Supporting information for

Efficient pyrido[1,2-*a*]benzimidazole formation from 2-aminopyridines and cyclohexanones under metal-free conditions

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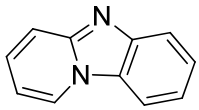
General information:

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 $SiMe_4$, chloroform signals. MS analyses were performed on Agilent 5975 GC-MS instrument (EI). The new compounds were characterized by ^{1}H NMR, ^{13}C NMR, MS and HRMS. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR and MS data with those of literature. All reagents were used as received from commercial sources without further purification.

General procedure (3a):

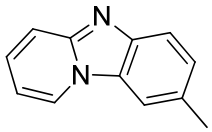
A 10 mL oven-dried reaction vessel was charged with I_2 (50.8 mg, 0.2 mmol), pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol). The reaction vessel was purged with oxygen for three times and was added cyclohexanone (**2a**, 31.2 μL, 0.3 mmol), 1,1,2,2-tetrachloroethane (0.9 mL) by syringe. The sealed vessel was stirred at 160 ^{o}C for 24 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and washed with saturated sodium hydroxide solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate for three times. The combined organic layer was dried over sodium sulfate, and evaporated under vacuum and the residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3a** as white solid; yield: 29.6 mg (88%), mp 130-132 °C.

Benzo[4,5]imidazo[1,2-*a*]pyridine (3a, CAS: 245-47-6)[1]



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.46 (d, J = 6.8 Hz, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 7.45-7.38 (m, 2H), 6.85 (t, J = 6.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.3, 144.3, 129.2, 128.5, 125.5, 125.1, 120.9, 119.7, 117.8, 110.3, 110.1; MS (EI) *m/z* (%) 168 (100), 140, 114, 84, 51.

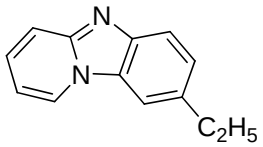
8-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3b)[2]



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-methylcyclohexanone (**2b**, 36.8 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 32.4 mg, 89% yield of **3b** as white solid, mp 73-74 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.38 (d, J = 6.8 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.67-7.65 (m, 2H), 7.39-7.35 (m, 2H), 6.81 (t, J = 6.8 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.9, 142.3, 130.8, 128.5, 128.47, 127.2, 124.7, 119.1, 117.6, 109.9, 109.8, 21.6; MS (EI) *m/z* (%) 182 (100), 154, 91, 78, 51.

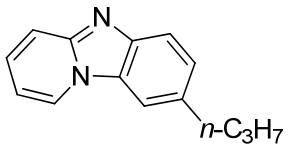
8-Ethylbenzo[4,5]imidazo[1,2-*a*]pyridine (3c)



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-ethylcyclohexanone (**2c**, 42.3 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 34.1 mg, 87% yield of **3c** as white solid, mp 38-39 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.42 (d, J = 6.8 Hz, 1H), 7.85 (d, J = 8. 4 Hz, 1H), 7.70-7.68 (m, 2H), 7.41-7.38 (m, 2H), 6.83 (t, J = 6.6 Hz, 1H), 2.89 (q, J = 6.8 Hz, 2H), 1.35 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.1, 142.5, 137.6, 128.7, 128.6, 126.3, 124.9, 119.3, 117.7, 109.9, 108.7, 29.1, 16.1; MS (EI) *m/z* (%) 196,181 (100), 90, 78, 51; HRMS calcd. for: $C_{13}H_{13}N_2$ $[M+H]^+$ 197.1073, found 197.1071.

8-Propylbenzo[4,5]imidazo[1,2-*a*]pyridine (3d)

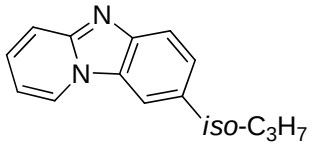


The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and

4-propylcyclohexanone (**2d**, 46.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 35.3 mg, 84% yield of **3d** as pale yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.41 (d, J = 6.8 Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.68-7.66 (m, 2H), 7.40-7.36 (m, 2H), 6.82 (t, J = 6.6 Hz, 1H), 2.82 (t, J = 7.6 Hz, 2H), 1.80-1.71 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.1, 142.6, 135.9, 128.6, 128.5, 126.7, 124.8, 119.2, 117.7, 109.8, 109.3, 38.2, 30.0, 13.6; MS (EI) *m/z* (%) 210, 195 (100), 168, 78, 51; HRMS calcd. for: $C_{14}H_{15}N_2$ $[M+H]^+$ 211.1230, found 211.1228.

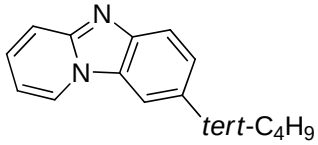
8-(*Iso*-propyl)benzo[4,5]imidazo[1,2-*a*]pyridine (3e)



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-isopropylcyclohexanone (**2e**, 46.5 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 34.9 mg, 83% yield of **3e** as white solid, mp 91-92 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.45 (d, J = 6.8 Hz, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.73-7.68 (m, 2H), 7.45-7.38 (m, 2H), 6.84 (t, J = 6.6 Hz, 1H), 3.19-3.12 (m, 1H), 1.37 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.2, 142.7, 142.4, 128.7, 128.6, 125.1, 124.9, 119.4, 117.8, 109.9, 107.2, 34.3, 24.4; MS (EI) *m/z* (%) 210, 195 (100), 181, 78, 51; HRMS calcd. for: $C_{14}H_{15}N_2$ $[M+H]^+$ 211.1230, found 211.1228.

8-(*Tert*-butyl)Benzo[4,5]imidazo[1,2-*a*]pyridine (3f, CAS: 1243272-97-0)[3]

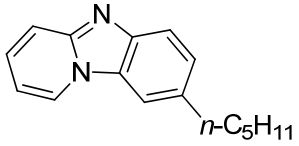


The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-(*tert*-butyl)cyclohexanone (**2f**, 51.9 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 37.2 mg, 83%

yield of **3f** as white solid, mp 90-92 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.47 (d, J = 6.8 Hz, 1H), 7.88-7.86 (m, 2H), 7.68-7.61 (m, 2H), 7.38 (t, J = 7.8 Hz, 1H), 6.82 (t, J = 6.4 Hz, 1H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.5, 144.8, 142.5, 128.7, 128.6, 125.0, 124.1, 119.2, 117.9, 110.0, 106.3, 35.1, 31.8; MS (EI) *m/z* (%) 224, 209 (100), 168, 78, 51.

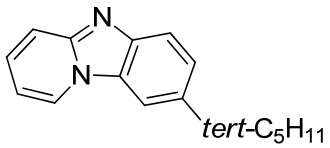
8-Pentylbenzo[4,5]imidazo[1,2-*a*]pyridine (3g)



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-pentylcyclohexanone (**2g**, 56.7 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 40.9 mg, 86% yield of **3g** as pale yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.41 (d, J = 6.4 Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.68-7.65 (m, 2H), 7.39-7.36 (m, 2H), 6.81 (t, J = 6.6 Hz, 1H), 2.83 (t, J = 7.6 Hz, 2H), 1.74-1.71 (m, 2H), 1.38-1.36 (m, 4H), 0.91 (t, J = 6.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.1, 142.6, 136.2, 128.6, 128.5, 126.7, 124.9, 119.2, 117.7, 109.8, 109.3, 36.1, 31.7, 31.3, 22.4, 13.9; MS (EI) *m/z* (%) 238, 209 (100), 193, 168, 51; HRMS calcd. for: $C_{14}H_{15}N_2$ $[M+H]^+$ 239.1543, found 239.1540.

8-(*Tert*-pentyl)Benzo[4,5]imidazo[1,2-*a*]pyridine (3h)

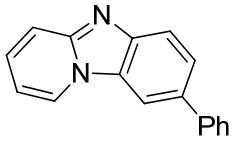


The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-(*tert*-pentyl)cyclohexanone (**2h**, 55.7 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 40.5 mg, 85% yield of **3h** as white solid, mp 91-92 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.47 (d, J = 6.4 Hz, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.80 (s,

1H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 6.83 (t, *J* = 6.4 Hz, 1H), 1.77 (q, *J* = 7.06 Hz, 2H), 1.42 (s, 6H), 0.7 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.3, 142.8, 142.3, 128.5, 128.4, 124.9, 124.3, 119.0, 117.7, 109.8, 107.1, 38.1, 37.0, 28.8, 9.1; MS (EI) *m/z* (%) 238, 209 (100), 181, 78, 51; HRMS calcd. for: $C_{14}H_{15}N_2$ $[M+H]^+$ 239.1543, found 239.1540.

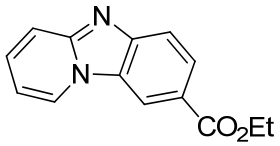
8-Phenylbenzo[4,5]imidazo[1,2-*a*]pyridine (3i)



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 4-phenylcyclohexanone (**2i**, 52.3 mg, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 42.9 mg, 88% yield of **3i** as white solid, mp 55-56 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.50 (d, *J* = 6.4 Hz, 1H), 8.07 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.74-7.69 (m, 3H), 7.51-7.36 (m, 4H), 6.88 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.7, 143.6, 141.1, 134.4, 129.3, 128.9, 128.7, 127.2, 126.8, 125.3, 125.0, 119.7, 117.7, 110.2, 108.5; MS (EI) *m/z* (%) 244 (100), 207, 122, 78, 51; HRMS calcd. for: $C_{14}H_{15}N_2$ $[M+H]^+$ 245.1073, found 245.1070.

Ethyl benzo[4,5]imidazo[1,2-*a*]pyridine-8-carboxylate (3j, CAS: 1312175-23-7)[1]

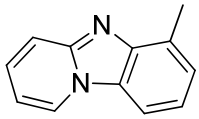


The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and ethyl 4-oxocyclohexanecarboxylate (**2j**, 47.8 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 39.8 mg, 83% yield of **3j** as white solid, mp 136-137 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (s, 1H), 8.58 (d, *J* = 6.4 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 9.2 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 6.96 (t, *J* = 6.6 Hz,

1H), 4.46 (q, *J* = 7.06 Hz, 2H), 1.46 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 166.5, 150.2, 147.4, 130.6, 128.1, 126.5, 125.4, 122.6, 118.9, 117.8, 112.7, 110.9, 60.8, 14.2; MS (EI) m/z (%) 240, 195 (100), 167, 140, 51.

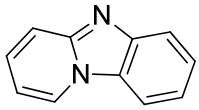
6-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3k)[3]



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 2-methylcyclohexanone (**2k**, 36.1 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 23.3 mg, 64% yield of **3k** as white solid, mp 137-139 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) *δ* 8.42 (d, *J* = 6.8 Hz, 1H), 7.76-7.72 (m, 2H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 6.84 (t, *J* = 6.6 Hz, 1H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.8, 143.7, 129.7, 128.9, 128.0, 125.5, 125.1, 120.9, 117.9, 110.1, 107.7, 17.1; MS (EI) m/z (%) 182 (100), 127, 91, 78, 51.

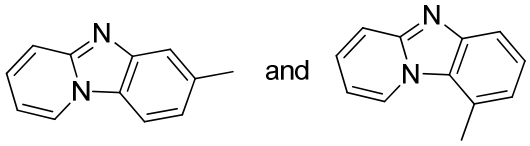
Benzo[4,5]imidazo[1,2-*a*]pyridine (3a, CAS: 245-47-6)[1]



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 2-chlorocyclohexanone (**2l**, 34.3 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 25.5 mg, 76% yield of **3a** as white solid, mp 130-132 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) *δ* 8.46 (d, *J* = 6.8 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.45-7.38 (m, 2H), 6.85 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) *δ* 148.3, 144.3, 129.2, 128.5, 125.5, 125.1, 120.9, 119.7, 117.8, 110.3, 110.1; MS (EI) *m/z* (%) 168 (100), 140, 114, 84, 51.

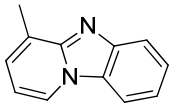
7-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine and 9-methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3m, CAS: 1243272-98-1 and 3m′, CAS: 474537-07-0)[2, 4]



The reaction was conducted with pyridin-2-amine (**1a**, 19.2 mg, 0.2 mmol) and 3-methylcyclohexanone (**2m**, 36.9 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 32.0 mg, 88% yield of **3m** and **3m′** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.78 (d, J = 6.8 Hz, 0.6H), 8.41 (d, J = 6.8 Hz, 0.4H), 7.81-7.67 (m, 2.4H), 7.43-7.38 (m, 1.6H), 7.19 (d, J = 8.4 Hz, 0.4H), 7.10 (d, J = 7.2 Hz, 0.6H), 6.85-6.79 (m, 1H), 2.92 (s, 1.8H), 2.57 (s, 1.2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.5, 144.6, 135.6, 128.9, 128.87, 128.5, 128.47, 127.4, 125.2, 125.0, 123.2, 122.6, 119.3, 117.9, 117.7, 117.5, 110.1, 110.06, 110.0, 109.96, 109.8, 109.78, 21.9, 19.6; MS (EI) m/z (%) 182 (100), 154, 91, 78, 51.

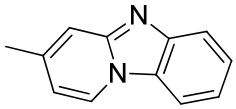
4-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3n, CAS: 23275-60-7)[2]



The reaction was conducted with 3-methylpyridin-2-amine (**1b**, 20.4 μL, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 29.1 mg, 80% yield of **3n** as white solid, mp 118-120 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.32 (d, J = 6.0 Hz, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.52 (t, J = 7.2 Hz, 1H), 7.36 (t, J = 7.0 Hz, 1H), 7.22 (d, J = 5.6 Hz, 1H), 6.77 (t, J = 6.2 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.9, 144.0, 129.02, 129.0, 127.5, 125.3, 122.7, 120.8, 119.7, 110.4, 110.2, 17.4; MS (EI) m/z (%) 182 (100), 129, 91, 77, 51.

3-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3o, CAS: 72570-64-0)[3]

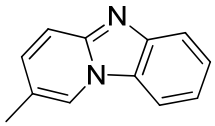


The reaction was conducted with 4-methylpyridin-2-amine (**1c**, 21.8 mg, 0.2 mmol) and

cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 30.2 mg, 83% yield of **3o** as white solid, mp 162-164 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.32 (d, J = 6.4 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.50 (t, J = 7.2 Hz, 1H), 7.44 (s, 1H), 7.33 (t, J = 7.4 Hz, 1H), 6.68 (d, J = 6.4 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.8, 144.4, 140.6, 128.4, 125.2, 124.0, 120.3, 119.3, 115.6, 112.9, 110.0, 21.7; MS (EI) m/z (%) 182 (100), 129, 91, 77, 51.

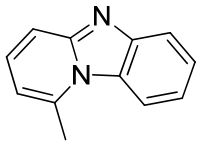
2-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3p, CAS: 88474-34-4)[2]



The reaction was conducted with 5-methylpyridin-2-amine (**1d**, 21.8 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 30.9 mg, 85% yield of **3p** as white solid, mp 144-145 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.22 (s, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.62 (d, J = 9.2 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.36-7.29 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.5, 144.4, 132.5, 128.4, 125.1, 122.4, 120.6, 119.7, 119.6, 117.0, 110.2, 17.9; MS (EI) m/z (%) 182 (100), 129, 91, 77, 51.

1-Methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3q)[2]

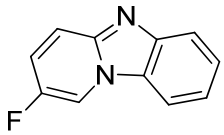


The reaction was conducted with 6-methylpyridin-2-amine (**1e**, 21.8 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 28.4 mg, 78% yield of **3q** as white solid, mp 96-98 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.15 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.54 (t, J = 7.6 Hz, 1H), 7.39-7.31 (m, 2H), 6.62 (d, J = 6.4 Hz, 1H), 3.05 (s, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$, ppm) δ 149.6, 144.9, 139.0, 129.9, 129.3, 125.1, 120.6, 119.6, 115.2, 114.7, 110.8, 21.3; MS (EI) m/z (%) 182 (100), 154, 91, 78, 51.

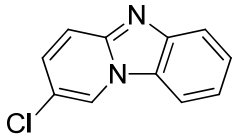
2-Fluorobenzo[4,5]imidazo[1,2-*a*]pyridine (3r, CAS: 1445436-70-3)[5]



The reaction was conducted with 5-fluoropyridin-2-amine (**1f**, 22.4 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 6:1) to provide 29.8 mg, 80% yield of **3r** as pale yellow solid, mp 200-201 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.38 (s, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.73-7.69 (m, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.42-7.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 151.5 (d, *J* = 235.8 Hz), 145.9, 145.1, 129.17 (d, *J* = 2.0 Hz), 125.7, 121.7 (d, *J* = 25.9 Hz), 121.4, 120.3, 118.5 (d, *J* = 8.4 Hz), 111.5 (d, *J* = 39.4 Hz), 110.4; MS (EI) m/z (%) 186 (100),158, 93, 76, 51; HRMS calcd. for: $C_{11}H_8N_2F$ $[M+H]^+$ 187.0666, found 187.0665.

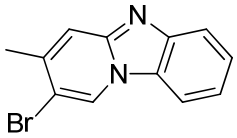
2-Chlorobenzo[4,5]imidazo[1,2-*a*]pyridine (3s)[6]



The reaction was conducted with 5-chloropyridin-2-amine (**1g**, 25.6 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 4:1) to provide 35.5 mg, 88% yield of **3s** as pale yellow solid, mp 202-204 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.50 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 9.6 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.43-7.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.4, 144.6, 130.6, 128.4, 126.0, 123.0, 121.7, 120.2, 118.3, 118.2, 110.3; MS (EI) m/z (%) 202 (100),182, 167, 76, 51.

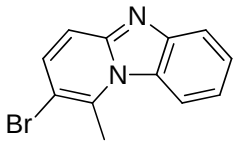
2-Bromo-3-methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3t)



The reaction was conducted with 5-bromo-4-methylpyridin-2-amine (**1h**, 37.2 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 6:1) to provide 42.6 mg, 82% yield of **3t** as pale yellow solid, mp 210-212 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.61 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.56-7.51 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.5, 144.7, 140.1, 128.1, 125.8, 125.2, 121.1, 119.9, 116.6, 110.2, 108.6, 23.1; MS (EI) m/z (%) 260 (100), 207, 181, 77, 51; HRMS calcd. for: $C_{12}H_{10}N_2Br$ $[M+H]^+$ 261.0022, found 261.0020.

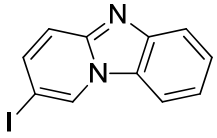
2-Bromo-1-methylbenzo[4,5]imidazo[1,2-*a*]pyridine (3u)



The reaction was conducted with 5-bromo-6-methylpyridin-2-amine (**1i**, 37.2 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 6:1) to provide 40.6 mg, 78% yield of **3u** as pale yellow solid, mp 157-158 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.14 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.55-7.48 (m, 3H), 7.35 (t, *J* = 7.4 Hz, 1H), 3.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.9, 144.9, 137.1, 133.1, 130.1, 125.2, 121.1, 119.8, 115.8, 114.7, 105.9, 20.4; MS (EI) m/z (%) 260 (100), 207, 181, 77, 51; HRMS calcd. for: $C_{12}H_{10}N_2Br$ $[M+H]^+$ 261.0022, found 261.0020.

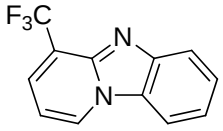
2-Iodobenzo[4,5]imidazo[1,2-*a*]pyridine (3v)



The reaction was conducted with 5-iodopyridin-2-amine (**1j**, 44.0 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 9:1) to provide 45.3 mg, 77% yield of **3v** as pale yellow solid, mp 188-189 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.69 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.57-7.50 (m, 3H), 7.40 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.6, 144.2, 136.8, 130.3, 127.9, 126.1, 121.7, 120.1, 119.1, 110.3, 71.8; MS (EI) m/z (%) 294 (100), 207, 167, 140, 51. HRMS calcd. for: $C_{11}H_8N_2I$ $[M+H]^+$ 294.9727, found 294.9722.

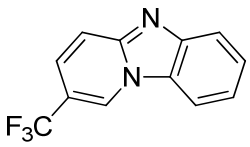
4-(Trifluoromethyl)benzo[4,5]imidazo[1,2-*a*]pyridine (3w)



The reaction was conducted with 3-(trifluoromethyl)pyridin-2-amine (**1k**, 32.4 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 9:1) to provide 41.5 mg, 88% yield of **3w** as pale yellow solid, mp 124-125 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.61 (d, *J* = 6.8 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 144.3, 143.4, 128.5, 128.1, 127.9 (q, *J* = 5.2 Hz), 126.4, 122.7 (q, *J* = 270.4 Hz), 122.1, 120.5, 118.9 (q, *J* = 33.5 Hz), 110.4, 108.3; MS (EI) m/z (%) 236 (100), 167, 118, 93, 51; HRMS calcd. for: $C_{12}H_8N_2F_3$ $[M+H]^+$ 237.0634, found 237.0632.

2-(Trifluoromethyl)benzo[4,5]imidazo[1,2-*a*]pyridine (3x, CAS: 1445436-74-7)[5]

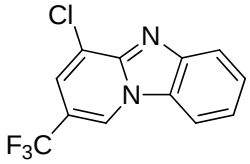


The reaction was conducted with 5-(trifluoromethyl)pyridin-2-amine (**1l**, 32.4 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column

chromatography on silica (petroleum ether/ethyl acetate = 9:1) to provide 42.5 mg, 90% yield of **3x** as pale yellow solid, mp 184-186 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.82 (s, 1H), 8.00-7.95 (m, 2H), 7.81 (d, *J* = 9.6 Hz, 1H), 7.63-7.55 (m, 2H), 7.48 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.4, 144.8, 128.5, 126.5, 124.6 (q, *J* = 2.5 Hz), 124.4 (q, *J* = 5.7 Hz), 123.4 (q, *J* = 269.1 Hz), 122.1, 120.3, 118.5, 114.3 (q, *J* = 34.2 Hz), 110.3; MS (EI) m/z (%) 236 (100), 167, 118, 93, 51.

4-Chloro-2-(trifluoromethyl)benzo[4,5]imidazo[1,2-*a*]pyridine (3y)



The reaction was conducted with 3-chloro-5-(trifluoromethyl)pyridin-2-amine (**1m**, 39.2 mg, 0.2 mmol) and cyclohexanone (**2a**, 31.2 μL, 0.3 mmol). The crude mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 9:1) to provide 49.7 mg, 92% yield of **3y** as pale yellow solid, mp 172-173 °C.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.76 (s, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.66-7.62 (m, 2H), 7.51 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 144.8, 144.3, 129.4, 126.9, 124.4, 123.2 (q, *J* = 1.8 Hz), 123.0, 122.9 (q, *J* = 5 Hz), 122.8 (q, *J* = 269.3 Hz), 120.9, 114.1 (q, *J* = 34.8 Hz), 110.6; MS (EI) m/z (%) 270 (100), 235, 135, 75, 51; HRMS calcd. for: $C_{12}H_7N_2ClF_3$ $[M+H]^+$ 271.0244, found 271.0242.

References

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[5] D. D. Liang, Y. M. He, L. Y. Liu, Q. Zhu, *Org. Lett*. **2013**, *15*, 3476.

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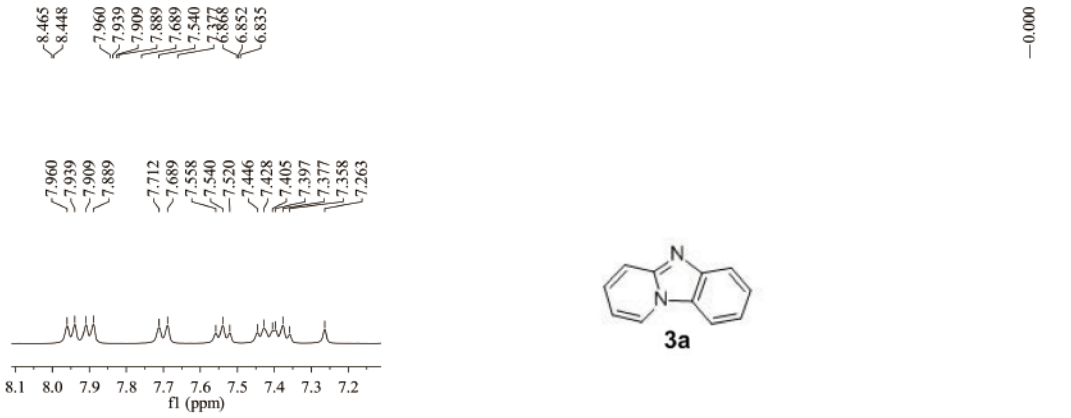
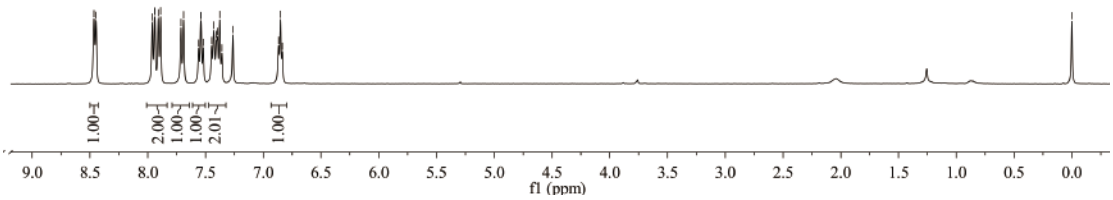
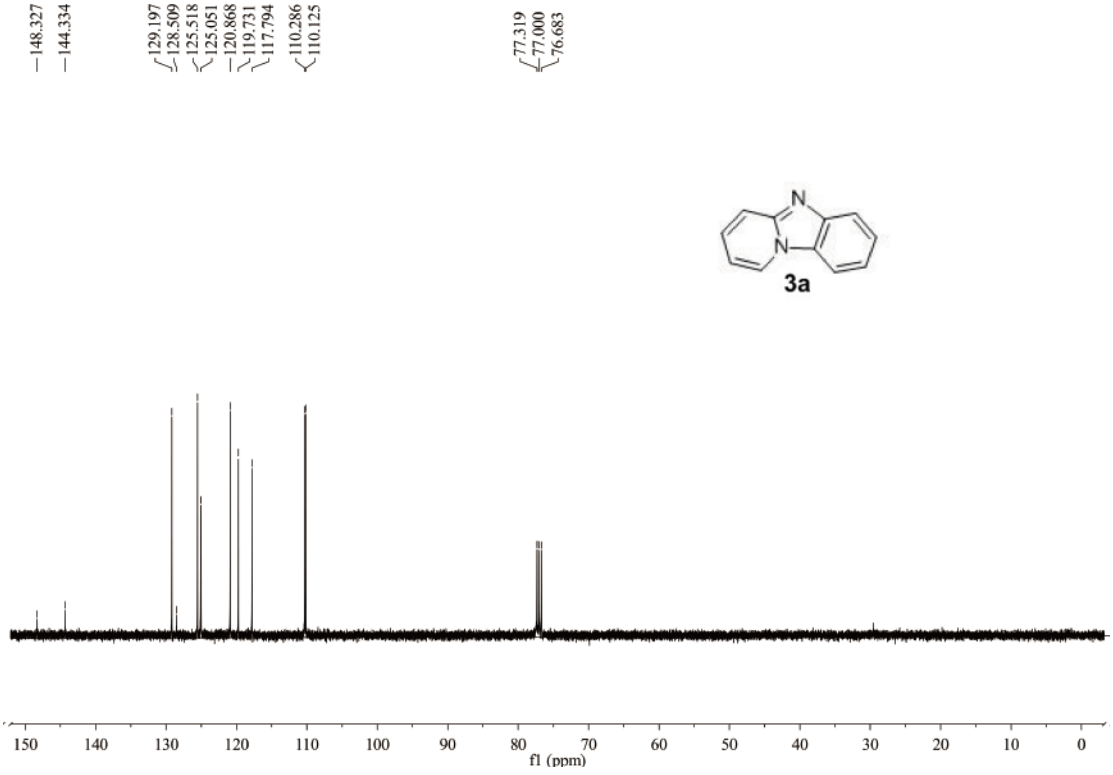
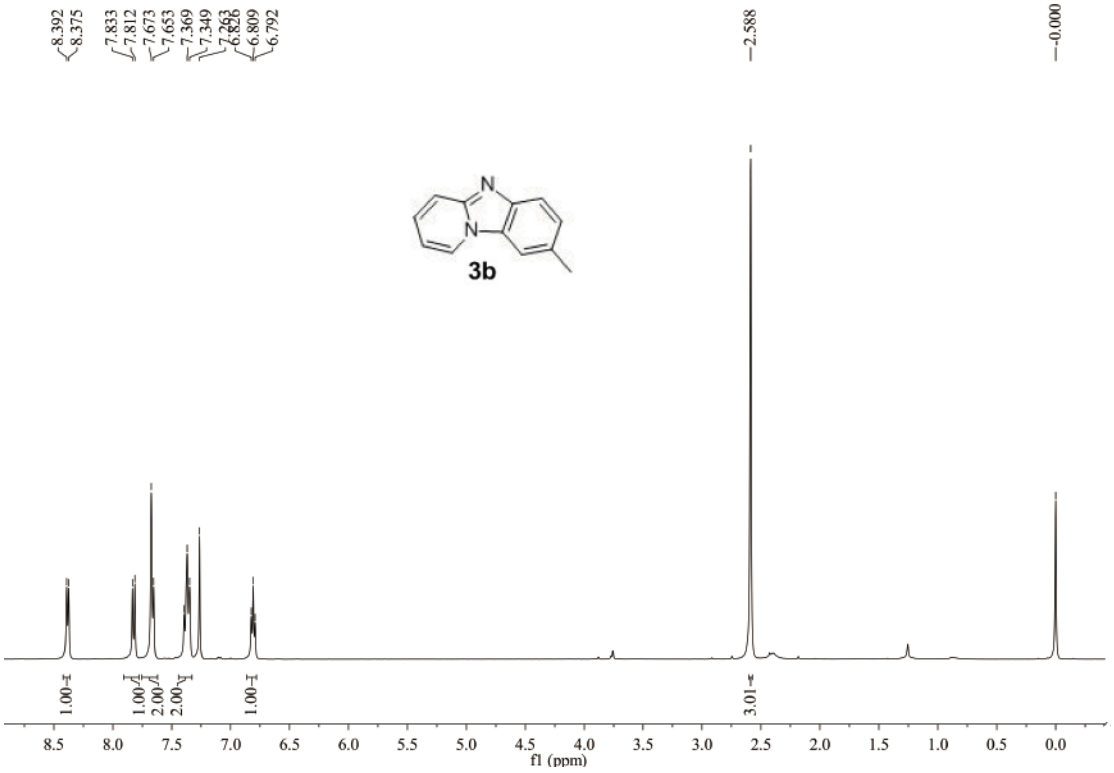
^{1}H and ^{13}C NMR spectra





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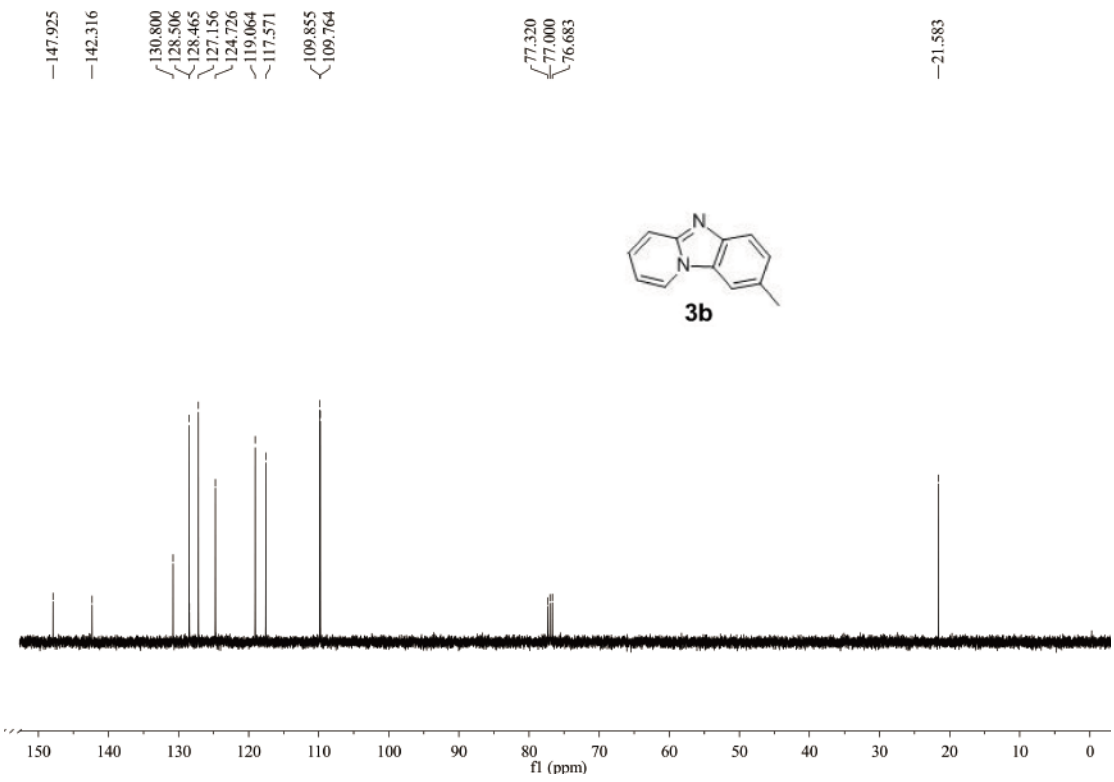
2.588
0.000
3b
1.00
1.00
2.00
2.00
1.00
3.01
fl (ppm)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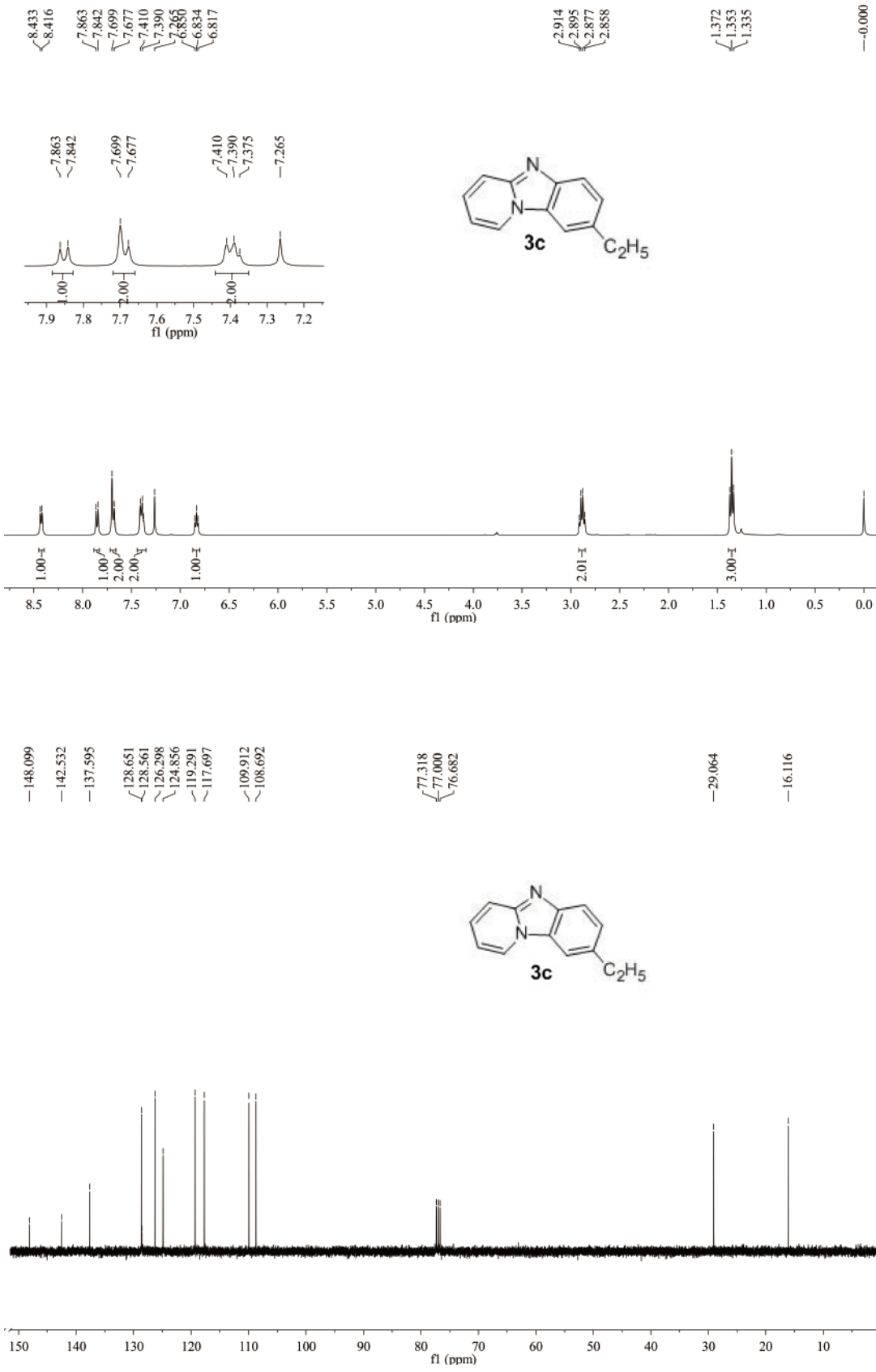
fl (ppm)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7.699
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3c
C2H5
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2.00
1.00
2.01
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
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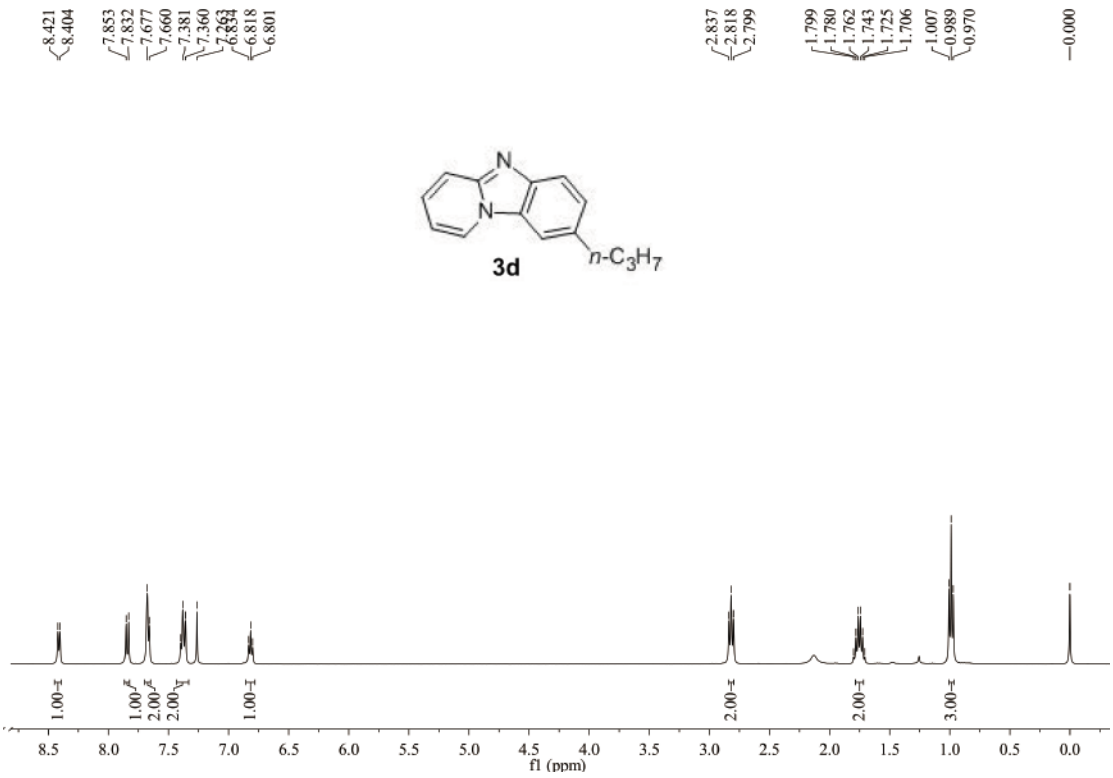
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3.00
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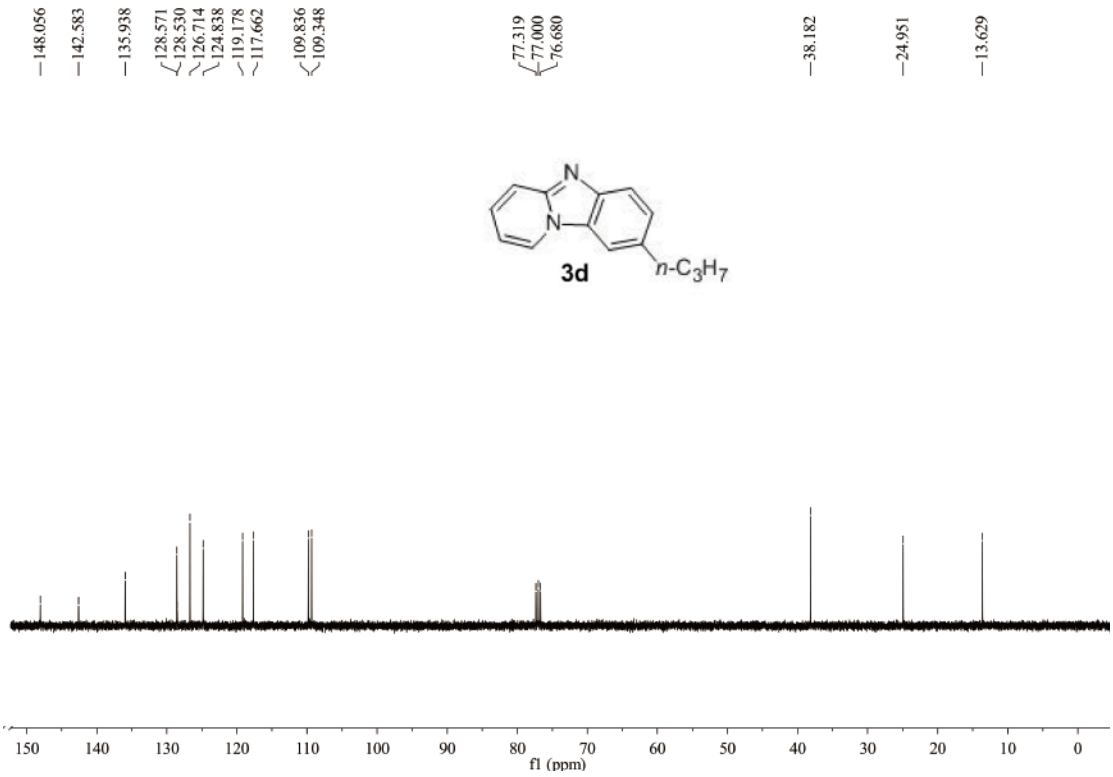
f1 (ppm)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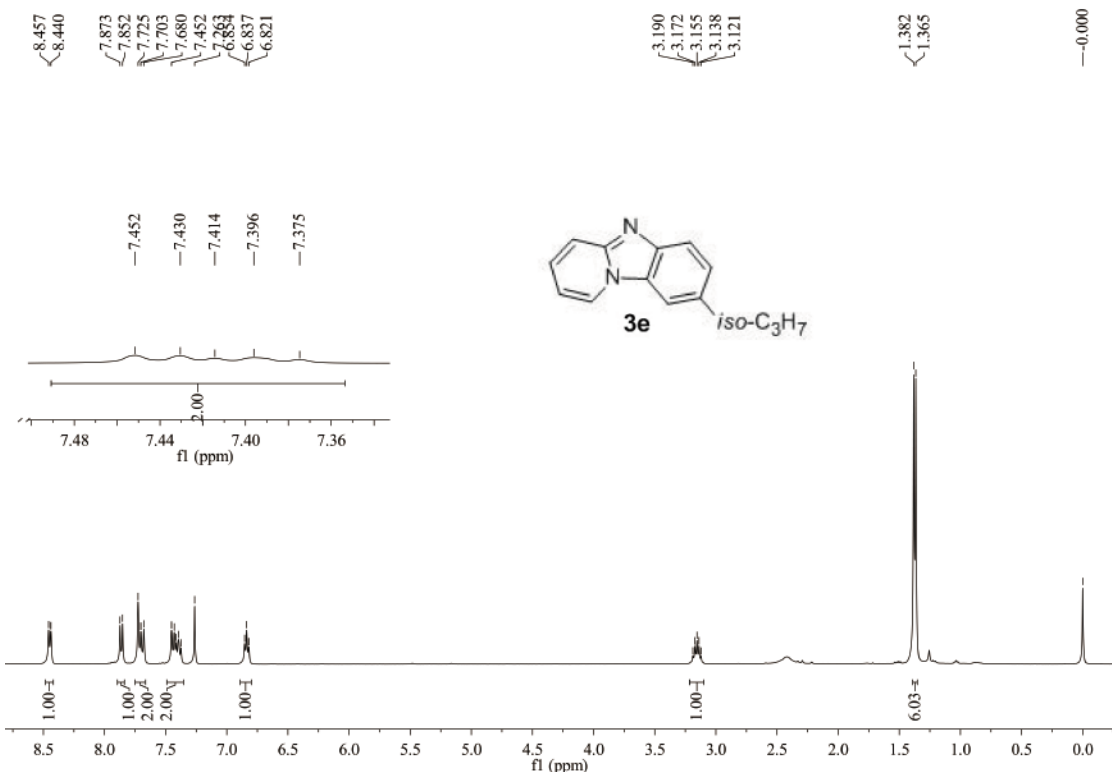
f1 (ppm)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3.121
1.382
1.365
0.000
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7.414
7.396
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7.44
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7.36
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2.00
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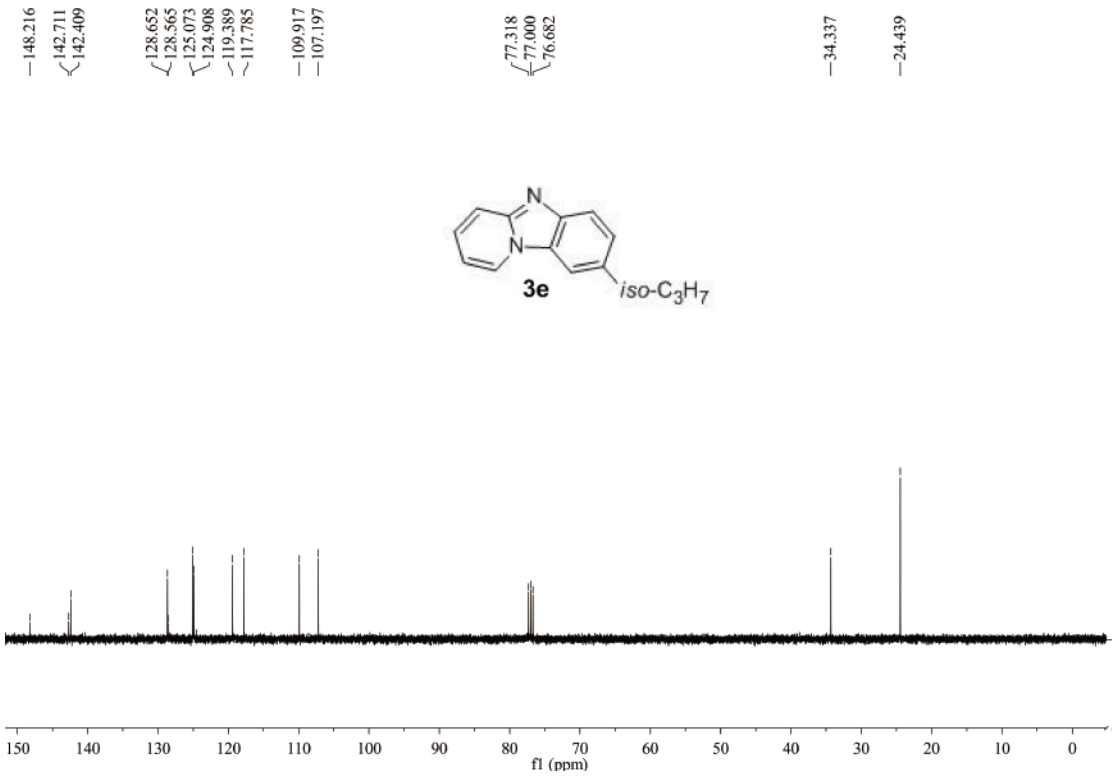
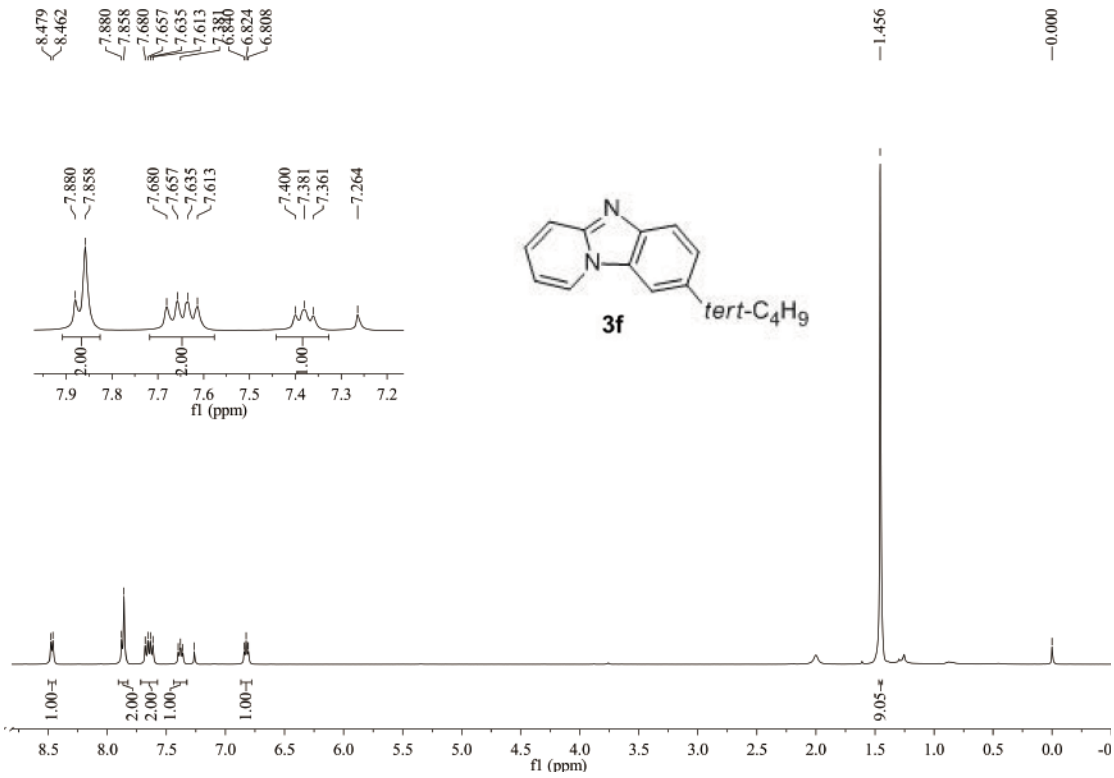
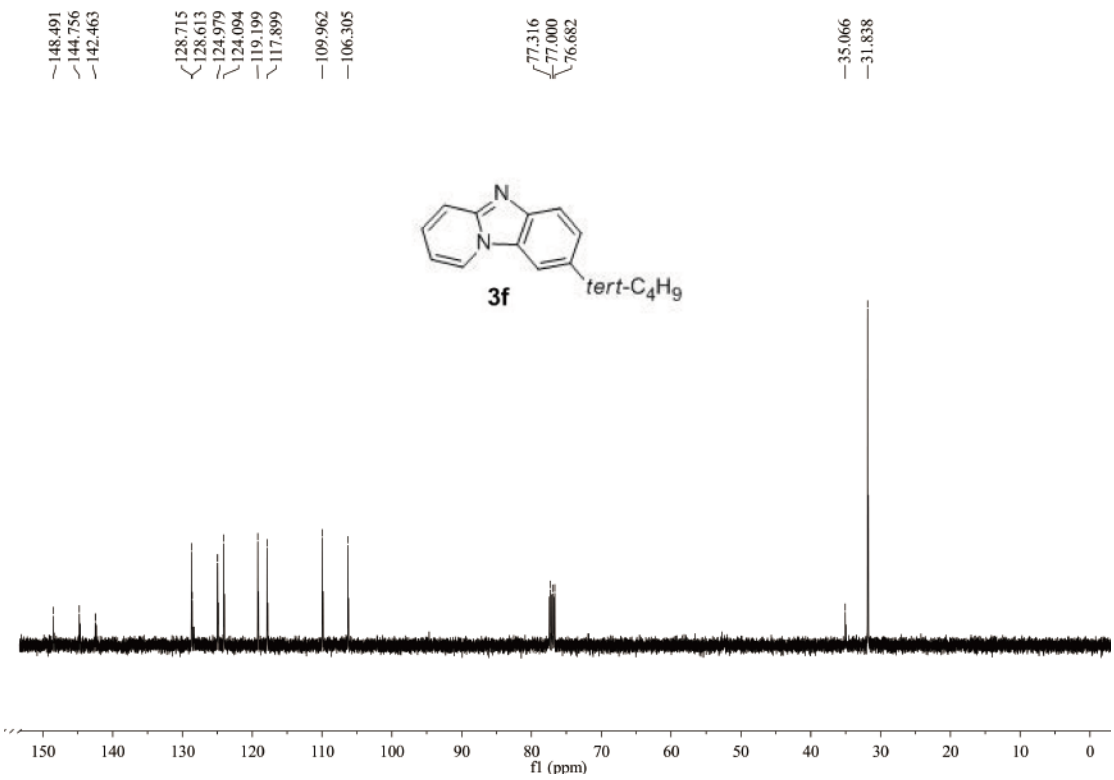
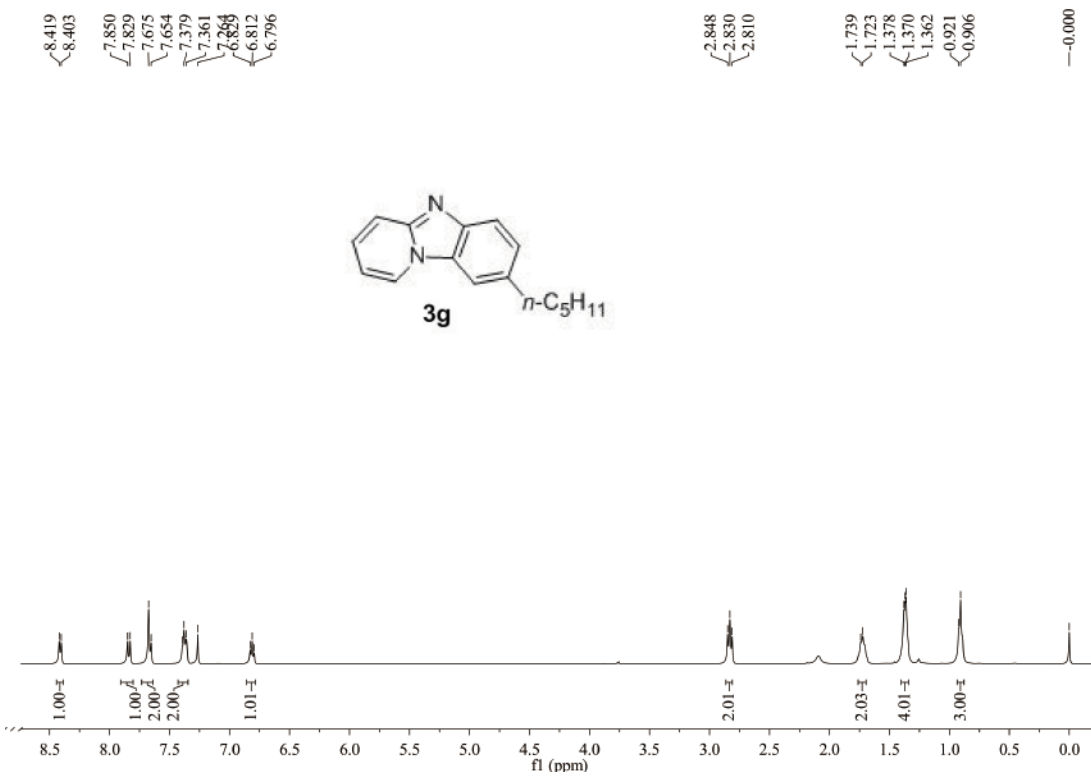
0.0
f1 (ppm)


148.216
142.711
142.409
128.652
128.565
125.073
124.908
119.389
117.785
109.917
107.197
77.318
77.000
76.682
34.337
24.439
3e
iso-C3H7
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.479
8.462
7.880
7.858
7.680
7.657
7.635
7.613
7.400
7.381
7.361
6.840
6.824
6.808
1.456
0.000
7.264
3f
tert-C4H9
fl (ppm)


148.491
144.756
142.463
128.715
128.613
124.979
124.094
119.199
117.899
109.962
106.305
77.316
77.000
76.682
35.066
31.838
3f
tert-C4H9
fl (ppm)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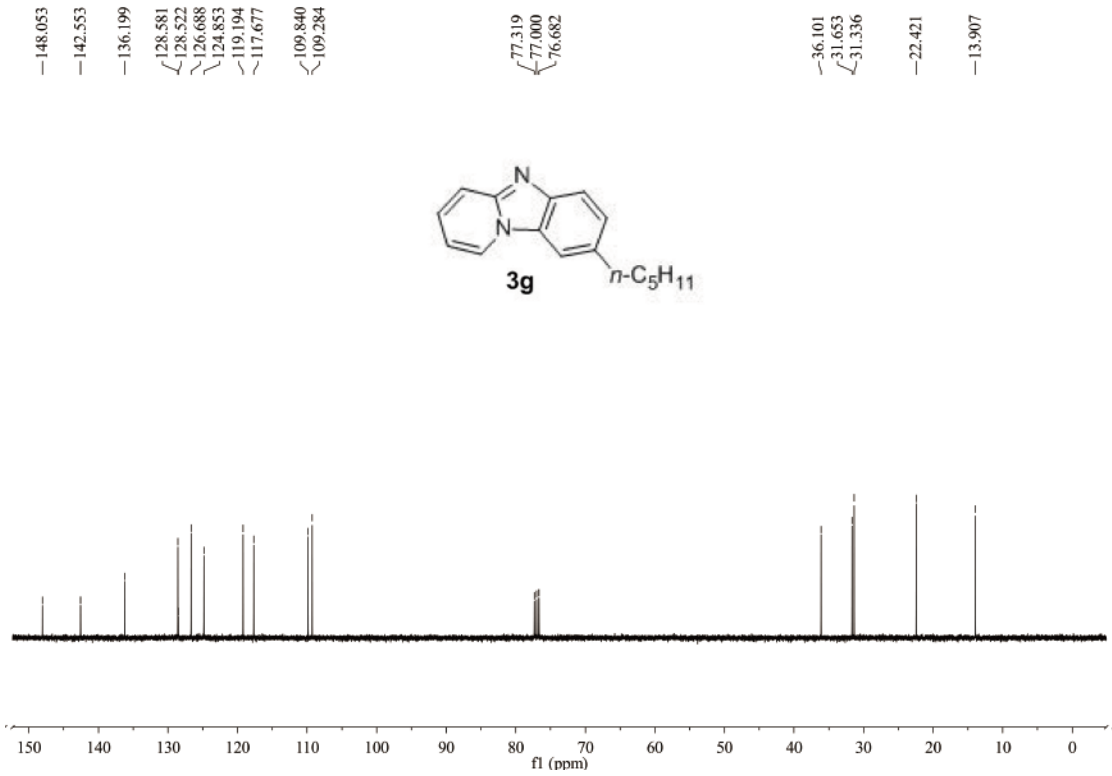
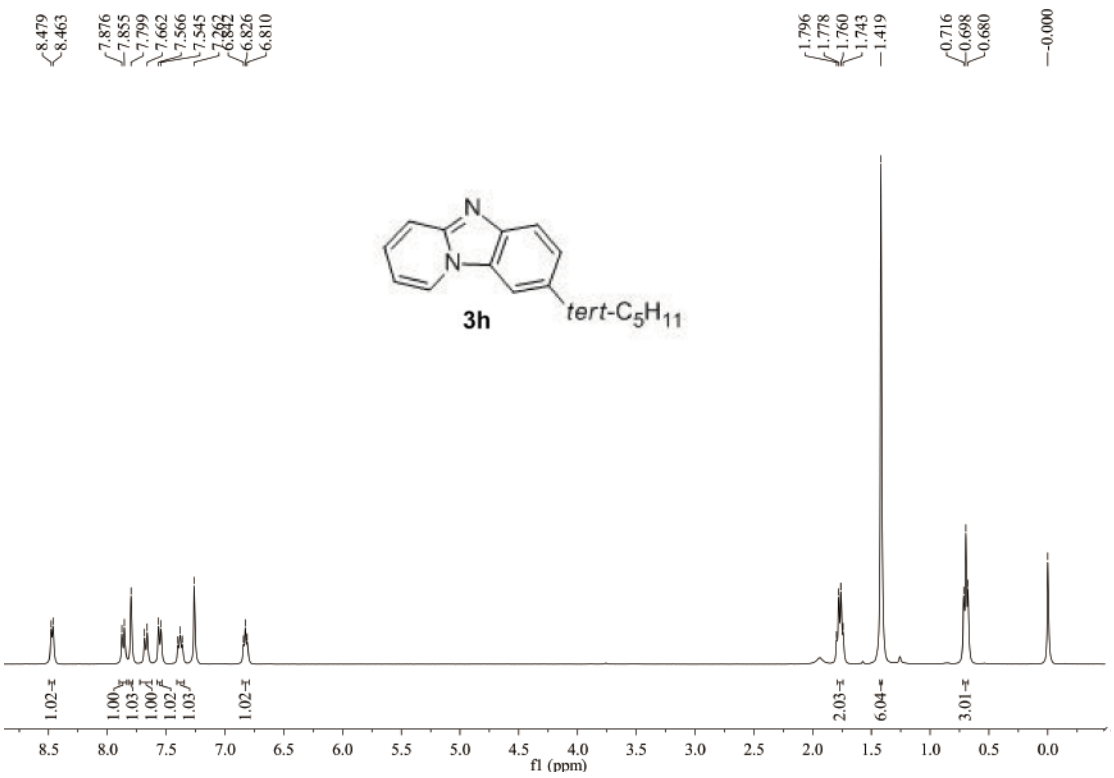
8.403
7.850
7.829
7.675
7.654
7.379
7.361
7.264
6.829
6.812
6.796
2.848
2.830
2.810
1.739
1.723
1.378
1.370
1.362
0.921
0.906
0.000
N
N
n-C5H11
3g
1.00
1.00
2.00
2.00
1.01
2.01
2.03
4.01
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.053
142.553
136.199
128.581
128.522
126.688
124.853
119.194
117.677
109.840
109.284
77.319
77.000
76.682
36.101
31.653
31.336
22.421
13.907
N
N
n-C5H11
3g
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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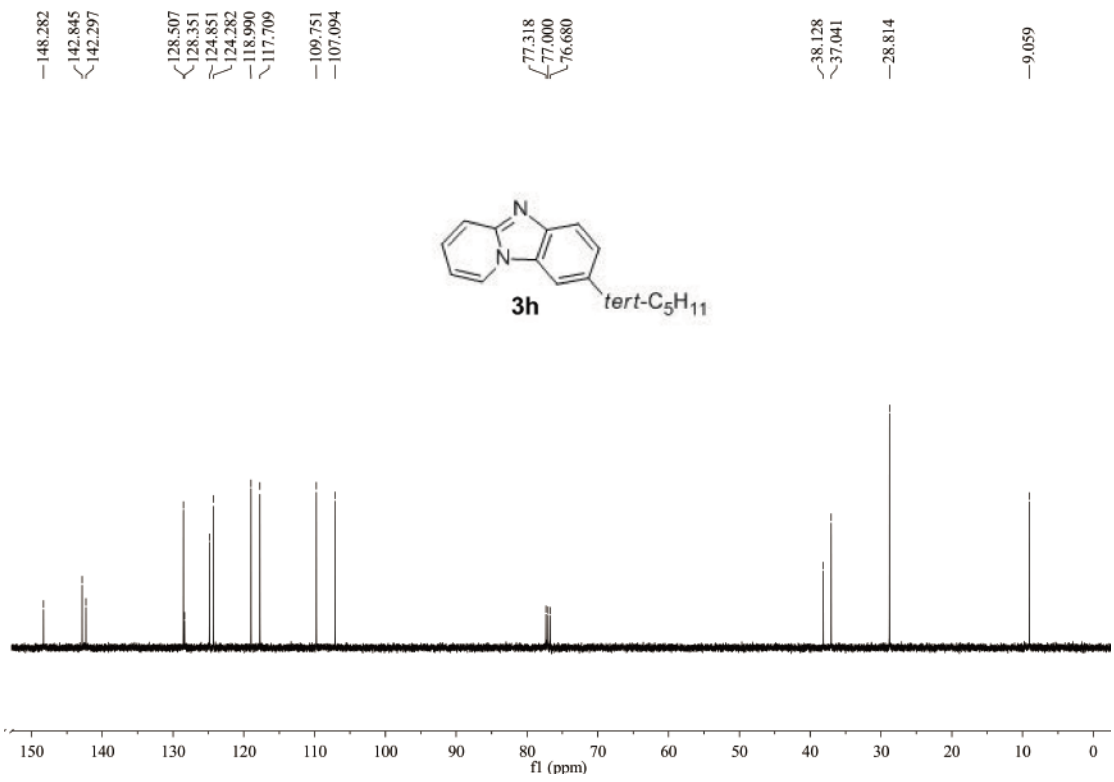
8.463
7.876
7.855
7.799
7.662
7.566
7.545
7.262
6.842
6.826
6.810
1.796
1.778
1.760
1.743
1.419
0.716
0.698
0.680
0.000
3h
tert-C5H11
1.02
1.00
1.03
1.00
1.02
1.03
1.02
2.03
6.04
3.01
fl (ppm)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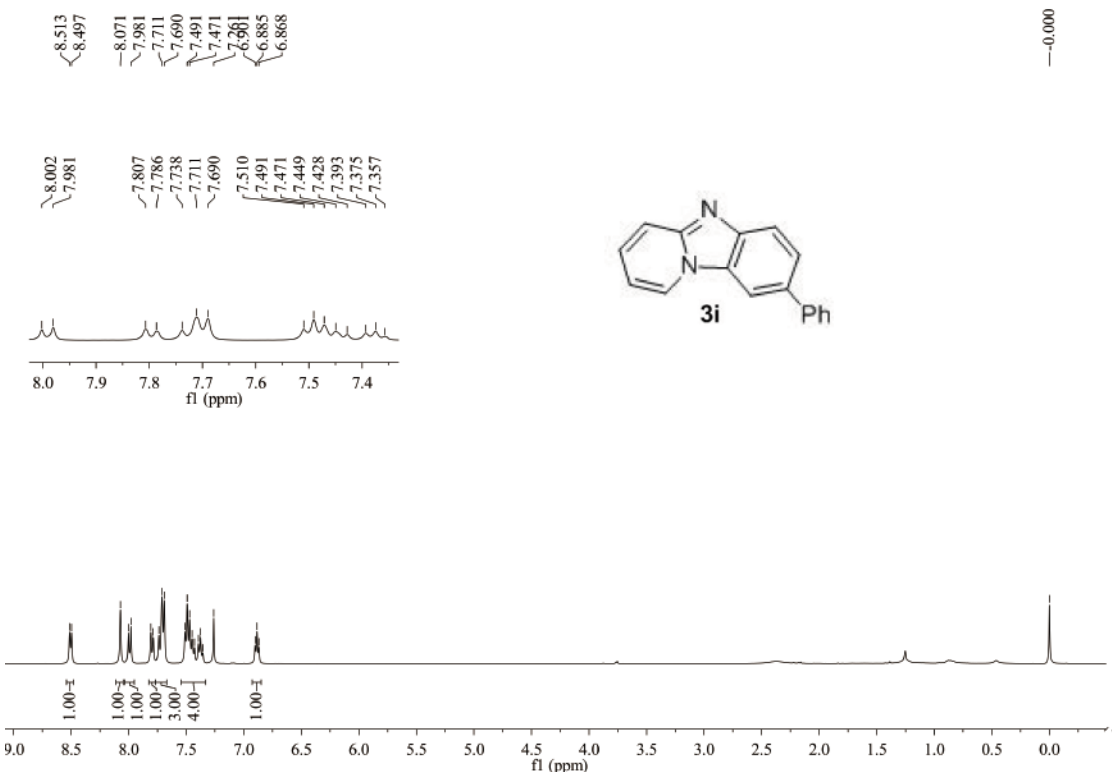
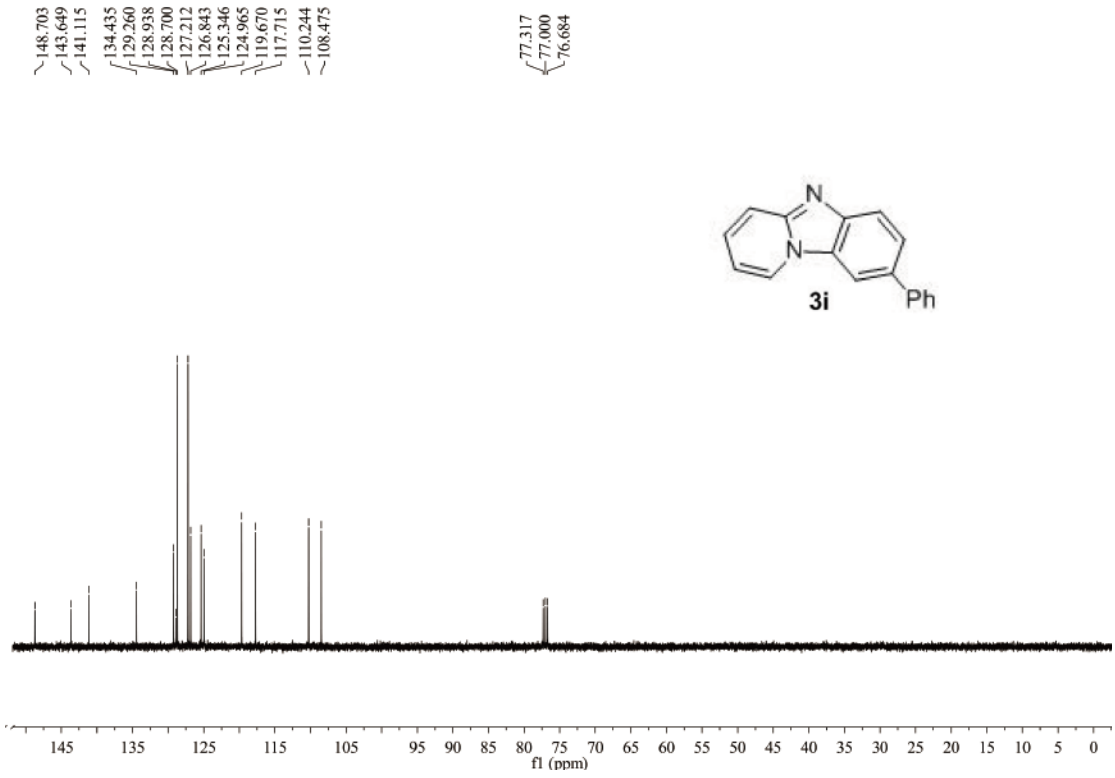
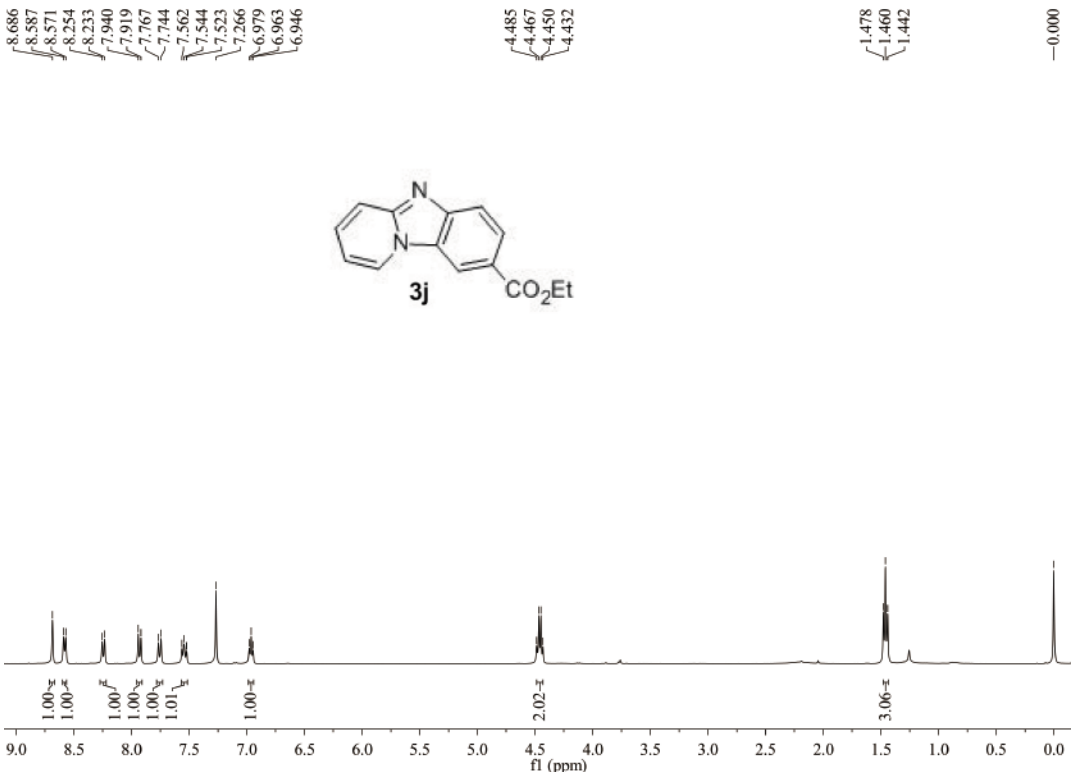
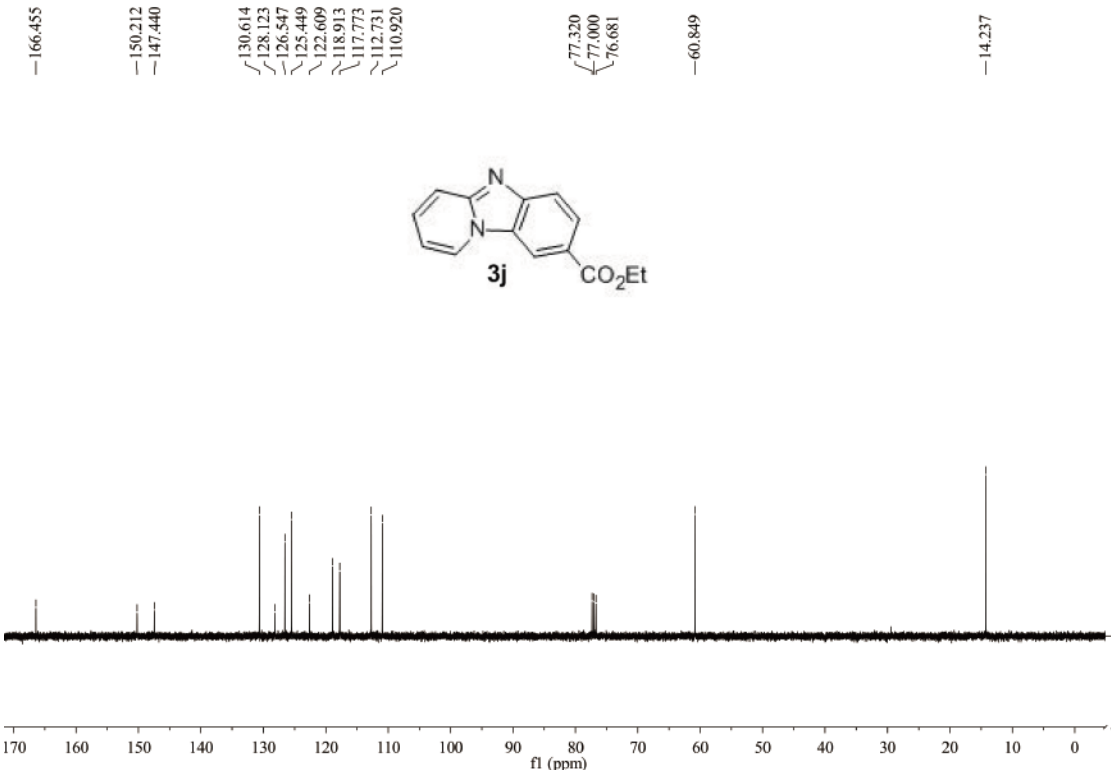
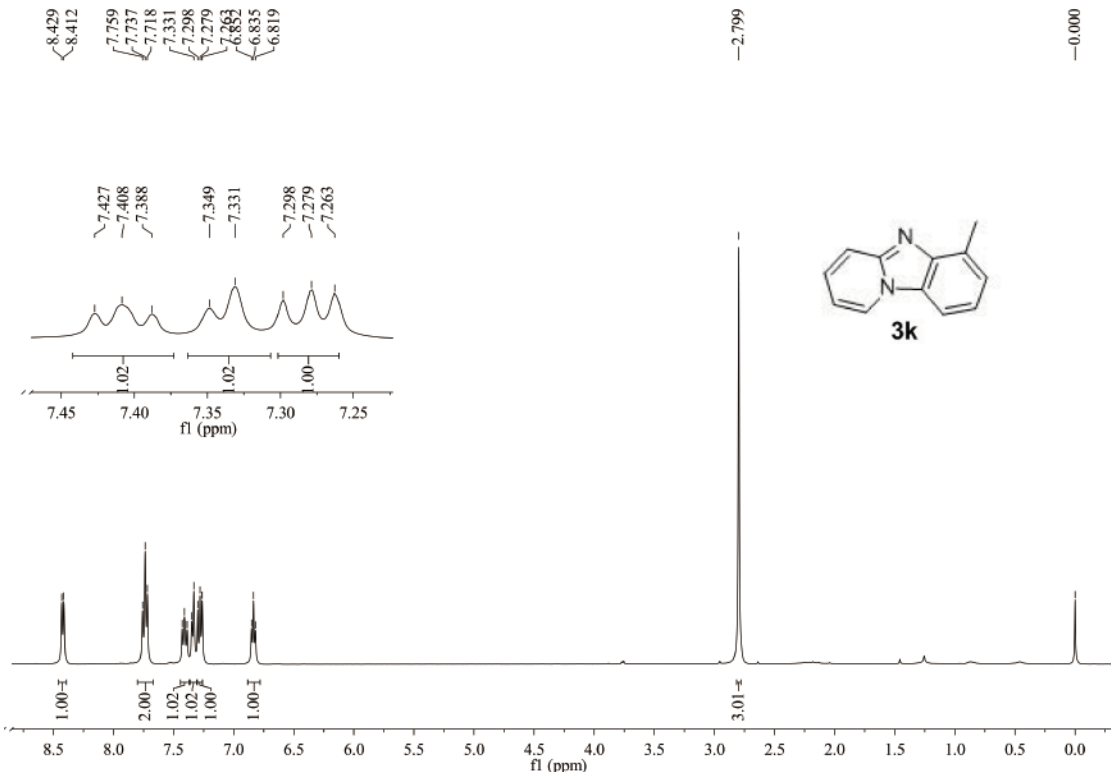
142.845
142.297
128.507
128.351
124.851
124.282
118.990
117.709
109.751
107.094
77.318
77.000
76.680
38.128
37.041
28.814
9.059
3h
tert-C5H11
fl (ppm)

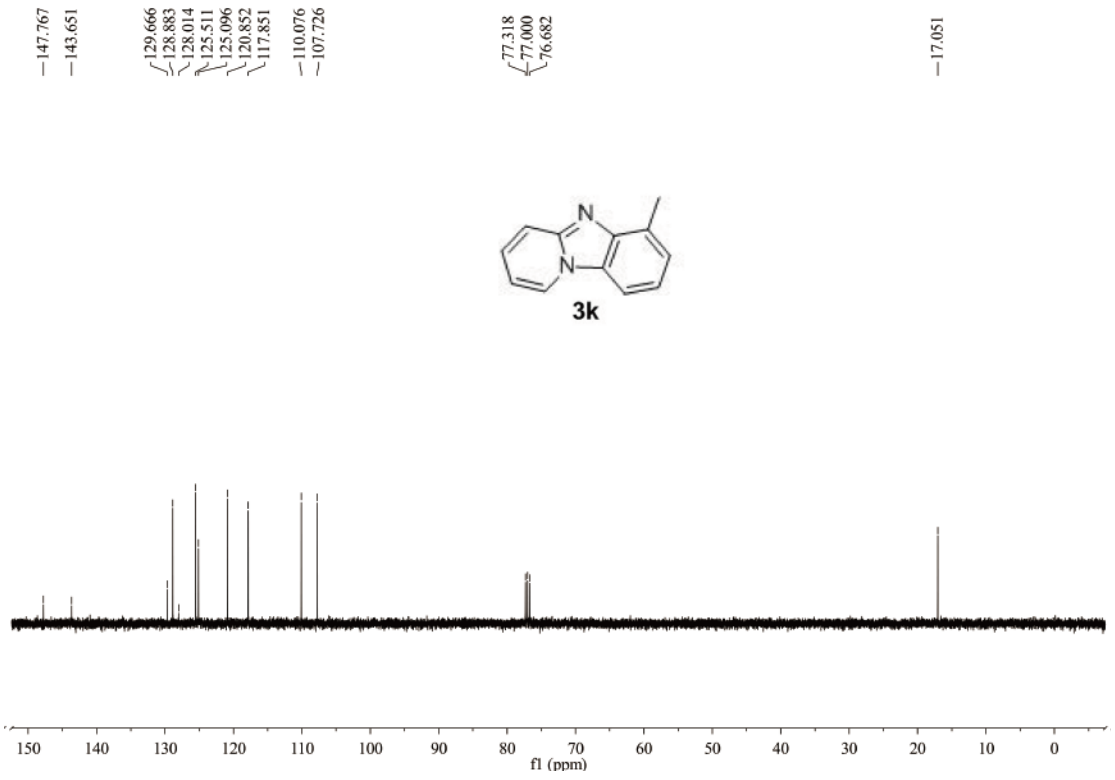

8.513
8.497
8.071
7.981
7.711
7.690
7.491
7.471
6.885
6.868
0.000
8.002
7.981
7.807
7.786
7.738
7.711
7.690
7.510
7.491
7.471
7.449
7.428
7.393
7.375
7.357
N
N
3i
Ph
8.0
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
1.00
1.00
1.00
3.00
4.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

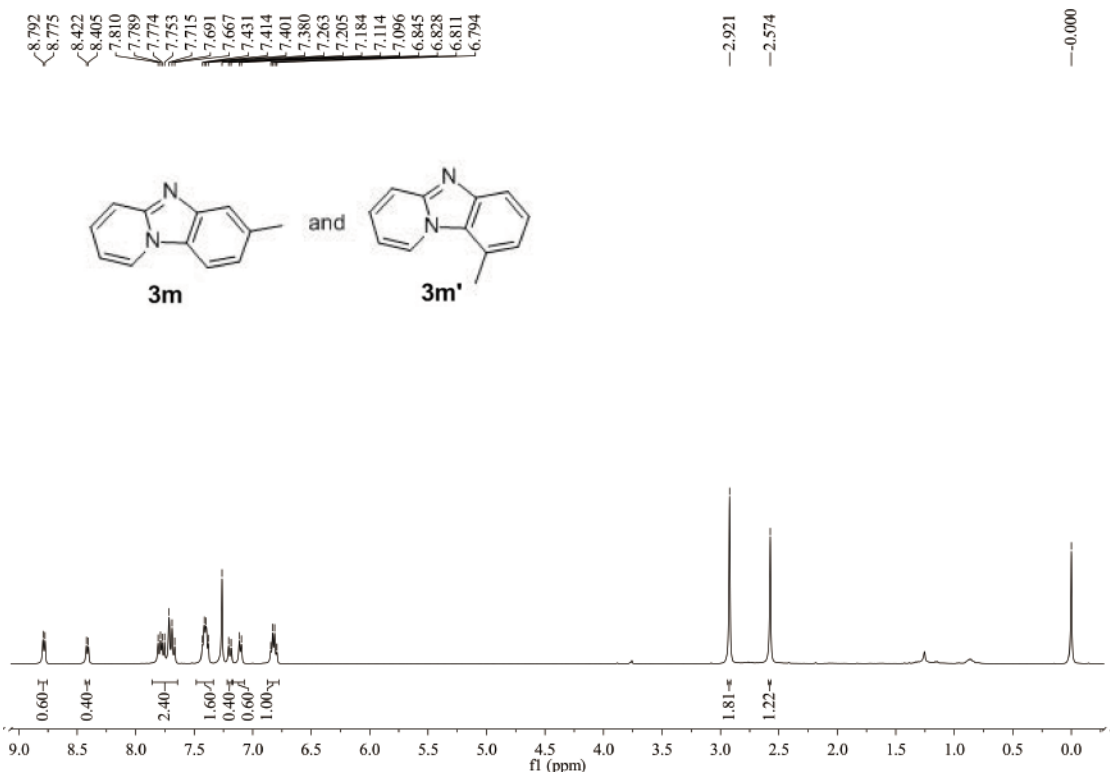

148.703
143.649
141.115
134.435
129.260
128.938
128.700
127.212
126.843
125.346
124.965
119.670
117.715
110.244
108.475
77.317
77.000
76.684
N
N
3i
Ph
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

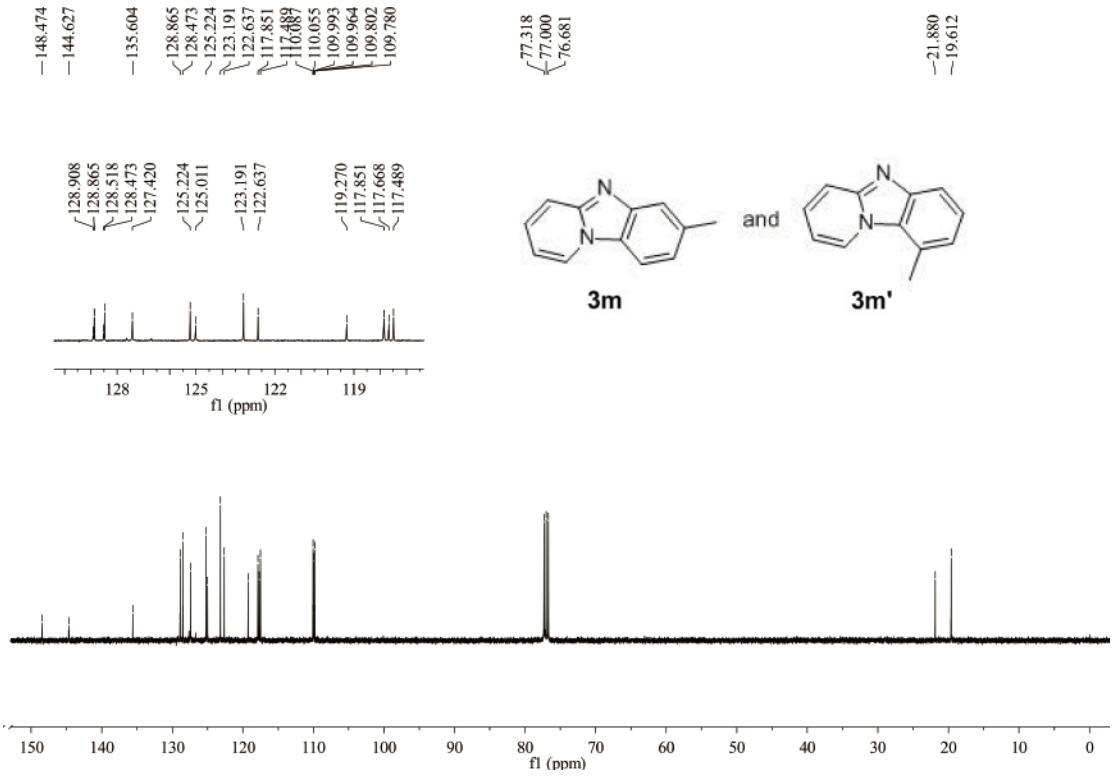

8.686
8.587
8.571
8.254
8.233
7.940
7.919
7.767
7.744
7.562
7.544
7.523
7.266
6.979
6.963
6.946
4.485
4.467
4.450
4.432
1.478
1.460
1.442
0.000
3j
CO2Et
1.00
1.00
1.00
1.00
1.00
1.01
1.00
2.02
3.06
fl (ppm)

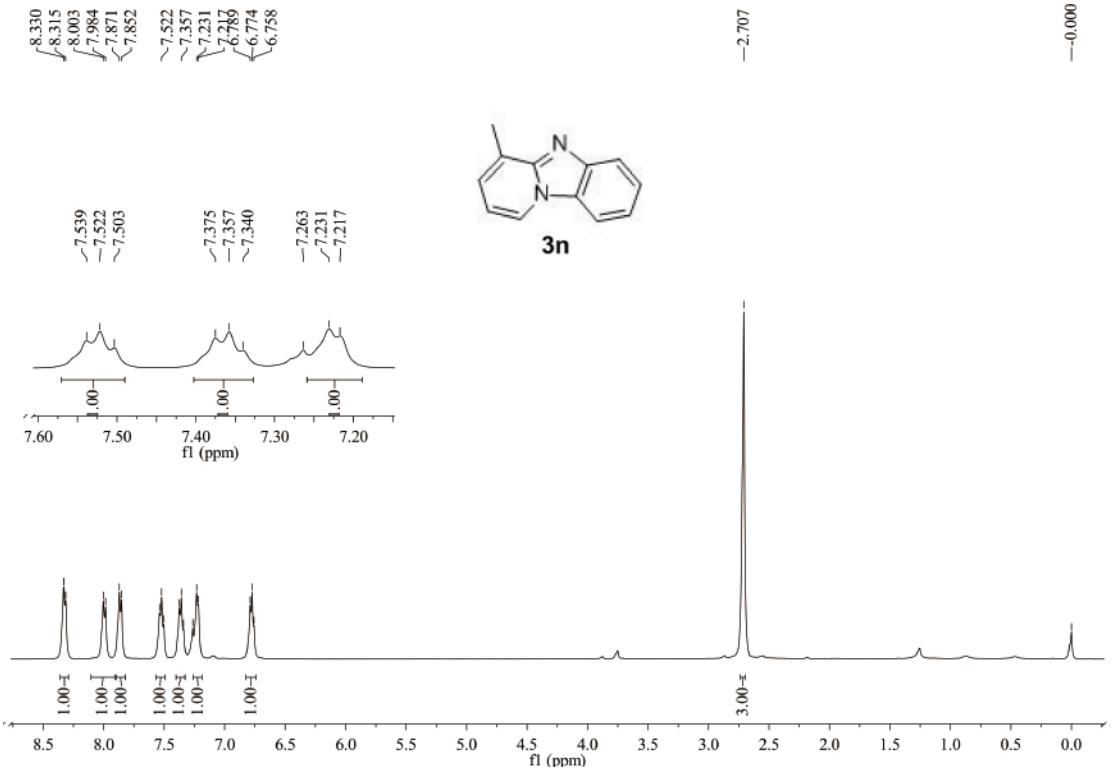

166.455
150.212
147.440
130.614
128.123
126.547
125.449
122.609
118.913
117.773
112.731
110.920
77.320
77.000
76.681
60.849
14.237
3j
CO2Et
fl (ppm)

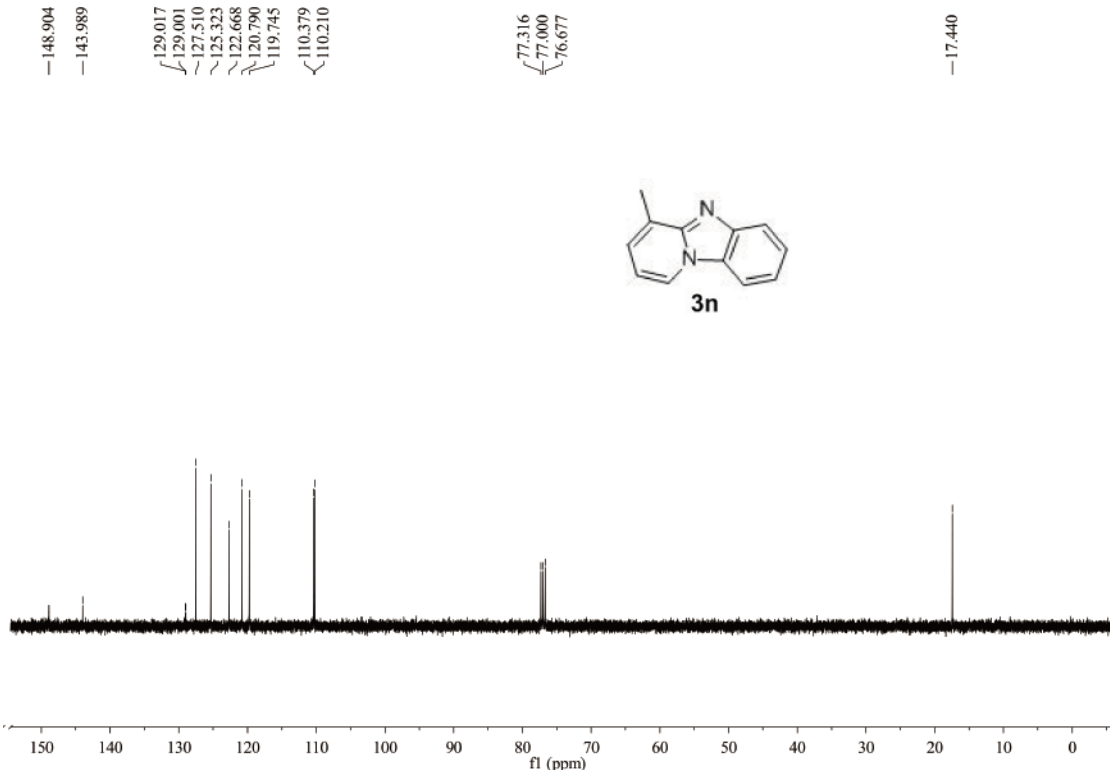

8.429
8.412
7.759
7.737
7.718
7.331
7.298
7.279
7.263
6.882
6.835
6.819
2.799
0.000
7.427
7.408
7.388
7.349
7.331
7.298
7.279
7.263
1.02
1.02
1.00
7.45
7.40
7.35
7.30
7.25
f1 (ppm)
N
N
3k
1.00
2.00
1.02
1.02
1.00
1.00
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

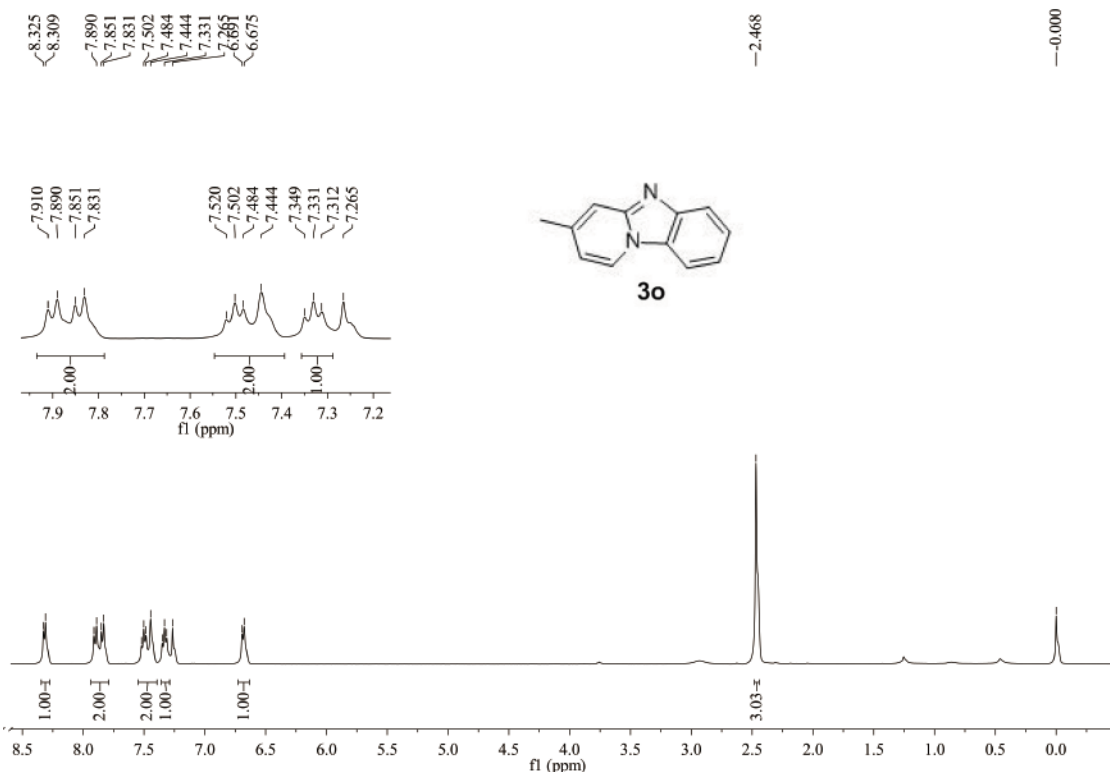

147.767
143.651
129.666
128.883
128.014
125.511
125.096
120.852
117.851
110.076
107.726
77.318
77.000
76.682
17.051
N
N
3k
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.792
8.775
8.422
8.405
7.810
7.789
7.774
7.753
7.715
7.691
7.667
7.431
7.414
7.401
7.380
7.263
7.205
7.184
7.114
7.096
6.845
6.828
6.811
6.794
2.921
2.574
0.000
and
3m
3m'
0.60
0.40
2.40
1.60
0.40
0.60
1.00
1.81
1.22
fl (ppm)


148.474
144.627
135.604
128.865
128.473
125.224
123.191
122.637
117.851
110.055
109.993
109.964
109.802
109.780
77.318
77.000
76.681
21.880
19.612
128.908
128.865
128.518
128.473
127.420
125.224
125.011
123.191
122.637
119.270
117.851
117.668
117.489
and
3m
3m'
fl (ppm)


8.330
8.315
8.003
7.984
7.871
7.852
7.522
7.357
7.231
7.217
6.789
6.774
6.758
2.707
0.000
N
N
3n
7.539
7.522
7.503
7.375
7.357
7.340
7.263
7.231
7.217
1.00
1.00
1.00
7.60
7.50
7.40
7.30
7.20
f1 (ppm)
1.00
1.00
1.00
1.00
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.904
143.989
129.017
129.001
127.510
125.323
122.668
120.790
119.745
110.379
110.210
77.316
77.000
76.677
17.440
N
N
3n
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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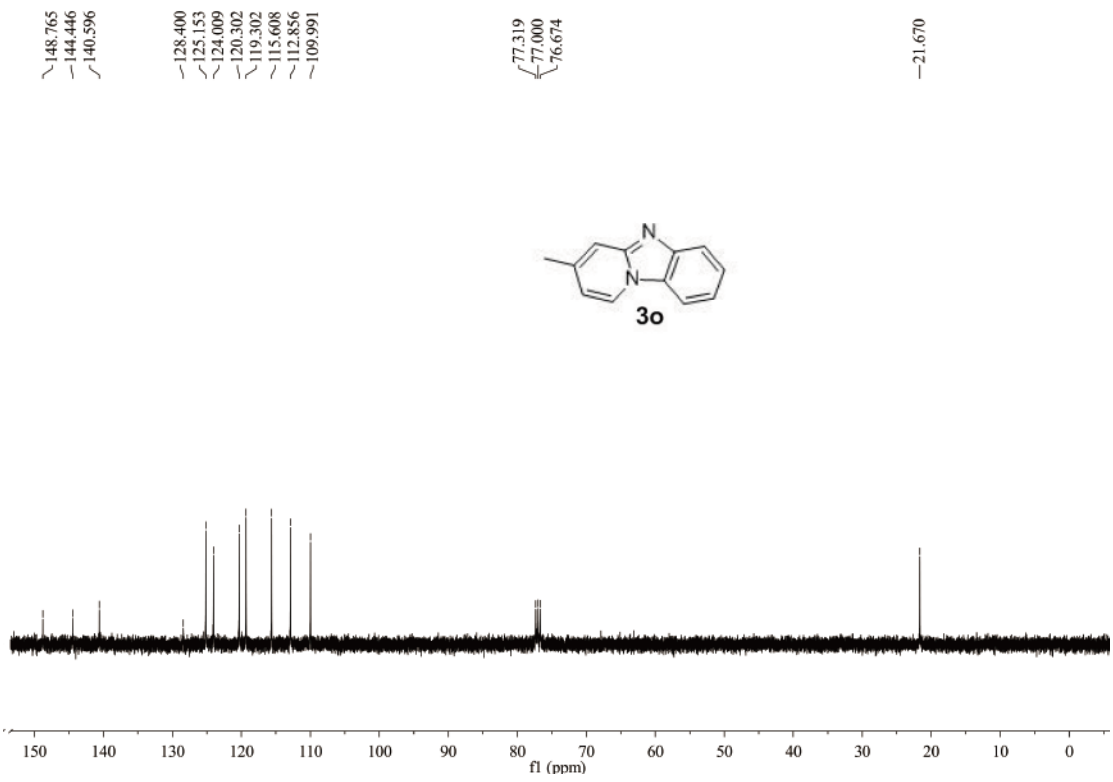
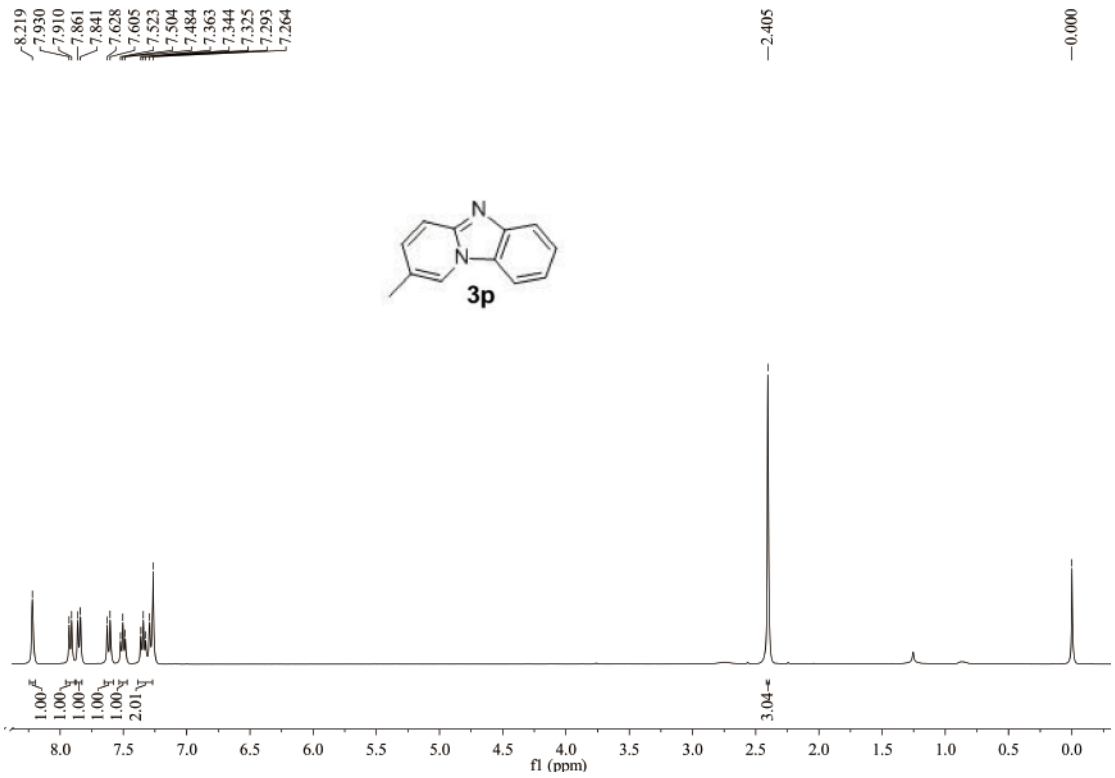
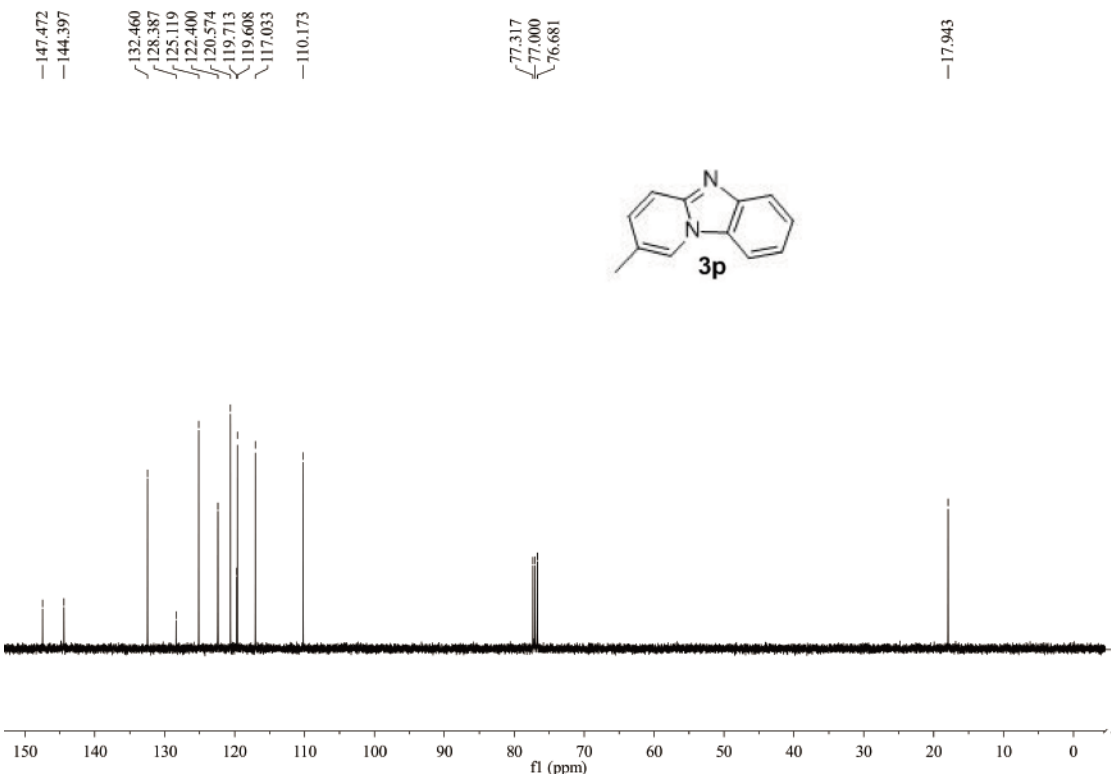
7.851
7.831
7.502
7.484
7.444
7.331
7.265
6.691
6.675
2.468
0.000
7.910
7.890
7.851
7.831
7.520
7.502
7.484
7.444
7.349
7.331
7.312
7.265
2.00
2.00
1.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
3o
1.00
2.00
2.00
1.00
1.00
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.765
144.446
140.596
128.400
125.153
124.009
120.302
119.302
115.608
112.856
109.991
77.319
77.000
76.674
21.670
3o
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.219
7.930
7.910
7.861
7.841
7.628
7.605
7.523
7.504
7.484
7.363
7.344
7.325
7.293
7.264
2.405
0.000
3p
1.00
1.00
1.00
1.00
1.00
2.01
3.04
f1 (ppm)


147.472
144.397
132.460
128.387
125.119
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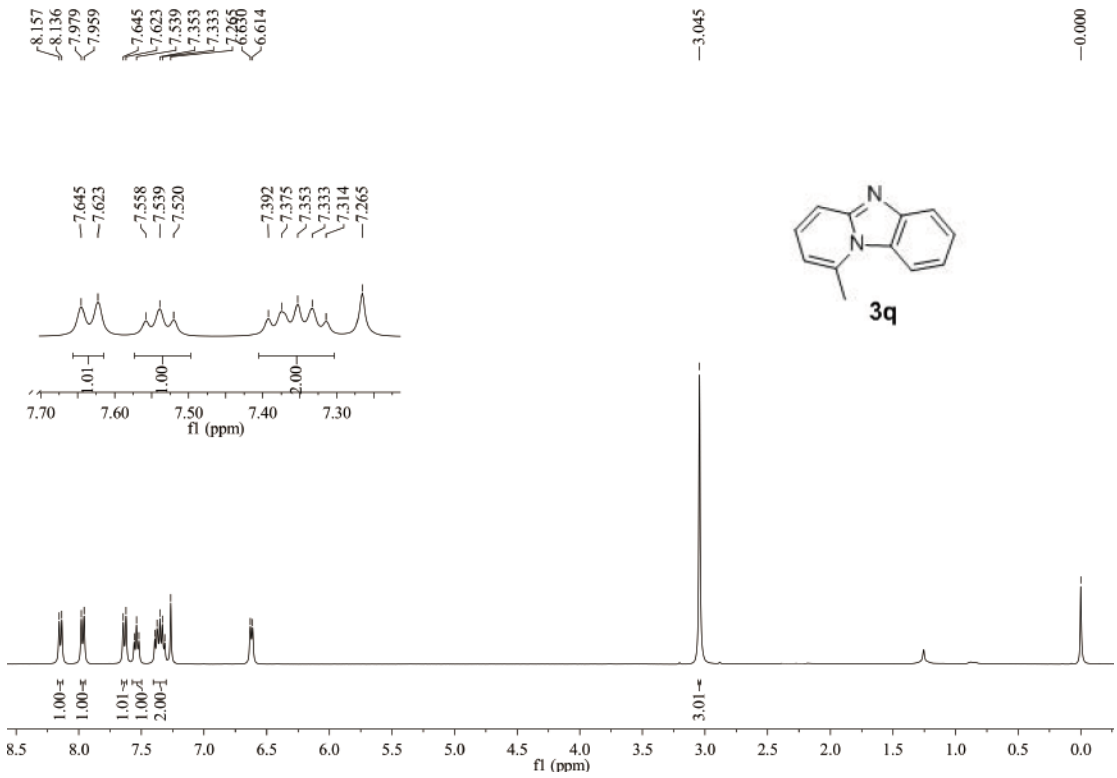
120.574
119.713
119.608
117.033
110.173
77.317
77.000
76.681
17.943
3p
f1 (ppm)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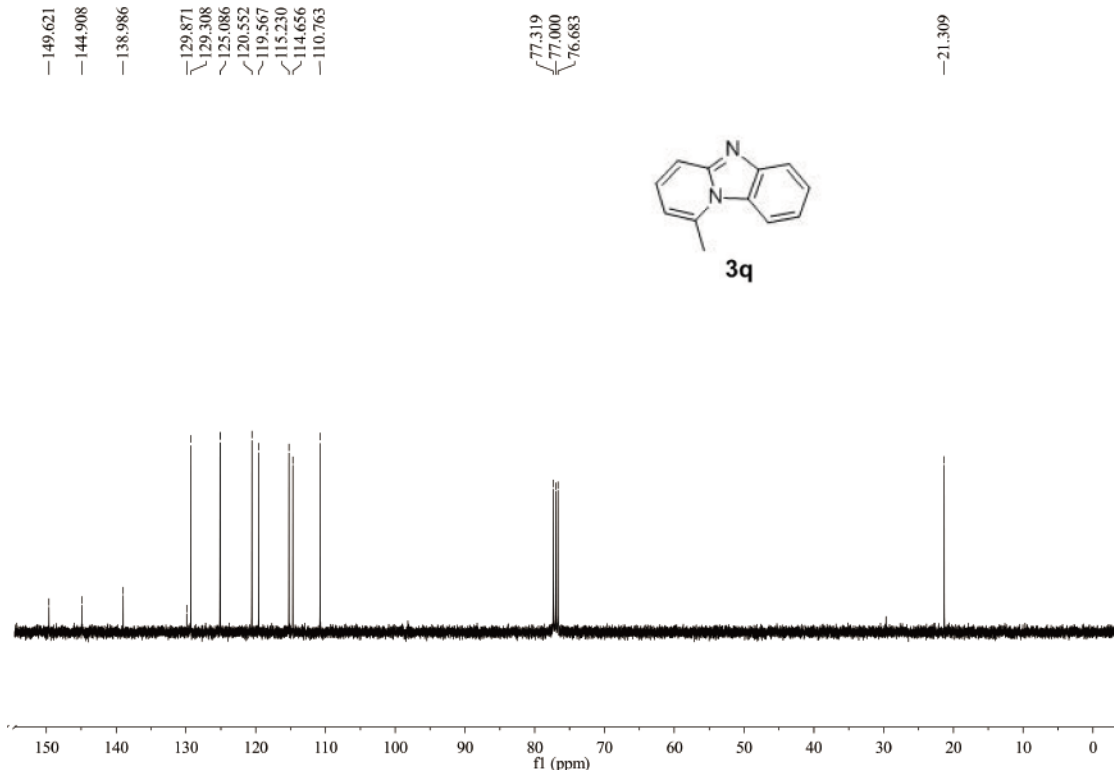
7.959
7.645
7.623
7.539
7.353
7.333
6.650
6.614
3.045
0.000
7.645
7.623
7.558
7.539
7.520
7.392
7.375
7.353
7.333
7.314
7.265
1.01
1.00
2.00
7.70
7.60
7.50
7.40
7.30
f1 (ppm)
3q
1.00
1.00
1.01
1.00
2.00
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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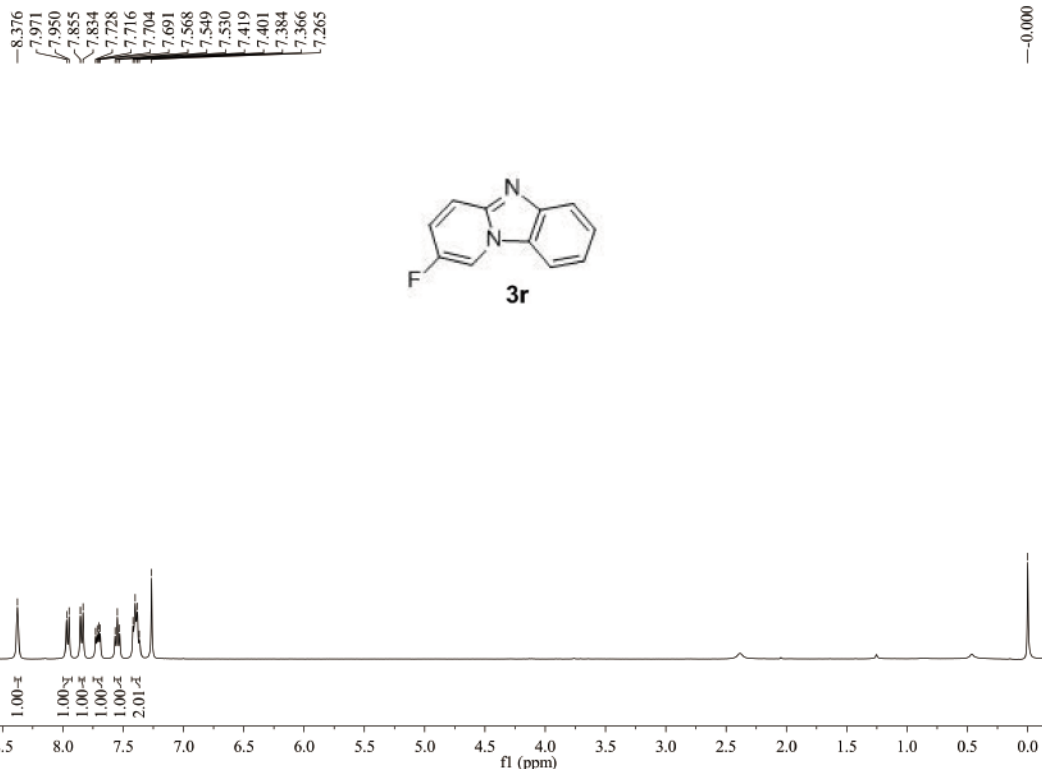
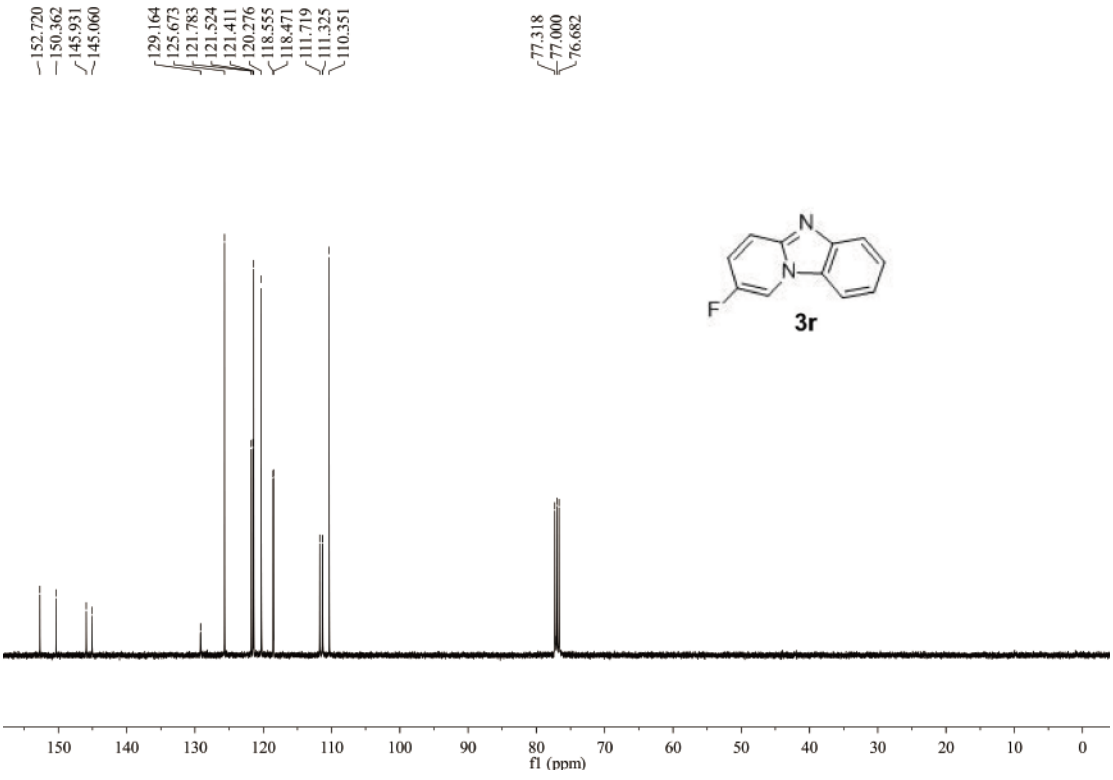
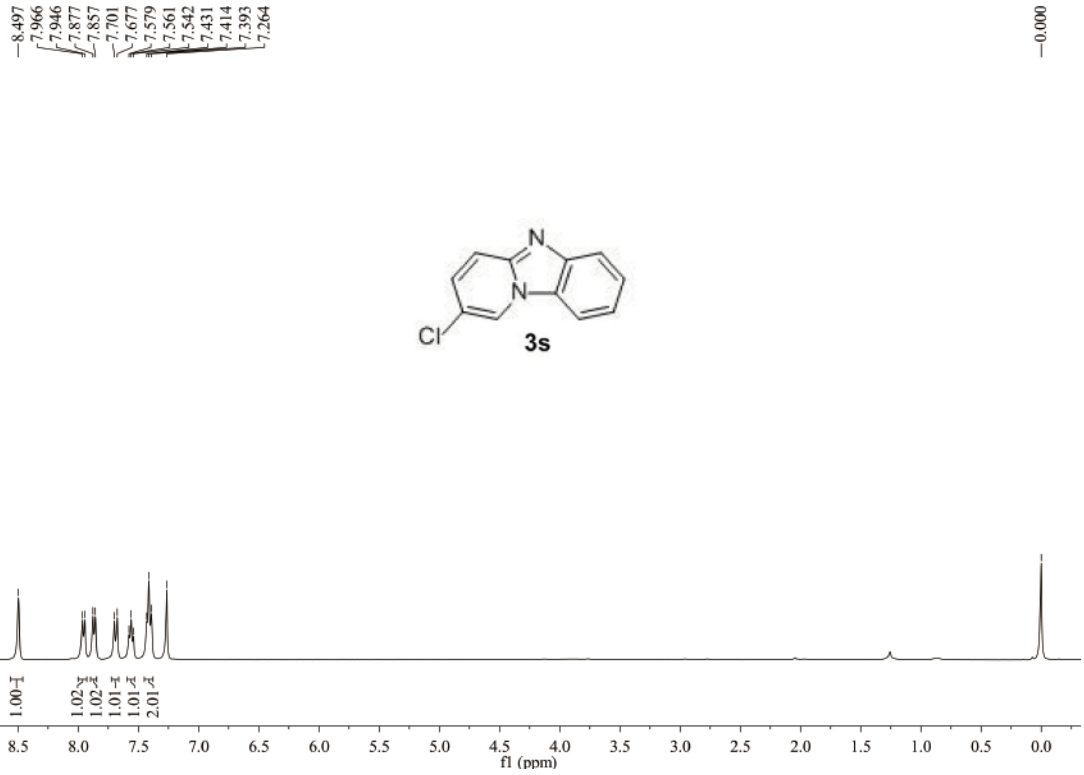
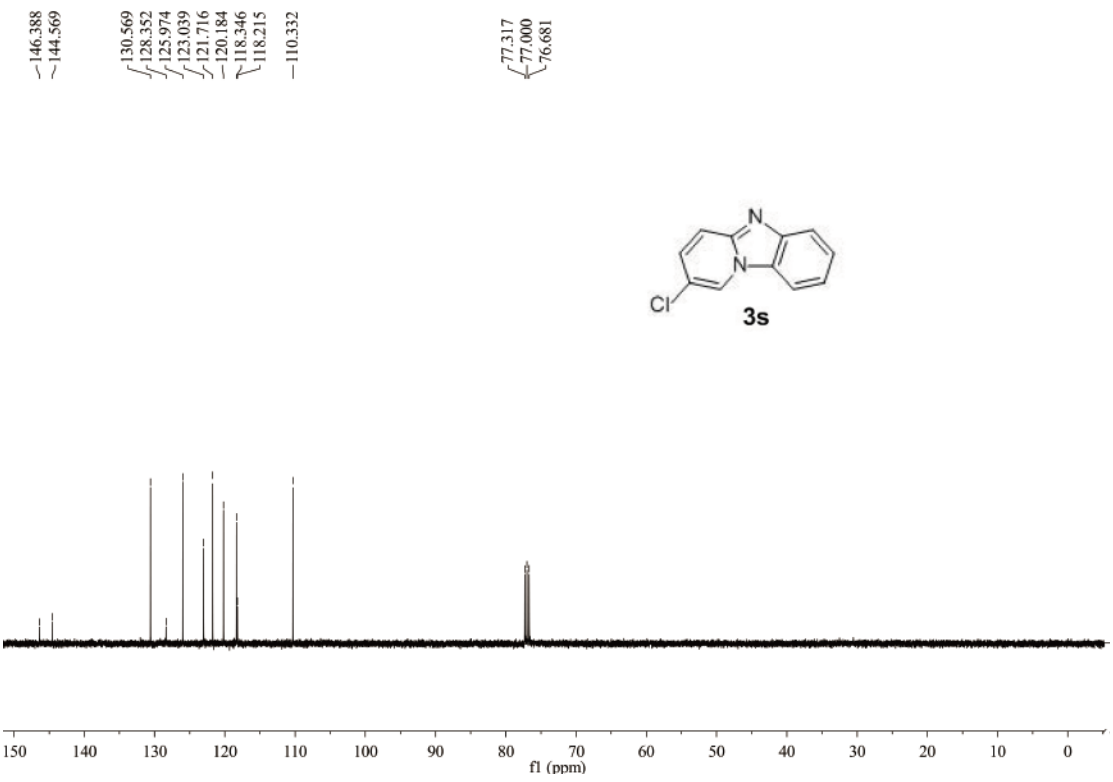
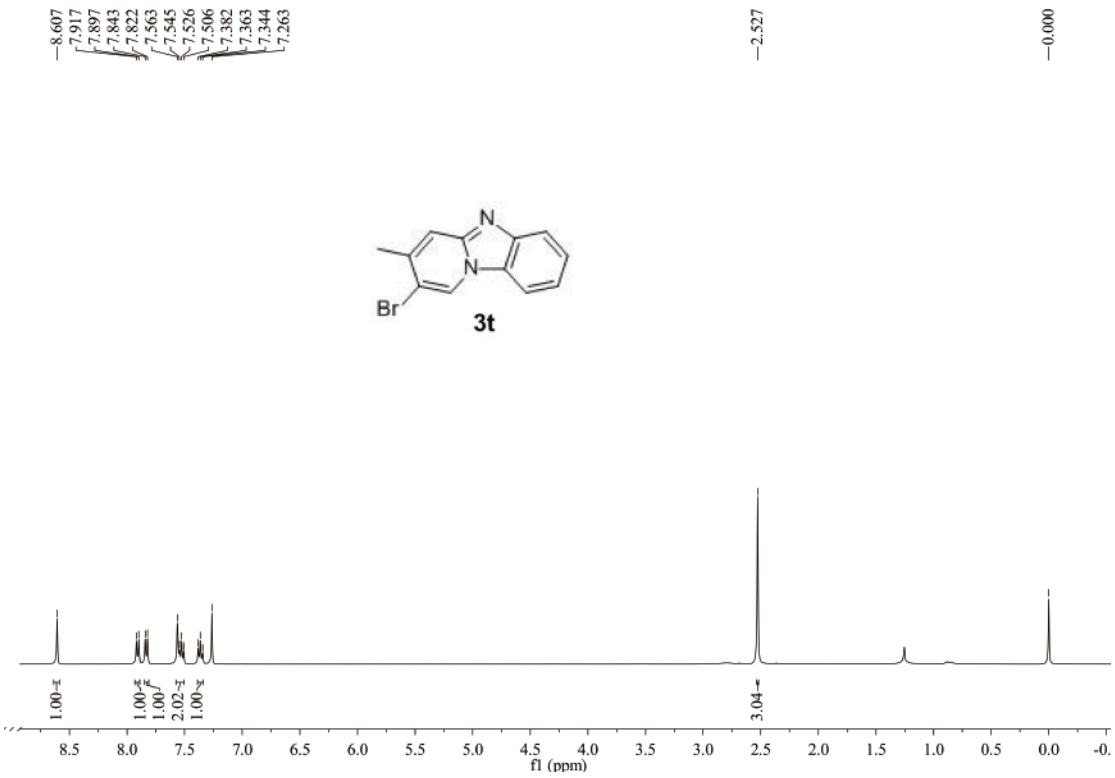
144.908
138.986
129.871
129.308
125.086
120.552
119.567
115.230
114.656
110.763
77.319
77.000
76.683
21.309
3q
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

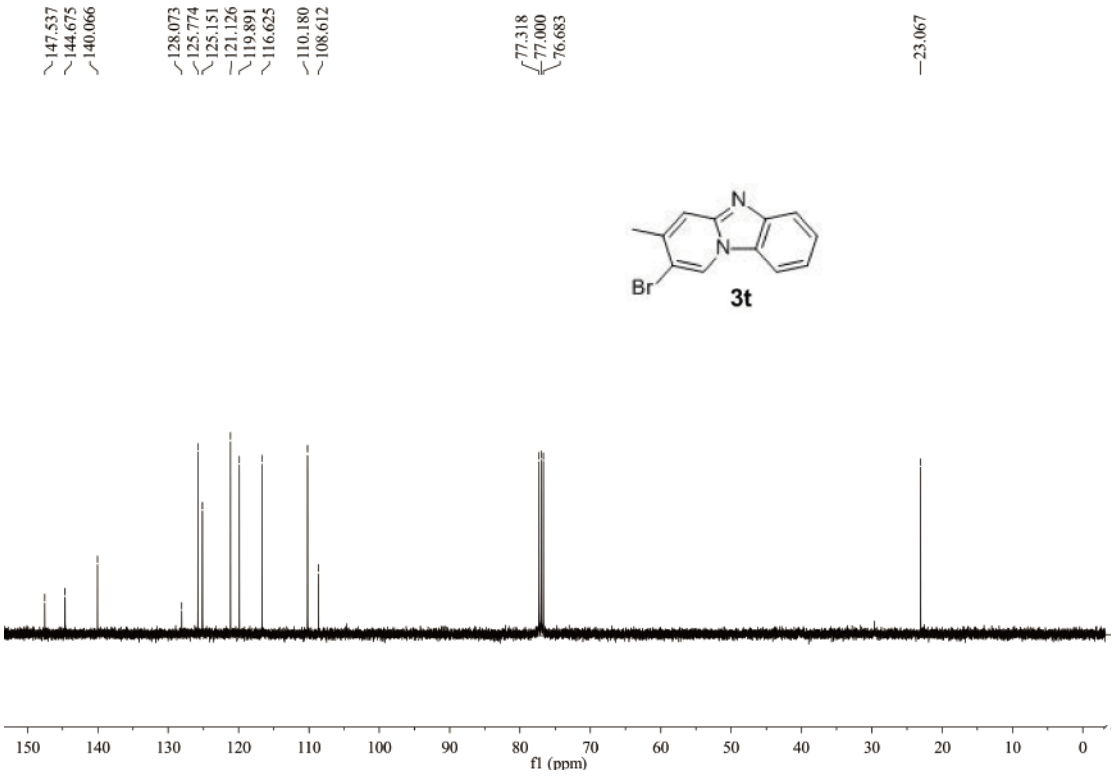

8.376
7.971
7.950
7.855
7.834
7.728
7.716
7.704
7.691
7.568
7.549
7.530
7.419
7.401
7.384
7.366
7.265
0.000
N
N
F
3r
1.00
1.00
1.00
1.00
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

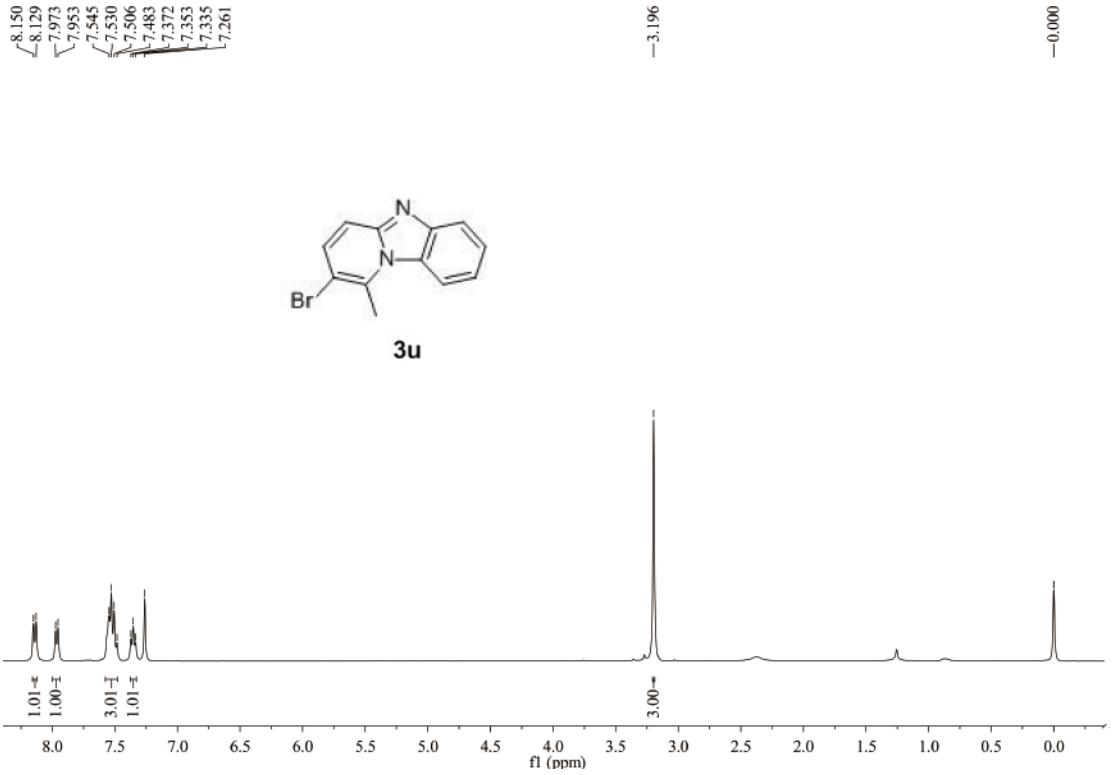

152.720
150.362
145.931
145.060
129.164
125.673
121.783
121.524
121.411
120.276
118.555
118.471
111.719
111.325
110.351
77.318
77.000
76.682
N
N
F
3r
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

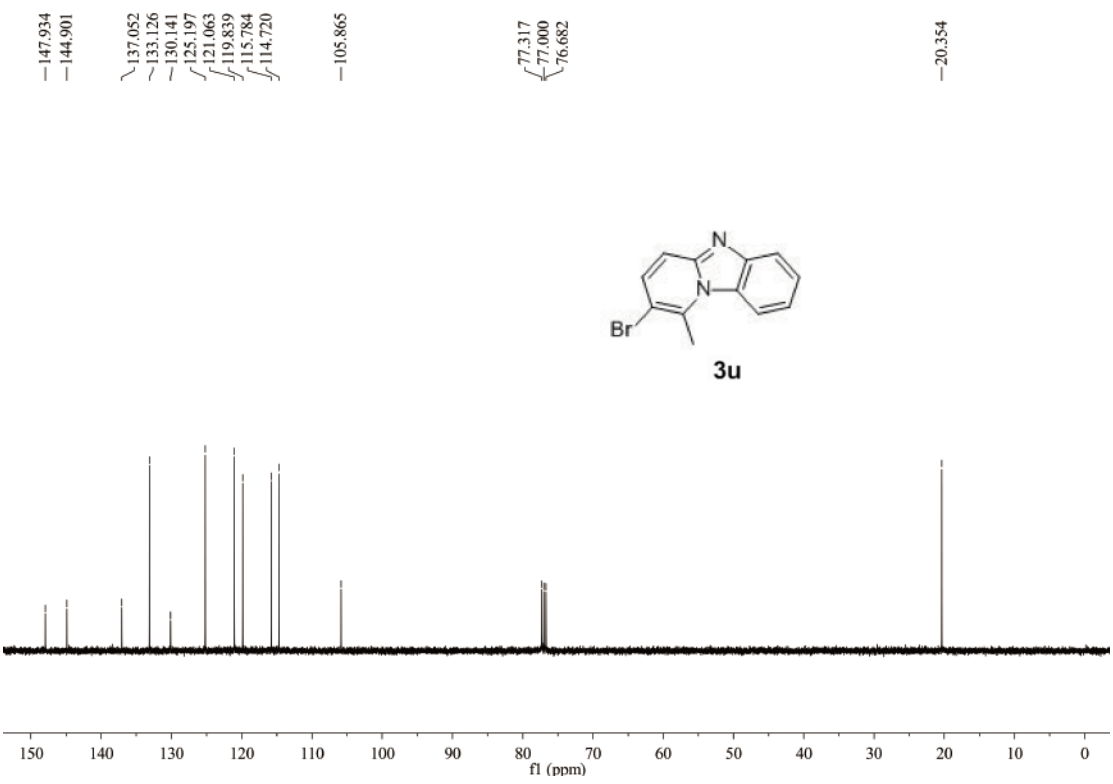

8.497
7.966
7.946
7.877
7.857
7.701
7.677
7.579
7.561
7.542
7.431
7.414
7.393
7.264
0.000
N
N
Cl
3s
1.00
1.02
1.02
1.01
1.01
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

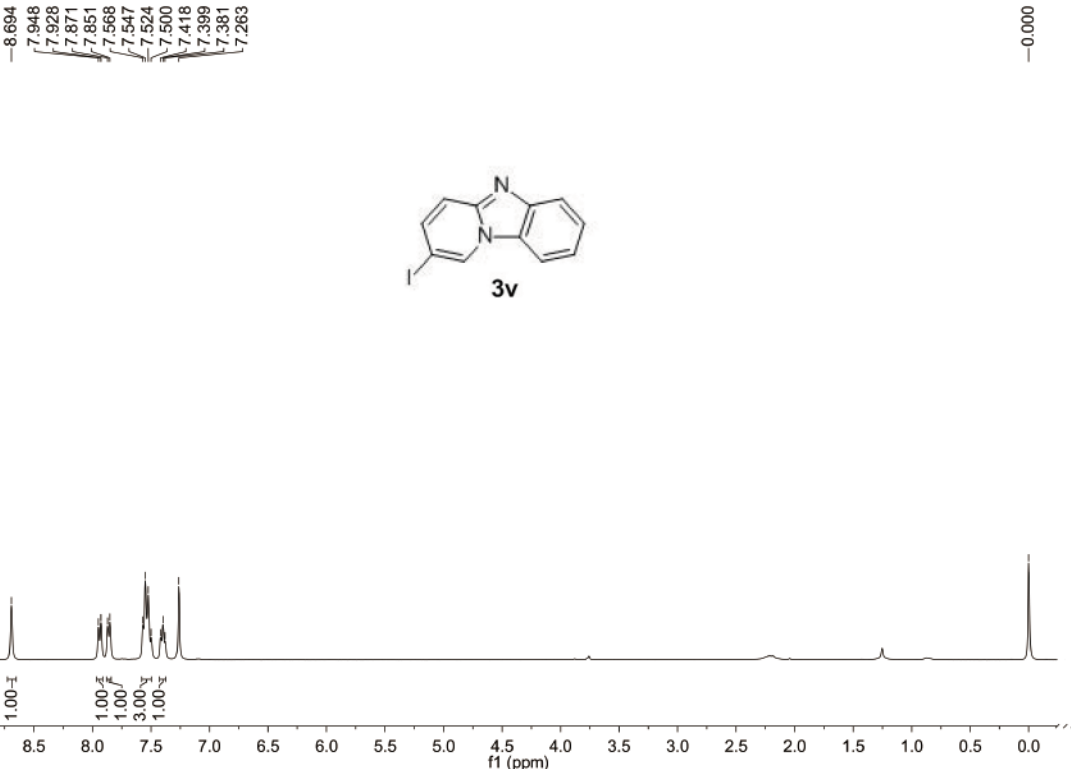

146.388
144.569
130.569
128.352
125.974
123.039
121.716
120.184
118.346
118.215
110.332
77.317
77.000
76.681
N
N
Cl
3s
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

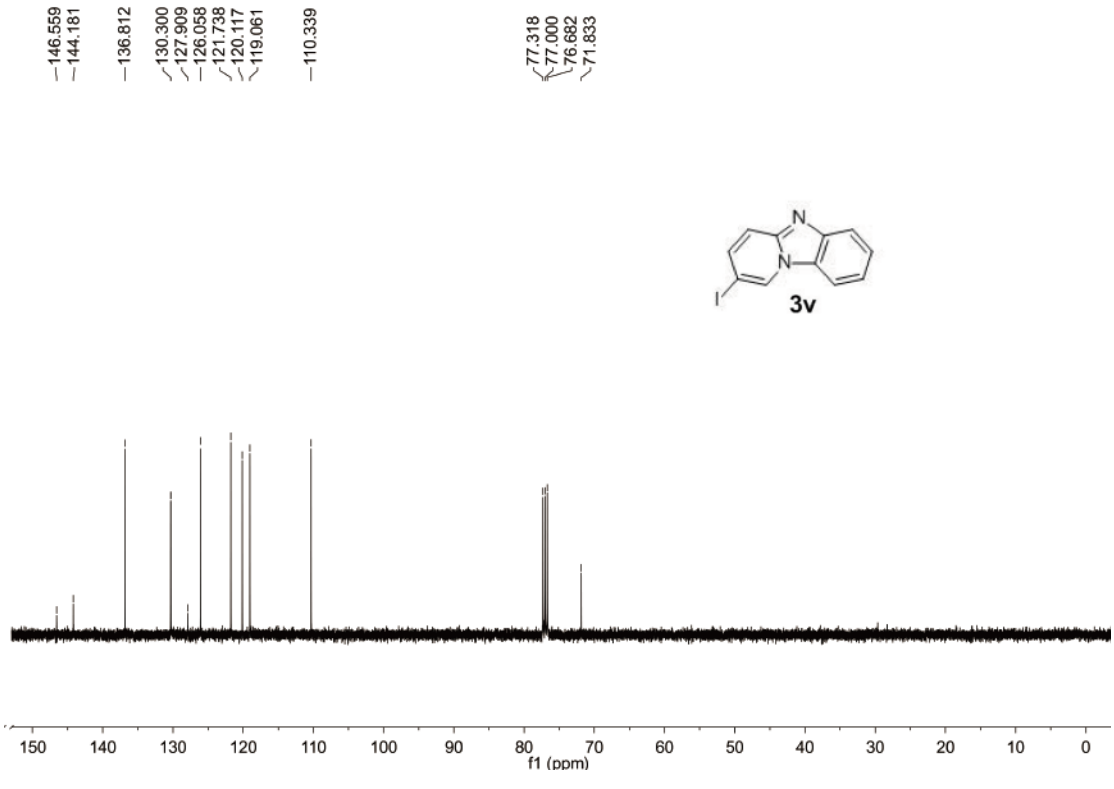

8.607
7.917
7.897
7.843
7.822
7.563
7.545
7.526
7.506
7.382
7.363
7.344
7.263
2.527
0.000
N
N
Br
3t
1.00
1.00
1.00
2.02
1.00
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

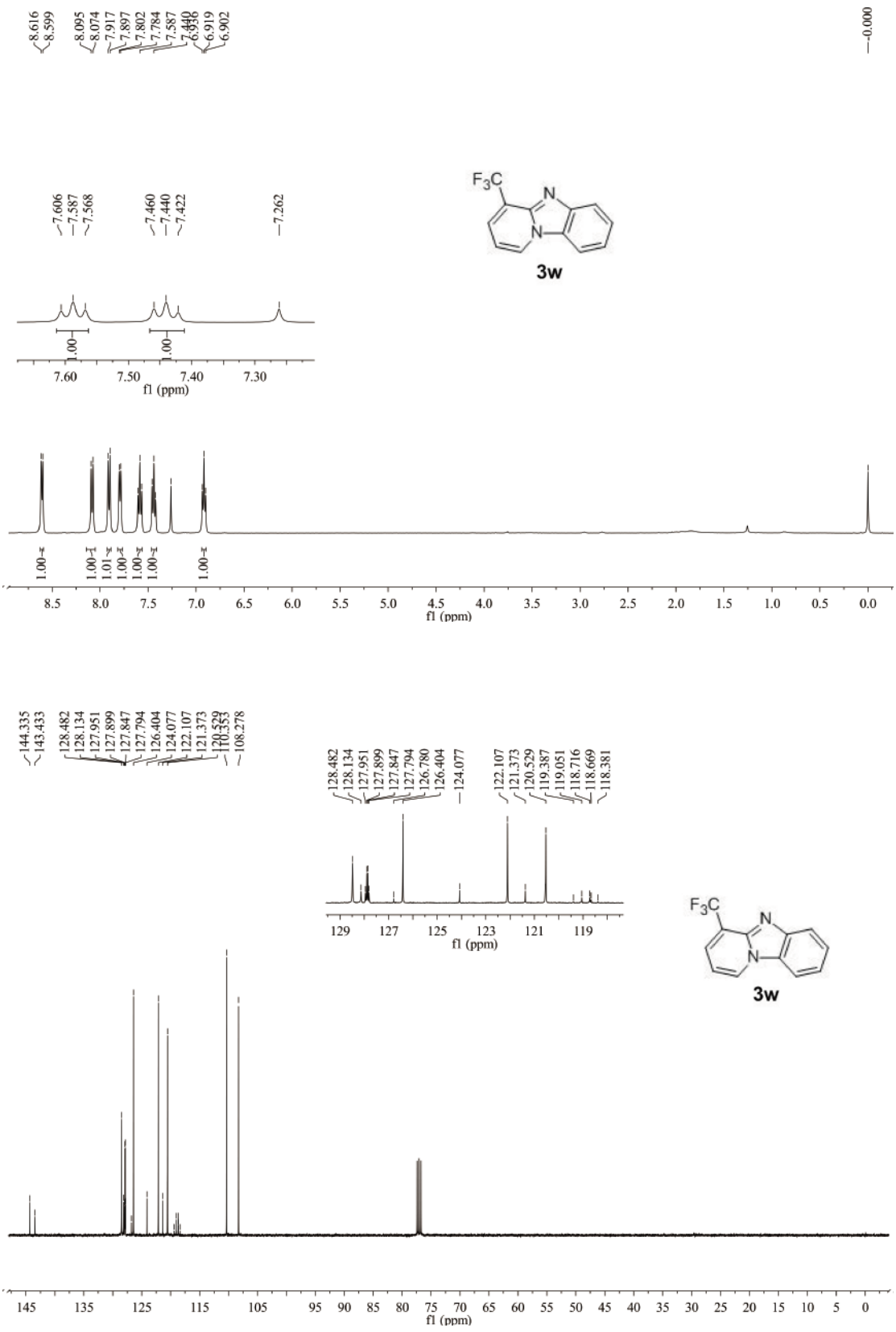

147.537
144.675
140.066
128.073
125.774
125.151
121.126
119.891
116.625
110.180
108.612
77.318
77.000
76.683
23.067
N
N
Br
3t
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

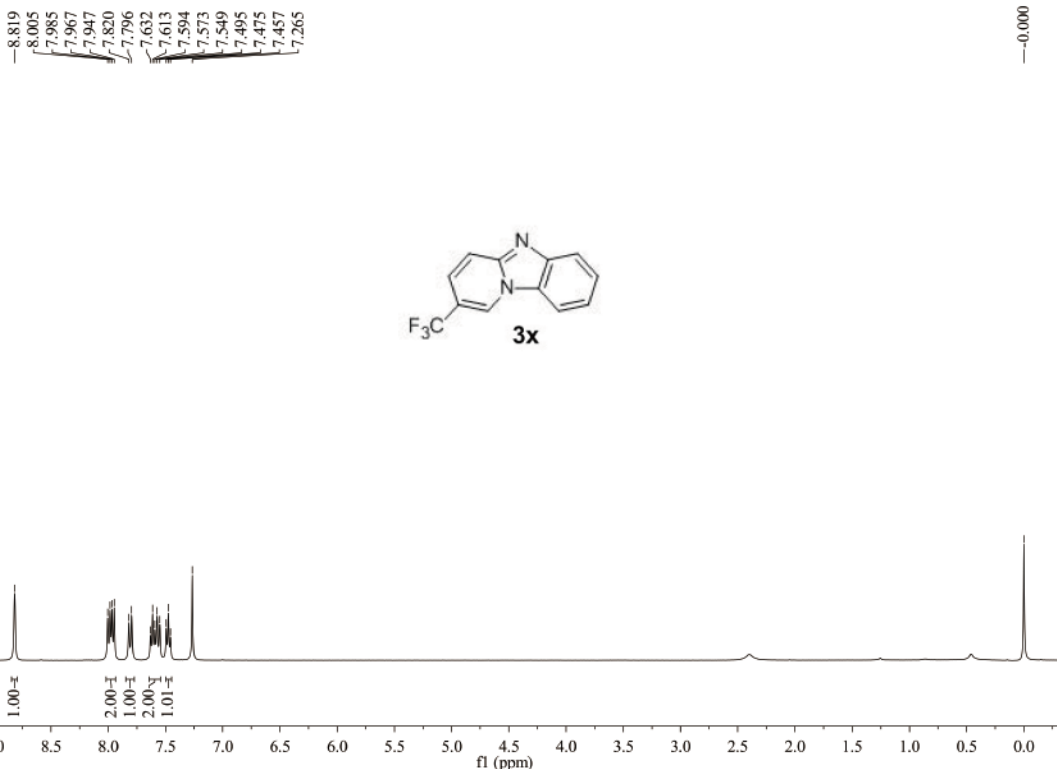

8.150
8.129
7.973
7.953
7.545
7.530
7.506
7.483
7.372
7.353
7.335
7.261
3.196
0.000
N
N
Br
3u
1.01
1.00
3.01
1.01
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

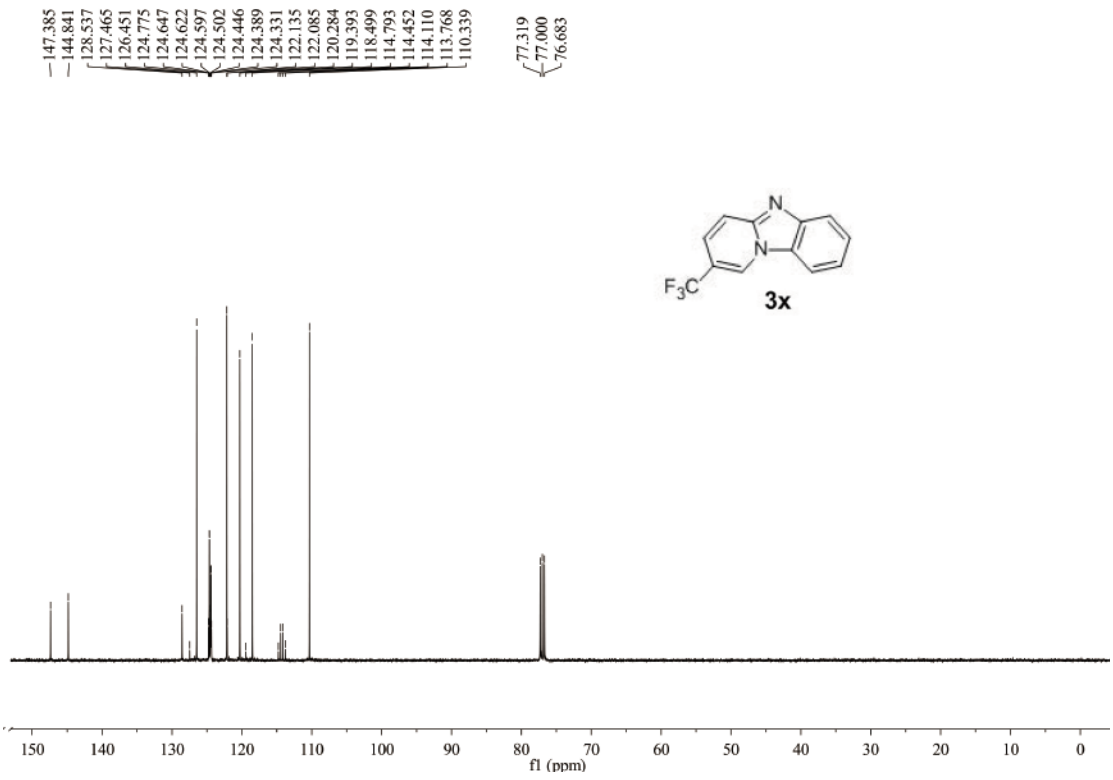

147.934
144.901
137.052
133.126
130.141
125.197
121.063
119.839
115.784
114.720
105.865
77.317
77.000
76.682
20.354
N
N
Br
3u
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

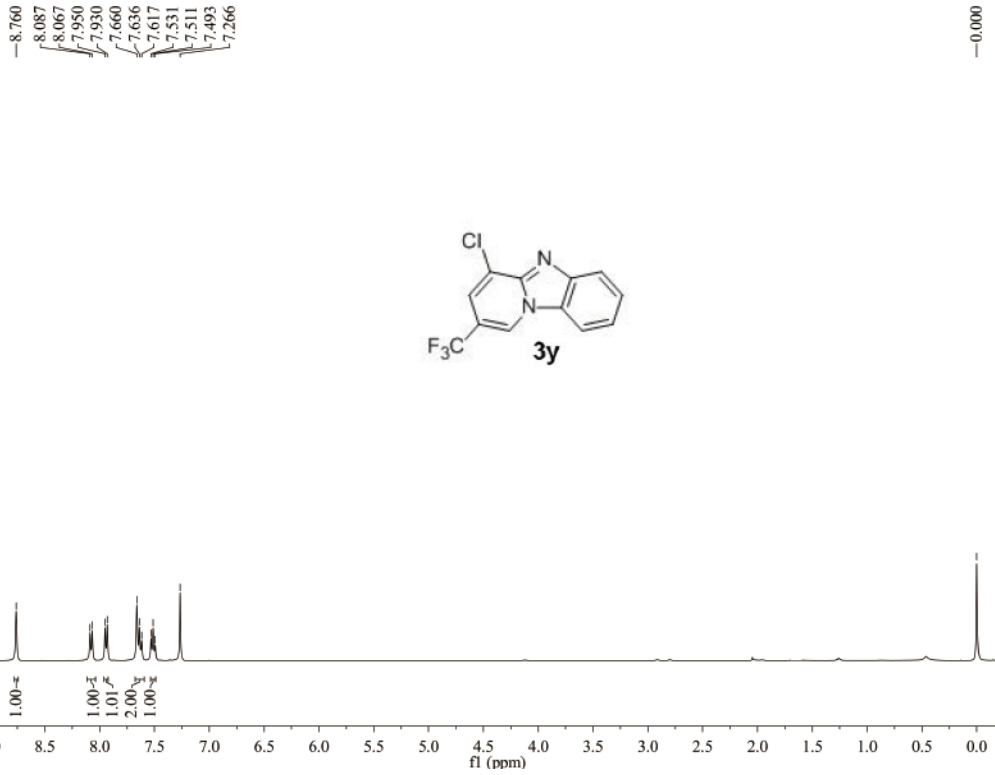

8.694
7.948
7.928
7.871
7.851
7.566
7.547
7.524
7.500
7.418
7.399
7.381
7.263
0.000
N
N
I
3v
1.00
1.00
1.00
3.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

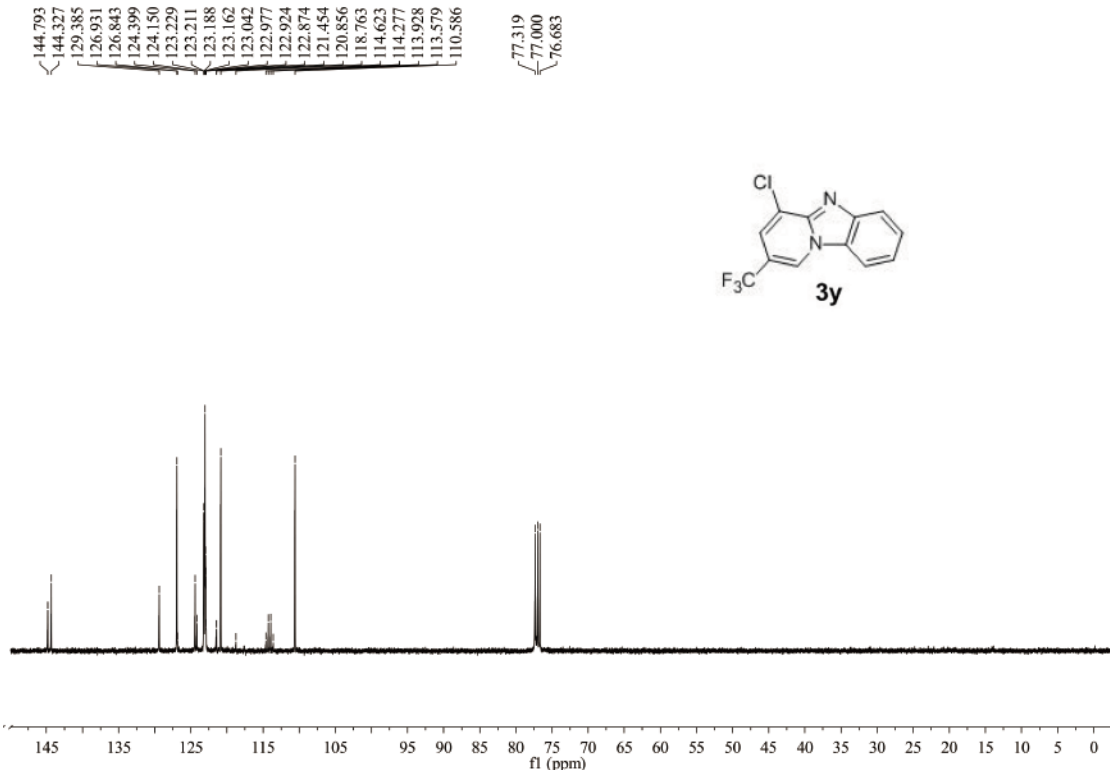

146.559
144.181
136.812
130.300
127.909
126.058
121.738
120.117
119.061
110.339
77.318
77.000
76.682
71.833
N
N
I
3v
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.616
8.599
8.095
8.074
7.917
7.897
7.802
7.784
7.587
7.440
6.938
6.919
6.902
0.000
7.606
7.587
7.568
7.460
7.440
7.422
7.262
F3C
N
N
3w
1.00
1.00
7.60
7.50
7.40
7.30
f1 (ppm)
1.00
1.00
1.01
1.00
1.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
144.335
143.433
128.482
128.134
127.951
127.899
127.847
127.794
126.404
124.077
122.107
121.373
108.278
128.482
128.134
127.951
127.899
127.847
127.794
126.780
126.404
124.077
122.107
121.373
120.529
119.387
119.051
118.716
118.669
118.381
129
127
125
123
121
119
f1 (ppm)
F3C
N
N
3w
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


8.819
8.005
7.985
7.967
7.947
7.820
7.796
7.632
7.613
7.594
7.573
7.549
7.495
7.475
7.457
7.265
0.000
N
N
F3C
3x
1.00
2.00
1.00
2.00
1.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.385
144.841
128.537
127.465
126.451
124.775
124.647
124.622
124.597
124.502
124.446
124.389
124.331
122.135
122.085
120.284
119.393
118.499
114.793
114.452
114.110
113.768
110.339
77.319
77.000
76.683
N
N
F3C
3x
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.760
8.087
8.067
7.950
7.930
7.660
7.636
7.617
7.531
7.511
7.493
7.266
0.000
Cl
N
N
F3C
3y
1.00
1.00
1.01
2.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


144.793
144.327
129.385
126.931
126.843
124.399
124.150
123.229
123.211
123.188
123.162
123.042
122.977
122.924
122.874
121.454
120.856
118.763
114.623
114.277
113.928
113.579
110.586
77.319
77.000
76.683
Cl
N
N
F3C
3y
145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)