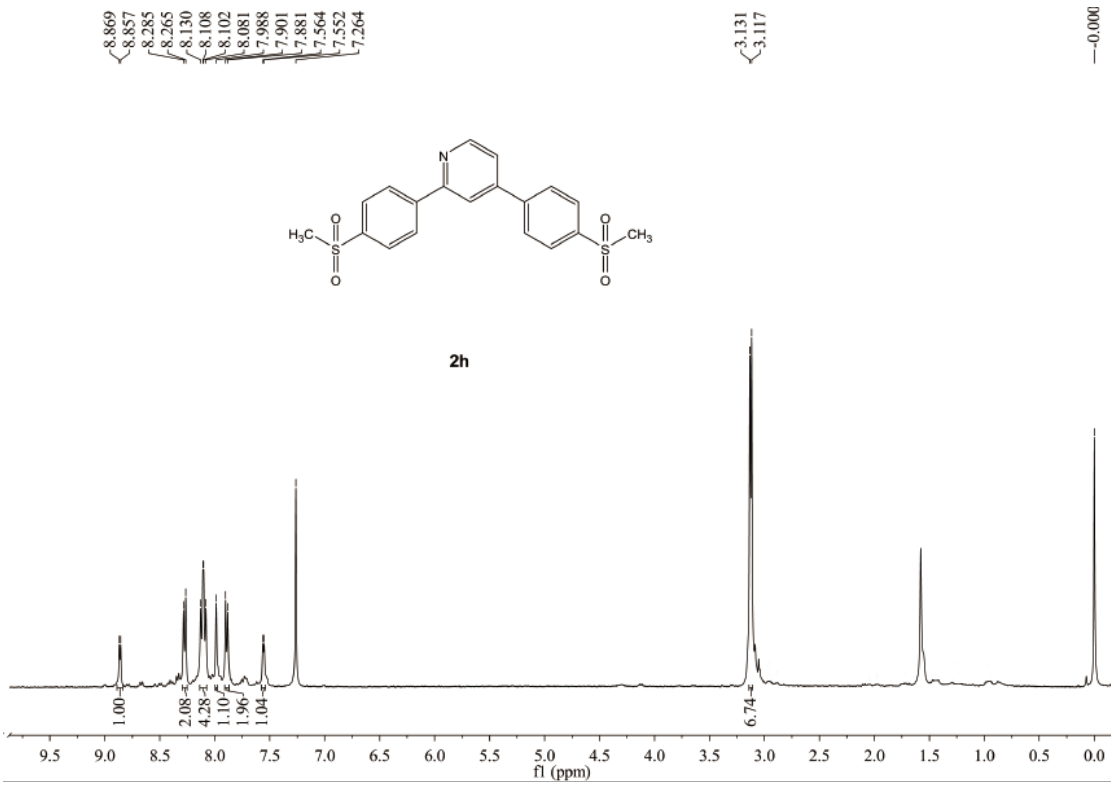
f1 (ppm)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8.081
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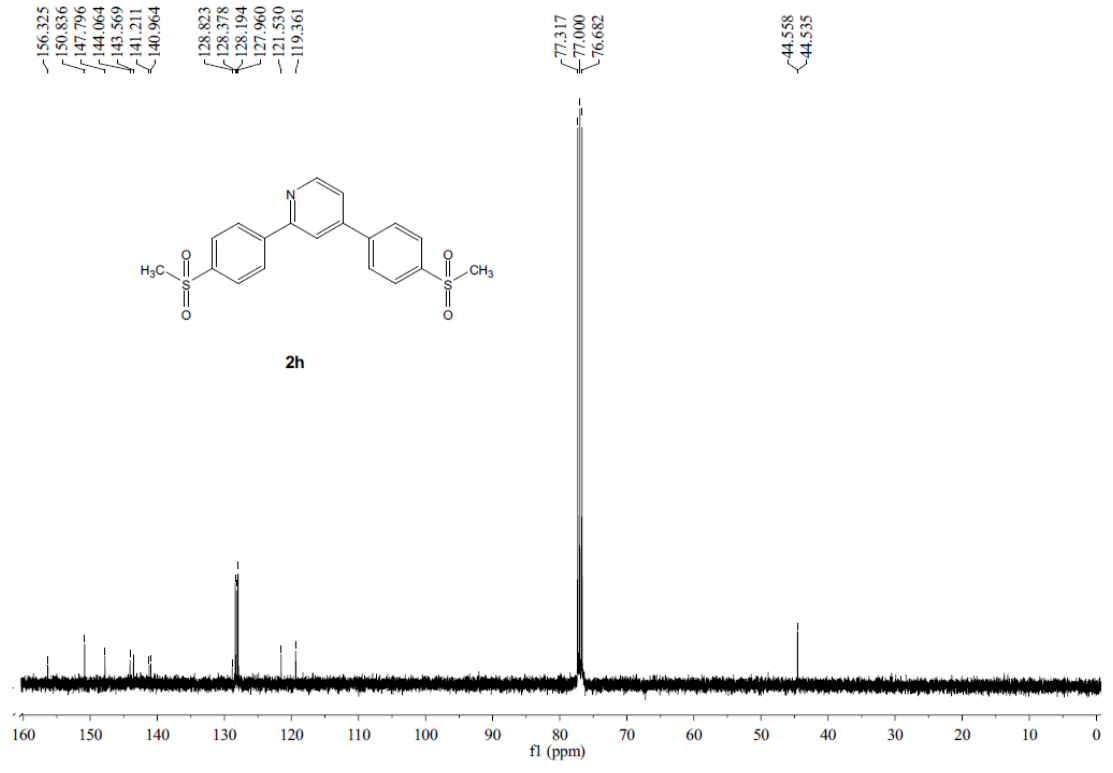
7.901
7.881
7.564
7.552
7.264
3.131
3.117
0.000
2h
1.00
2.08
4.28
1.10
1.96
1.04
6.74
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.378
128.194
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2h
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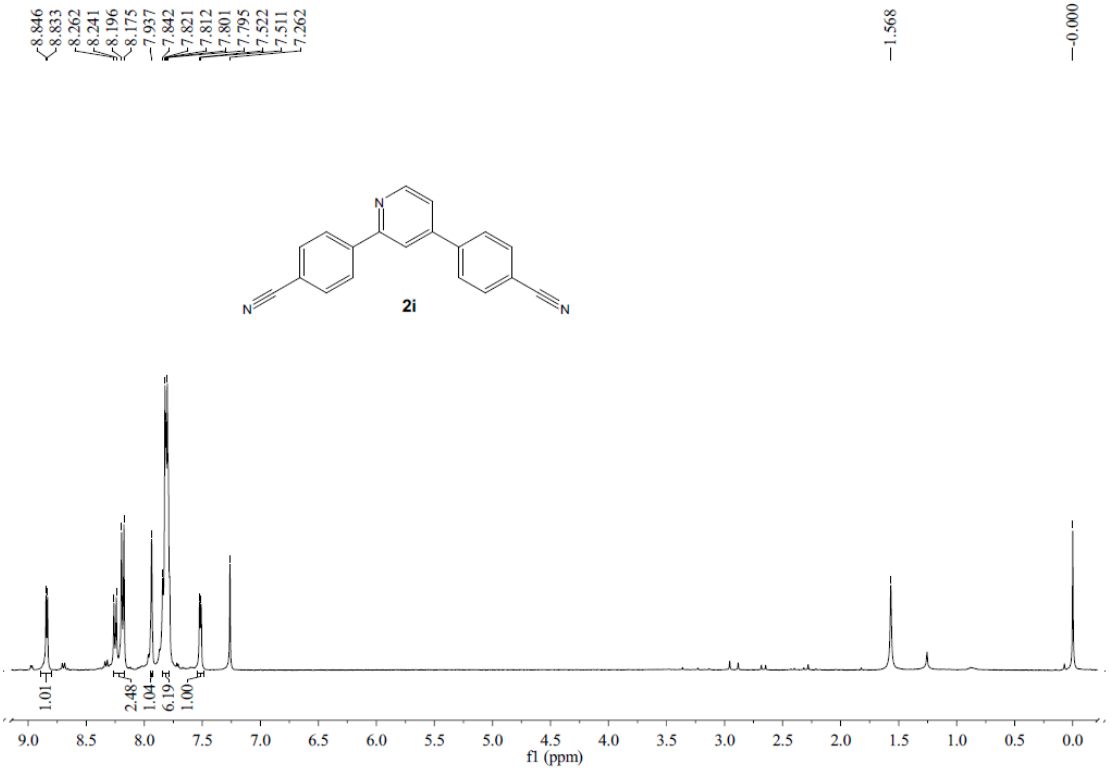
f1 (ppm)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7.842
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7.812
7.801
7.795
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7.262
1.568
0.000
2i
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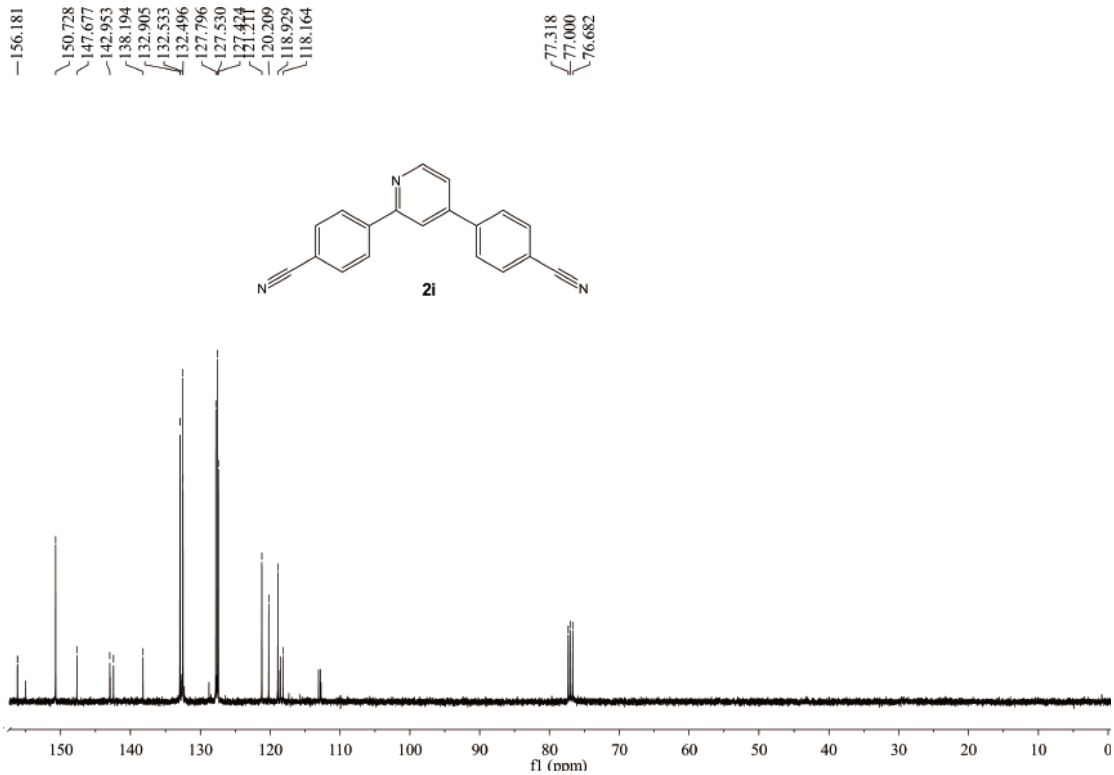
2.48
1.04
6.19
1.00
fl (ppm)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118.929
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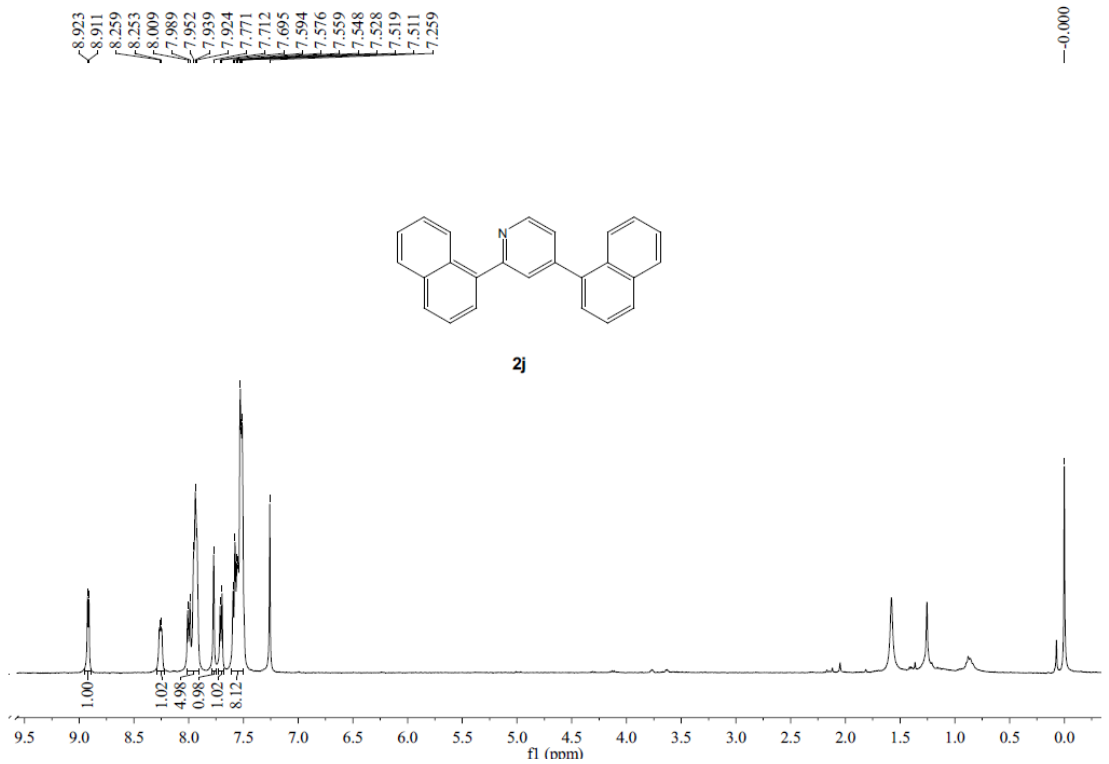
77.318
77.000
76.682
2i
fl (ppm)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7.952
7.939
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7.771
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7.594
7.576
7.559
7.548
7.528
7.519
7.511
7.259
-0.000
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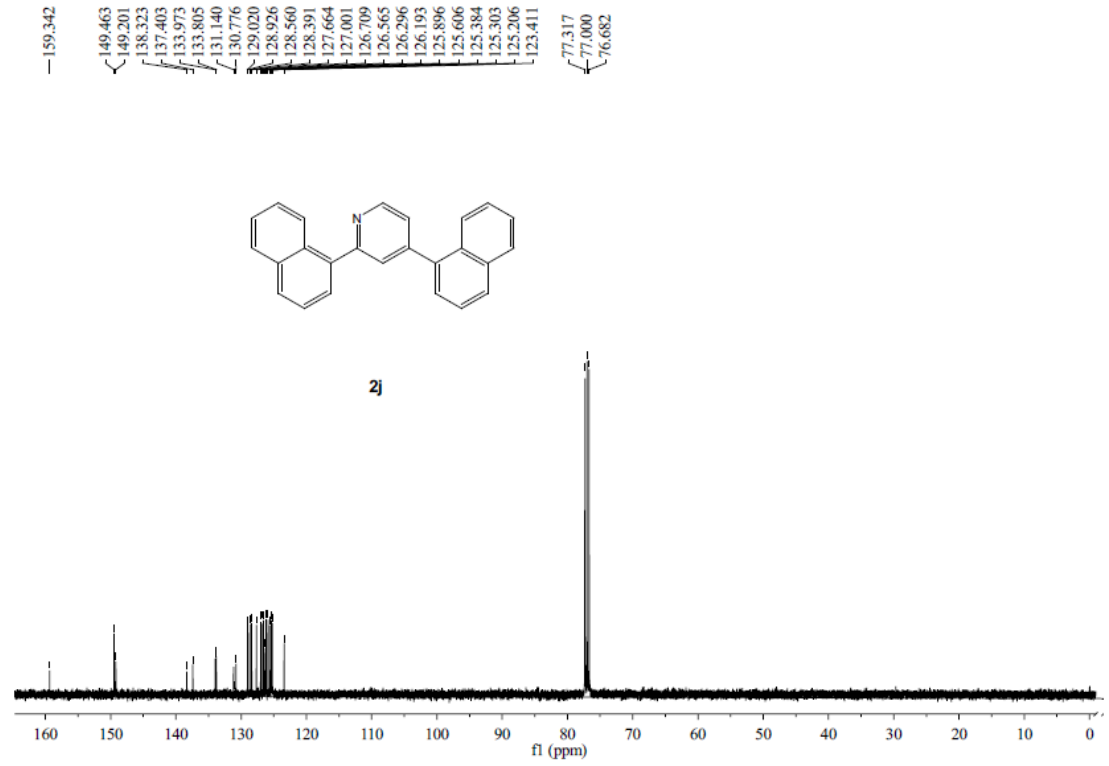
2j
1.00
1.02
4.98
0.98
1.02
8.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.001
126.709
126.565
126.296
126.193
125.896
125.606
125.384
125.303
125.206
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77.317
77.000
76.682
N
2j
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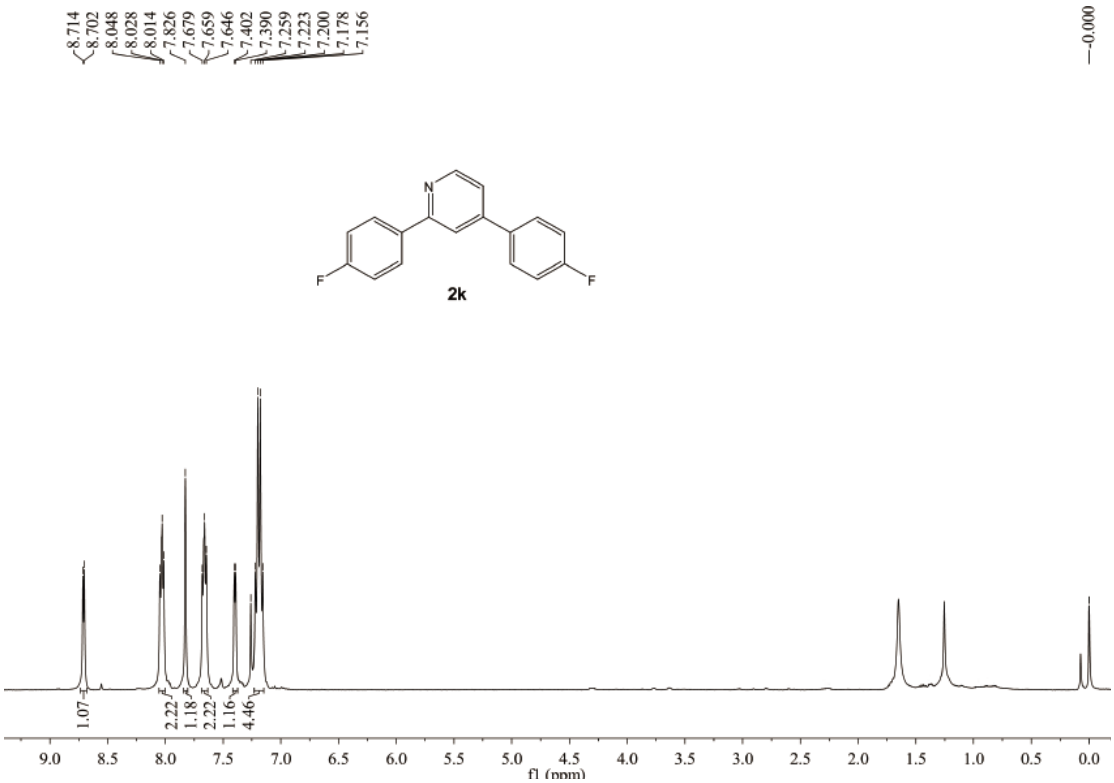
f1 (ppm)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7.223
7.200
7.178
7.156
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N
F
F
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1.07
2.22
1.18
2.22
1.16
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9.0
8.5
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7.5
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6.5
6.0
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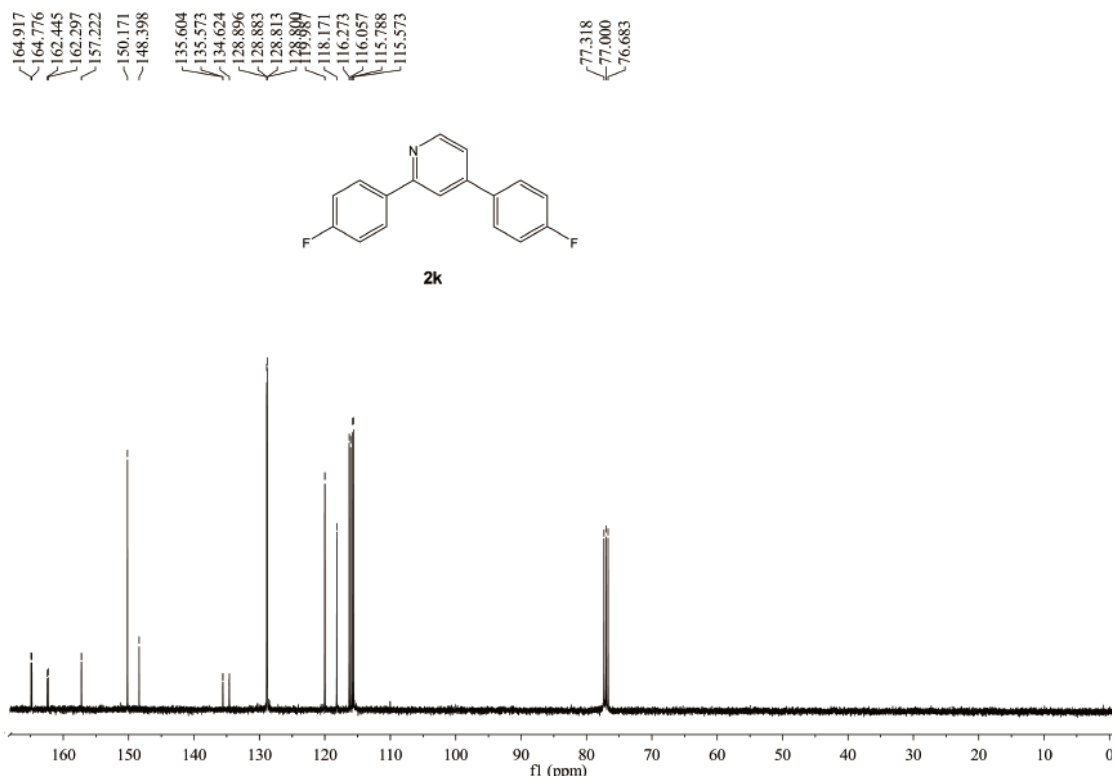
f1 (ppm)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128.813
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116.273
116.057
115.788
115.573
77.318
77.000
76.683
N
F
F
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130
120
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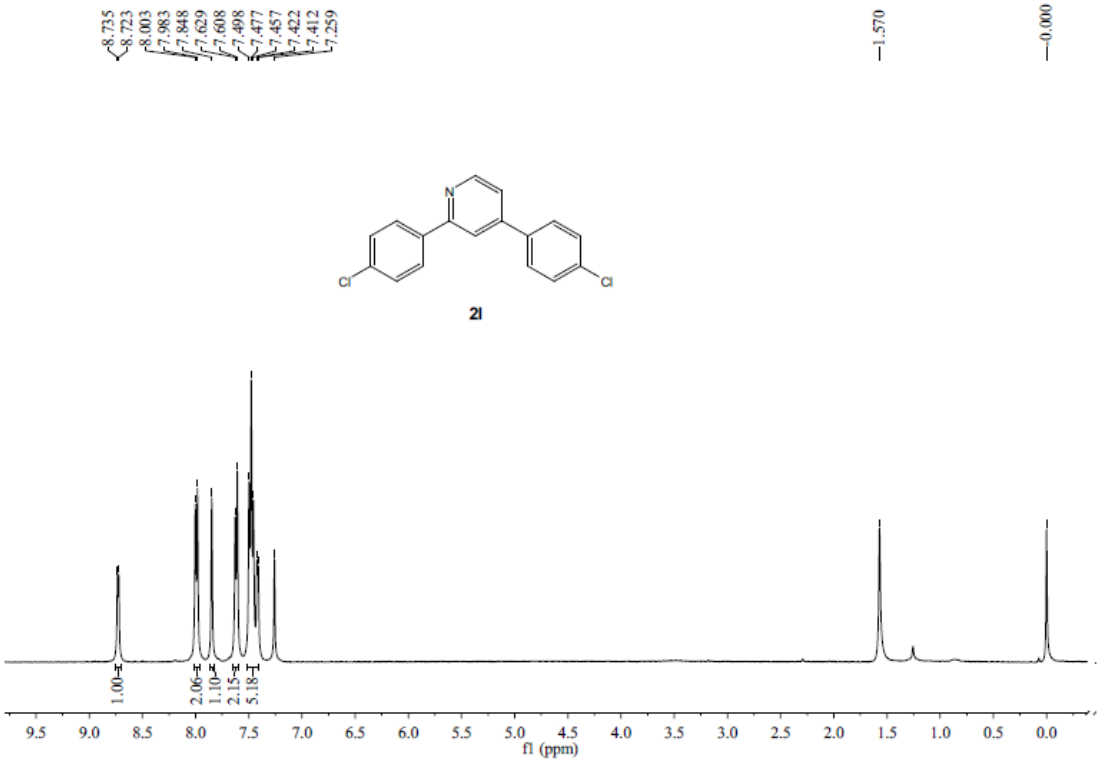
20
10
f1 (ppm)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7.412
7.259
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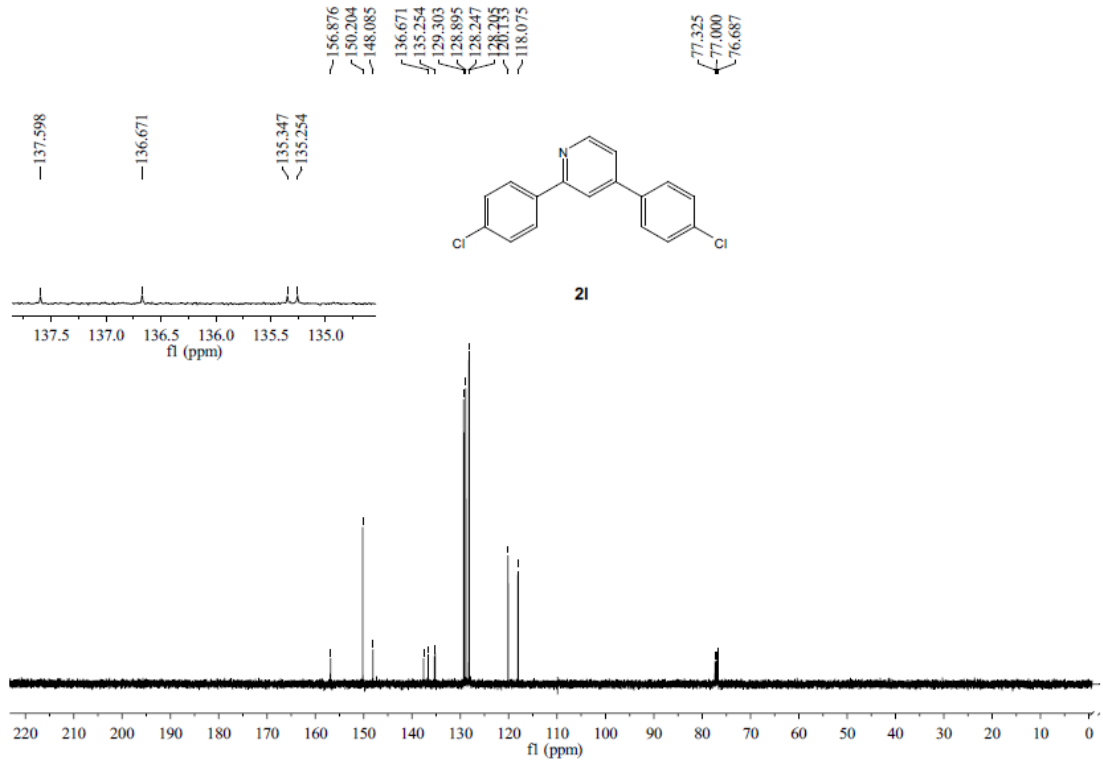
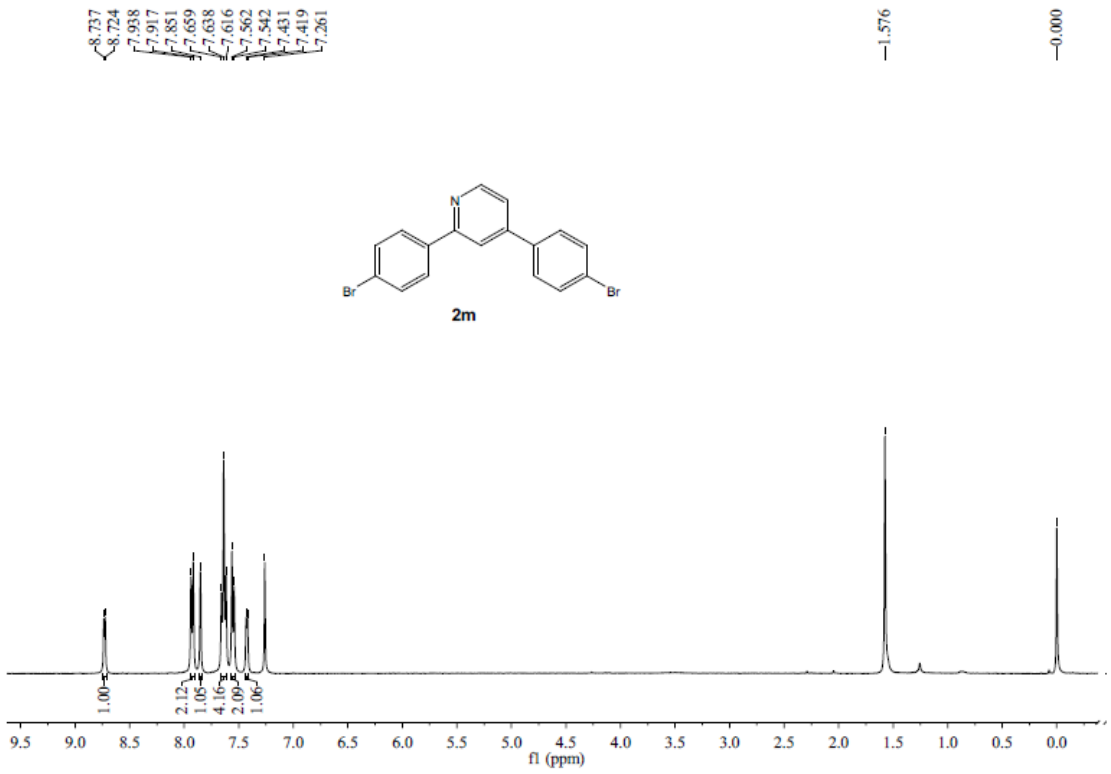
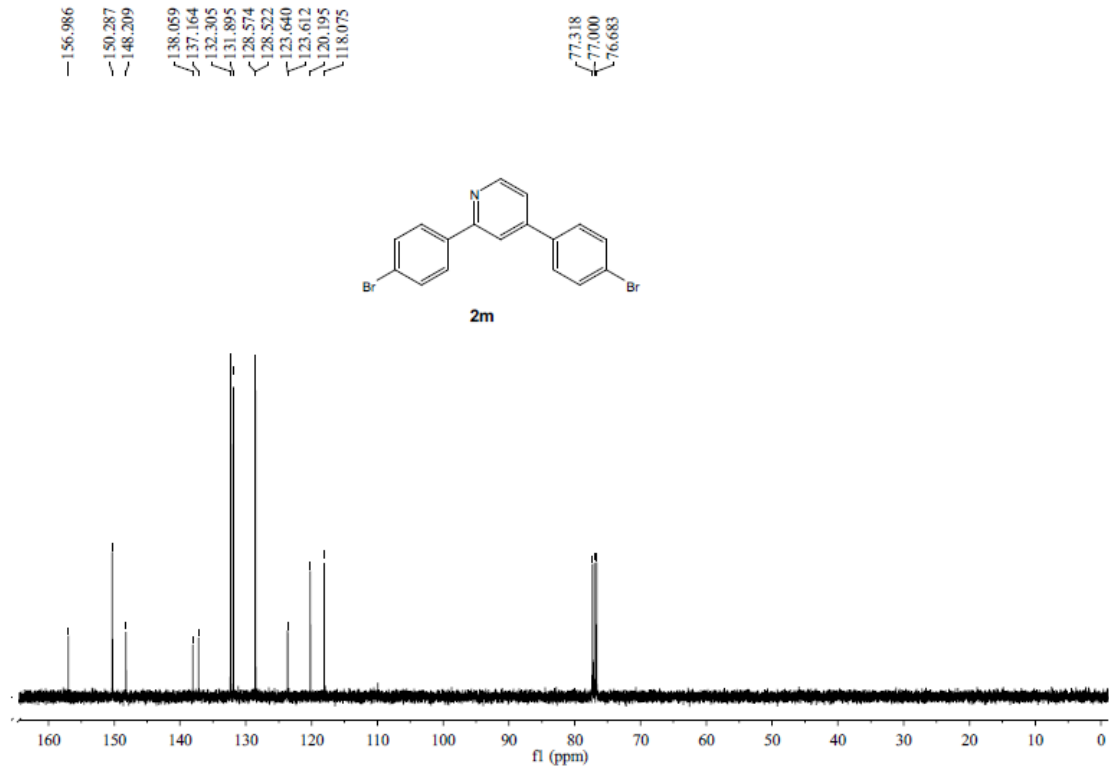
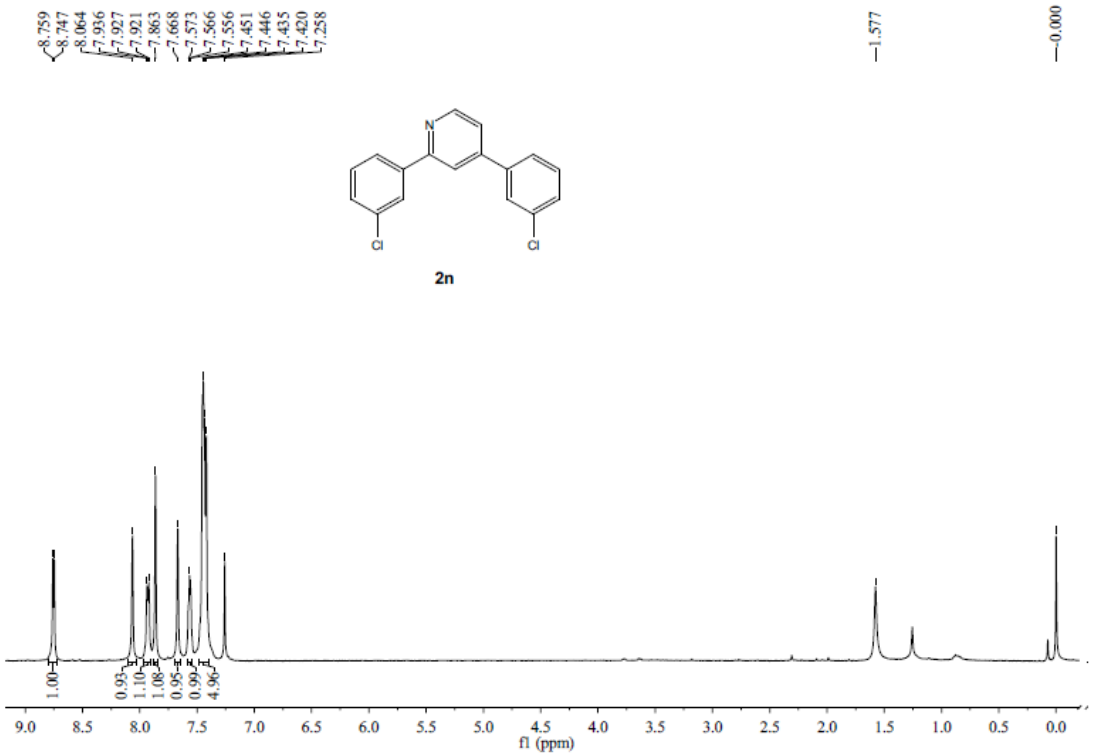
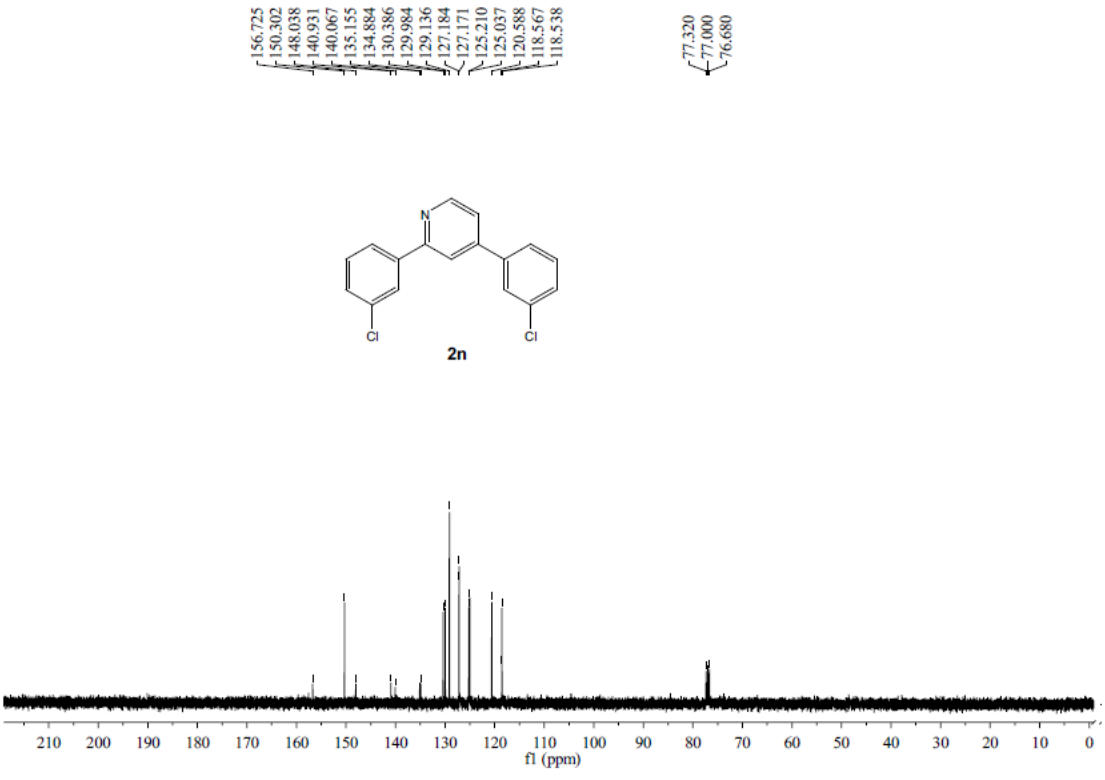
N
Cl
Cl
2l
1.00
2.06
1.10
2.15
5.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

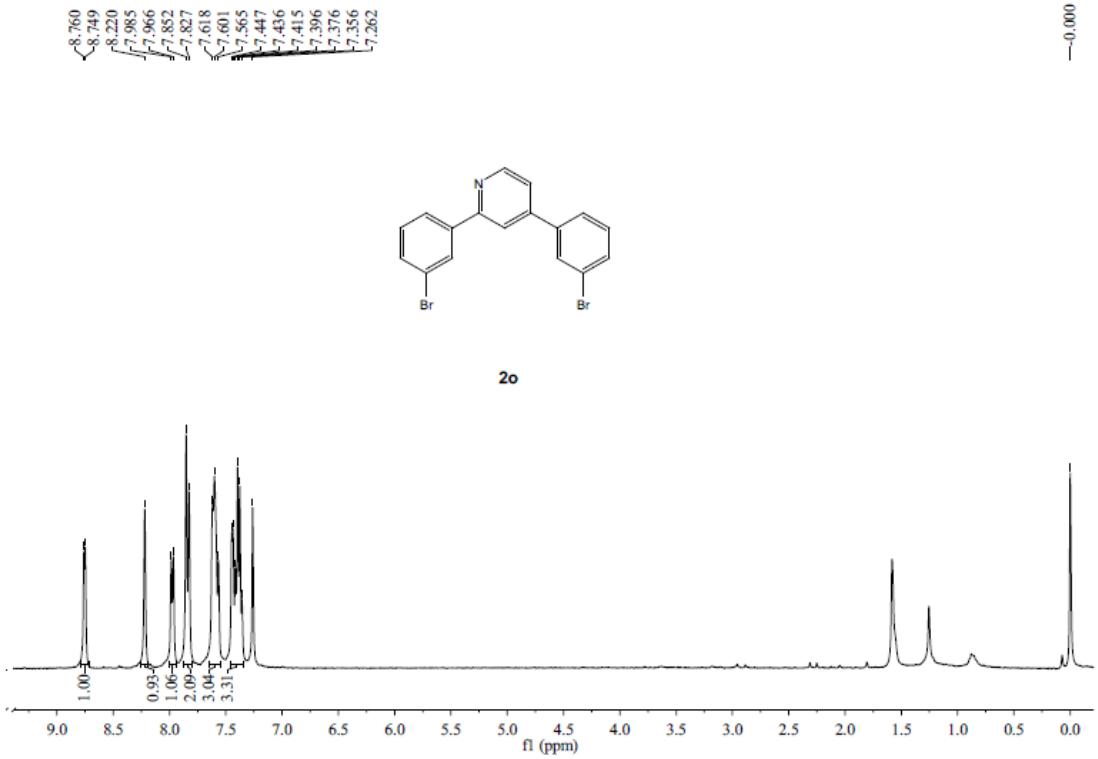

156.876
150.204
148.085
136.671
135.254
129.303
128.895
128.247
128.205
120.133
118.075
77.325
77.000
76.687
137.598
136.671
135.347
135.254
N
Cl
Cl
2l
137.5 137.0 136.5 136.0 135.5 135.0
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

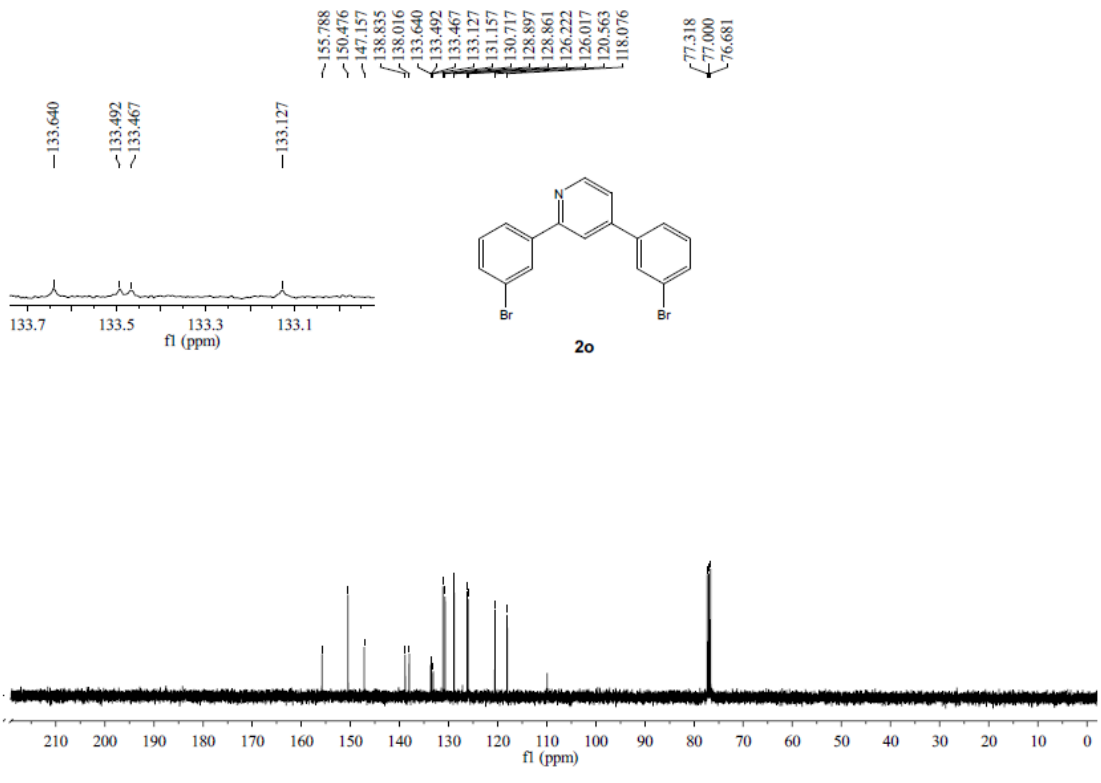

8.737
8.724
7.938
7.917
7.851
7.659
7.638
7.616
7.562
7.542
7.431
7.419
7.261
1.576
0.000
N
Br
Br
2m
1.00
2.12
1.05
4.16
2.00
1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


156.986
150.287
148.209
138.059
137.164
132.305
131.895
128.574
128.522
123.640
123.612
120.195
118.075
77.318
77.000
76.683
N
Br
Br
2m
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

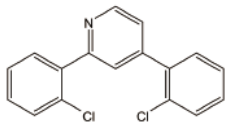

8.759
8.747
8.064
7.936
7.927
7.921
7.863
7.668
7.573
7.566
7.556
7.451
7.446
7.435
7.420
7.258
1.577
0.000
N
Cl
Cl
2n
1.00
0.93
1.10
1.08
0.95
0.99
4.96
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


156.725
150.302
148.038
140.931
140.067
135.155
134.884
130.386
129.984
129.136
127.184
127.171
125.210
125.037
120.588
118.567
118.538
77.320
77.000
76.680
N
Cl
Cl
2n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

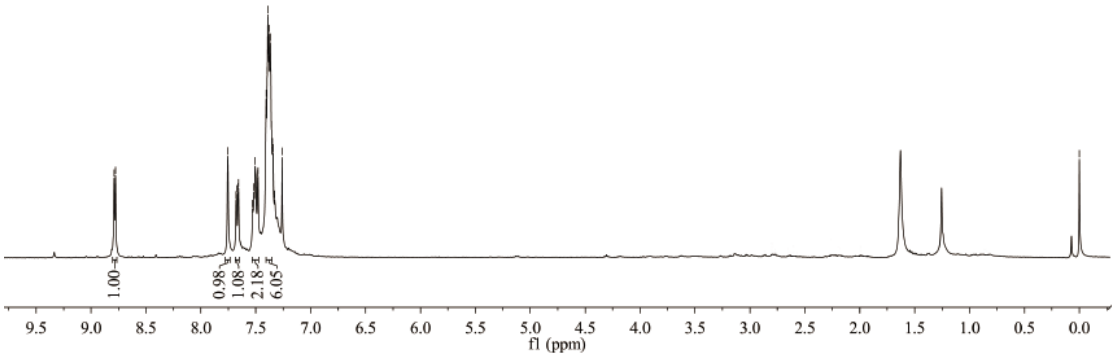

8.760
8.749
8.220
7.985
7.966
7.852
7.827
7.618
7.601
7.565
7.447
7.436
7.415
7.396
7.376
7.356
7.262
0.000
N
Br
Br
2o
1.00
0.93
1.06
2.09
3.04
3.31
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

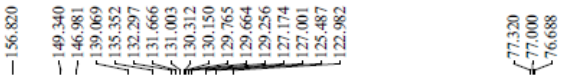

155.788
150.476
147.157
138.835
138.016
133.640
133.492
133.467
133.127
131.157
130.717
128.897
128.861
126.222
126.017
120.563
118.076
77.318
77.000
76.681
133.640
133.492
133.467
133.127
133.7
133.5
133.3
133.1
f1 (ppm)
N
Br
Br
2o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

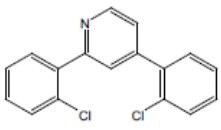

8.790
8.778
7.756
7.678
7.674
7.660
7.656
7.528
7.523
7.516
7.504
7.484
7.481
7.405
7.395
7.390
7.384
7.378
7.366
7.356
7.348
7.343
7.329
7.260
0.000


N
Cl
Cl

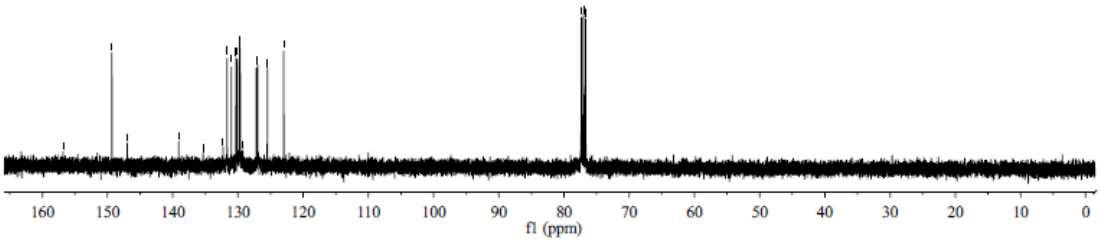
2p

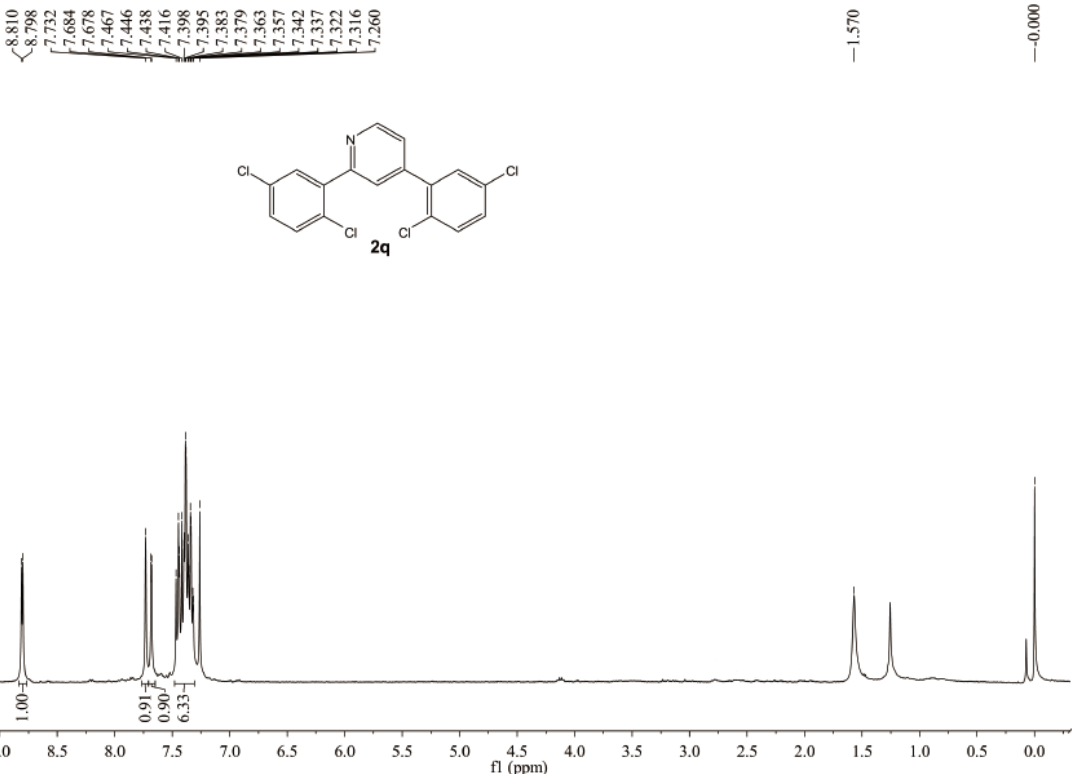

1.00
0.98
1.08
2.18
6.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

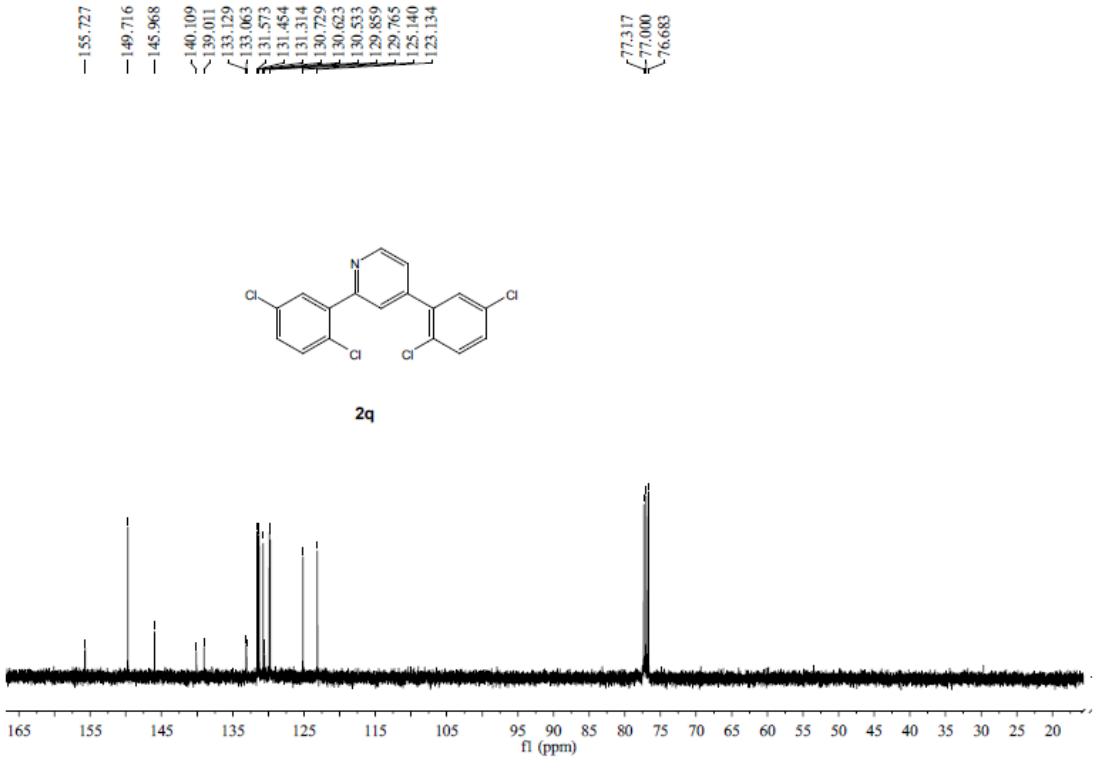

156.820
149.340
146.981
139.069
135.352
132.297
131.666
131.003
130.312
130.150
129.765
129.664
129.256
127.174
127.001
125.487
122.982
77.320
77.000
76.688

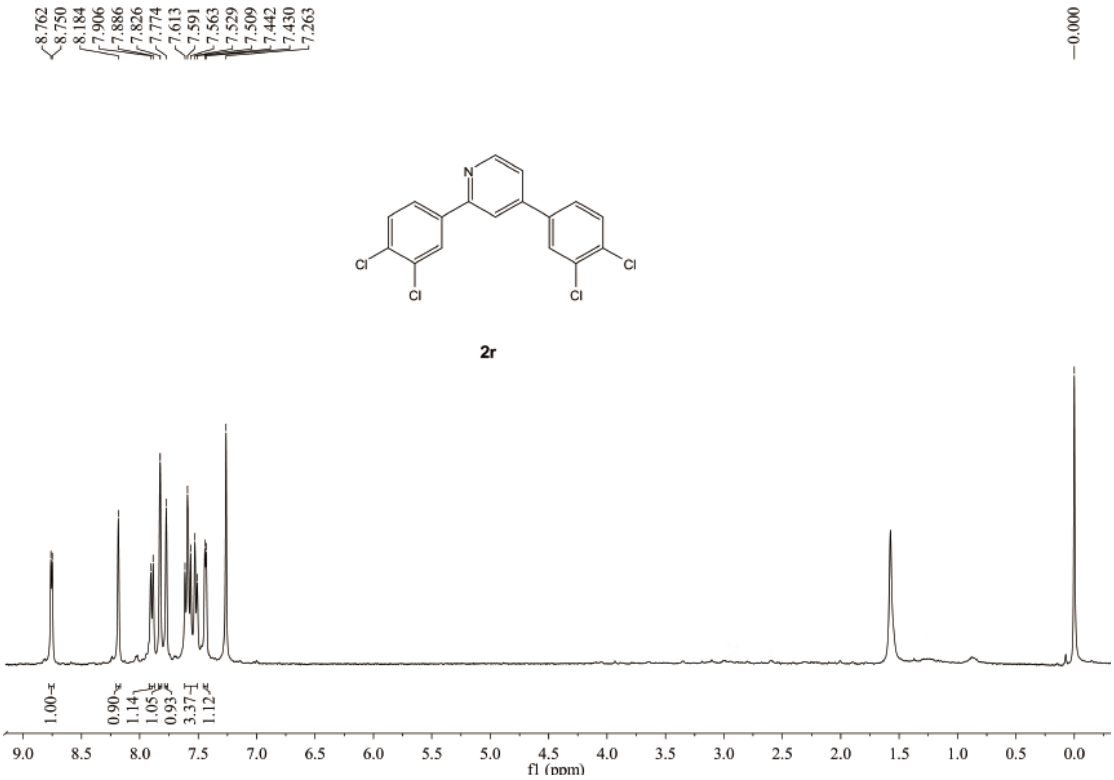

N
Cl
Cl

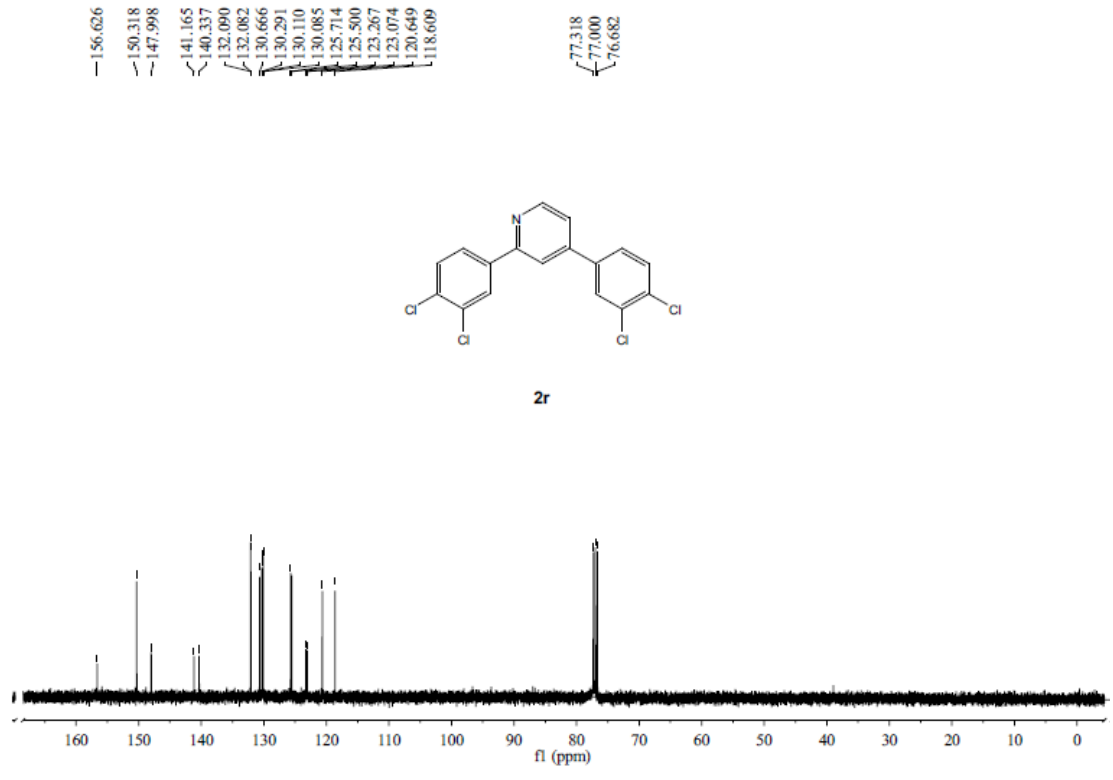
2p

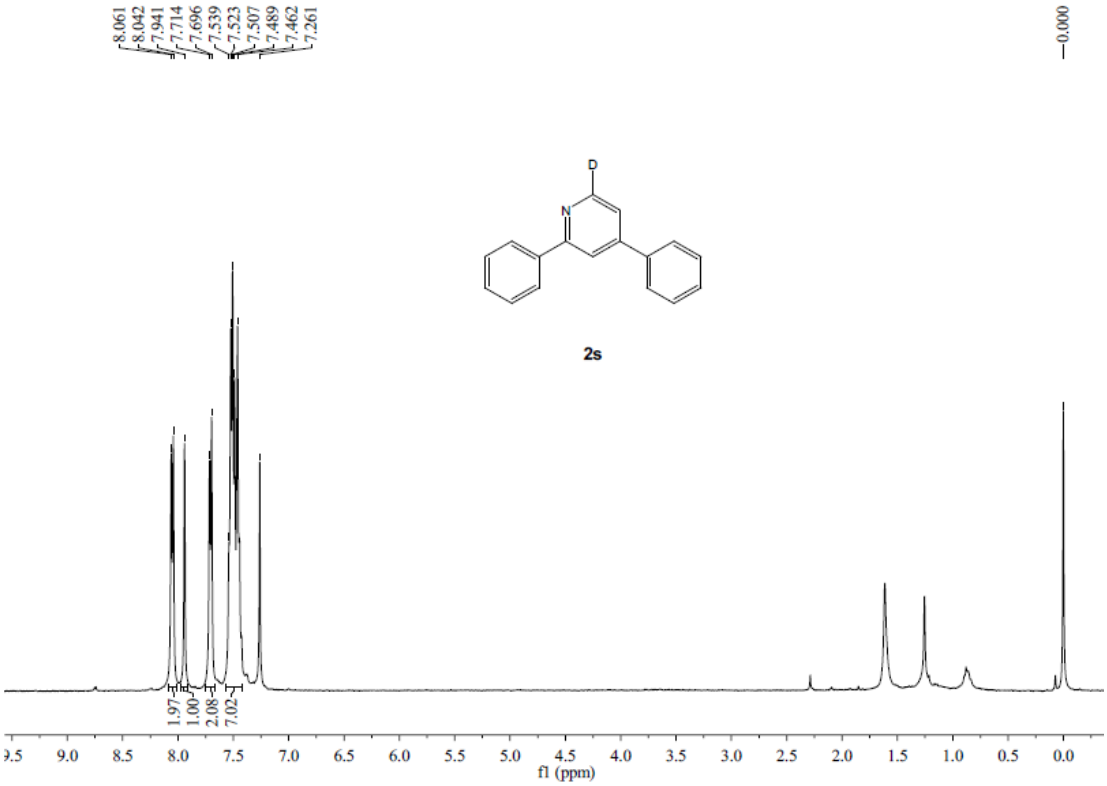

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

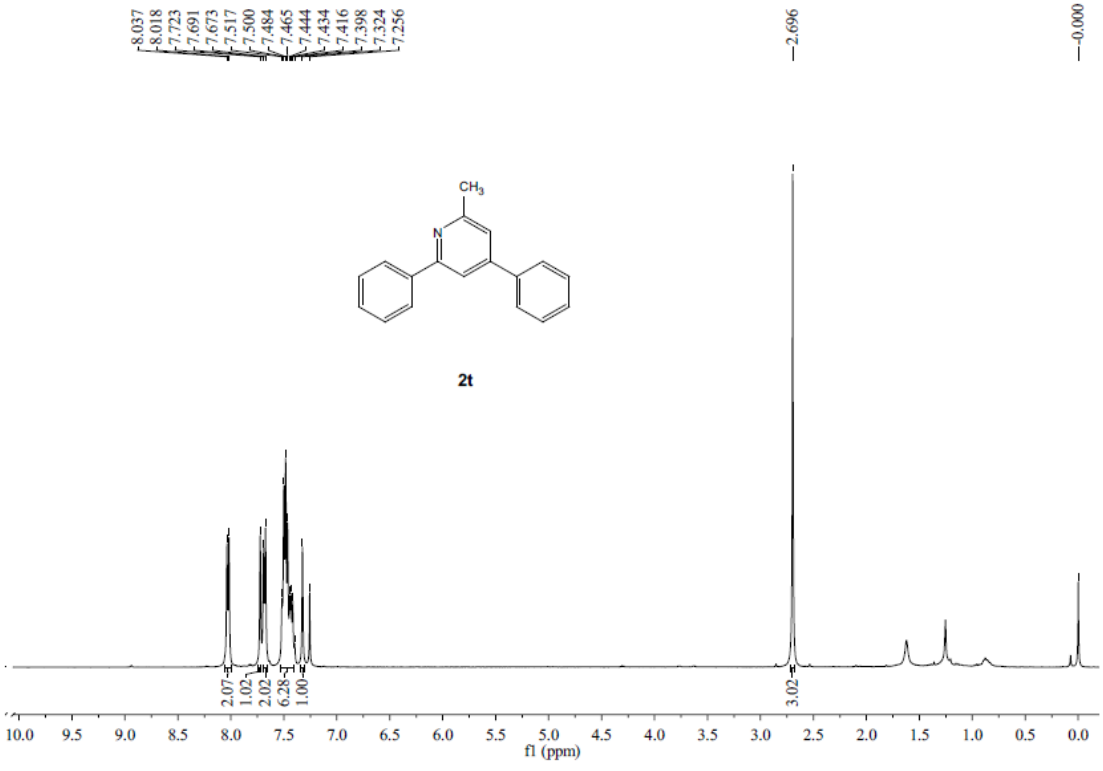

8.810
8.798
7.732
7.684
7.678
7.467
7.446
7.438
7.416
7.398
7.395
7.383
7.379
7.363
7.357
7.342
7.337
7.322
7.316
7.260
1.570
0.000
N
Cl
Cl
Cl
Cl
2q
1.00
0.91
0.90
6.33
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

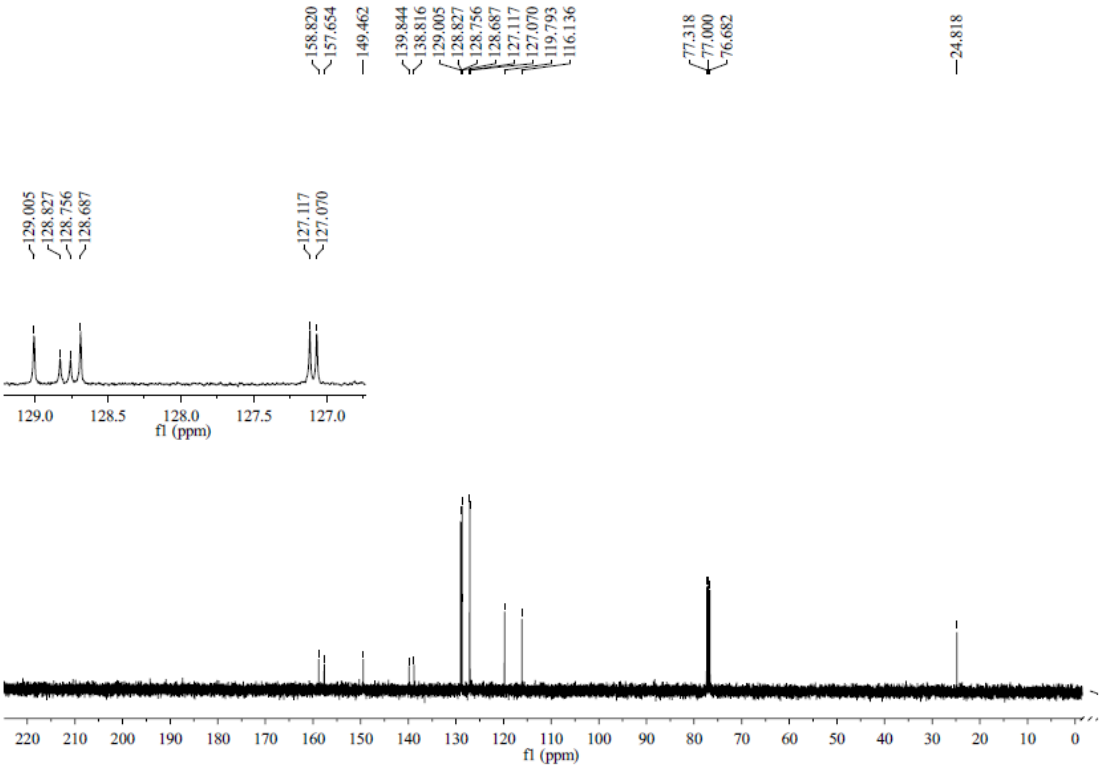

155.727
149.716
145.968
140.109
139.011
133.129
133.063
131.573
131.454
131.314
130.729
130.623
130.533
129.859
129.765
125.140
123.134
77.317
77.000
76.683
N
Cl
Cl
Cl
Cl
2q
165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)


8.762
8.750
8.184
7.906
7.886
7.826
7.774
7.613
7.591
7.563
7.529
7.509
7.442
7.430
7.263
0.000
N
Cl
Cl
Cl
Cl
2r
1.00
0.90
1.14
1.05
0.93
3.37
1.12
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)


156.626
150.318
147.998
141.165
140.337
132.090
132.082
130.666
130.291
130.110
130.085
125.714
125.500
123.267
123.074
120.649
118.609
77.318
77.000
76.682
N
Cl
Cl
Cl
Cl
2r
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.061
8.042
7.941
7.714
7.696
7.539
7.523
7.507
7.489
7.462
7.261
0.000
D
N
2s
1.97
1.00
2.08
7.02
fl (ppm)


8.037
8.018
7.723
7.691
7.673
7.517
7.500
7.484
7.465
7.444
7.434
7.416
7.398
7.324
7.256
2.696
0.000
CH3
N
2t
2.07
1.02
2.02
6.28
1.00
3.02
fl (ppm)


158.820
157.654
149.462
139.844
138.816
129.005
128.827
128.756
128.687
127.117
127.070
119.793
116.136
77.318
77.000
76.682
24.818
129.005
128.827
128.756
128.687
127.117
127.070
129.0
128.5
128.0
127.5
127.0
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)