Supporting Information

Metal- and Base-Free Synthesis of Imidazo[1,2-a]pyridines through Elemental Sulfur-Initiated Oxidative Annulation of 2-Aminopyridines and Aldehydes

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1. General information

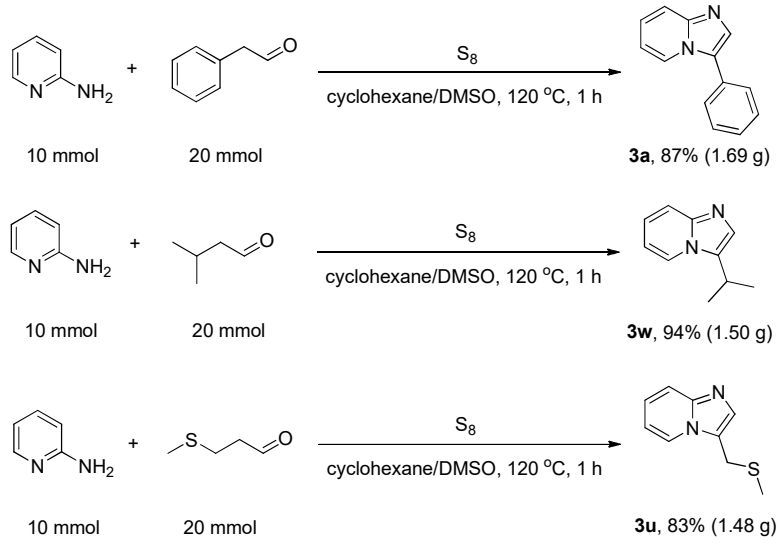
All reactions were carried out under air atmosphere unless otherwise noted. Column chromatography was performed using aluminum oxide (neutral) (100-200 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at the Institute of Chemistry, Chinese Academy of Sciences. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. All reagents were obtained from commercial suppliers and used without further purification.

2. General procedure for the synthesis of imidazo[1,2-*a*]pyridines

3a for example: Pyridin-2-amine (**1a**, 19.5 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol) were added to a 10 mL reaction vessel. Cyclohexane (0.2 mL) and DMSO (0.4 mL) were then added by syringe. The sealed reaction vessel under air atmosphere was stirred at 120 ^{o}C for 1 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and washed with saturated salt water. 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 the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:2, R_f = 0.60) to yield the desired product **3a** as brown solid (33.4 mg, 86% yield), mp 95-97 ^{o}C.

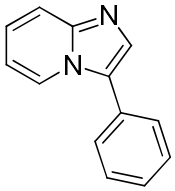
3. Procedure for gram-scale reactions

Pyridin-2-amine (**1a**, 0.96 g, 10 mmol), aldehyde (**2**, 20 mmol) and sulfur powder (0.64 g, 20 mmol) were added to a round bottomed flask (50 mL). To the reaction vessel cyclohexane (3.0 mL) and DMSO (6.0 mL) were added by measuring cylinder. The reaction mixture was stirred at 120 ^{o}C under air conditions for 1 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (15 mL) and washed with saturated salt water. 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 the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:2) to yield the desired product.



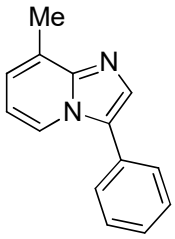
4. Characterization data of products

3-Phenylimidazo[1,2-*a*]pyridine (3a, CAS: 92961-15-4)[1]



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.35 (d, J = 6.6 Hz, 1H), 7.70-7.65 (m, 2H), 7.58-7.53 (m, 4H), 7.43 (t, J = 6.1 Hz, 1H), 7.21 (t, J = 6.1 Hz, 1H), 6.82 (t, J = 6.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.8, 132.1, 128.98, 128.96, 127.9, 127.7, 125.5, 124.0, 123.1, 117.9, 112.3.

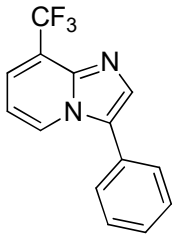
8-Methyl-3-phenylimidazo[1,2-*a*]pyridine (3b)[2]



The reaction was conducted with 3-methylpyridin-2-amine (**1b**, 22.0 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3b** as brown oily liquid (39.9 mg, 96% yield. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.21 (d, J = 6.9 Hz, 1H), 7.69 (s, 1H), 7.56-7.48 (m, 4H), 7.40 (t, J = 7.2 Hz, 1H), 7.00 (d, J = 6.7 Hz, 1H), 6.72 (t, J = 6.8 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.4, 131.7, 129.5, 129.1, 128.2, 128.1, 127.9, 126.1, 123.1, 121.2, 112.6,17.0.

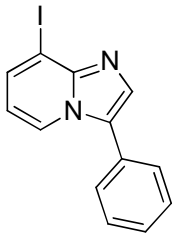
3-Phenyl-8-(trifluoromethyl)imidazo[1,2-*a*]pyridine (3c)



The reaction was conducted with 3-(trifluoromethyl)pyridin-2-amine (**1c**, 32.4 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3c** as brown solid (21.5 mg, 41% yield), mp 82-83 ^{o}C. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.47 (d, J = 6.9 Hz, 1H), 7.82 (s, 1H), 7.58-7.54 (m, 5H), 7.49-7.46 (m, 1H), 6.90 (t, J = 7.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 141.2, 133.4, 129.4, 128.9, 128.4, 128.3, 126.7, 126.6, 122.9 (q, J = 270 Hz), 122.8 (q, J = 4 Hz), 119.7 (q, J = 33 Hz), 110.9; HRMS (ESI) m/z calcd for $C_{14}H_{10}F_3N_2^+$ $(M+H)^+$ 263.07906, found 263.07922.

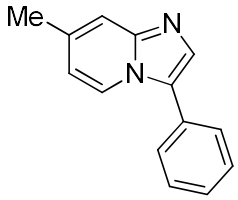
8-Iodo-3-phenylimidazo[1,2-*a*]pyridine (3d)



The reaction was conducted with 3-iodopyridin-2-amine (**1d**, 44.0 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3d** as white solid (48.6 mg, 76% yield), mp 123-124 ^{o}C. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.32 (dd, J = 6.9 Hz, 1.0 Hz, 1H), 7.77 (s, 1H), 7.71 (dd, J = 7.1 Hz, 1.0 Hz, 1H), 7.56-7.50 (m, 4H), 7.47-7.42 (m, 1H), 6.58 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.2, 133.6, 132.7, 129.3, 128.9, 128.6, 128.2, 127.7, 123.6, 113.3, 84.9; HRMS calcd. for $C_{13}H_{10}IN_2^+$ $(M+H)^+$ 320.98832, found 320.98853.

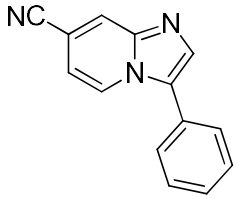
7-Methyl-3-phenylimidazo[1,2-*a*]pyridine (3e, CAS: 882187-78-2)[2]



The reaction was conducted with 4-methylpyridin-2-amine (**1e**, 21.6 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3e** as brown oily liquid (31.2 mg, 75% yield). R_f = 0.55 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.23 (d, J = 7.1 Hz, 1H), 7.62 (s, 1H), 7.56-7.49 (m, 4H), 7.44-7.38 (m, 2H), 6.65 (dd, J = 7.1 Hz, 1.5 Hz, 1H) ; ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.5, 135.3, 132.0, 129.4, 129.2, 128.0, 127.9, 125.2, 122.6, 116.5, 115.2, 21.2.

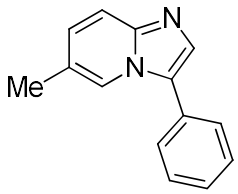
3-Phenylimidazo[1,2-*a*]pyridine-7-carbonitrile (3f)



The reaction was conducted with 2-aminoisonicotinonitrile (**1f**, 24.0 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3f** as brown solid (35.0 mg, 80% yield), mp 123-125 ^{o}C. R_f = 0.45 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.40 (d, J = 7.2 Hz, 1H), 8.12 (s, 1H), 7.92 (s, 1H), 7.60-7.50 (m, 5H), 6.98 (dd, J = 7.2 Hz, 1.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.5, 136.4, 132.1, 128.8, 128.2, 126.9, 123.9, 123.2, 122.5, 117.7, 112.2, 30.2; HRMS (ESI) m/z calcd for $C_{14}H_{10}N_3^+$ $(M+H)^+$ 220.08692, found 220.08652.

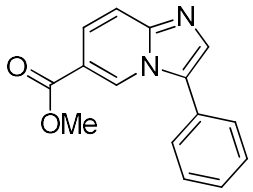
6-Methyl-3-phenylimidazo[1,2-*a*]pyridine (3g, CAS: 1338248-70-6)[2]



The reaction was conducted with 5-methylpyridin-2-amine (**1g**, 21.6 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3g** as brown oily liquid (32.4 mg, 78% yield). R_f = 0.55 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.11 (s, 1H), 7.65 (s, 1H), 7.61 (d, J = 9.2 Hz, 1H), 7.57-7.50 (m, 4H), 7.44-7.40 (m, 1H), 7.07 (dd, J = 9.2 Hz, 1.4 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.1, 132.0, 129.4, 129.2, 128.1, 127.6, 125.4, 122.3, 120.9, 117.4, 18.4. HRMS (ESI) m/z calcd for $C_{14}H_{13}N_2^+$ $(M+H)^+$ 209.10732, found 209.10722.

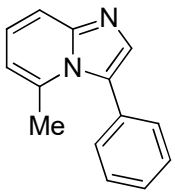
Methyl 3-phenylimidazo[1,2-*a*]pyridine-6-carboxylate (3h, CAS:1338248-82-0)[2]



The reaction was conducted with methyl 6-aminonicotinate (**1h**, 30.4 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3h** as brown solid (30.2 mg, 60% yield), mp 84-86 ^{o}C. R_f = 0.35 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.47 (s, 1H), 8.38 (d, J = 7.3 Hz, 1H), 7.88 (s, 1H), 7.58-7.54 (m, 4H), 7.49-7.45 (m, 2H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.6, 144.9, 134.7, 129.4, 128.8, 128.4, 128.1, 127.3, 125.7, 122.9, 120.9, 111.9, 52.5. HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_2^+$ $(M+H)^+$ 253.09715, found 253.09770.

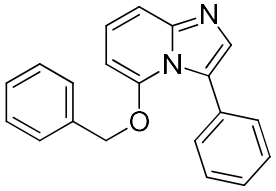
5-Methyl-3-phenylimidazo[1,2-*a*]pyridine (3i, CAS: 1338248-81-9)[2]



The reaction was conducted with 6-methylpyridin-2-amine (**1i**, 21.6 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3i** as yellow solid (25.0 mg, 60% yield), mp 63-65 ^{o}C. R_f = 0.50 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.60 (d, J = 9.0 Hz, 1H), 7.54 (s, 1H), 7.46-7.38 (m, 5H), 7.14-7.10 (m, 1H), 6.51 (d, J = 6.8 Hz, 1H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.8, 136.4, 134.0, 131.8, 131.6, 128.4, 127.4, 126.2, 124.5, 115.9, 113.4, 21.7.

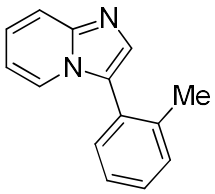
5-(Benzyloxy)-3-phenylimidazo[1,2-*a*]pyridine (3j)



The reaction was conducted with 6-(benzyloxy)pyridin-2-amine (**1j**, 40.0 mg, 0.2 mmol), 2-phenylacetaldehyde (**2a**, 46.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3j** as yellow solid (55.8 mg, 93% yield), mp 108-110 ^{o}C. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.95 (d, J = 6.8 Hz, 1H), 7.66 (s, 1H), 7.56-7.48 (m, 6H), 7.42-7.29 (m, 4H), 6.65 (t, J = 7.2 Hz, 1H), 6.51 (d, J = 7.5 Hz, 1H), 5.35 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 148.2, 140.5, 136.1, 131.4, 129.3, 129.1, 128.5, 128.1, 128.1, 128.0, 127.3, 126.7, 116.5, 112.4, 102.6, 70.6. HRMS (ESI) m/z calcd for $C_{20}H_{17}N_2O^+$ $(M+H)^+$ 301.13354, found 301.13394.

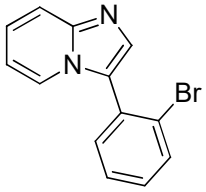
3-(*o*-Tolyl)imidazo[1,2-*a*]pyridine (3k)[3]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(o-tolyl)acetaldehyde (**2b**, 53.6 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3k** as faint yellow oily liquid (35.4 mg, 85% yield). R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.77 (d, J = 6.9 Hz, 1H), 7.70 (d, J = 9.1 Hz, 1H), 7.62 (s, 1H), 7.39-7.32 (m, 4H), 7.27- 7.19 (m, 1H), 6.78 (t, J = 6.8 Hz, 1H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.4, 138.2, 132.7, 131.1, 130.7, 129.1, 128.1, 126.2, 124.6, 124.0, 123.6, 117.9, 112.2, 19.7.

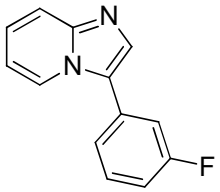
3-(2-Bromophenyl)imidazo[1,2-*a*]pyridine (3l)



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(2-bromophenyl)acetaldehyde (**2c**, 79.2 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3l** as yellow oily liquid (37.1 mg, 67% yield). R_f = 0.55 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.82 (d, J = 6.8 Hz, 1H), 7.78-7.72 (m, 3H), 7.47-7.46 (m, 2H), 7.39-7.34 (m, 1H), 7.27 (t, J = 7.9 Hz, 1H), 6.84 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.5, 133.4, 133.2, 133.1, 130.6, 130.1, 127.8, 125.1, 124.6, 124.4, 124.3, 117.9, 112.3; HRMS (ESI) m/z calcd for $C_{13}H_{10}BrN_2^+$ $(M+H)^+$ 273.00219, found 273.00186.

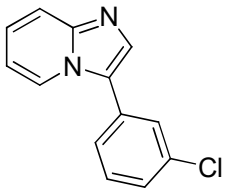
3-(3-Fluorophenyl)imidazo[1,2-*a*]pyridine (3m, CAS: 1560900-40-4)[4]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 3-methylstyrene (**2d**, 55.2 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3m** as yellow oily liquid (12.7 mg, 30% yield). R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.37 (d, J = 6.9 Hz, 1H), 7.73- 7.70 (m, 2H), 7.53-7.47 (m, 1H), 7.37 (d, J = 7.7 Hz, 1H), 7.30-7.23 (m, 2H), 7.12 (t, J = 8.2 Hz, 1H), 6.87 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 163.2 (d, J = 247 Hz), 146.3, 132.9, 131.3 (d, J = 8 Hz), 130.9 (d, J = 9 Hz), 124.67, 124.56, 123.5 (d, J = 3 Hz), 123.3, 118.4, 115.1(d, J = 21 Hz), 114.7 (d, J = 22 Hz), 112.9; HRMS (ESI) m/z calcd for $C_{13}H_{10}FN_2^+$ $(M+H)^+$ 213.08225, found 213.08157.

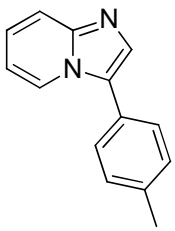
3-(3-Chlorophenyl)imidazo[1,2-*a*]pyridine (3n, CAS: 1361328-90-6)[5]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(3-chlorophenyl)acetaldehyde (**2e**, 61.6 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3n** as yellow oily liquid (27.8 mg, 61% yield). R_f = 0.5 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.34 (d, J = 6.9 Hz, 1H), 7.73-7.71 (m, 2H), 7.56 (s, 1H), 7.47-7.46 (m, 2H), 7.41-7.40 (m, 1H), 7.27-7.24 (m, 1H), 6.88 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.2, 135.2, 132.7, 131.0, 130.5, 128.3, 127.8, 126.0, 124.8, 124.3, 123.2, 118.3, 113.0; HRMS (ESI) m/z calcd for $C_{13}H_{10}ClN_2^+$ $(M+H)^+$ 229.05270, found 229.05258.

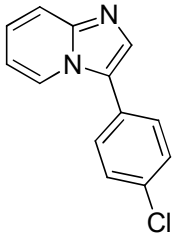
3-(p-Tolyl)imidazo[1,2-*a*]pyridine (3o, CAS: 1338248-67-1)[1]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(p-tolyl)acetaldehyde (**2f**, 53.6 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3o** as yellow oily liquid (30.8 mg, 74% yield). R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.32 (d, J = 6.9 Hz, 1H), 7.71-7.67 (m, 2H), 7.46 (d, J = 7.4 Hz, 2H), 7.33 (d, J = 7.7 Hz, 2H), 7.23-7.19 (m, 1H), 6.82 (t, J = 6.8 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.8, 138.3, 131.8, 130.0, 128.1, 126.2, 125.8, 124.3, 123.4, 118.1, 112.6, 21.3.

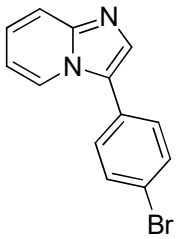
3-(4-Chlorophenyl)imidazo[1,2-*a*]pyridine (3p) [6]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(4-chlorophenyl)acetaldehyde (**2g**, 71.5 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3p** as yellow solid (37.8 mg, 83% yield), mp 94-96 ^{o}C. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.29 (d, J = 6.8 Hz, 1H), 7.73-7.70 (m, 2H), 7.50 (s, 4H), 7.27-7.23(m, 1H), 6.86 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.9, 134.2, 131.8, 129.5, 129.3, 127.4, 125.0, 124.7, 123.2, 118.1, 113.1; HRMS (ESI) m/z calcd for $C_{13}H_{10}ClN_2^+$ $(M+H)^+$ 229.05270, found 229.05324.

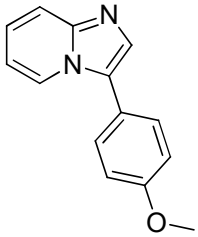
3-(4-Bromophenyl)imidazo[1,2-*a*]pyridine (3q, CAS: 1338248-68-2)[1]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(4-bromophenyl)acetaldehyde (**2h**, 79.2 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3q** as yellowish solid (43.5 mg, 80% yield), mp 95-97 ^{o}C. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.30 (d, J = 6.9 Hz, 1H), 7.80 (d, J = 9.0 Hz, 1H), 7.74 (s, 1H), 7.67 (d, J = 8.1 Hz, 2H), 7.44 (d, J = 8.2 Hz, 2H), 7.32-7.27 (m, 1H), 6.90 (t, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.6, 140.9, 132.5, 131.3, 129.6, 125.4, 124.6, 123.2, 122.5, 118.0, 113.4.

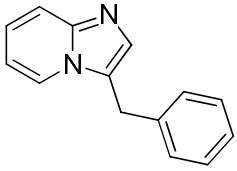
3-(4-Methoxyphenyl)imidazo[1,2-*a*]pyridine (3r, CAS: 1338248-76-2)[1]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 2-(4-methoxyphenyl)acetaldehyde (**2i**, 60.0 mg, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3r** as yellowish solid (35.8 mg, 80% yield), mp 110-112 ^{o}C. R_f = 0.40 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.27 (d, J = 6.9 Hz, 1H), 7.68 (d, J = 9.1 Hz, 1H), 7.64 (s, 1H), 7.48 (d, J = 8.5 Hz, 2H), 7.21-7.18 (m, 1H), 7.06 (d, J = 8.5 Hz, 2H), 6.81 (t, J = 6.8 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 159.7, 145.6, 131.7, 129.7, 125.5, 124.1, 123.3, 121.4, 118.1, 114.7, 112.5, 55.4.

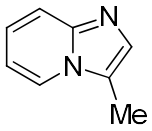
3-Benzylimidazo[1,2-*a*]pyridine (3s)[7]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 3-phenylpropanal (**2j**, 55.4 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3s** as brown solid (39.9 mg, 96% yield), mp 110-112 ^{o}C. R_f = 0.70 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.77 (d, J = 6.9 Hz, 1H), 7.68 (d, J = 9.1 Hz, 1H), 7.49 (s, 1H), 7.32-7.25 (m, 3H), 7.19-7.15 (m, 3H), 6.74 (t, J = 6.8 Hz, 1H), 4.25 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.3, 136.3, 131.6, 128.8, 128.3, 127.0, 124.2, 123.3, 122.6, 117.6, 112.4, 30.2; HRMS (ESI) m/z calcd for $C_{14}H_{13}N_2^+$ $(M+H)^+$ 209.10732, found 209.10799

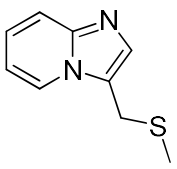
3-Methylimidazo[1,2-*a*]pyridine (3t)[8]



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), propionaldehyde (**2k**, 31.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3t** as brown oily liquid (25.6 mg, 97% yield). R_f = 0.65 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.88 (d, J = 6.9 Hz, 1H), 7.62 (d, J = 9.1 Hz, 1H), 7.42 (s, 1H), 7.18-7.14 (m, 1H), 6.84 (t, J = 6.8 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.1, 131.2, 123.1, 122.7, 119.8, 117.7, 112.0, 9.0; HRMS (ESI) m/z calcd for $C_8H_9N_2^+$ $(M+H)^+$ 133.07602, found 133.07640.

3-((Methylthio)methyl)imidazo[1,2-*a*]pyridine (3u)

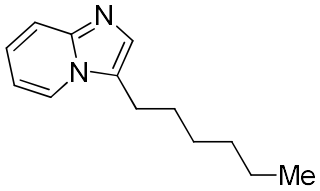


The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol),

3-(methylthio)propanal (**2l**, 41.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3u** as brown solid (28.5 mg, 80% yield), mp 58-60 ^{o}C. R_f = 0.25 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.13 (dd, J = 6.9 Hz, 1.0 Hz, 1H), 7.63 (dd, J = 9.1 Hz, 1.0 Hz, 1H), 7.53 (s, 1H), 7.23-7.18 (m, 1H), 6.85 (t, J = 6.8 Hz, 1H), 3.99 (s, 2H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.1, 133.1, 123.9, 123.8, 118.5, 117.7, 111.9, 26.7, 14.5; HRMS calcd. for $C_9H_{11}N_2S$ $[M+H]^+$ 179.06375, found 179.06369.

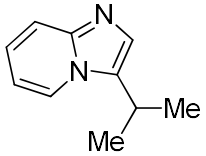
3-Hexylimidazo[1,2-*a*]pyridine (3v)



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), octanal (**2m**, 64.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3v** as yellow oily liquid (32.7 mg, 81% yield). R_f = 0.55 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.92 (d, J = 6.8 Hz, 1H), 7.66 (d, J = 9.1 Hz, 1H), 7.42 (s, 1H), 7.19-7.15 (m, 1H), 6.84 (t, J = 6.7 Hz, 1H), 2.82 (t, J = 7.6 Hz, 2H), 1.79-1.75 (m, 2H), 1.46-1.42 (m, 2H), 1.34-1.32 (m, 4H), 0.90 (t, J = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 144.9, 130.0, 124.6, 123.5, 122.9, 117.7, 112.1, 31.5, 29.1, 26.8, 23.8, 22.5, 14.0; HRMS (ESI) m/z calcd for $C_{13}H_{19}N_2^+$ $(M+H)^+$ 203.15428, found 203.15417.

3-Isopropylimidazo[1,2-*a*]pyridine (3w, CAS: 78132-60-2)[9]

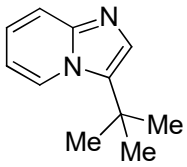


The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 3-methylbutanal (**2n**, 43.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3w** as

brown oily liquid (31.0 mg, 97% yield). R_f = 0.50 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.93 (d, J = 6.9 Hz, 1H), 7.61 (d, J = 9.1 Hz, 1H), 7.41 (s, 1H), 7.14-7.10 (m, 1H), 6.81-6.78 (m, 1H), 3.20-3.13 (m, 1H), 1.38 (d, J = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.2, 130.3, 128.5, 122.9, 122.9, 117.8, 111.7, 23.9, 20.6; HRMS (ESI) m/z calcd for $C_{10}H_{13}N_2^+$ $(M+H)^+$ 161.10732, found 161.10686.

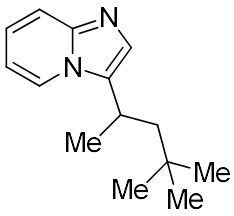
3-(*tert*-Butyl)imidazo[1,2-*a*]pyridine (3x)



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 3,3-dimethylbutanal (**2o**, 51.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3x** as yellowish solid (33.4 mg, 96% yield), mp 85-86 ^{o}C. R_f = 0.65 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.24 (d, J = 7.0 Hz, 1H), 7.64 (d, J = 9.1 Hz, 1H), 7.39 (s, 1H), 7.16-7.12 (m, 1H), 6.79 (t, J = 6.8 Hz, 1H), 1.49 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.2, 132.7, 129.1, 125.3, 122.8, 118.2, 111.5, 30.8, 28.0; HRMS (ESI) m/z calcd for $C_{11}H_{15}N_2^+$ $(M+H)^+$ 175.12297, found 175.12238

3-(4,4-Dimethylpentan-2-yl)imidazo[1,2-a]pyridine (3y)



The reaction was conducted with pyridin-2-amine (**1a**, 19.8 mg, 0.2 mmol), 3,5,5-trimethylhexanal (**2p**, 73.0 μL, 0.4 mmol) and sulfur powder (12.8 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1:1) to yield the desired product **3y** as yellowish solid (42.3 mg, 98% yield), mp 95-96 ^{o}C. R_f = 0.60 (1:2 petroleum ether/EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.00 (d, J = 6.9 Hz, 1H), 7.65 (d, J = 9.1 Hz, 1H), 7.43 (s, 1H), 7.16 (t, J = 7.8 Hz, 1H), 6.84 (t, J = 6.7 Hz, 1H), 3.19-3.16 (m, 1H), 1.91 (dd, J = 14.1 Hz, 6.4 Hz, 1H), 1.56 (dd, J = 14.1 Hz, 5.4 Hz, 1H), 1.37 (d, J = 6.9 Hz, 3H), 0.90 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 144.9, 130.8, 129.2, 123.2, 123.0, 118.0, 112.0, 49.0, 31.1, 29.9, 25.9, 22.0; HRMS (ESI) m/z calcd for $C_{14}H_{21}N_2^+$ $(M+H)^+$ 217.16993, found 217.16982.

5. References

[1] B. B. Touré, B. S. Lane, D.Sames, *Org. Lett.* **2006**, *8*, 1979.

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[4] N. P. Grimster, C. Gauntlett, C. R. A. Godfrey, M. J. Gaunt, *Angew. Chem. Int. Ed*. **2005**, *44,* 3125.

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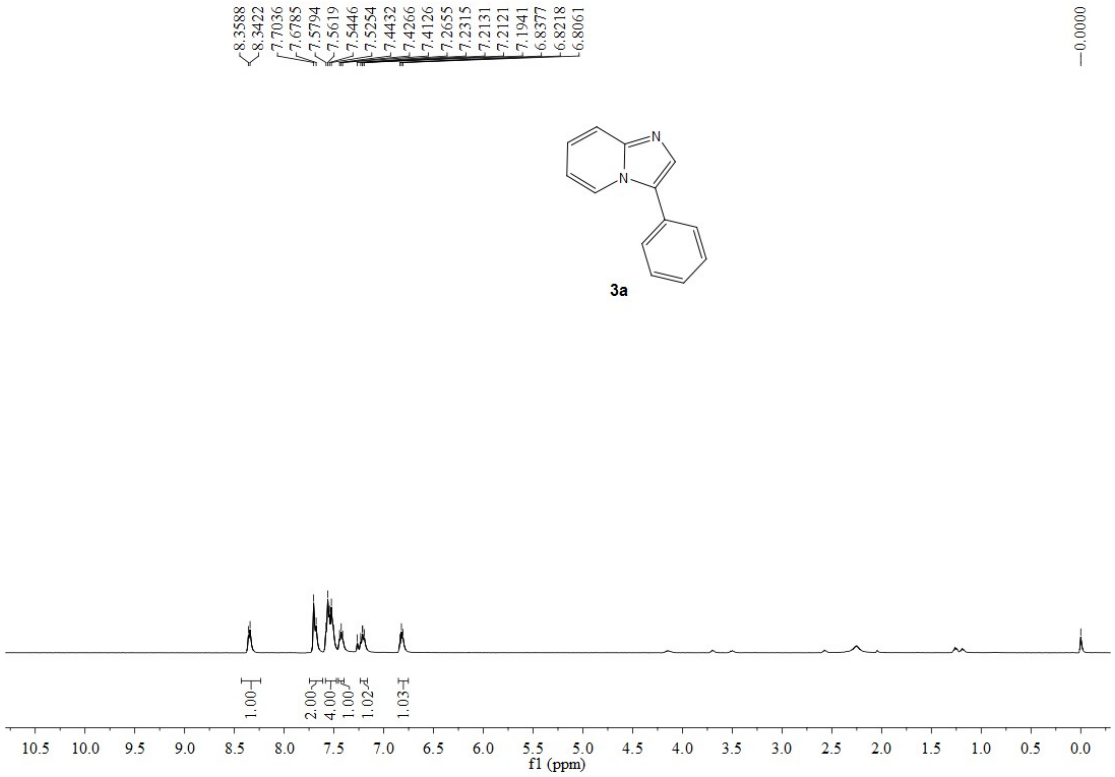
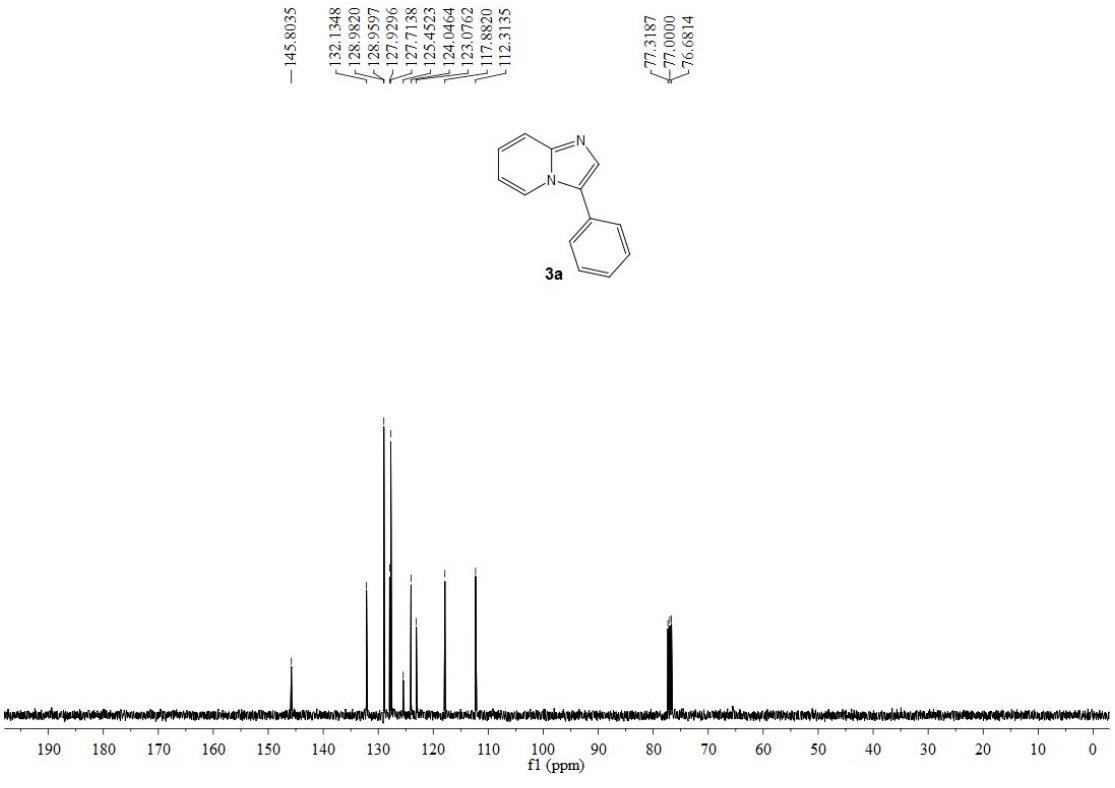
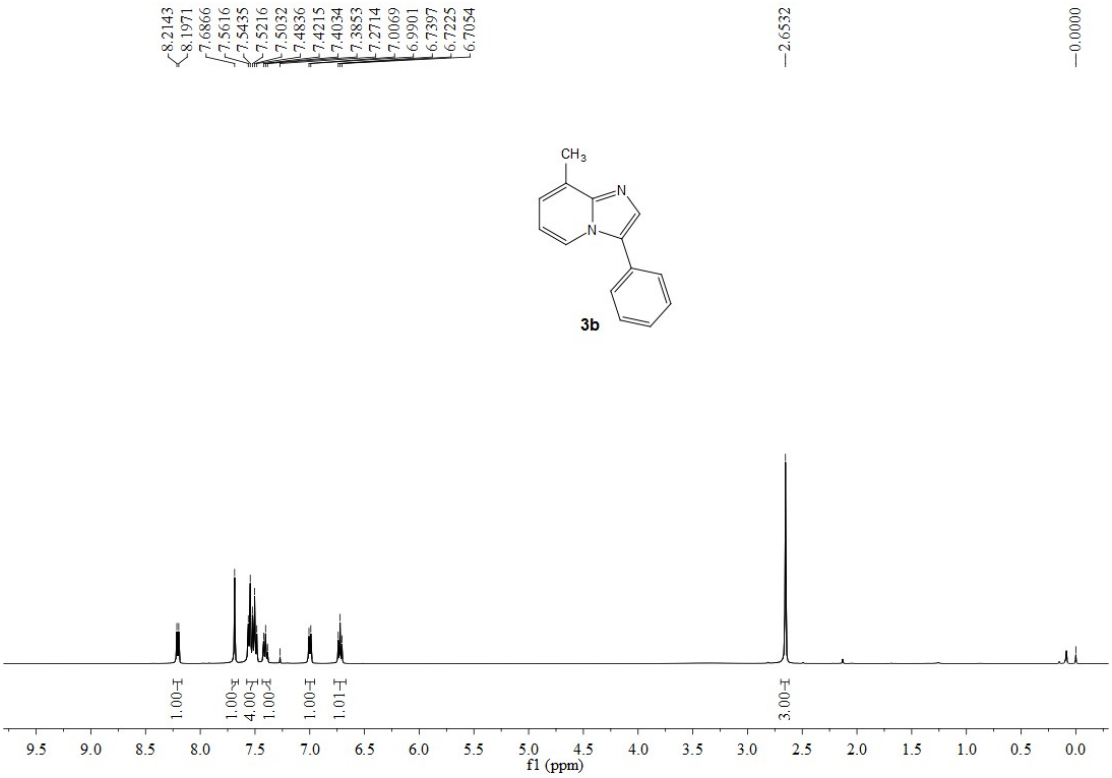
[9] G. Maury, C.Pigiere, *Tetrahedron*, **1981**, *7*, 83.

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



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7.0069
6.9901
6.7397
6.7225
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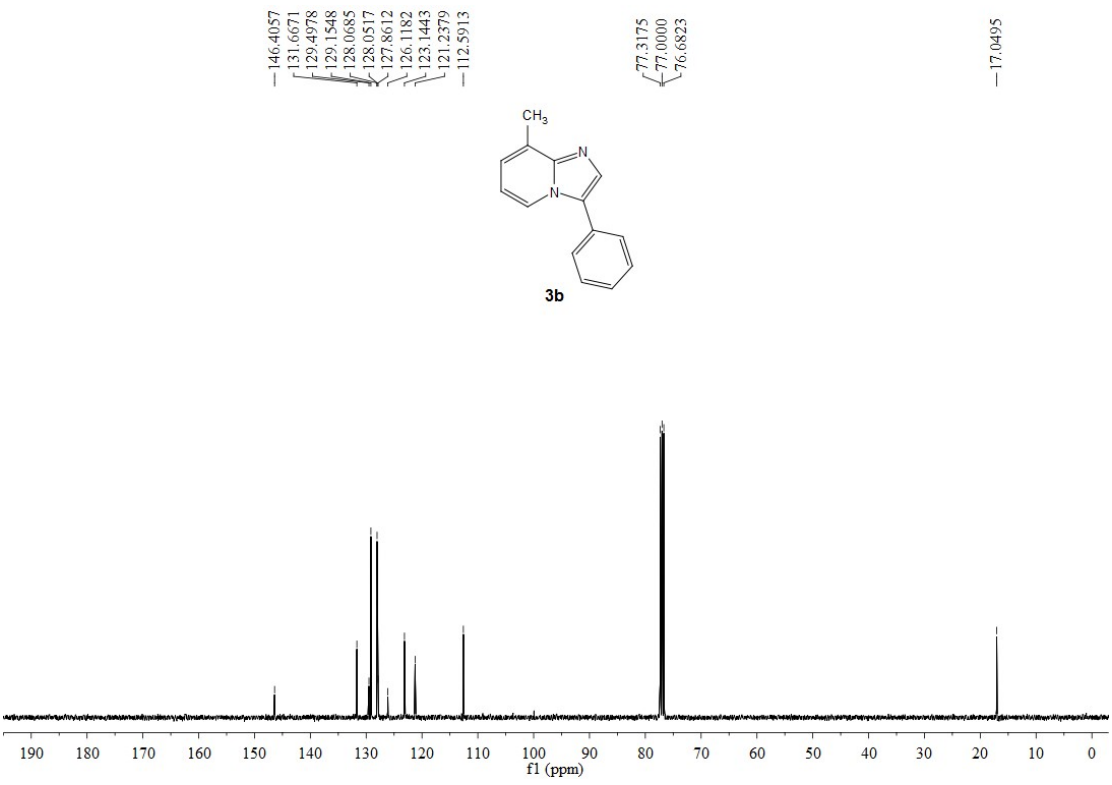
2.6532
0.0000
CH3
N
N
3b
1.00
1.00
4.00
1.00
1.00
1.01
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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CH3
N
N
3b
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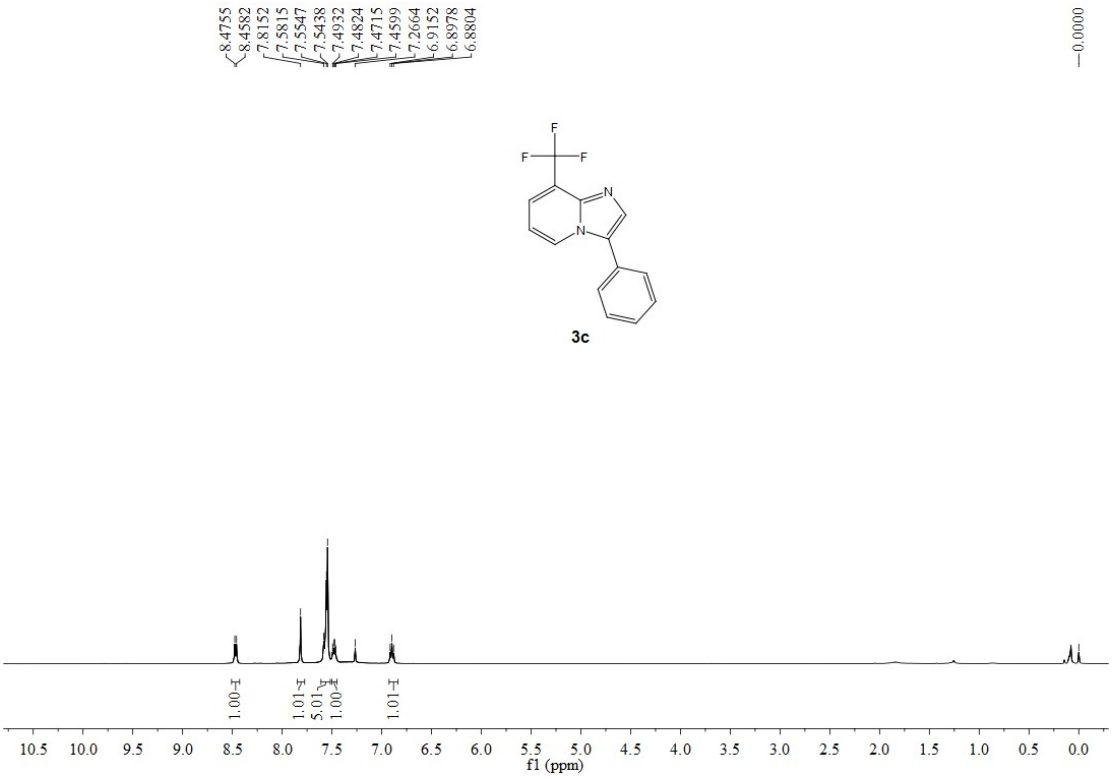
f1 (ppm)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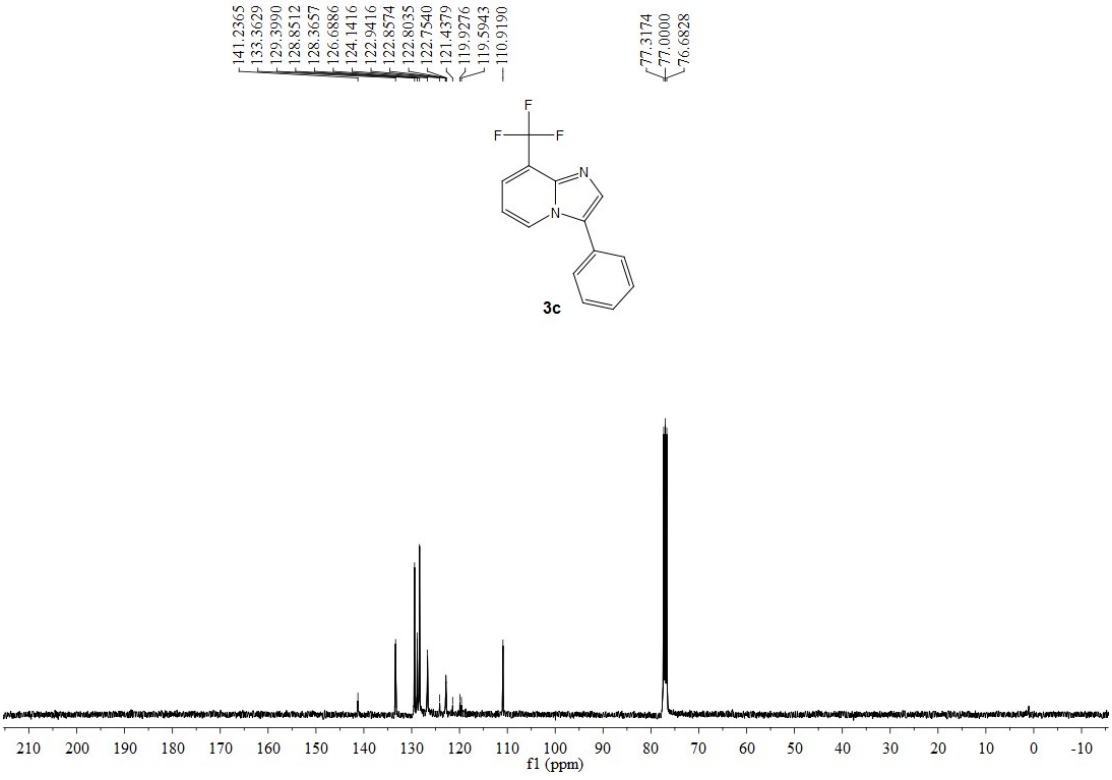
F
F
F
N
N
3c
1.00
1.01
5.01
1.00
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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F
F
N
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3c
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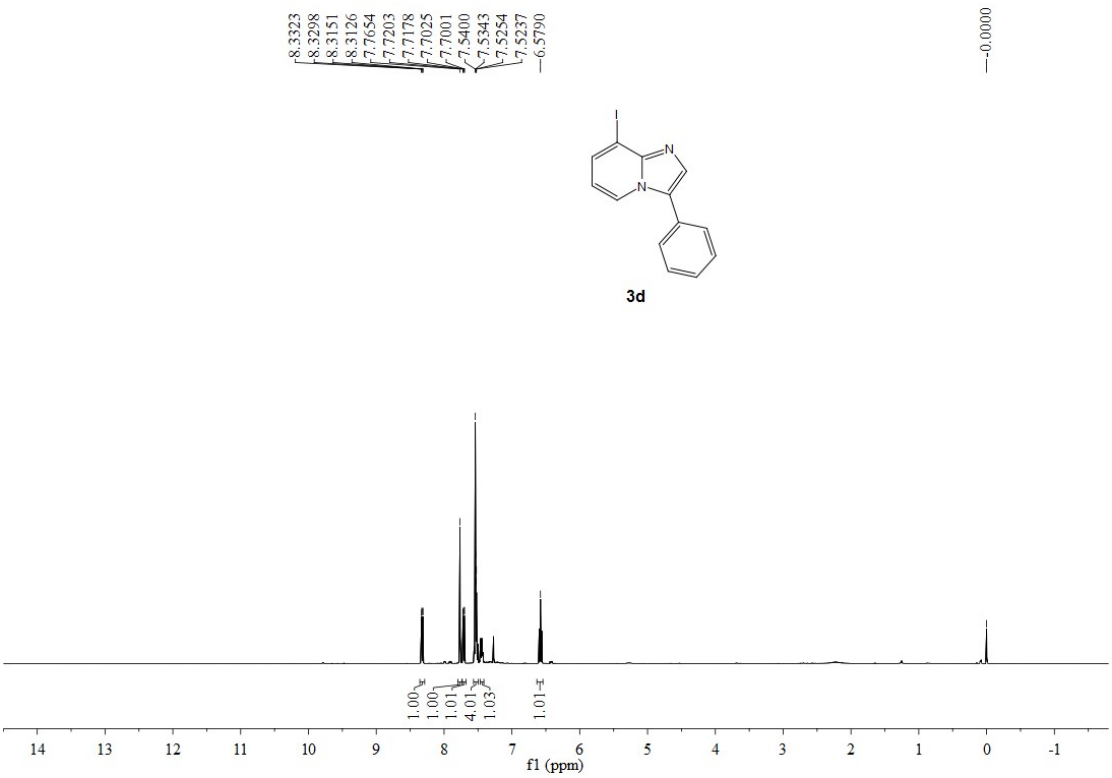
f1 (ppm)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1.01
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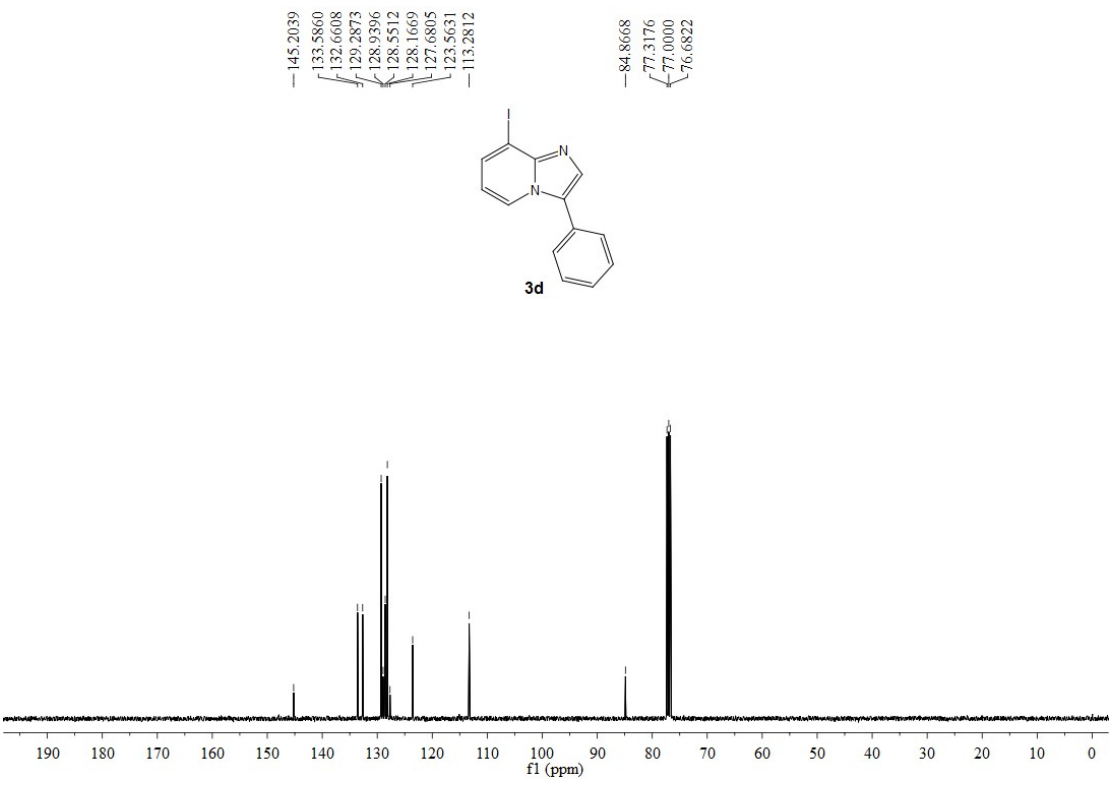
1.03
1.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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129.2873
128.9396
128.5512
128.1669
127.6805
123.5631
113.2812
84.8668
77.3176
77.0000
76.6822
3d
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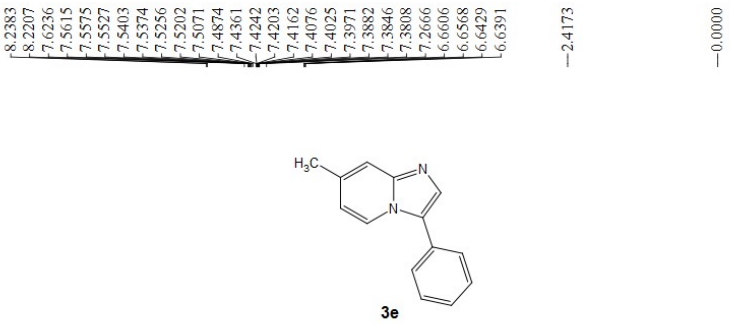
f1 (ppm)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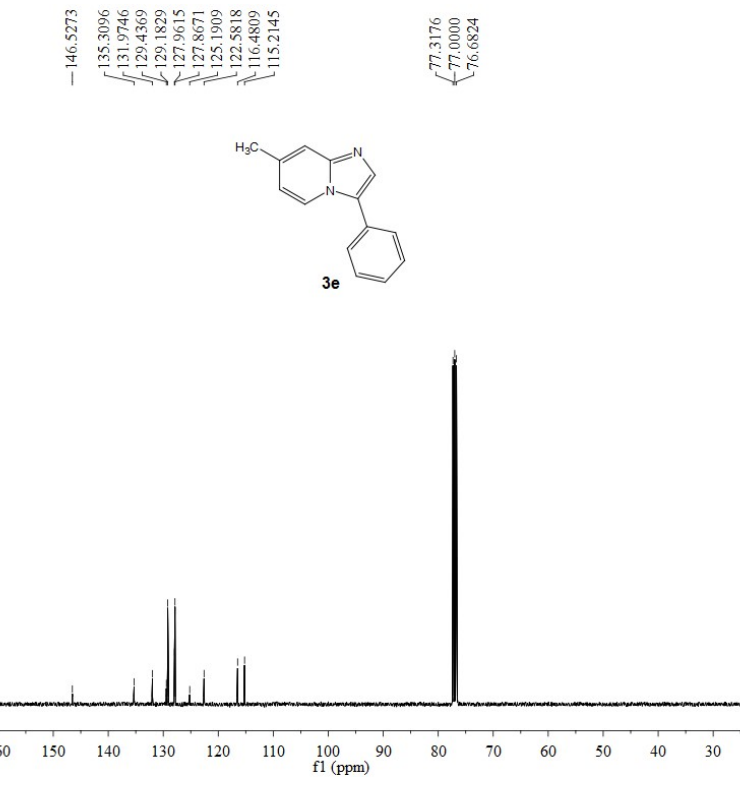
7.6236
7.5615
7.5575
7.5527
7.5403
7.5374
7.5256
7.5202
7.5071
7.4874
7.4361
7.4242
7.4203
7.4162
7.4076
7.4025
7.3971
7.3882
7.3846
7.3808
7.2666
7.6606
7.6568
7.6429
7.6391
2.4173
0.0000
H3C
N
N
3e
1.00
1.04
4.00
2.00
1.00
3.00
f1 (ppm)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115.2145
77.3176
77.0000
76.6824
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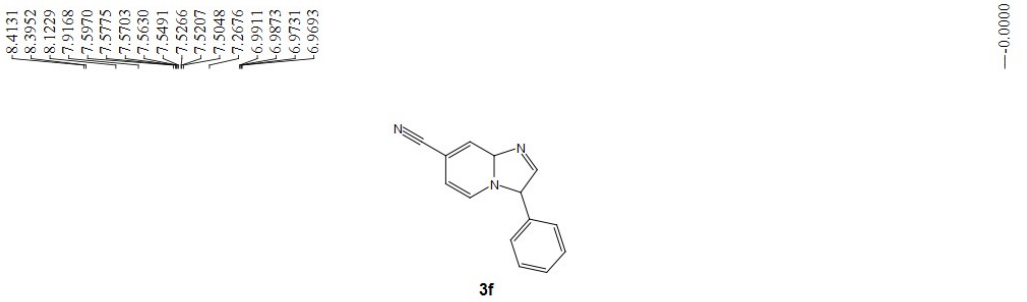
H3C
N
N
3e
f1 (ppm)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8.3952
8.1229
7.9168
7.5970
7.5775
7.5703
7.5630
7.5491
7.5266
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7.5048
7.2676
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6.9873
6.9731
6.9693
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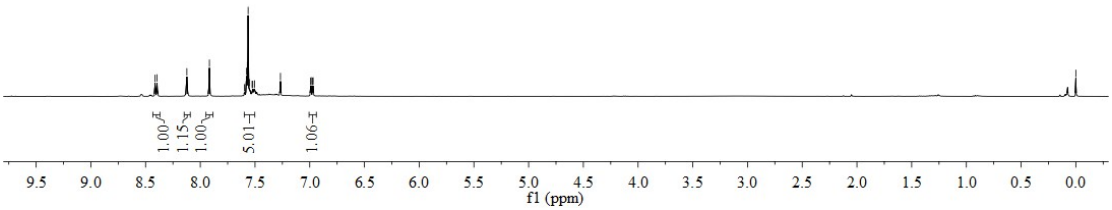
N
N
N

3f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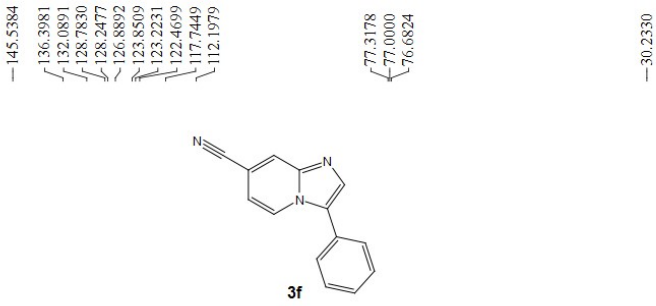
1.15
1.00
5.01
1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.0891
128.7830
128.2477
126.8892
123.8509
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117.7449
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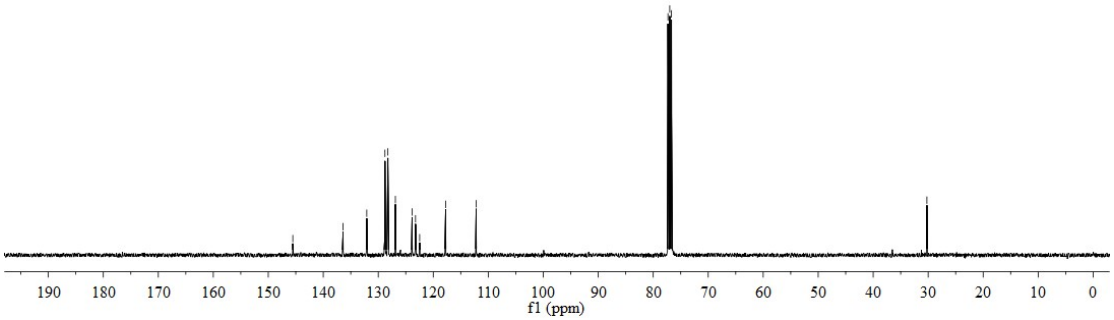
77.3178
77.0000
76.6824
30.2330
N
N
N

3f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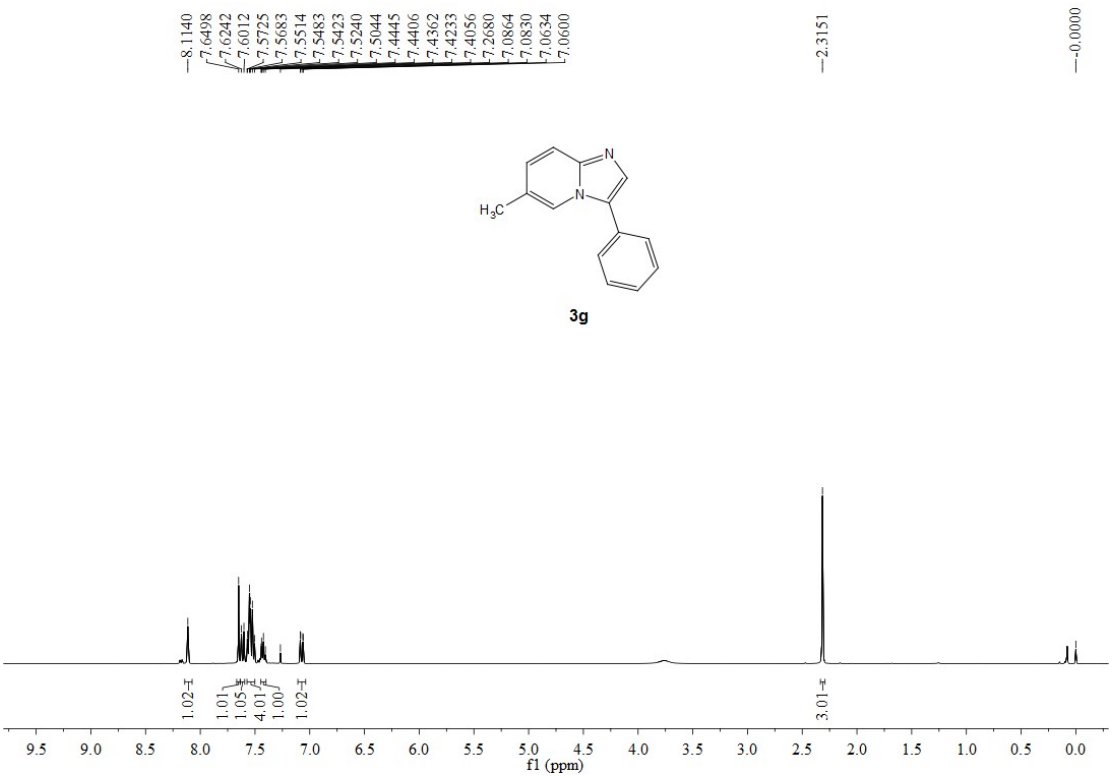
f1 (ppm)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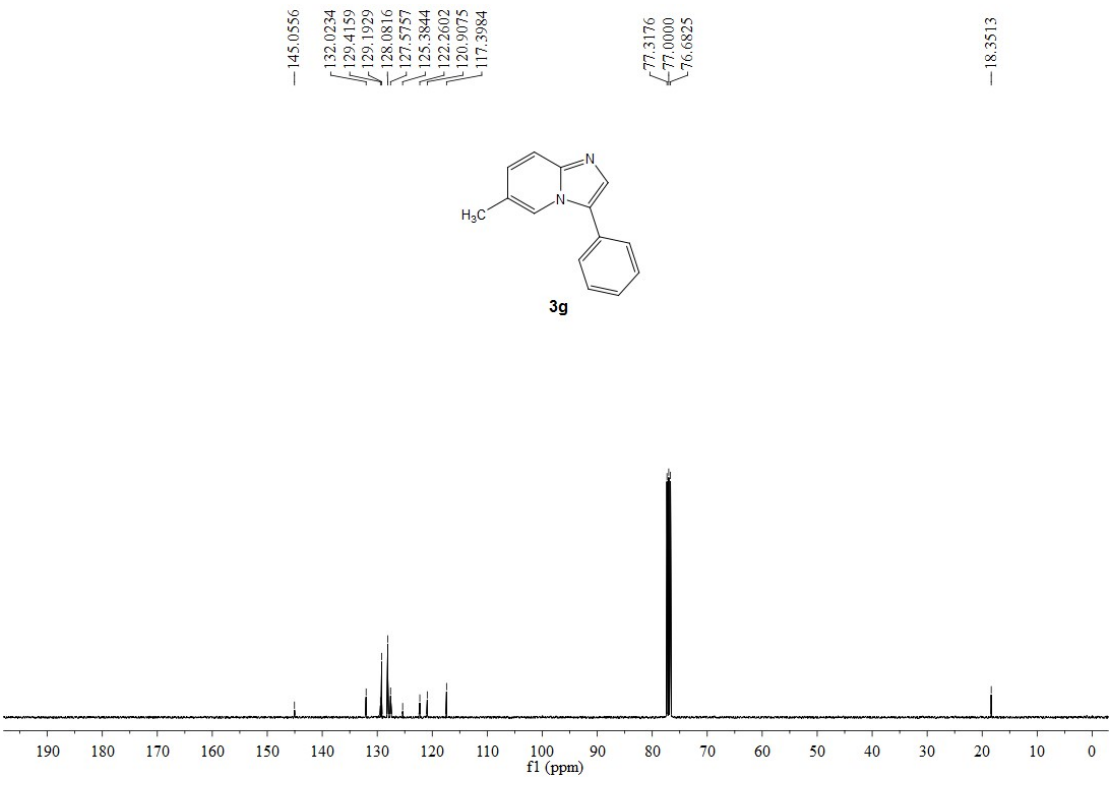
7.6498
7.6242
7.6012
7.5725
7.5683
7.5514
7.5483
7.5423
7.5240
7.5044
7.4445
7.4406
7.4362
7.4233
7.4056
7.2680
7.0864
7.0830
7.0634
7.0600
2.3151
-0.0000
N
N
H3C
1.02
1.01
1.05
4.01
1.00
1.02
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3g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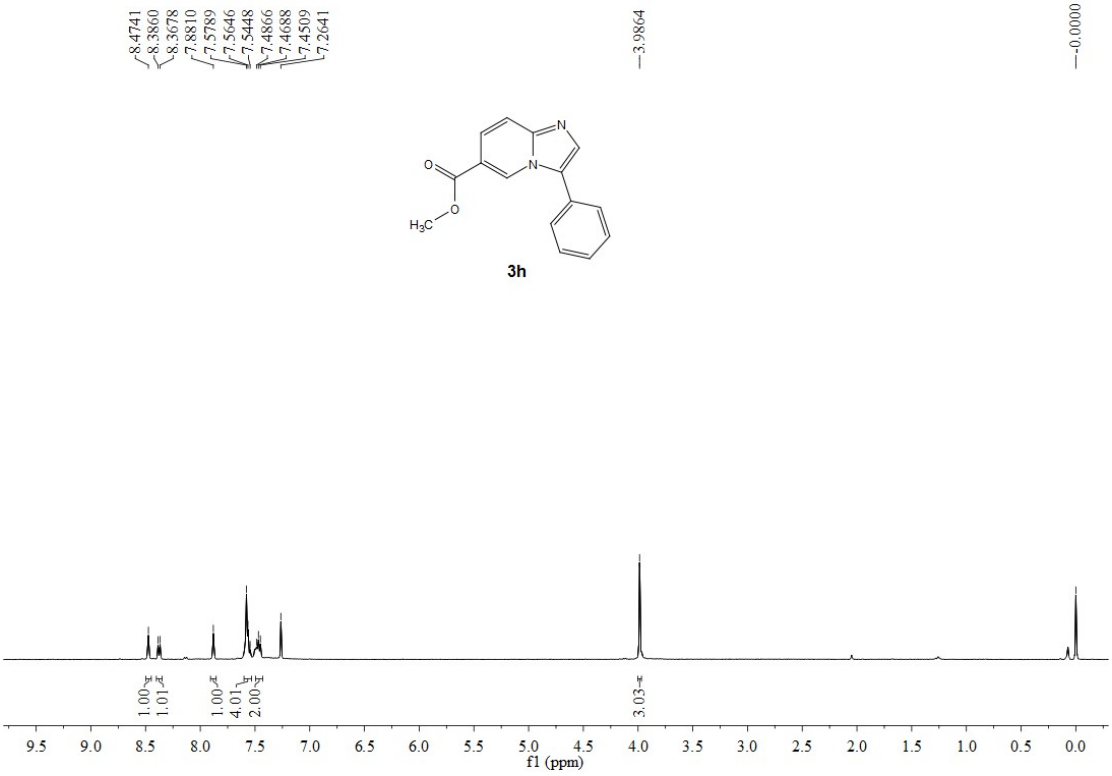
132.0234
129.4159
129.1929
128.0816
127.5757
125.3844
122.2602
120.9075
117.3984
77.3176
77.0000
76.6825
18.3513
N
N
H3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3g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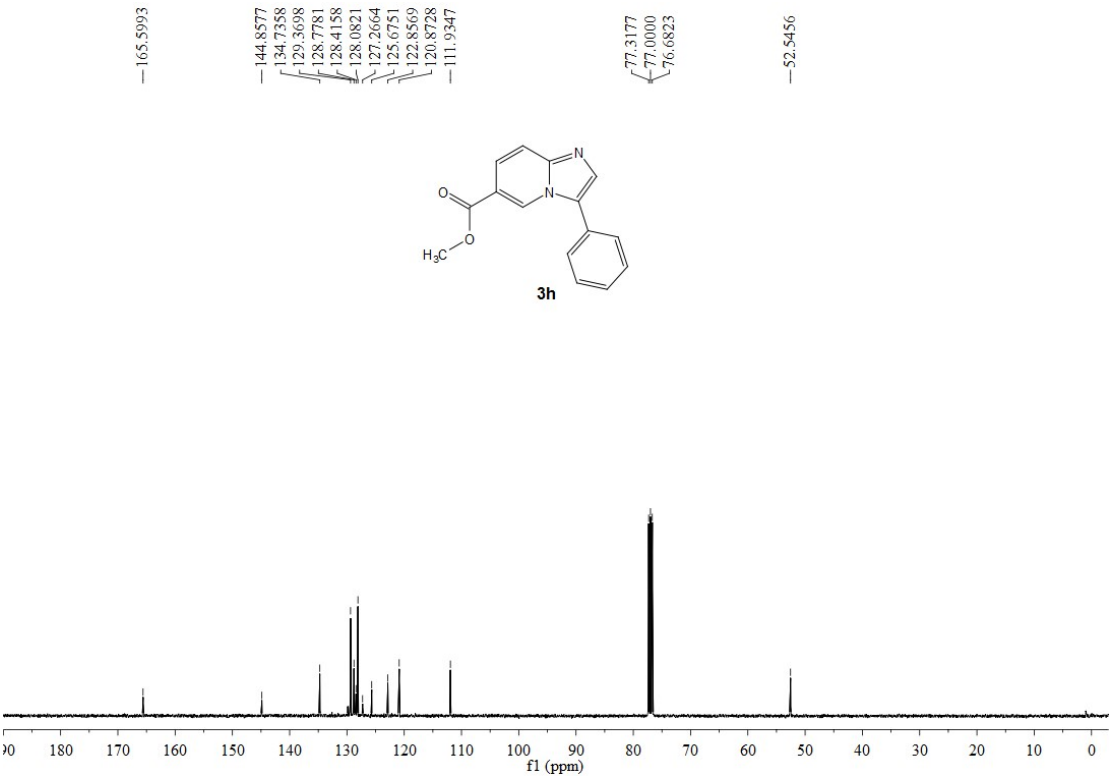
8.3860
8.3678
7.8810
7.5789
7.5646
7.5448
7.4866
7.4688
7.4509
7.2641
3.9864
0.0000
O
N
N
O
H3C
3h
1.00
1.01
1.00
4.01
2.00
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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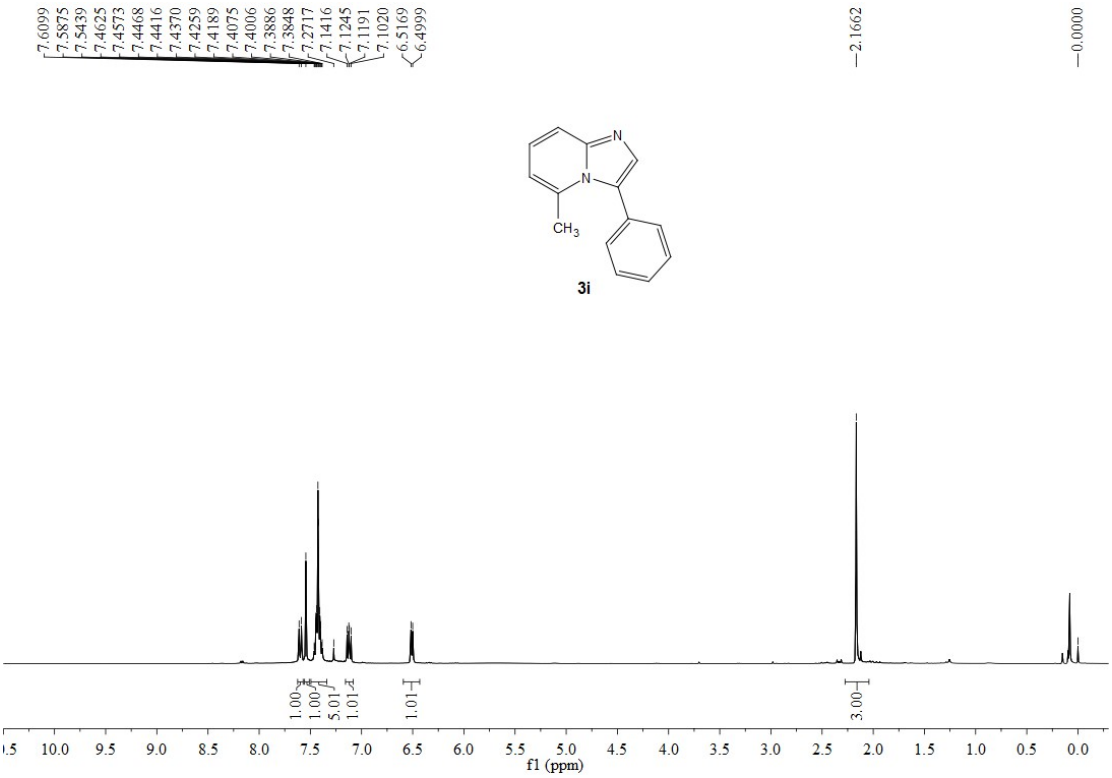
144.8577
134.7358
129.3698
128.7781
128.4158
128.0821
127.2664
125.6751
122.8569
120.8728
111.9347
77.3177
77.0000
76.6823
52.5456
O
N
N
O
H3C
3h
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5875
7.5439
7.4625
7.4573
7.4468
7.4416
7.4370
7.4259
7.4189
7.4075
7.4006
7.3886
7.3848
7.2717
7.1416
7.1245
7.1191
7.1020
6.5169
6.4999
2.1662
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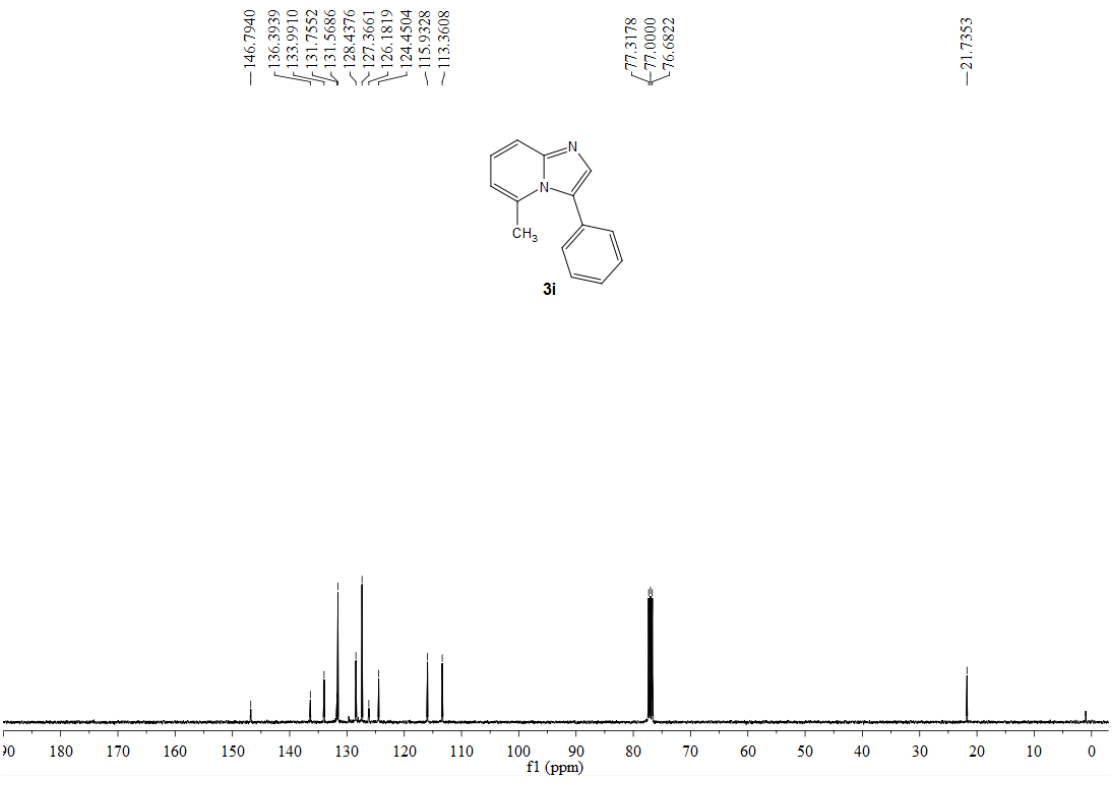
N
N
CH3
1.00
1.00
5.01
1.01
1.01
3.00
f1 (ppm)

3i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133.9910
131.7552
131.5686
128.4376
127.3661
126.1819
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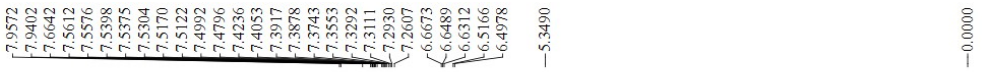
113.3608
77.3178
77.0000
76.6822
21.7353
N
N
CH3
f1 (ppm)

3i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7.9402
7.6642
7.5612
7.5576
7.5398
7.5375
7.5304
7.5170
7.5122
7.4992
7.4796
7.4236
7.4053
7.3917
7.3878
7.3743
7.3553
7.3292
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7.2607
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6.6489
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5.3490
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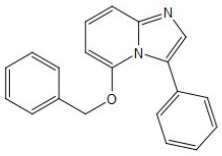
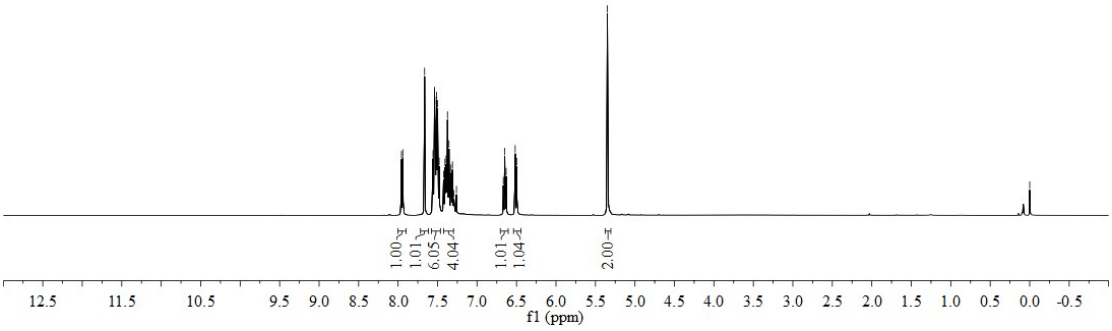


3j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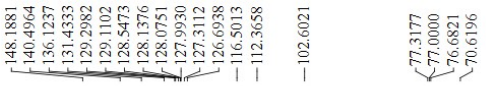
1.01
6.05
4.04
1.01
1.04
2.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


148.1881
140.4964
136.1237
131.4333
129.2982
129.1102
128.5473
128.1376
128.0751
127.9930
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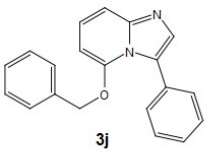
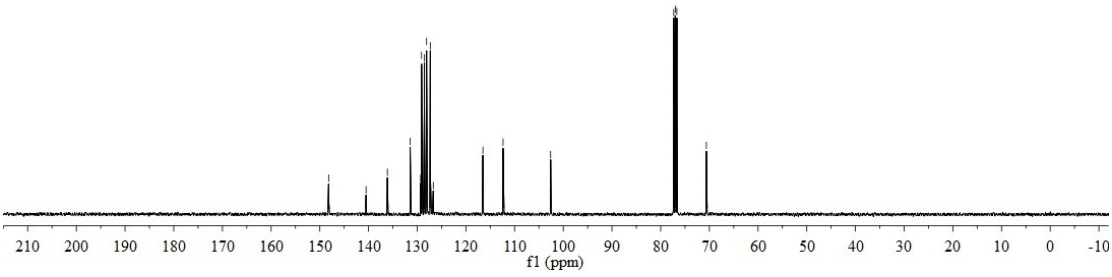
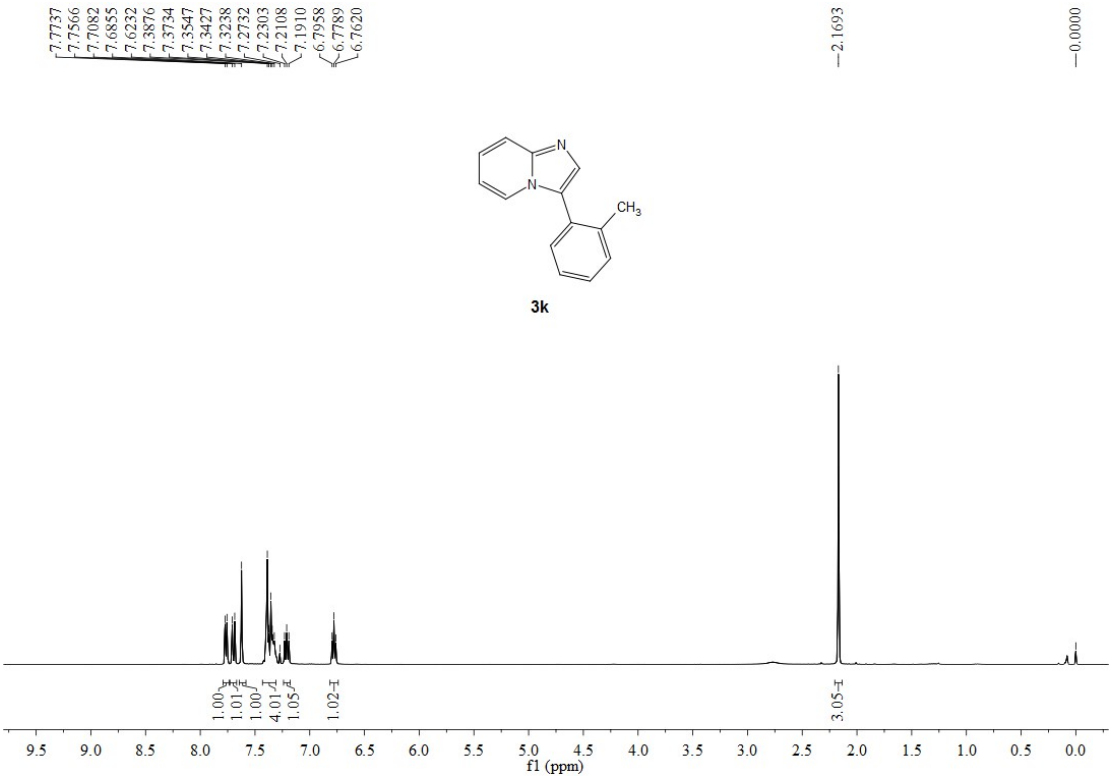
126.6938
116.5013
112.3658
102.6021
77.3177
77.0000
76.6821
70.6196



3j


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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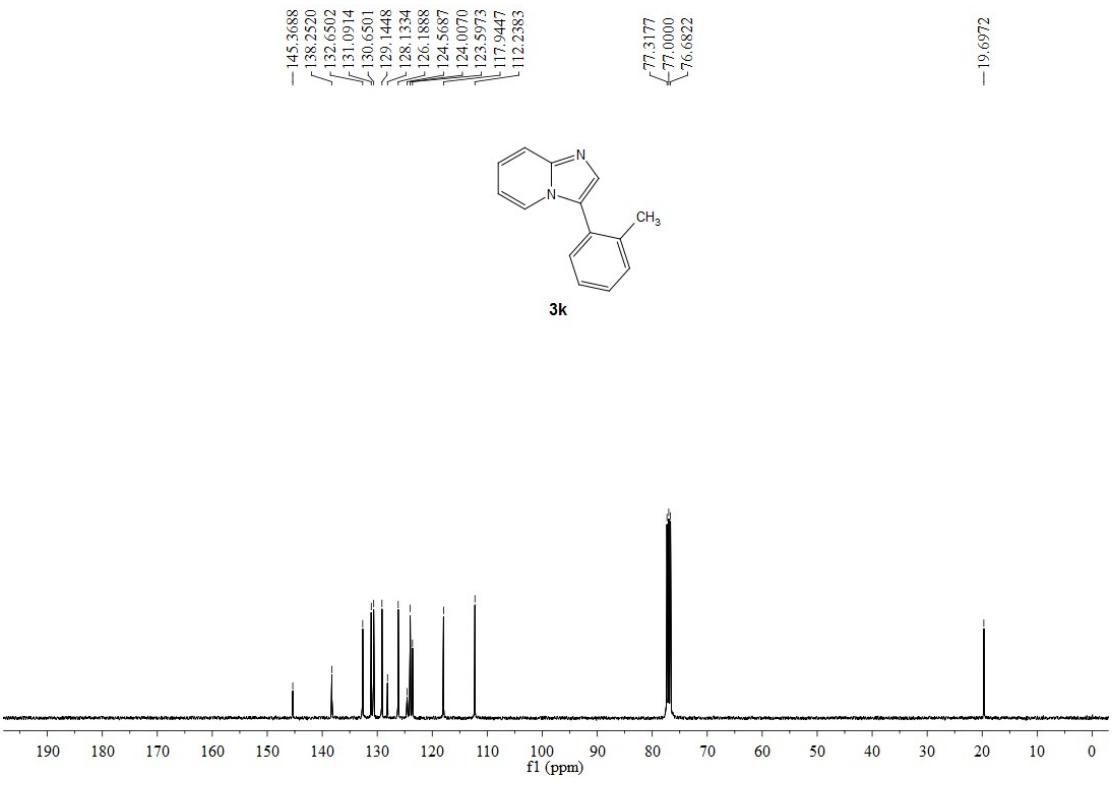
7.6232
7.3876
7.3734
7.3547
7.3427
7.3238
7.2732
7.2303
7.2108
7.1910
6.7958
6.7789
6.7620
2.1693
0.0000
N
N
CH3
1.00
1.01
1.00
4.01
1.05
1.02
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3k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128.1334
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124.5687
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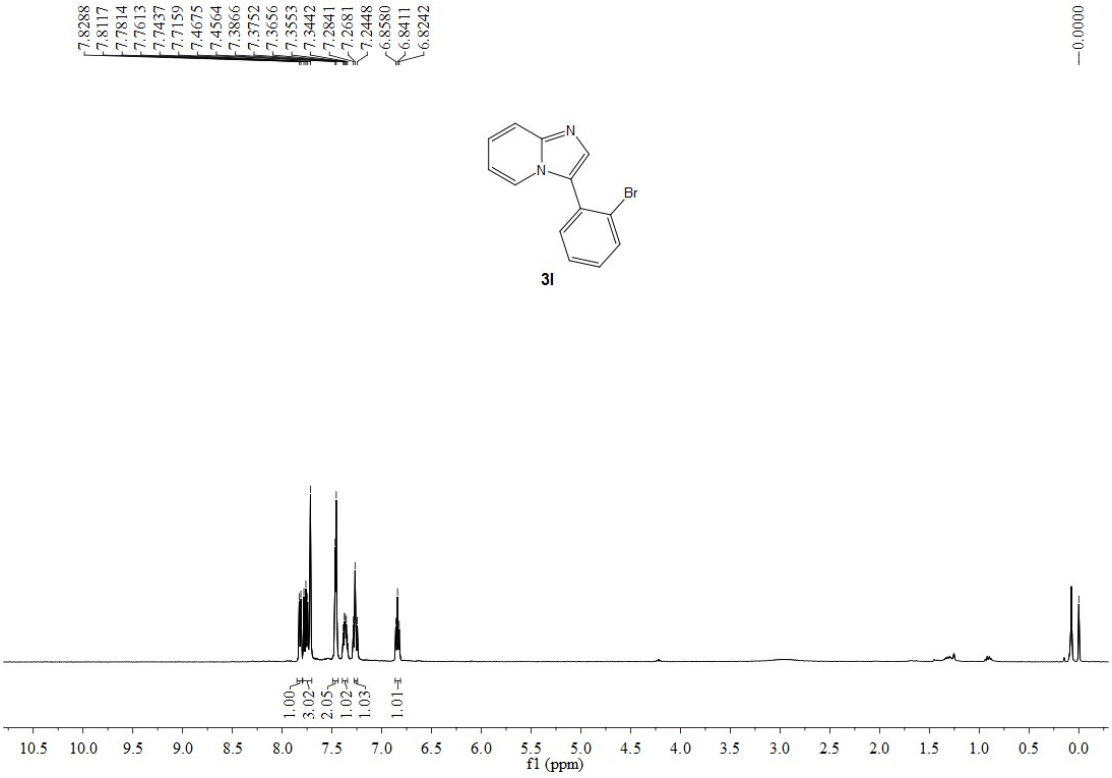
123.5973
117.9447
112.2383
77.3177
77.0000
76.6822
19.6972
N
N
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3k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7.7437
7.7159
7.4675
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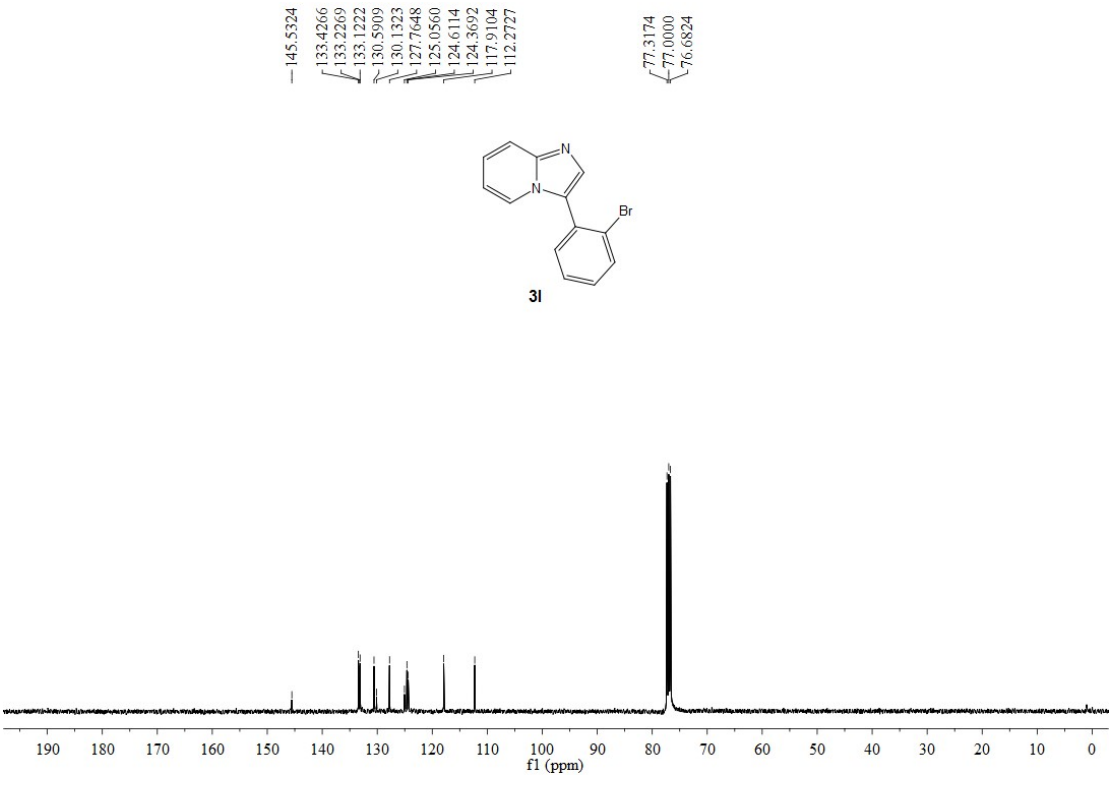
7.3866
7.3752
7.3656
7.3553
7.3442
7.2841
7.2681
7.2448
6.8580
6.8411
6.8242
0.0000
N
N
Br
3l
1.00
3.02
2.05
1.02
1.03
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.2269
133.1222
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130.1323
127.7648
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124.6114
124.3692
117.9104
112.2727
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76.6824
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N
Br
3l
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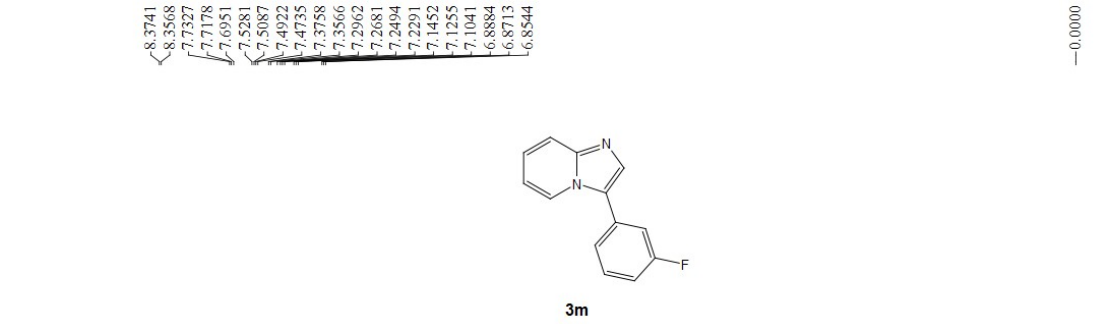
f1 (ppm)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8.3568
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7.7178
7.6951
7.5281
7.5087
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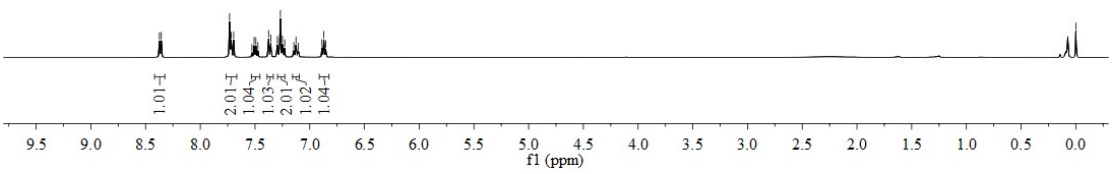
7.4735
7.3758
7.3566
7.2962
7.2681
7.2494
7.2291
7.1452
7.1255
7.1041
6.8884
6.8713
6.8544
0.0000
N
N
F

3m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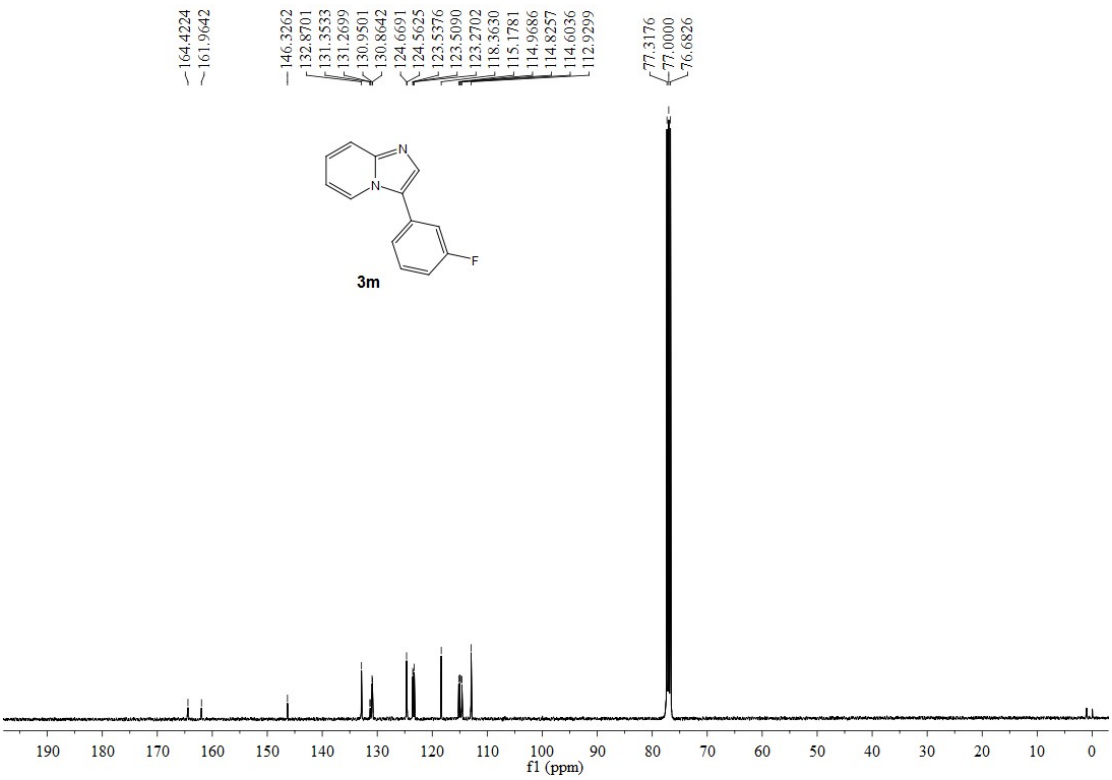
2.01
1.04
1.03
2.01
1.02
1.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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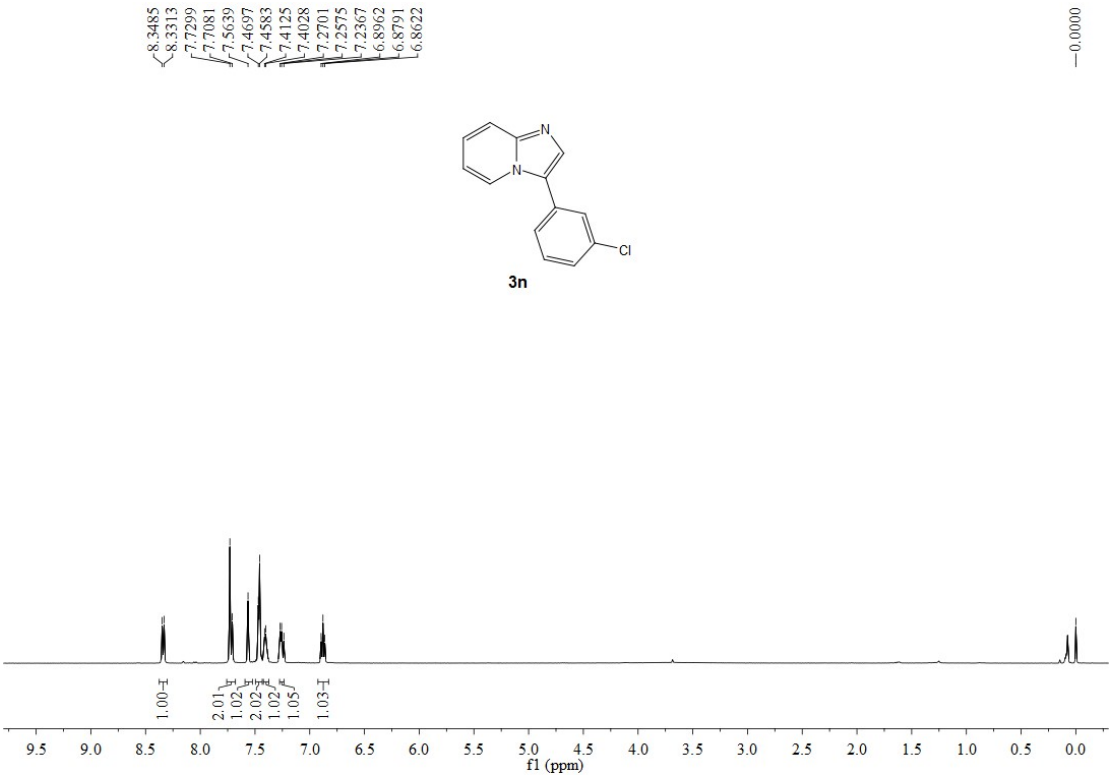
123.5376
123.5090
123.2702
118.3630
115.1781
114.9686
114.8257
114.6036
112.9299
77.3176
77.0000
76.6826
N
N
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3m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7.7299
7.7081
7.5639
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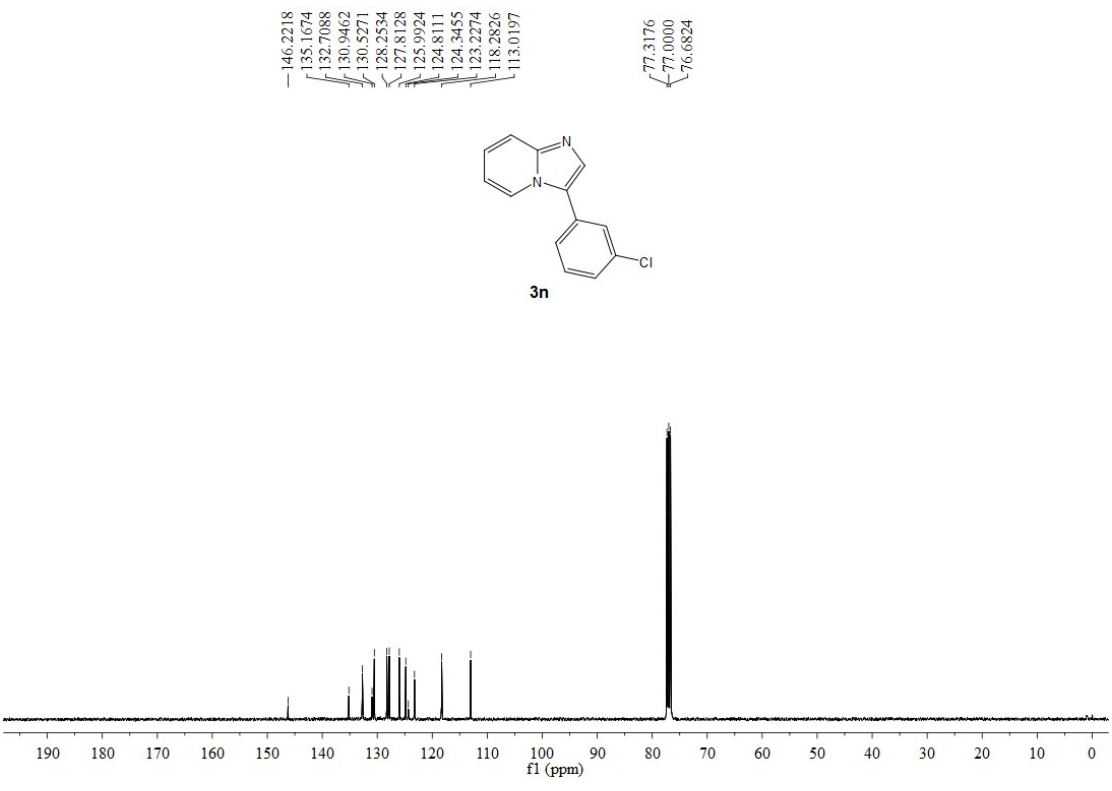
7.4583
7.4125
7.4028
7.2701
7.2575
7.2367
6.8962
6.8791
6.8622
0.0000
N
N
Cl
3n
1.00
2.01
1.02
2.02
1.02
1.05
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.7088
130.9462
130.5271
128.2534
127.8128
125.9924
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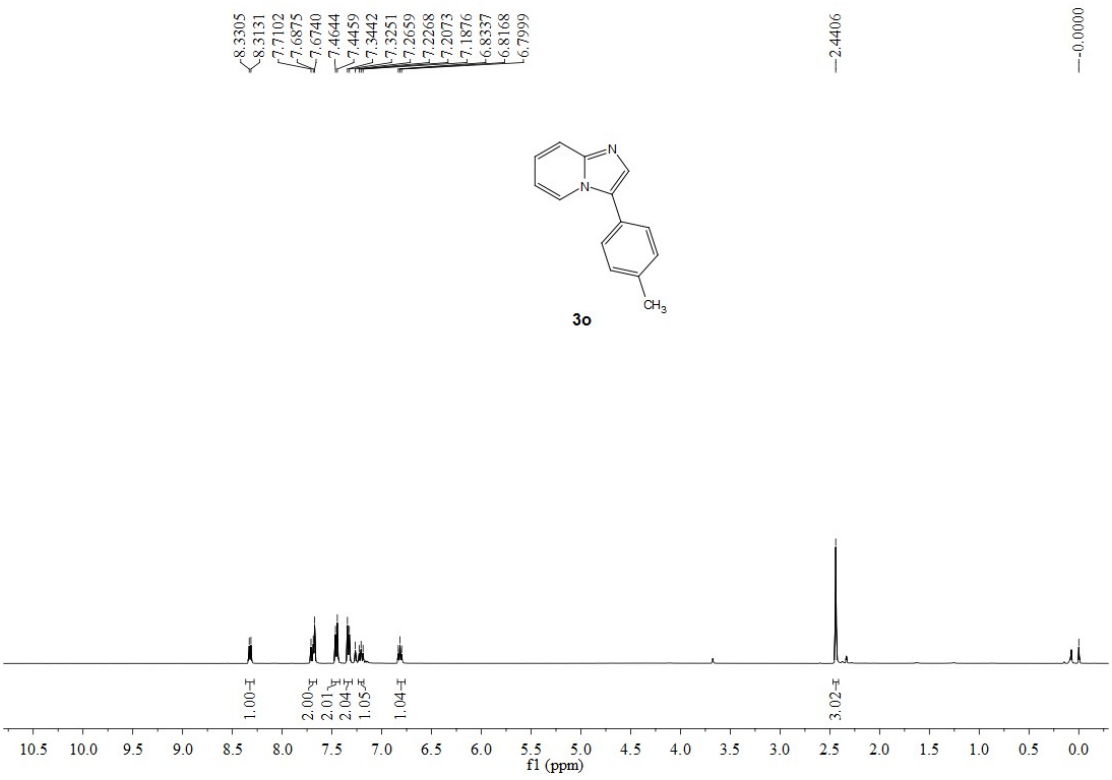
124.3455
123.2274
118.2826
113.0197
77.3176
77.0000
76.6824
N
N
Cl
3n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4644
7.4459
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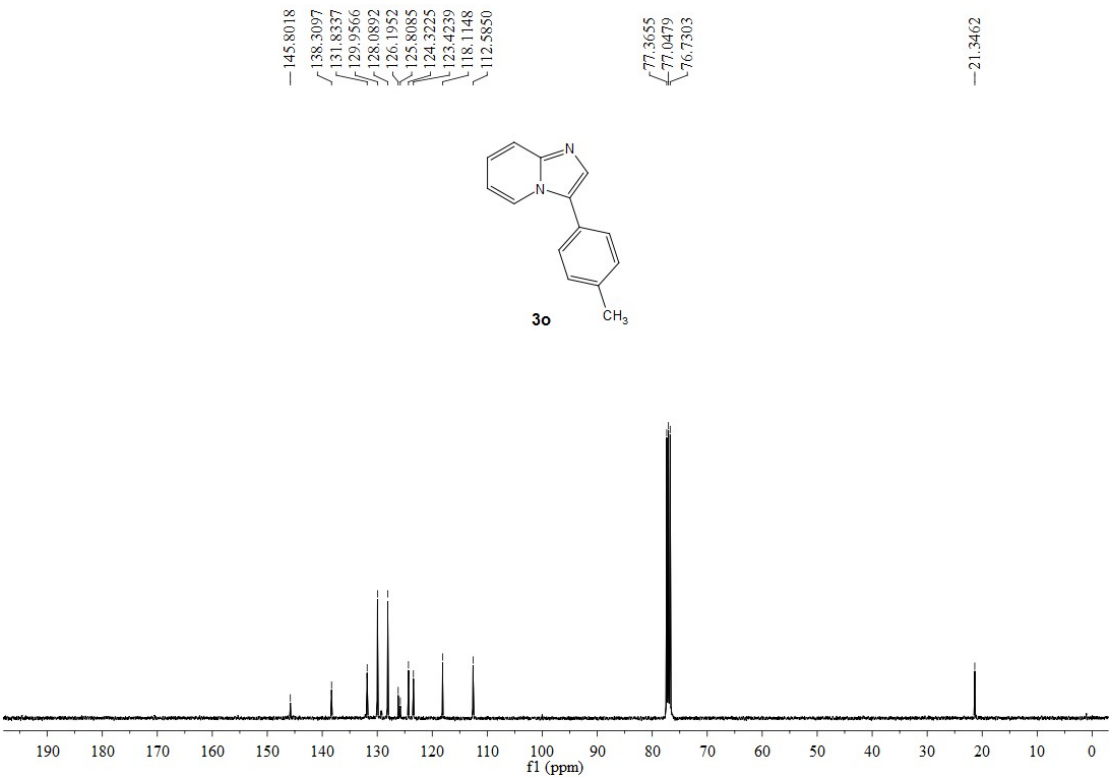
7.2659
7.2268
7.2073
7.1876
6.8337
6.8168
6.7999
2.4406
0.0000
N
N
CH3
3o
1.00
2.00
2.01
2.04
1.05
1.04
3.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.8085
124.3225
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118.1148
112.5850
77.3655
77.0479
76.7303
21.3462
N
N
CH3
3o
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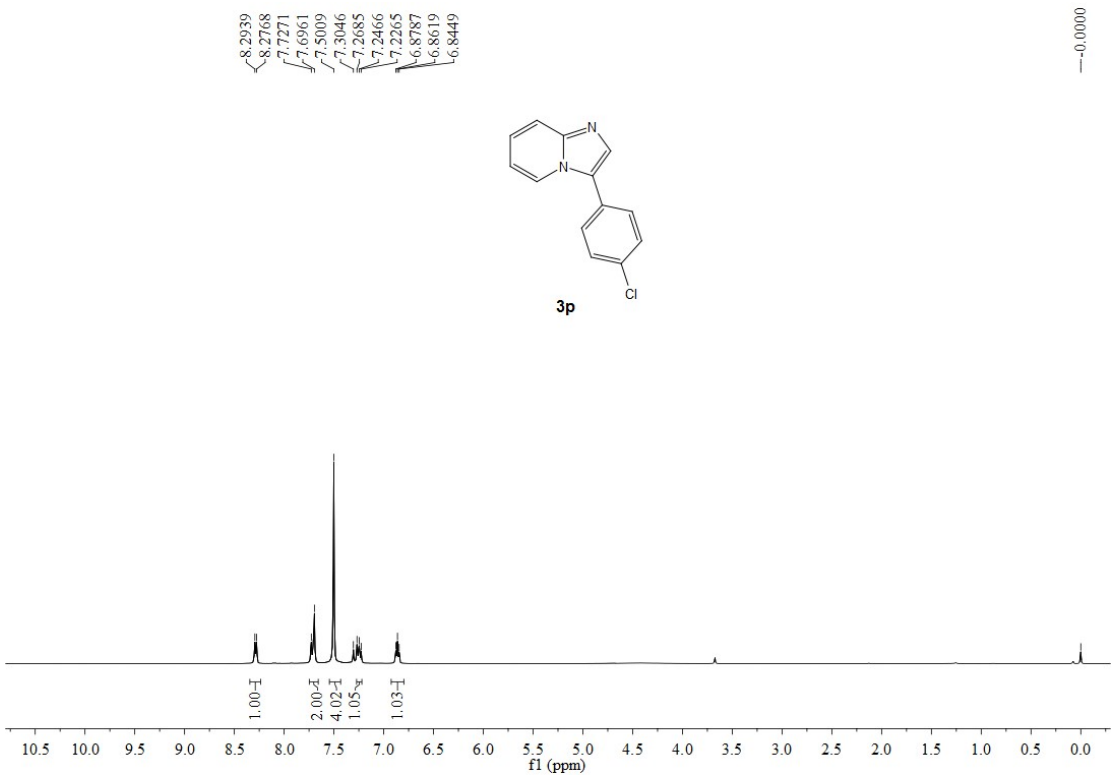
f1 (ppm)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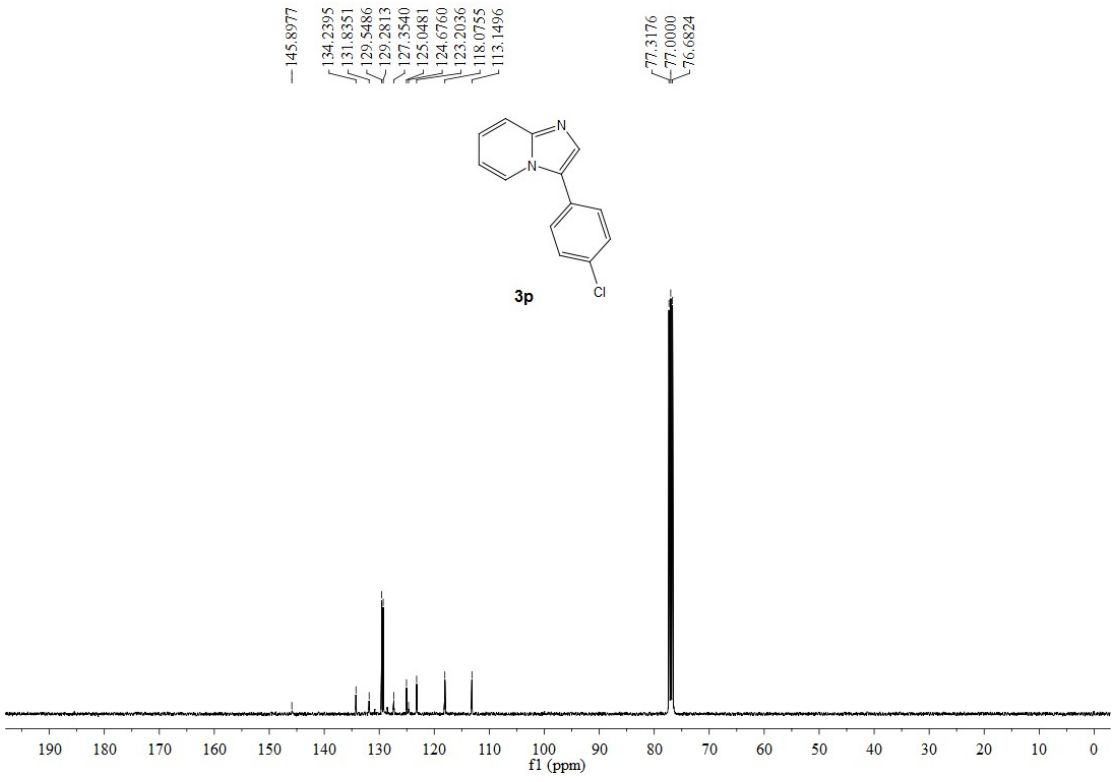
7.7271
7.6961
7.5009
7.3046
7.2685
7.2466
7.2265
6.8787
6.8619
6.8449
-0.0000
N
N
Cl
3p
1.00
2.00
4.02
1.05
1.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.8351
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129.2813
127.3540
125.0481
124.6760
123.2036
118.0755
113.1496
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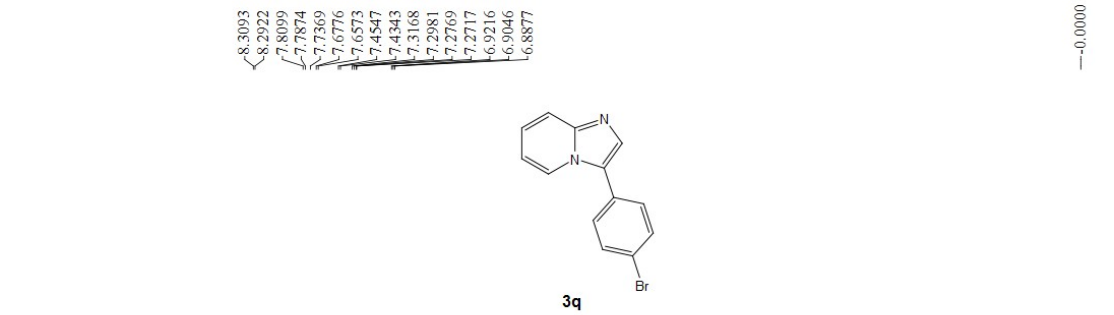
77.0000
76.6824
N
N
Cl
3p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.2922
7.8099
7.7874
7.7369
7.6776
7.6573
7.4547
7.4343
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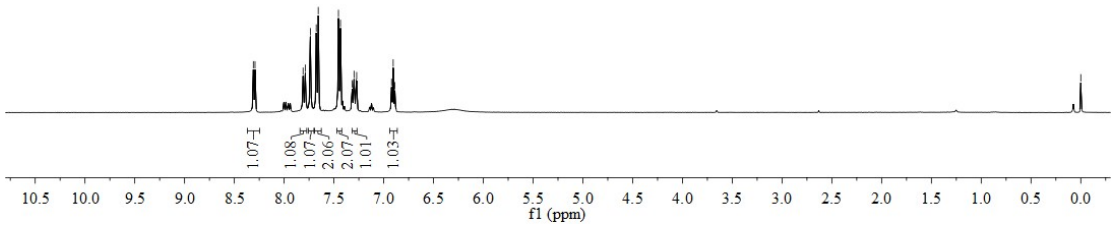
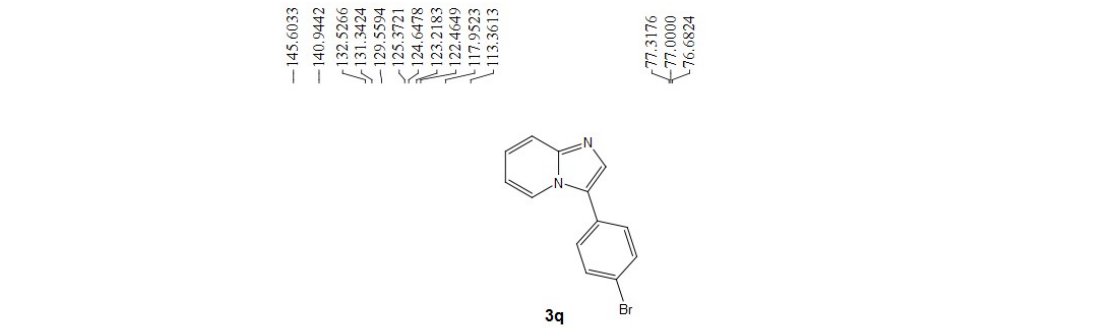
7.2769
7.2717
6.9216
6.9046
6.8877
0.0000
N
N
Br

3q


1.07
1.08
1.07
2.06
2.07
1.01
1.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.5266
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129.5594
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77.0000
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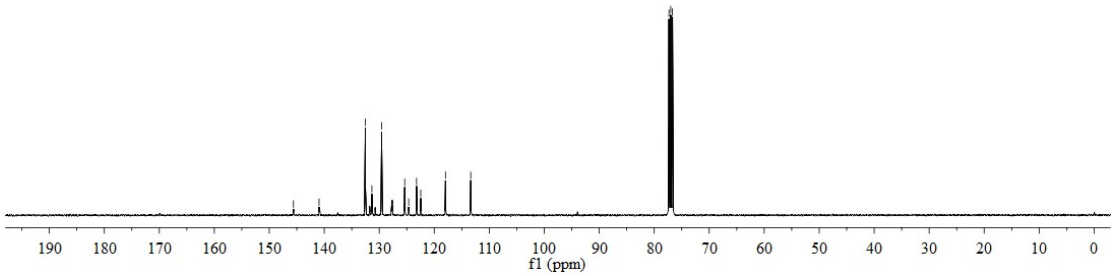
N
N
Br

3q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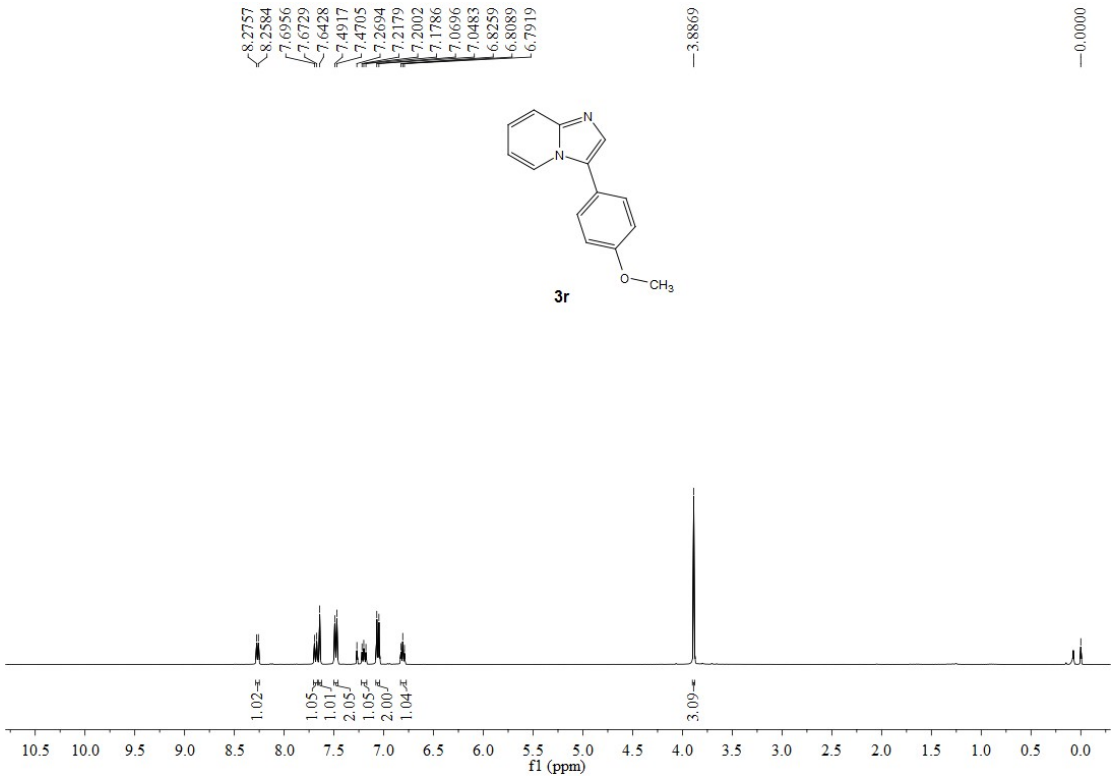
f1 (ppm)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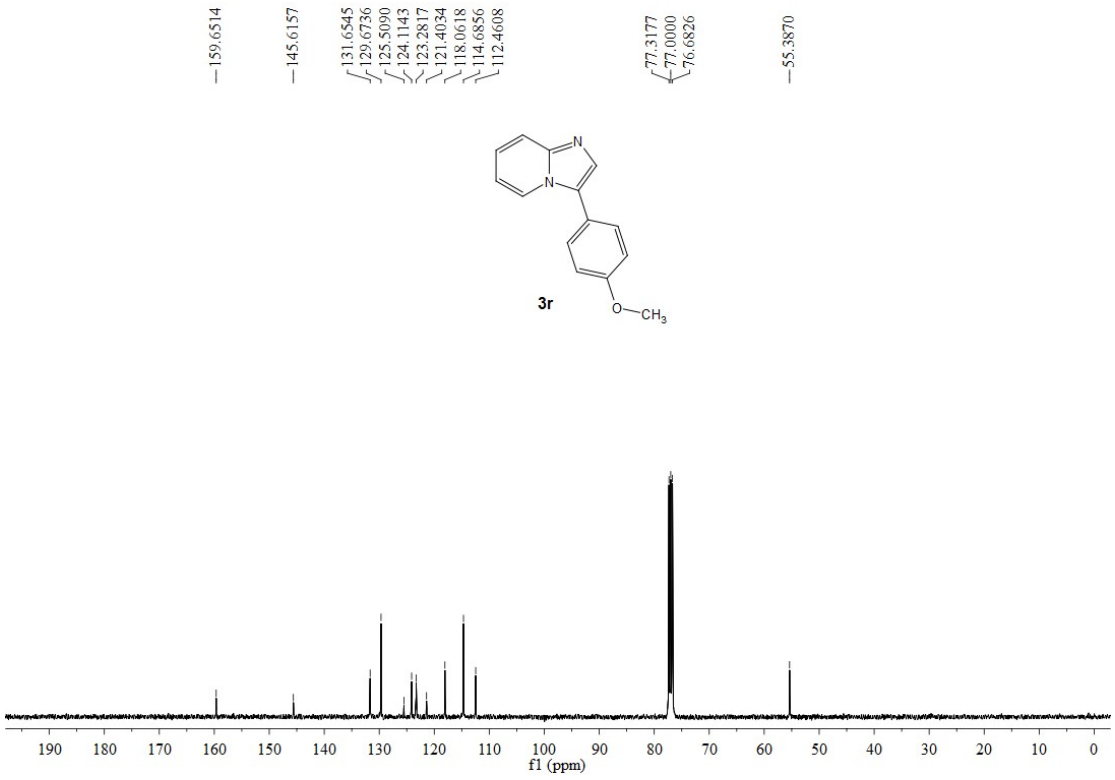
7.6956
7.6729
7.6428
7.4917
7.4705
7.2694
7.2179
7.2002
7.1786
7.0696
7.0483
6.8259
6.8089
6.7919
3.8869
0.0000
3r
1.02
1.05
1.01
2.05
1.05
2.00
1.04
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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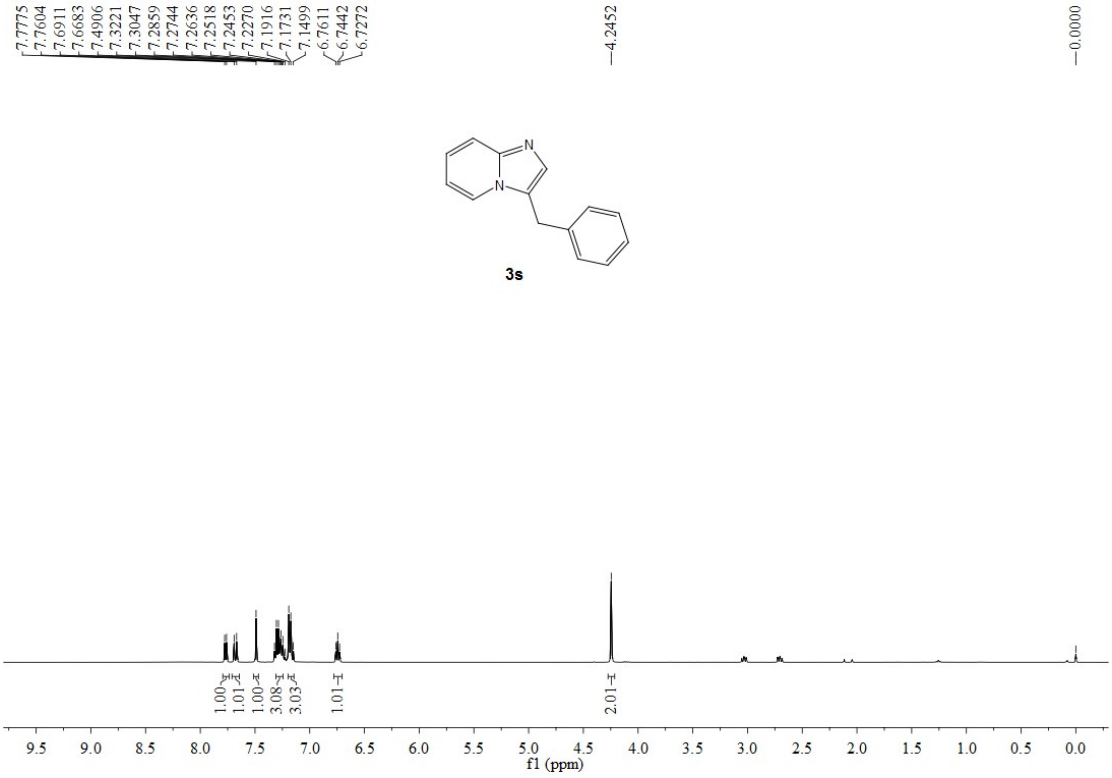
131.6545
129.6736
125.5090
124.1143
123.2817
121.4034
118.0618
114.6856
112.4608
77.3177
77.0000
76.6826
55.3870
3r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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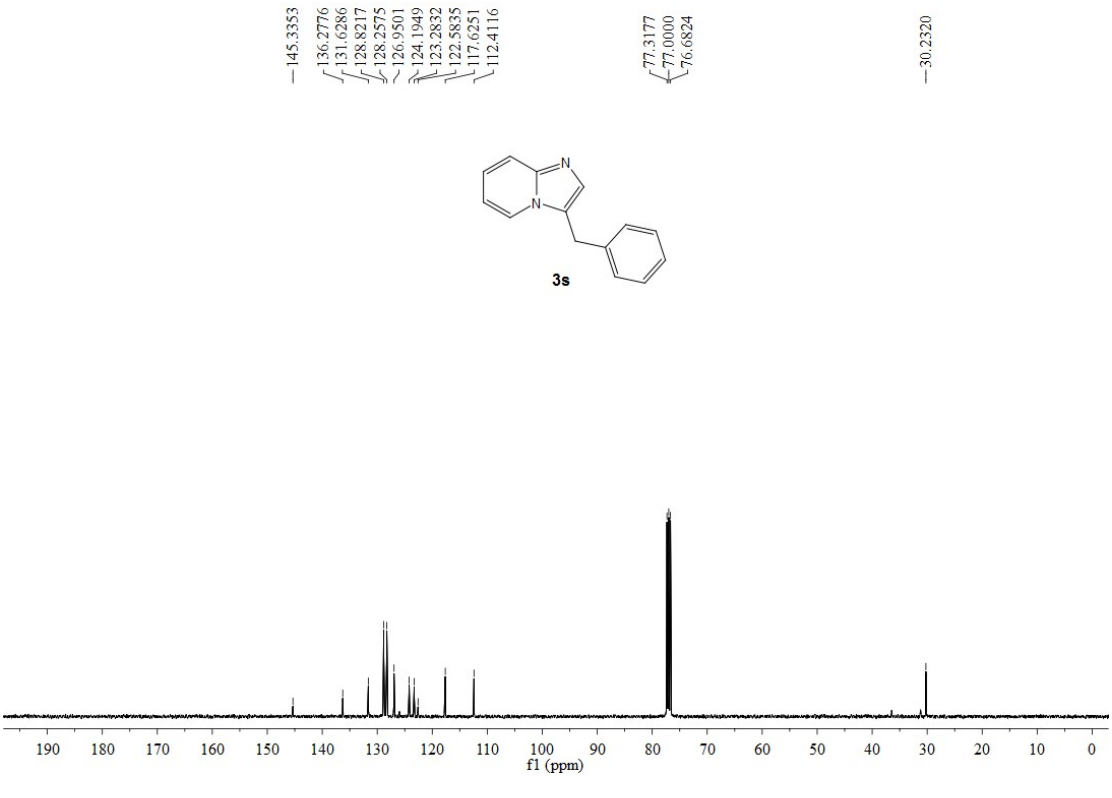
7.7604
7.6911
7.6683
7.4906
7.3221
7.3047
7.2859
7.2744
7.2636
7.2518
7.2453
7.2270
7.1916
7.1731
7.1499
6.7611
6.7442
6.7272
4.2452
0.0000
3s
1.00
1.01
1.00
3.08
3.03
1.01
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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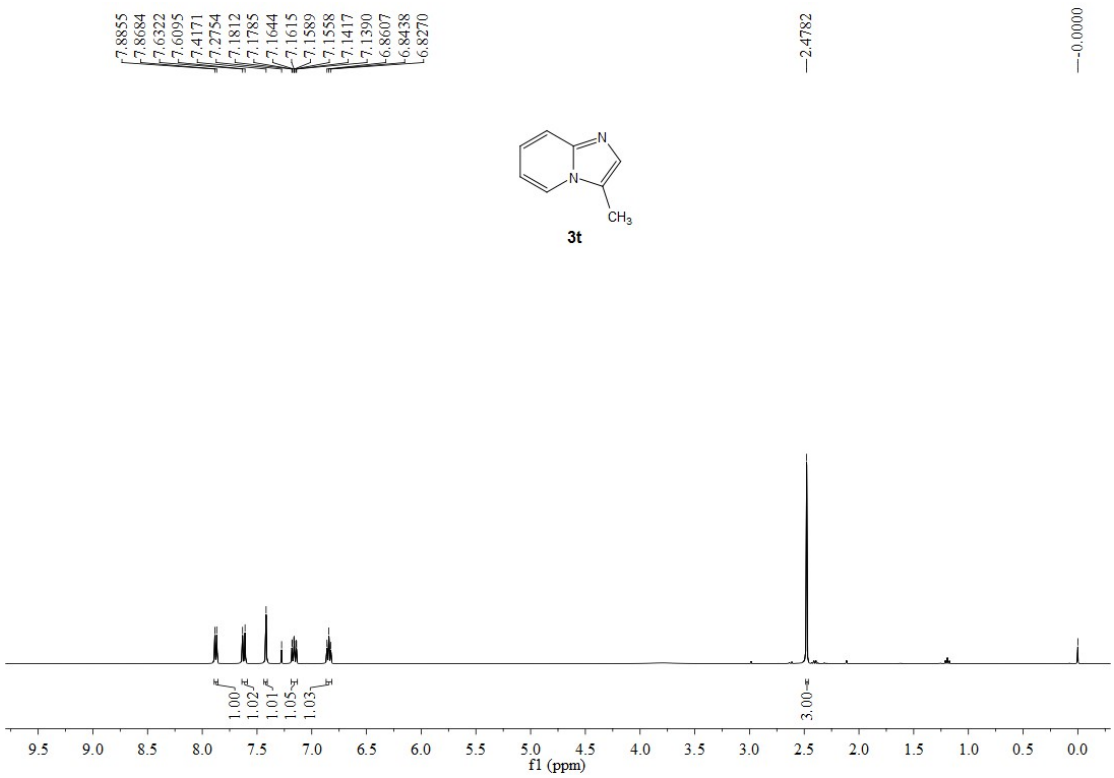
128.2575
126.9501
124.1949
123.2832
122.5835
117.6251
112.4116
77.3177
77.0000
76.6824
30.2320
3s
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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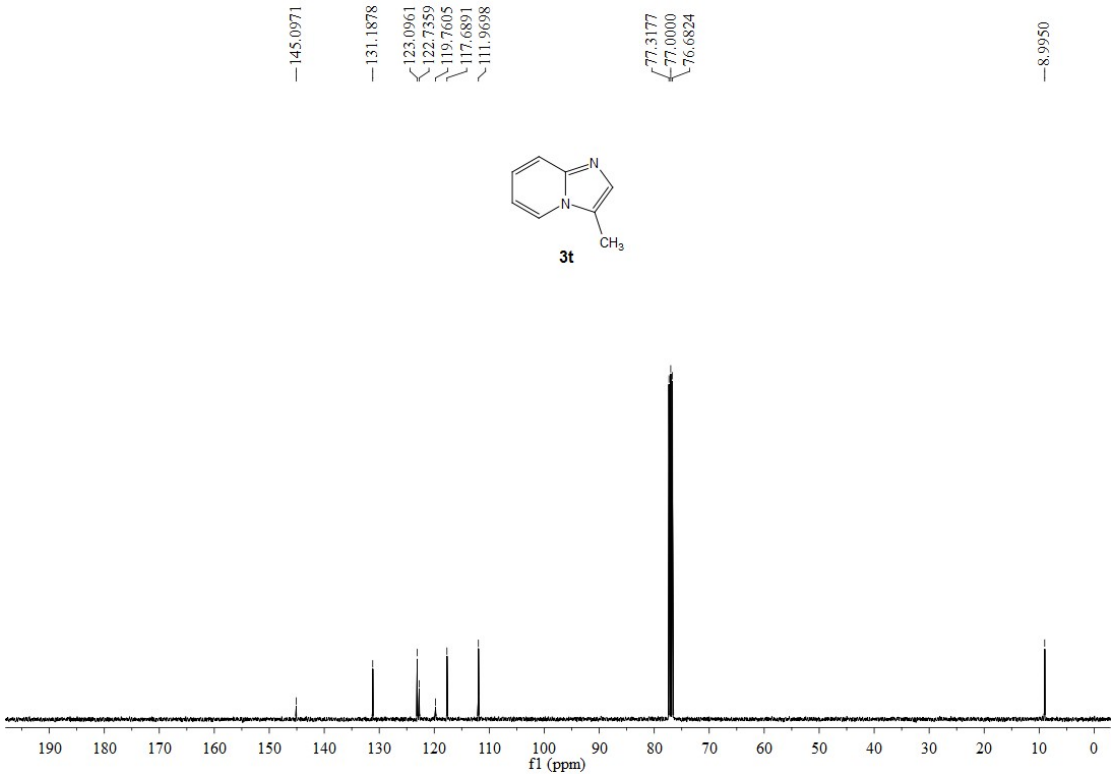
7.8684
7.6322
7.6095
7.4171
7.2754
7.1812
7.1785
7.1644
7.1615
7.1589
7.1558
7.1417
7.1390
6.8607
6.8438
6.8270
2.4782
-0.0000
N
N
CH3
3t
1.00
1.02
1.01
1.05
1.03
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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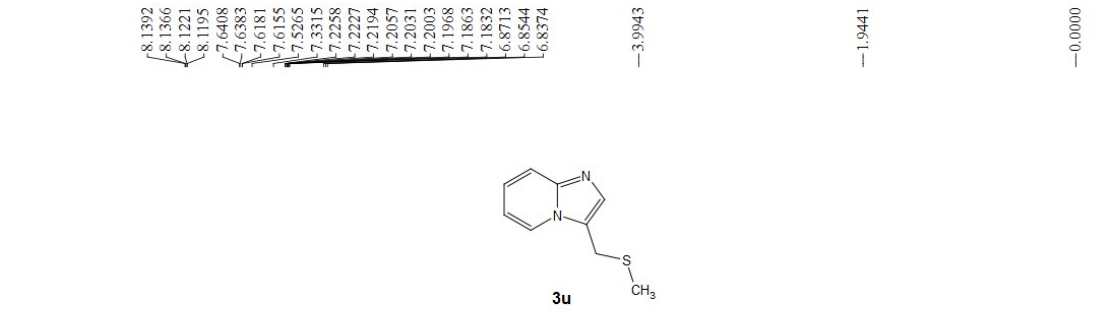
8.9950
N
N
CH3
3t
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.1366
8.1221
8.1195
7.6408
7.6383
7.6181
7.6155
7.5265
7.3315
7.2258
7.2227
7.2194
7.2057
7.2031
7.2003
7.1968
7.1863
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6.8544
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3.9943
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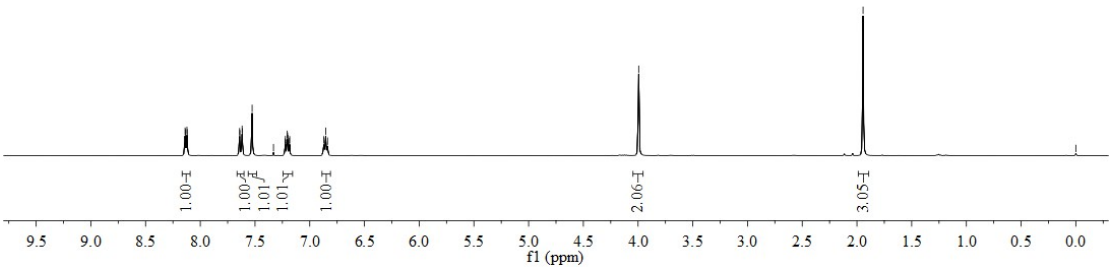
N
N
S
CH3

3u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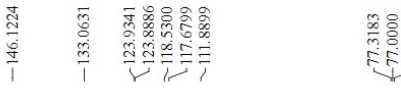
1.00
1.01
1.01
1.00
2.06
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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111.8899
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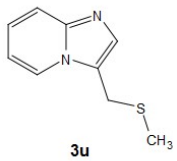
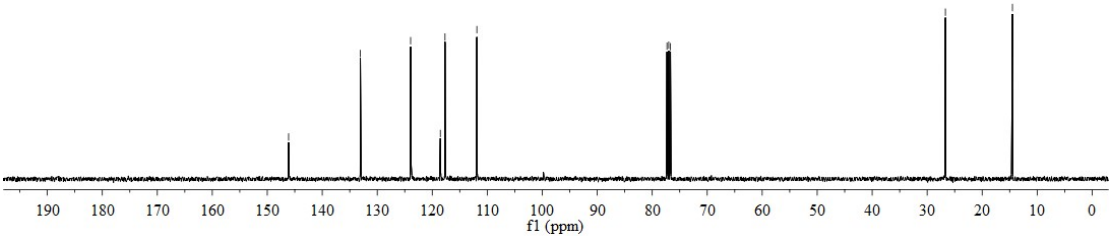
77.0000
76.6815
26.6860
14.4960


N
N
S
CH3

3u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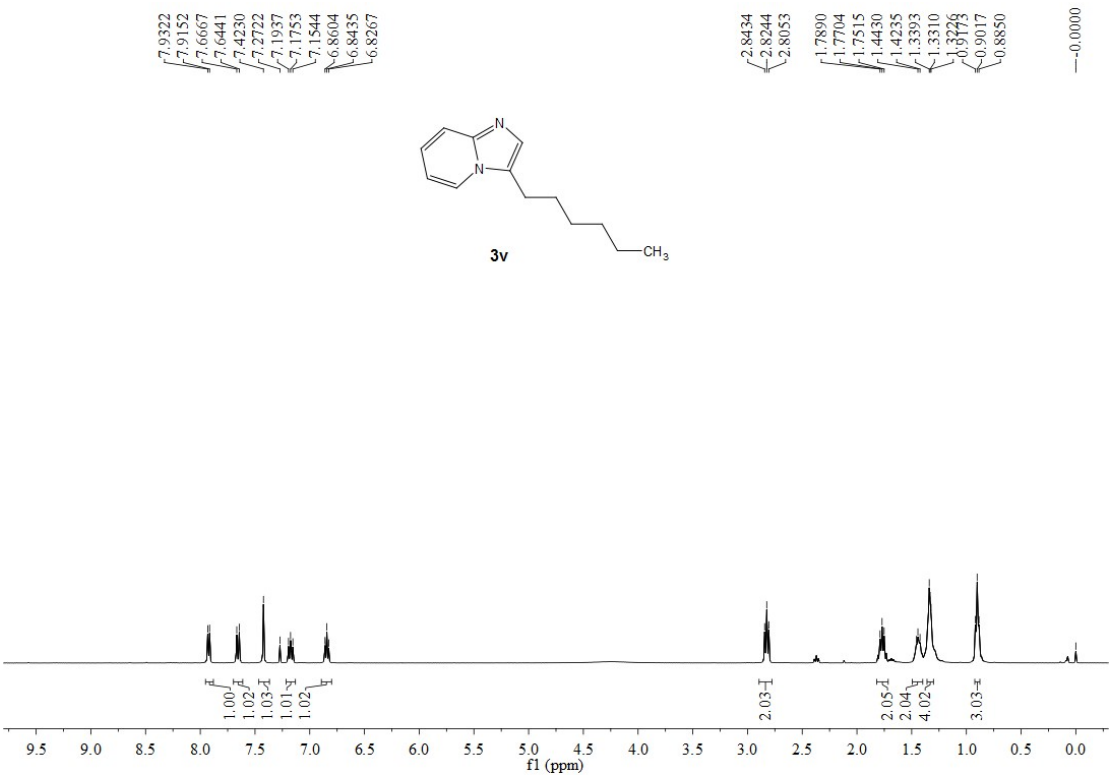
f1 (ppm)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7.1937
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7.1544
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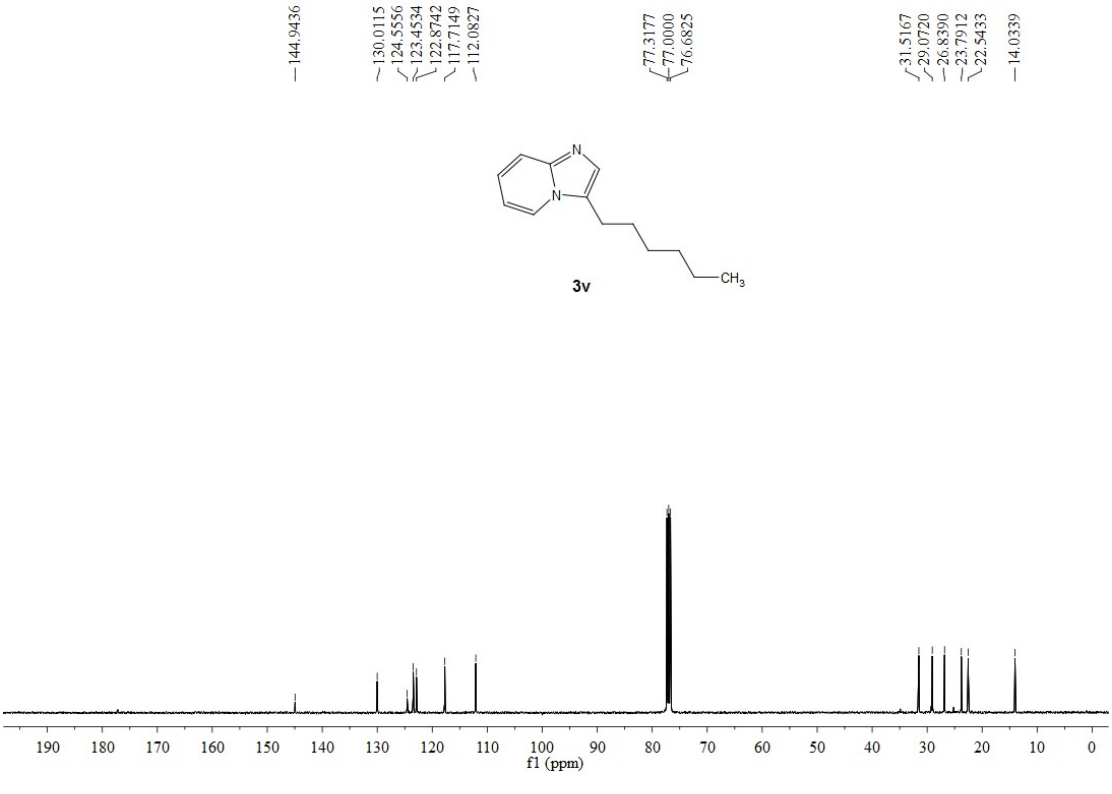
6.8267
2.8434
2.8244
2.8053
1.7890
1.7704
1.7515
1.4430
1.4235
1.3393
1.3310
0.9017
0.8850
-0.0000
N
N
CH3
3v
1.00
1.02
1.03
1.01
1.02
2.03
2.05
2.04
4.02
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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29.0720
26.8390
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14.0339
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N
CH3
3v
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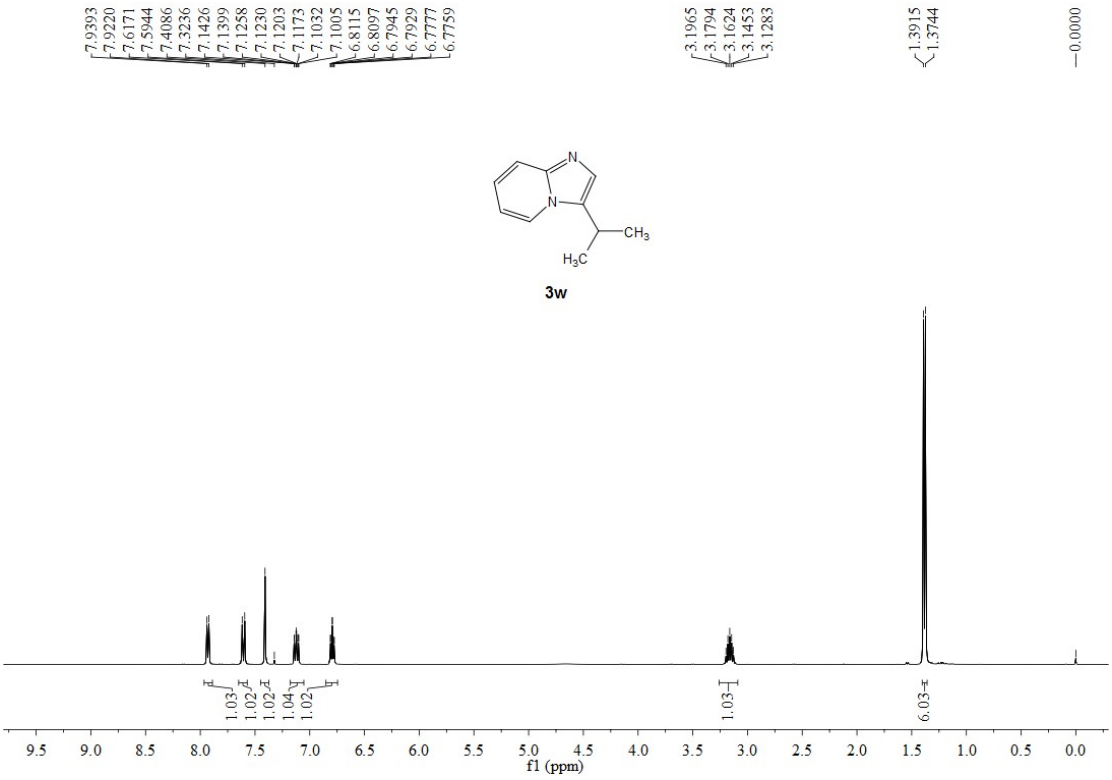
f1 (ppm)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7.1173
7.1032
7.1005
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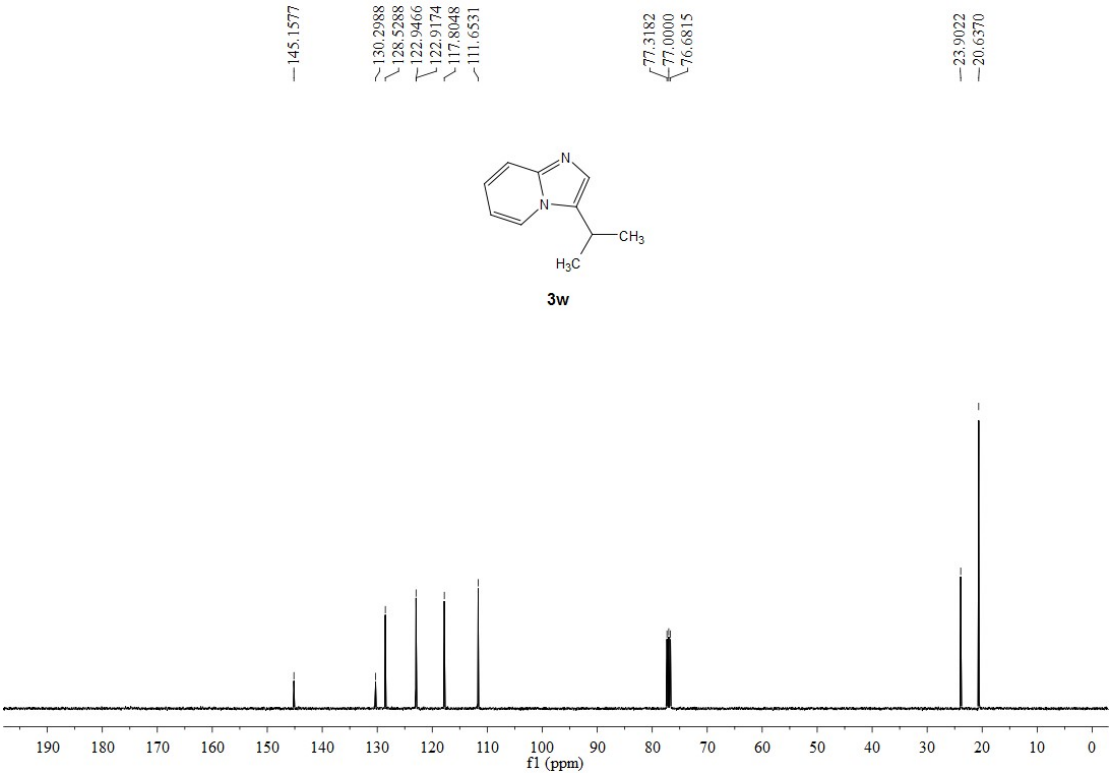
6.7945
6.7929
6.7777
6.7759
3.1965
3.1794
3.1624
3.1453
3.1283
1.3915
1.3744
0.0000
N
N
CH3
H3C
1.03
1.02
1.02
1.04
1.02
1.03
6.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3w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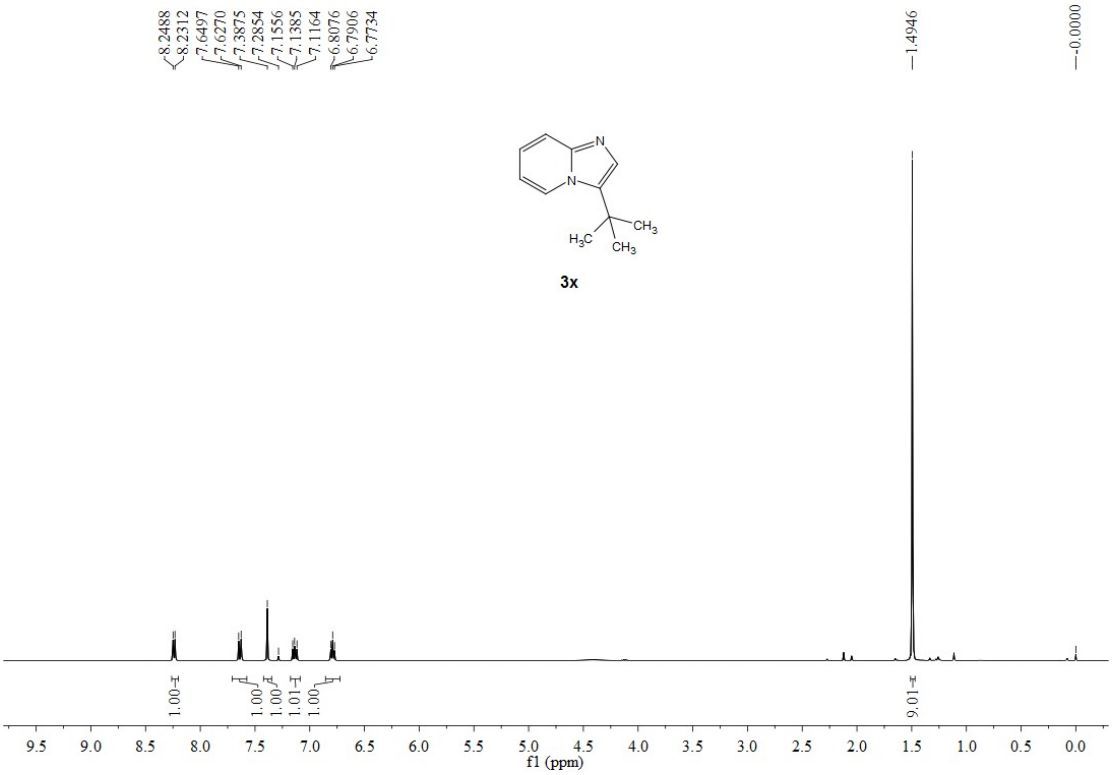
N
N
CH3
H3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3w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7.1164
6.8076
6.7906
6.7734
1.4946
0.0000
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N
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CH3
CH3
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1.00
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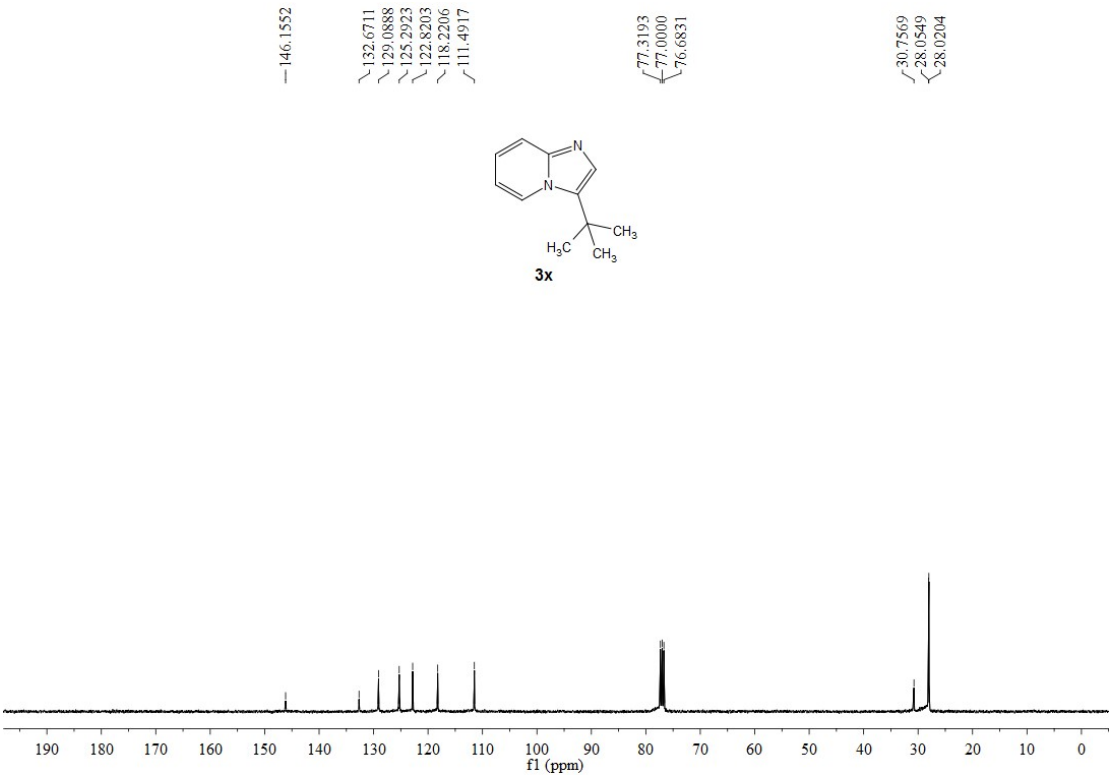
1.01
1.00
9.01
f1 (ppm)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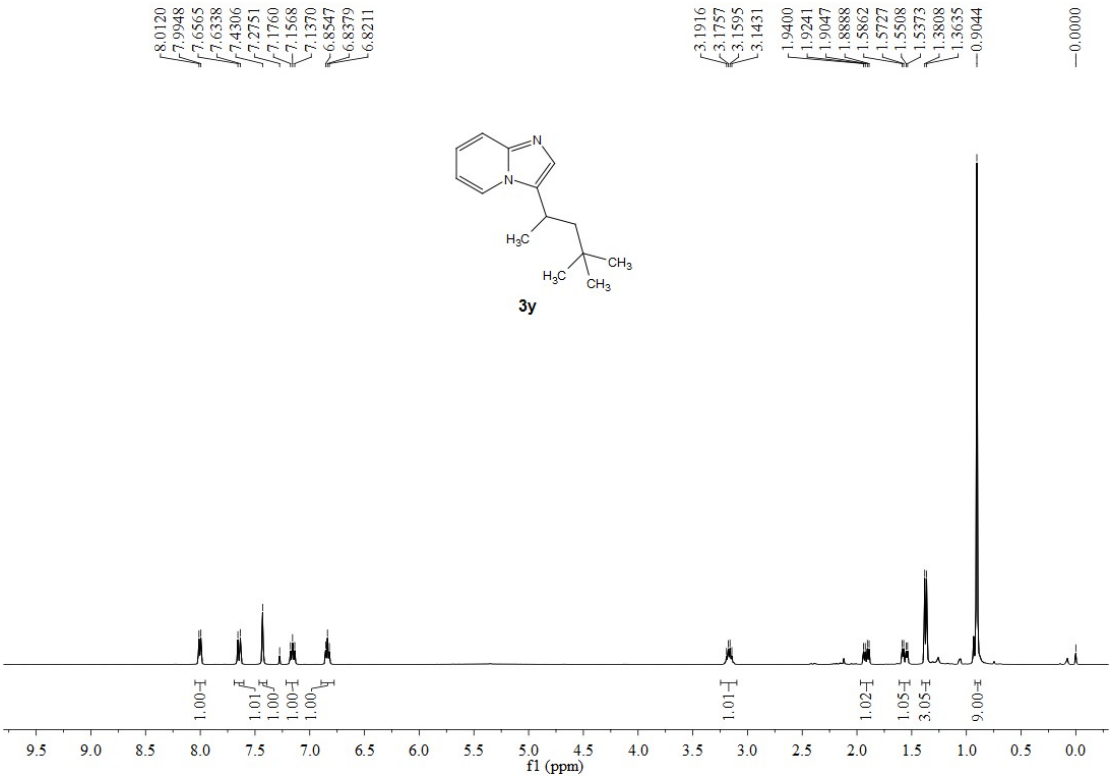
N
H3C
CH3
CH3
3x
f1 (ppm)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7.4306
7.2751
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7.1370
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6.8379
6.8211
3.1916
3.1757
3.1595
3.1431
1.9400
1.9241
1.9047
1.8888
1.5862
1.5727
1.5508
1.5373
1.3808
1.3635
0.9044
0.0000
3y
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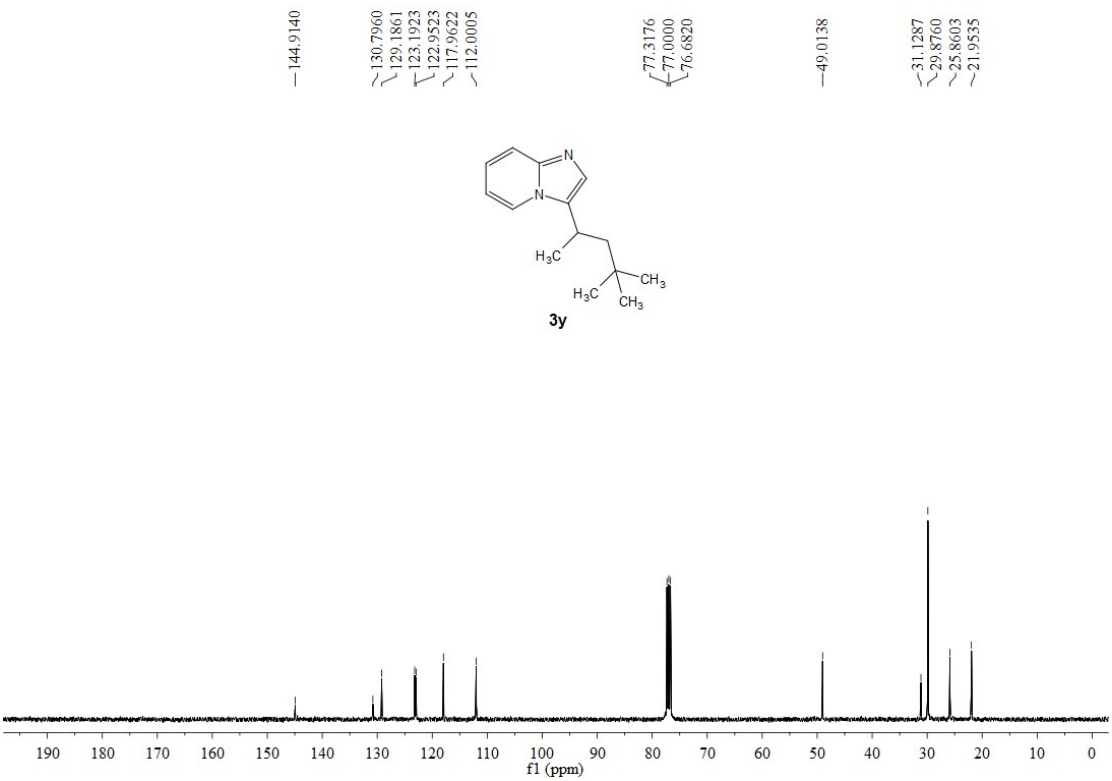
1.00
1.00
1.00
1.01
1.02
1.05
3.05
9.00
f1 (ppm)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29.8760
25.8603
21.9535
3y
f1 (ppm)