Supporting Information for

Copper-Catalyzed C–H Acyloxylation of 2-Phenylpyridine Using Oxygen as Oxidant

Feifan Wang, Zhiyang Lin, Weisheng Yu, Qingdong Hu, Chao Shu, and Wu Zhang*

Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, China.

Table of Contents

General Information

All starting materials and reagents were commercially available and used directly without further purification. Most of 2-phenylpyridines were synthesized by the reactions between the corresponding 2-bromopyridine or 2-Iodopyridine and phenylboronic acids according to the literature procedures.[1] All known products gave satisfactory analytical data by NMR spectra, corresponding to the reported literature values. In addition, unknown compounds were confirmed by HRMS. Melting points were determined using X-4 micro melting point apparatus and are uncorrected. NMR spectra were recorded at room temperature on a Bruker Avance-300 or Bruker Avance-500 at 300 MHz or 500 MHz with tetramethylsilane (TMS) as an internal standard. Chemical shifts are given in δ relative to TMS, the coupling constants *J* are given in Hz. High-resolution mass spectra (HRMS) were recorded on Agilent 6200 LC/MS TOF using APCI or ESI in positive mode.

General Procedures

General Procedure for Copper-Catalyzed C–H Acyloxylation

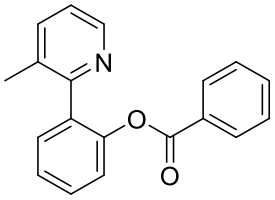
To a 10 mL reaction tube was added 3-methyl-2-phenylpyridine **1a** (0.2 mmol), acid (0.3 mmol), CuBr (2.9 mg, 10 mol %), and chlorobenzene (2 mL) under oxygen atmosphere. The mixture was stirred at 130 ℃ for 24 h. The reaction mixture was then cooled to room temperature, diluted with ethyl acetate and quenched with saturated sodium chloride. The aqueous phase was extracted with ethyl acetate (3×10 mL). The organic layer was dried over Na_2SO_4. After concentration, the resulting residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 12/1) to afford the product.

Copper-Catalyzed C–H Acyloxylation of 1a with benzoic acid (4 mmol scale)

To a 50 mL reaction tube was added 3-methyl-2-phenylpyridine **1a** (676.9 mg, 4 mmol), benzoic acid **2a** (732.8 mg, 6 mmol), CuBr (57.4 mg, 10 mol %), chlorobenzene (15 mL) under oxygen atmosphere. The mixture was stirred at 130 ℃ for 24 h. The reaction mixture was then cooled to room temperature, diluted with ethyl acetate and quenched with saturated sodium chloride. The aqueous phase was extracted with ethyl acetate (3 × 40 mL). The organic layer was dried over Na_2SO_4. After concentration, the resulting residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 12/1) to afford the desired product **3aa** (936.8 mg, 81%) as a white solid.

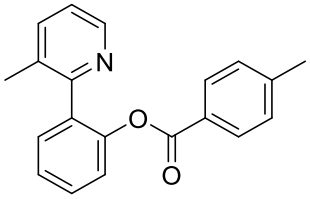
(1) Rao, X. F.; Liu, C.; Qiu, J. S.; Jin, Z. L. *Org. Biomol. Chem*. **2012**, *10*, 7875.

2-(3-Methylpyridin-2-yl)phenyl benzoate 3aa



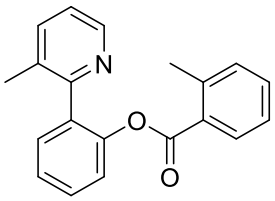
White solid. Mp = 93.8–94.6 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.44 (d, *J* = 3.3 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 2H), 7.54–7.29 (m, 8H), 7.11–7.07 (m, 1H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.6, 155.4, 148.3, 146.6, 137.9, 133.5, 133.4, 132.3, 130.5, 129.9, 129.3, 128.4, 128.1, 126.0, 122.8, 122.5, 19.1. HRMS (APCI): Calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$ 290.1181, found 290.1183.

2-(3-Methylpyridin-2-yl)phenyl-4-methylbenzoate 3ab



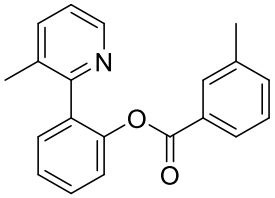
White solid. Mp = 100.6–101.5 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.44 (d, *J* = 3.6 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.48–7.33 (m, 5H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.12–7.08 (m, 1H), 2.37 (s, 3H), 2.21 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.6, 155.5, 148.4, 146.6, 144.1, 137.8, 133.6, 132.3, 130.4, 130.0, 129.3, 129.1, 126.6, 125.9, 122.8, 122.5, 21.7, 19.1. HRMS (APCI): Calcd for $C_{20}H_{18}NO_2$ $[M + H]^+$ 304.1337, found 304.1341.

2-(3-Methylpyridin-2-yl)phenyl-2-methylbenzoate 3ac



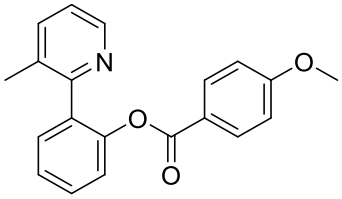
White solid. Mp = 91.7–93.0 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.46 (d, *J* = 3.9 Hz, 1H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.56–7.45 (m, 2H), 7.44–7.39 (m, 1H), 7.40–7.31 (m, 3H), 7.22–7.08 (m, 3H), 2.43 (s, 3H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.3, 155.7, 148.4, 146.6, 140.8, 137.9, 133.7, 132.3, 131.6, 130.7, 130.4, 129.3, 128.6, 125.9, 125.6, 123.0, 122.5, 21.4, 19.1. HRMS (APCI): Calcd for $C_{20}H_{18}NO_2$ $[M + H]^+$ 304.1337, found 304.1335.

2-(3-Methylpyridin-2-yl)phenyl-3-methylbenzoate 3ad



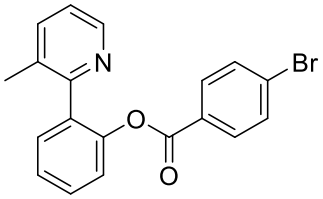
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.45 (d, *J* = 3.9 Hz, 1H), 7.72–7.64 (m, 2H), 7.54–7.47 (m, 2H), 7.47–7.43 (m, 1H), 7.43–7.39 (m, 1H), 7.39–7.31 (m, 2H), 7.29–7.22 (m, 1H), 7.13–7.09 (m, 1H), 2.34 (s, 3H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.7, 155.6, 148.4, 146.6, 138.2, 137.8, 134.1, 133.6, 132.3, 130.5, 130.4, 129.3, 128.2, 127.0, 125.9, 122.8, 122.4, 21.2, 19.1. HRMS (APCI): Calcd for $C_{20}H_{18}NO_2$ $[M + H]^+$ 304.1337, found 304.1342.

2-(3-Methylpyridin-2-yl)phenyl-4-methoxybenzoate 3ae



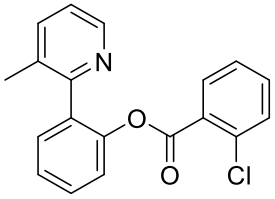
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.49–8.39 (m, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.54–7.31 (m, 5H), 7.17–7.04 (m, 1H), 6.85 (d, *J* = 8.4 Hz, 2H), 3.83 (s, 3H), 2.21 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.2, 163.7, 155.6, 148.4, 146.6, 137.8, 133.6, 132.2, 132.0, 130.4, 129.2, 125.8, 122.9, 122.4, 121.6, 113.6, 55.4, 19.1. HRMS (APCI): Calcd for $C_{20}H_{18}NO_3$ $[M + H]^+$ 320.1287, found 320.1284.

2-(3-Methylpyridin-2-yl)phenyl-4-bromobenzoate 3af



Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.43 (d, *J* = 3.6 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.61–7.46 (m, 4H), 7.45–7.33 (m, 3H), 7.16–7.07 (m, 1H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 162.9, 154.3, 147.1, 145.6, 136.9, 132.4, 131.2, 130.7, 130.4, 129.4, 128.4, 127.6, 127.2, 125.1, 121.7, 121.6, 18.1. HRMS (APCI): Calcd for $C_{19}H_{15}NO_2Br$ $[M + H]^+$ 368.0286, found 368.0285.

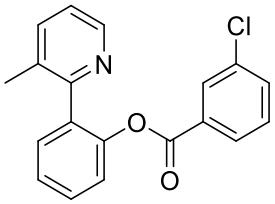
2-(3-Methylpyridin-2-yl)phenyl-2-chlorobenzoate 3ag



White solid. Mp = 81.7–82.6 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.47 (d, *J* = 3.9 Hz, 1H), 7.61–7.45 (m, 3H), 7.44–7.30 (m, 5H), 7.25–7.07 (m, 2H), 2.22 (s, 3H). **^{13}C**

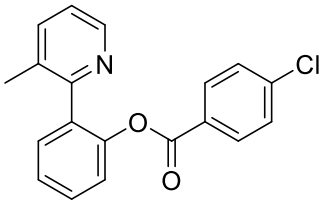
NMR (75 MHz, $CDCl_3$): δ 163.4, 155.5, 148.1, 146.6, 138.0, 134.0, 133.6, 132.8, 132.5, 131.4, 131.0, 130.5, 129.4, 129.2, 126.5, 126.2, 122.9, 122.7, 19.2. HRMS (APCI): Calcd for $C_{19}H_{15}NO_2Cl$ $[M + H]^+$ 324.0791, found 324.0798.

2-(3-Methylpyridin-2-yl)phenyl-3-chlorobenzoate 3ah



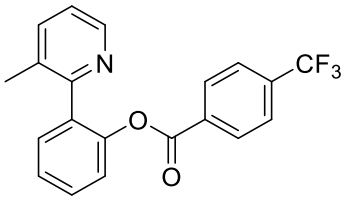
White solid. Mp = 84.6–86.4 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.48–8.39 (m, 1H), 7.83 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.57–7.43 (m, 4H), 7.43–7.36 (m, 2H), 7.35–7.25 (m, 1H), 7.15–7.08 (m, 1H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 163.4, 155.3, 148.1, 146.7, 137.9, 134.5, 133.4, 133.3, 132.2, 131.1, 130.5, 129.9, 129.7, 129.4, 128.0, 126.1, 122.6, 19.1. HRMS (APCI): Calcd for $C_{19}H_{15}NO_2Cl$ $[M + H]^+$ 324.0791, found 324.0799.

2-(3-Methylpyridin-2-yl)phenyl-4-chlorobenzoate 3ai



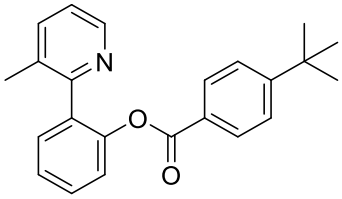
White solid. Mp = 76.1–77.3 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.40–8.29 (m, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.47–7.38 (m, 2H), 7.37–7.21 (m, 5H), 7.08–6.98 (m, 1H), 2.14 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 162.7, 154.3, 147.1, 145.6, 138.8, 136.9, 132.4, 131.2, 130.2, 129.4, 128.3, 127.7, 126.7, 125.1, 121.7, 121.5, 18.1. HRMS (APCI): Calcd for $C_{19}H_{15}NO_2Cl$ $[M + H]^+$ 324.0791, found 324.0792.

2-(3-Methylpyridin-2-yl)phenyl-4-(trifluoromethyl)benzoate 3aj



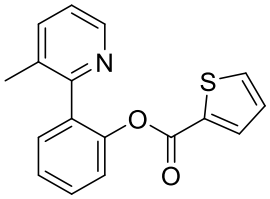
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.47–8.37 (m, 1H), 8.03–7.93 (m, 2H), 7.64 (d, *J* = 7.8 Hz, 2H), 7.55–7.45 (m, 2H), 7.44–7.33 (m, 3H), 7.15–7.06 (m, 1H), 2.23 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 163.4, 155.3, 148.1, 146.7, 138.0, 134.7 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 133.4, 132.6, 132.2, 130.5, 130.3, 129.4, 126.2, 125.4 (q, $^3J_{C\text{-}F}$ = 3.5 Hz), 123.5 (q, $^1J_{C\text{-}F}$ = 271.6 Hz), 122.7, 122.6, 19.1. HRMS (APCI): Calcd for $C_{20}H_{15}NO_2F_3$ $[M + H]^+$ 358.1055, found 358.1052.

2-(3-Methylpyridin-2-yl)phenyl-4-(tert-butyl)benzoate 3ak



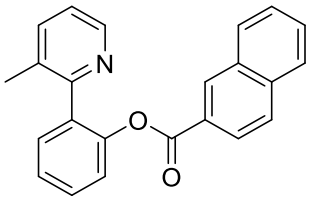
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.49–8.42 (m, 1H), 7.82 (d, *J* = 8.1 Hz, 2H), 7.54–7.42 (m, 3H), 7.42–7.34 (m, 4H), 7.15–7.07 (m, 1H), 2.22 (s, 3H), 1.31 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.5, 157.1, 155.6, 148.4, 146.7, 137.8, 133.6, 132.2, 130.4, 129.8, 129.3, 126.6, 125.8, 125.4, 122.8, 122.5, 35.1, 31.1, 19.1. HRMS (APCI): Calcd for $C_{23}H_{24}NO_2$ $[M + H]^+$ 346.1807, found 346.1803.

2-(3-Methylpyridin-2-yl)phenyl thiophene-2-carboxylate 3al



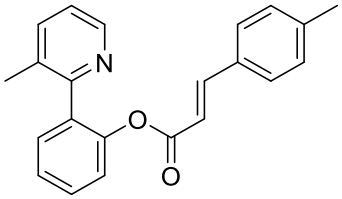
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.48–8.40 (m, 1H), 7.70 (dd, *J* = 3.6, 0.9 Hz, 1H), 7.55–7.48 (m, 2H), 7.48–7.31 (m, 4H), 7.15–7.07 (m, 1H), 7.06–6.98 (m, 1H), 2.23 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 159.8, 155.3, 147.9, 146.7, 137.8, 134.4, 133.5, 133.3, 132.5, 132.3, 130.5, 129.3, 127.8, 126.1, 122.7, 122.5, 19.1. HRMS (APCI): Calcd for $C_{17}H_{14}NO_2S$ $[M + H]^+$ 296.0745, found 296.0744.

2-(3-Methylpyridin-2-yl)phenyl-2-naphthoate 3am



Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.50–8.39 (m, 2H), 7.93–7.76 (m, 4H), 7.62–7.42 (m, 6H), 7.42–7.34 (m, 1H), 7.14–7.03 (m, 1H), 2.25 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.7, 155.5, 148.5, 146.7, 137.9, 135.7, 133.6, 132.4, 132.3, 131.7, 130.5, 129.4, 129.4, 128.5, 128.2, 127.7, 126.7, 126.6, 126.0, 125.3, 122.8, 122.5, 19.2. HRMS (APCI): Calcd for $C_{23}H_{18}NO_2$ $[M + H]^+$ 340.1337, found 340.1331.

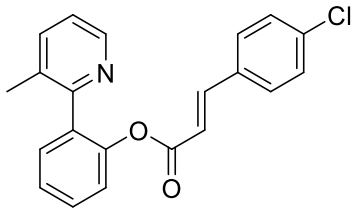
2-(3-Methylpyridin-2-yl)phenyl-(E)-3-(p-tolyl)acrylate 3an



White solid. Mp = 64.2–65.6 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.55–8.43 (m, 1H), 7.64–7.50 (m, 2H), 7.50–7.40 (m, 2H), 7.40–7.28 (m, 4H), 7.23–7.06 (m, 3H), 6.31 (d,

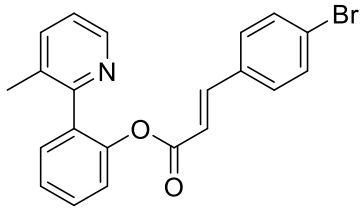
J = 15.9 Hz, 1H), 2.36 (s, 3H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.9, 155.5, 148.2, 146.6, 146.3, 141.2, 137.9, 133.5, 132.3, 131.4, 130.5, 129.7, 129.3, 128.2, 125.8, 122.8, 122.5, 115.8, 21.5, 19.1. HRMS (APCI): Calcd for $C_{22}H_{20}NO_2$ $[M + H]^+$ 330.1494, found 330.1492.

2-(3-Methylpyridin-2-yl)phenyl-(E)-3-(4-chlorophenyl)acrylate 3ao



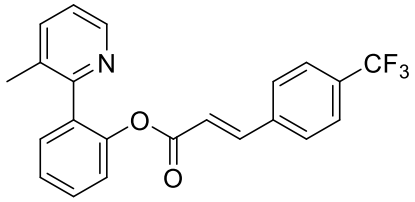
White solid. Mp = 128.3–129.6 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.86–8.38 (m, 1H), 7.64–7.50 (m, 2H), 7.48–7.27 (m, 8H), 7.22–7.09 (m, 1H), 6.33 (d, *J* = 15.9 Hz, 1H), 2.23 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.5, 155.5, 148.1, 146.7, 144.8, 137.9, 136.5, 133.5, 132.6, 132.3, 130.5, 129.4, 129.3, 129.2, 125.9, 122.7, 122.5, 117.5, 19.1. HRMS (APCI): Calcd for $C_{21}H_{17}NO_2Cl$ $[M + H]^+$ 350.0948, found 350.0950.

2-(3-Methylpyridin-2-yl)phenyl-(E)-3-(4-bromophenyl)acrylate 3ap



White solid. Mp = 113.2–114.5 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.54–8.41 (m, 1H), 7.59–7.52 (m, 1H), 7.52–7.42 (m, 3H), 7.42–7.21 (m, 6H), 7.20–7.08 (m, 1H), 6.34 (d, *J* = 15.9 Hz, 1H), 2.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.5, 155.5, 148.1, 146.6, 144.9, 138.0, 133.4, 133.0, 132.3, 132.2, 130.5, 129.6, 129.3, 125.9, 124.9, 122.7, 122.6, 117.6, 19.1. HRMS (APCI): Calcd for $C_{21}H_{17}NO_2Br$ $[M + H]^+$ 394.0443, found 394.0447.

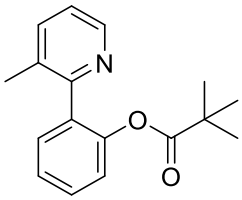
2-(3-Methylpyridin-2-yl)phenyl-(E)-3-(4-(trifluoromethyl)phenyl)acrylate 3aq



White solid. Mp = 81.6–82.3 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.49 (d, *J* = 4.0 Hz, 1H), 7.67–7.60 (m, 3H), 7.59–7.50 (m, 3H), 7.50–7.44 (m, 1H), 7.44–7.39 (m, 1H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.35–7.29 (m, 1H), 7.15 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.43 (d, *J* = 16.0 Hz, 1H), 2.24 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 164.2, 155.5, 148.0,

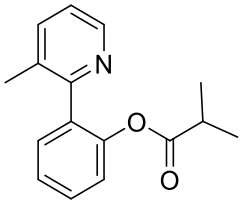
146.7, 144.3, 138.0, 137.4, 133.5, 132.3, 132.0 (q, $^{2}J_{C\text{-}F}$ = 32.4 Hz), 130.5, 129.3, 128.3, 126.0, 125.9 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 123.8 (q, $^{1}J_{C\text{-}F}$ = 270.6 Hz), 122.7, 122.6, 119.5, 19.1. HRMS (ESI): Calcd for $C_{22}H_{17}NO_2F_3$ $[M + H]^+$ 384.1211, found 384.1208.

2-(3-Methylpyridin-2-yl)phenyl pivalate 3ar



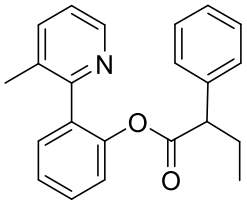
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.54–8.42 (m, 1H), 7.63–7.49 (m, 1H), 7.46–7.38 (m, 1H), 7.37–7.28 (m, 2H), 7.22–7.11 (m, 2H), 2.18 (s, 3H), 1.00 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 176.3, 155.7, 148.3, 146.5, 137.7, 133.7, 132.5, 130.0, 129.2, 125.7, 122.8, 122.5, 38.8, 26.8, 19.0. HRMS (APCI): Calcd for $C_{17}H_{20}NO_2$ $[M + H]^+$ 270.1494, found 270.1491.

2-(3-Methylpyridin-2-yl)phenyl isobutyrate 3as



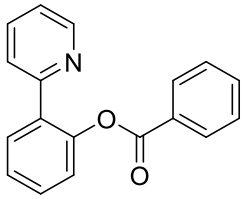
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.54–8.44 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.47–7.38 (m, 1H), 7.38–7.29 (m, 2H), 7.23–7.14 (m, 2H), 2.61–2.43 (m, 1H), 2.19 (s, 3H), 0.94 (d, *J* = 6.9 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 175.0, 155.6, 148.1, 146.5, 137.8, 133.7, 132.5, 130.2, 129.2, 125.8, 122.8, 122.5, 33.9, 19.0, 18.5. HRMS (APCI): Calcd for $C_{16}H_{18}NO_2$ $[M + H]^+$ 256.1337, found 256.1334.

2-(3-Methylpyridin-2-yl)phenyl-2-phenylbutanoate 3at



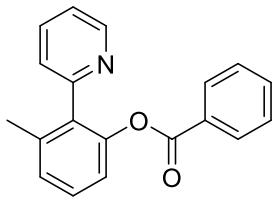
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.39–8.28 (m, 1H), 7.45–7.33 (m, 3H), 7.32–7.26 (m, 2H), 7.24–7.17 (m, 3H), 7.14–7.01 (m, 3H), 3.42 (t, *J* = 7.8 Hz, 1H), 2.03 (s, 3H), 1.98–1.83 (m, 1H), 1.73–1.55 (m, 1H), 0.72 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 171.8, 155.1, 148.0, 146.4, 138.2, 137.7, 133.6, 132.2, 130.3, 129.2, 128.6, 127.8, 127.1, 125.9, 122.6, 122.5, 53.2, 26.4, 18.9, 11.9. HRMS (APCI): Calcd for $C_{22}H_{22}NO_2$ $[M + H]^+$ 332.1650, found 332.1648.

2-(Pyridin-2-yl)phenyl benzoate 3ba



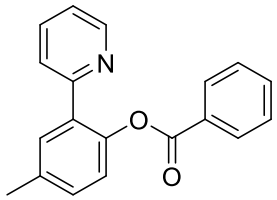
White solid. Mp = 91.4–92.6 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.59 (d, *J* = 4.5 Hz, 1H), 8.18–7.99 (m, 2H), 7.78 (d, *J* = 6.0 Hz, 1H), 7.70–7.53 (m, 3H), 7.53–7.36 (m, 4H), 7.34–7.27 (m, 1H), 7.20–7.09 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.2, 155.5, 149.6, 148.3, 136.2, 133.5, 133.3, 130.9, 130.2, 129.8, 129.5, 128.5, 126.4, 123.7, 123.4, 122.2. HRMS (APCI): Calcd for $C_{18}H_{14}NO_2$ $[M + H]^+$ 276.1024, found 276.1018.

3-Methyl-2-(pyridin-2-yl)phenyl benzoate 3ca



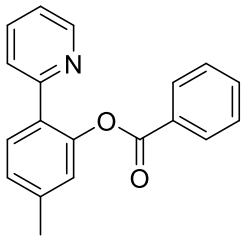
Yellow liquid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.66–8.62 (m, 1H), 7.88–7.80 (m, 2H), 7.67–7.57 (m, 1H), 7.55–7.47 (m, 1H), 7.40–7.32 (m, 3H), 7.31–7.27 (m, 1H), 7.24–7.20 (m, 1H), 7.18–7.12 (m, 2H), 2.19 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 164.1, 154.7, 148.4, 147.6, 137.2, 135.1, 132.6, 132.3, 128.9, 128.3, 127.9, 127.3, 126.9, 123.8, 121.1, 119.1, 18.9. HRMS (APCI): Calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$ 290.1181, found 290.1175.

4-Methyl-2-(pyridin-2-yl)phenyl benzoate 3da



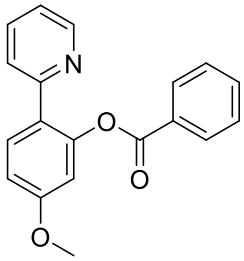
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.70–8.54 (m, 1H), 8.08 (d, *J* = 7.5 Hz, 2H), 7.71–7.51 (m, 4H), 7.49–7.38 (m, 2H), 7.32–7.22 (m, 1H), 7.21–7.07 (m, 2H), 2.43 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.3, 155.6, 149.6, 146.0, 136.1, 133.4, 132.8, 131.3, 130.4, 130.1, 129.5, 128.5, 123.7, 123.0, 122.1, 20.9. HRMS (APCI): Calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$ 290.1181, found 290.1188.

5-Methyl-2-(pyridin-2-yl)phenyl benzoate 3ea



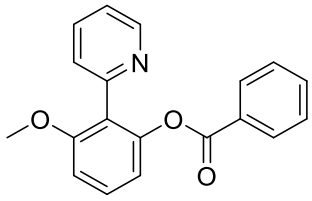
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.64–8.52 (m, 1H), 8.09 (d, *J* = 6.6 Hz, 2H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.65–7.51 (m, 3H), 7.50–7.40 (m, 2H), 7.30–7.17 (m, 1H), 7.17–7.07 (m, 2H), 2.43 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.2, 154.5, 148.4, 147.1, 139.2, 135.1, 132.4, 129.6, 129.3, 129.1, 128.5, 127.4, 126.2, 122.7, 122.5, 120.9, 20.1. HRMS (APCI): Calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$ 290.1181, found 290.1184.

5-Methoxy-2-(pyridin-2-yl)phenyl benzoate 3fa



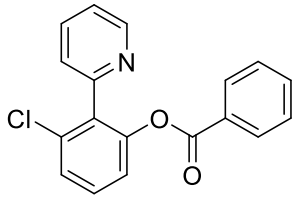
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.62–8.52 (m, 1H), 8.10 (d, *J* = 6.6 Hz, 2H), 7.742 (d, *J* = 8.4 Hz, 1H), 7.66–7.52 (m, 3H), 7.52–7.41 (m, 2H), 7.17–7.07 (m, 1H), 7.01–6.91 (m, 1H), 6.85 (s, 1H), 3.87 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.1, 160.7, 155.3, 149.5, 149.2, 136.2, 133.5, 131.6, 130.2, 129.4, 128.5, 128.2, 123.4, 121.7, 112.6, 108.7, 55.6. HRMS (APCI): Calcd for $C_{19}H_{16}NO_3$ $[M + H]^+$ 306.1130, found 306.1125.

3-Methoxy-2-(pyridin-2-yl)phenyl benzoate 3ga



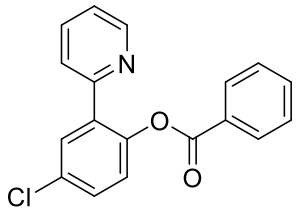
White solid. Mp = 82.6–84.2 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.66–8.53 (m, 1H), 7.89 (d, *J* = 7.5 Hz, 2H), 7.71–7.58 (m, 1H), 7.58–7.48 (m, 1H), 7.47–7.31 (m, 4H), 7.19–7.09 (m, 1H), 8.96 (d, *J* = 2.7 Hz, 1H), 6.94 (d, *J* = 3.3 Hz, 1H), 3.80 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.0, 158.0, 153.2, 149.6, 149.2, 135.7, 133.3, 130.0, 129.6, 129.3, 128.3, 125.8, 123.5, 122.0, 115.4, 108.9, 56.1. HRMS (APCI): Calcd for $C_{19}H_{16}NO_3$ $[M + H]^+$ 306.1130, found 306.1122.

3-Chloro-2-(pyridin-2-yl)phenyl benzoate 3ha



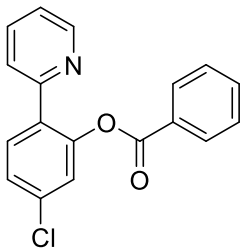
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.67–8.56 (m, 1H), 7.94–7.78 (m, 2H), 7.73–7.61 (m, 1H), 7.58–7.48 (m, 1H), 7.47–7.42 (m, 1H), 7.42–7.31 (m, 4H), 7.30–7.23 (m, 1H), 7.23–7.13 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.7, 153.6, 149.7, 149.4, 136.1, 134.0, 133.6, 133.3, 130.0, 129.7, 128.8, 128.4, 127.4, 125.4, 122.7, 121.7. HRMS (APCI): Calcd for $C_{18}H_{13}NO_2Cl$ $[M + H]^+$ 310.0634, found 310.0635.

4-Chloro-2-(pyridin-2-yl)phenyl benzoate 3ia



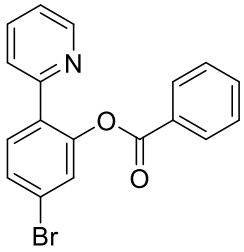
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.71–8.56 (m, 1H), 8.15–8.01 (m, 2H), 7.86–7.77 (m, 1H), 7.70–7.52 (m, 3H), 7.52–7.39 (m, 3H), 7.32–7.23 (m, 1H), 7.23–7.15 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 163.9, 153.1, 148.7, 145.7, 135.4, 133.6, 132.7, 130.8, 129.8, 129.2, 128.6, 128.0, 127.5, 123.7, 122.7, 121.6. HRMS (APCI): Calcd for $C_{18}H_{13}NO_2Cl$ $[M + H]^+$ 310.0634, found 310.0631.

5-Chloro-2-(pyridin-2-yl)phenyl benzoate 3ja



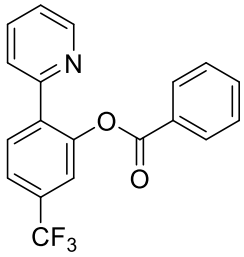
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.65–8.52 (m, 1H), 8.07 (d, *J* = 7.5 Hz, 2H), 7.80–7.69 (m, 1H), 7.67–7.57 (m, 2H), 7.57–7.30 (m, 5H), 7.22–7.11 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.8, 154.5, 149.7, 148.7, 136.3, 134.9, 133.7, 131.9, 131.8, 130.2, 129.2, 128.6, 126.7, 123.8, 123.6, 122.4. HRMS (APCI): Calcd for $C_{18}H_{13}NO_2Cl$ $[M + H]^+$ 310.0634, found 310.0640.

5-Bromo-2-(pyridin-2-yl)phenyl benzoate 3ka



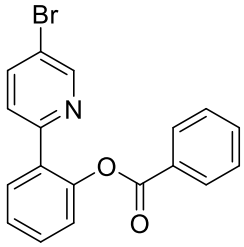
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.71–8.48 (m, 1H), 8.06 (d, *J* = 6.6 Hz, 2H), 7.74–7.58 (m, 3H), 7.58–7.38 (m, 5H), 7.24–7.11 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ 163.8, 153.5, 148.7, 147.6, 135.3, 132.7, 131.3, 131.0, 129.2, 128.6, 127.9, 127.6, 125.6, 122.6, 121.6, 121.4. HRMS (APCI): Calcd for $C_{18}H_{13}NO_2Br$ $[M + H]^+$ 354.0129, found 354.0133.

2-(Pyridin-2-yl)-5-(trifluoromethyl)phenyl benzoate 3la



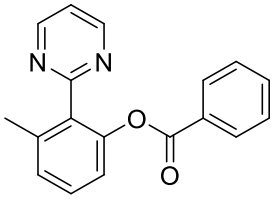
Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.71–8.56 (m, 1H), 8.07 (d, *J* = 7.2 Hz, 2H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.73–7.56 (m, 5H), 7.53–7.41 (m, 2H), 7.24–7.16 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 164.8, 154.2, 149.9, 148.4, 136.8, 136.4, 133.8, 132.0, 131.6, 131.1, 130.2, 128.9, 128.6, 123.7, 123.5 (q, $^{1}J_{C\text{-}F}$ = 271.1 Hz), 123.1 (q, $^{3}J_{C\text{-}F}$ = 3.4 Hz), 122.8, 120.9 (q, $^{2}J_{C\text{-}F}$ = 3.7 Hz). HRMS (APCI): Calcd for $C_{19}H_{13}NO_2F_3$ $[M + H]^+$ 344.0898, found 344.0900.

2-(5-Bromopyridin-2-yl)phenyl benzoate 3ma



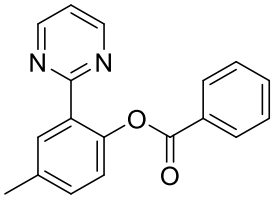
Yellow solid. Mp = 82.6–84.2 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.72–8.57 (m, 1H), 8.96 (d, *J* = 7.2 Hz, 2H), 7.86–7.68 (m, 2H), 7.67–7.56 (m, 1H), 7.55–7.23 (m, 5H), 7.33–7.23 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.1, 154.0, 150.7, 148.2, 138.8, 133.7, 132.1, 130.8, 130.2, 129.3, 128.6, 126.6, 124.8, 123.5, 119.6. HRMS (APCI): Calcd for $C_{18}H_{13}NO_2Br$ $[M + H]^+$ 354.0129, found 354.0121.

3-Methyl-2-(pyrimidin-2-yl)phenyl benzoate 3na



White solid. Mp = 83–84 ℃. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.82–8.67 (m, 2H), 7.95–7.84 (m, 2H), 7.60–7.48 (m, 1H), 7.45–7.32 (m, 3H), 7.26–7.18 (m, 2H), 7.18–7.11 (m, 1H), 2.28 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 163.9, 163.8, 155.9, 147.8, 137.1, 132.2, 131.0, 128.9, 128.4, 128.4, 127.8, 127.3, 127.1, 119.5, 118.0, 18.8. HRMS (APCI): Calcd for $C_{18}H_{15}N_2O_2$ $[M + H]^+$ 291.1133, found 291.1130.

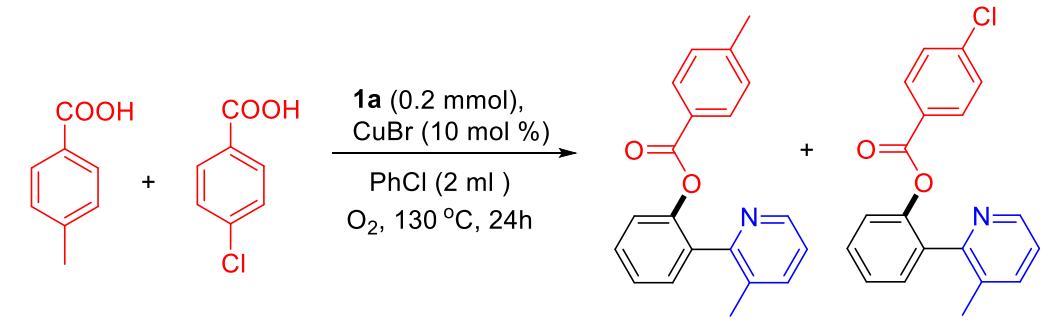
4-Methyl-2-(pyrimidin-2-yl)phenyl benzoate 3oa



Yellow liquid. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.15 (d, *J* = 7.5 Hz, 2H), 8.05 (s, 1H), 7.67–7.55 (m, 1H), 7.54–7.42 (m, 2H), 7.40–7.31 (m, 1H), 7.23–7.15 (m, 1H), 7.09 (t, *J* = 5.1 Hz, 1H), 2.46 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.0, 162.9, 155.9, 146.4, 135.0, 132.5, 132.0, 131.0, 130.8, 129.2, 129.1, 127.4, 127.3, 122.8, 117.9, 19.9. HRMS (APCI): Calcd for $C_{18}H_{15}N_2O_2$ $[M + H]^+$ 291.1133, found 291.1128.

Intermolecular Competition Experiments

(a) *intermolecular competition experiments between acids* ***2***

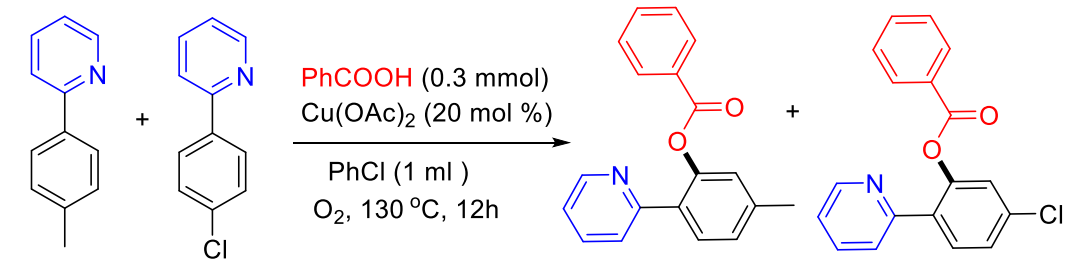


2b (0.3 mmol) **2i** (0.3 mmol) **3ab**, 36% **3ai**, 41%

Scheme S1

To a 10 mL reaction tube was added 3-methyl-2-phenylpyridine **1a** (0.2 mmol), *p*-toluylic acid **2b** (0.3 mmol), *p*-chlorobenzoic acid **2i** (0.3 mmol), CuBr (2.9 mg, 10 mol %), and chlorobenzene (2 mL) under oxygen atmosphere. The mixture was stirred at 130 ℃ for 24 h. The reaction mixture was then cooled to room temperature, diluted with ethyl acetate and quenched with saturated sodium chloride. The aqueous phase was extracted with ethyl acetate (3 × 10 mL). The organic layer was dried over Na_2SO_4. After concentration, the resulting residue was purified by flash chromatography to afford the product **3ab** (21.8 mg, 36%) and **3ai** (26.5 mg, 41%).

(b) *intermolecular competition experiments between arenes* ***1***

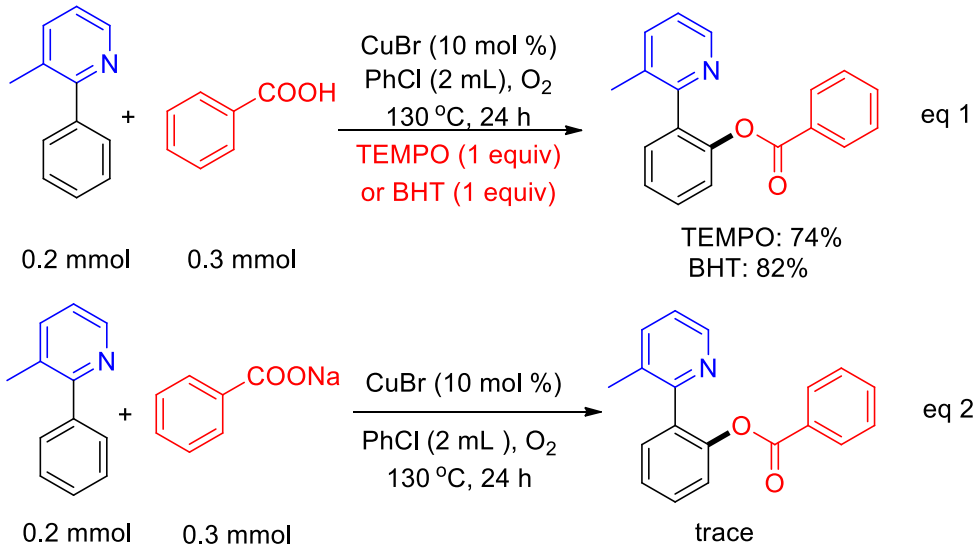


1e (0.1 mmol) **1j** (0.1 mmol) **3ea**, 22% **3ja**, 7%

Scheme S2

To a 10 mL reaction tube was added 2-(p-tolyl)pyridine **1e** (0.1 mmol), 2-(4-chlorophenyl)pyridine **1j** (0.1 mmol), benzoic acid **2a** (0.3 mmol), $Cu(OAc)_2$ (3.6 mg, 20 mol %), and chlorobenzene (1 mL) under oxygen atmosphere. The mixture was stirred at 130 ℃ for 12 h. The reaction mixture was then cooled to room temperature, diluted with ethyl acetate and quenched with saturated sodium chloride. The aqueous phase was extracted with ethyl acetate (3 × 10 mL). The organic layer was dried over Na_2SO_4. After concentration, the resulting residue was purified by flash chromatography to afford the product **3ea** (6.4 mg, 22%) and **3ja** (2.3 mg, 7%).

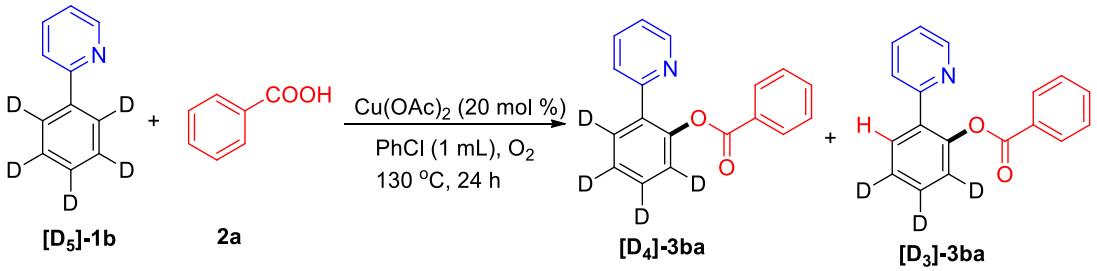
Control Experiments



Scheme S3

Isotopic Labeling Experiments

To a 10 mL reaction tube was added $[D]_5$-**1b** (0.2 mmol), benzoic acid **2a** (0.3 mmol), $Cu(OAc)_2$ (3.6 mg, 20 mol %), and chlorobenzene (1 mL) under oxygen atmosphere. The mixture was stirred at 130 ℃ for 24 h. The reaction mixture was then cooled to room temperature, diluted with ethyl acetate and quenched with saturated sodium chloride. The aqueous phase was extracted with ethyl acetate (3×10 mL). The organic layer was dried over Na_2SO_4. After concentration, the resulting residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 12/1) to afford the product. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.61 (d, *J* = 4.5 Hz, 1H), 8.09 (d, *J* = 7.5 Hz, 2H), 7.79 (s, 0.57 H), 7.68–7.53 (m, 3H), 7.51–7.41 (m, 2H), 7.21–7.12 (m, 1H).



[D_3]-3ba/[D_4]-3ba = 0.57/0.43=1.3

Scheme S4

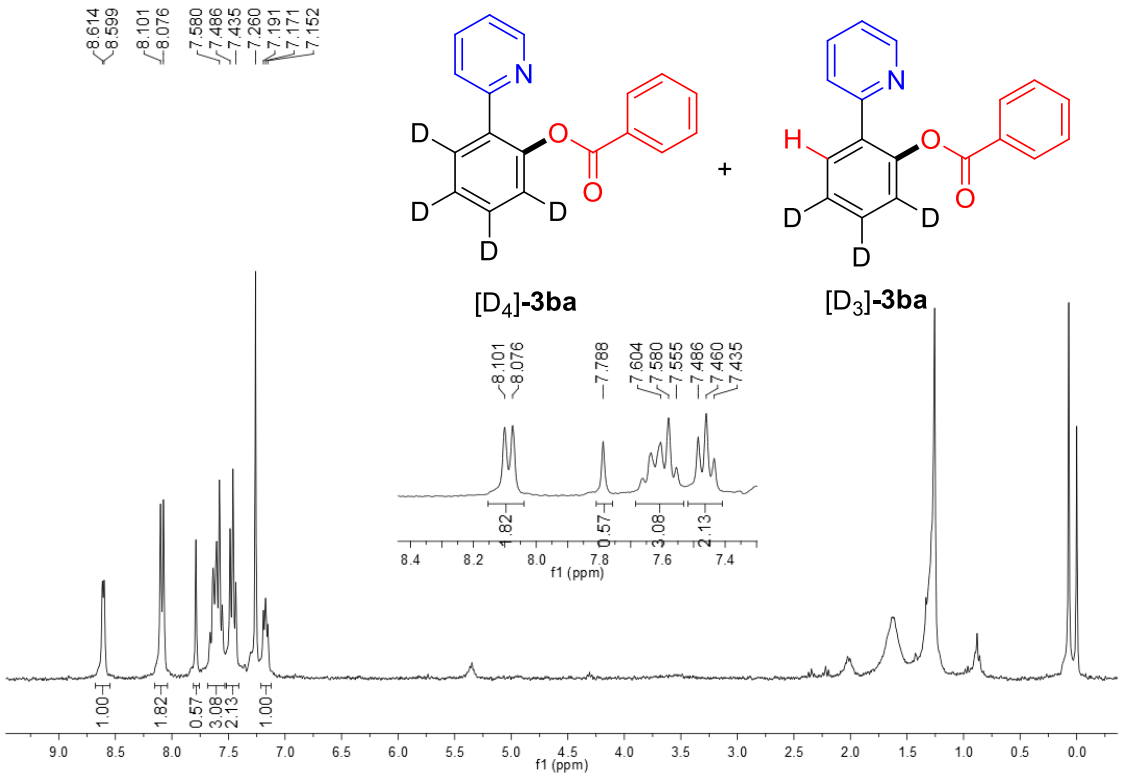
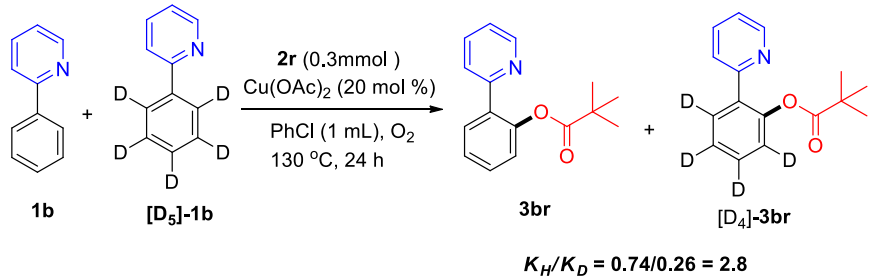


Figure S1

Kinetic Isotop Effect Experiments

To a 10 mL reaction tube was added **1b** (0.1 mmol), $[D]_5$-**1b** (0.1 mmol), pivalic acid **2r** (0.3 mmol), $Cu(OAc)_2$ (3.6 mg, 20 mol %), and chlorobenzene (1 mL) under oxygen atmosphere. The mixture was stirred at 130 ℃ for 24 h. The reaction mixture was then cooled to room temperature, diluted with ethyl acetate and quenched with saturated sodium chloride. The aqueous phase was extracted with ethyl acetate (3×10 mL). The organic layer was dried over Na_2SO_4. After concentration, the resulting residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 12/1) to afford the product. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.69 (d, *J* = 4.2 Hz, 1H), 7.77–7.67 (m, 1H), 7.67–7.61 (m, 0.77H), 7.53–7.46 (m, 1H), 7.46–7.38 (m, 1H), 7.37–7.30 (m, 1H), 7.25–7.20 (m, 1H), 7.15–7.07 (m, 0.74H), 1.20 (s, 9H).



K_H/K_D = 0.74/0.26 = 2.8

Scheme S5

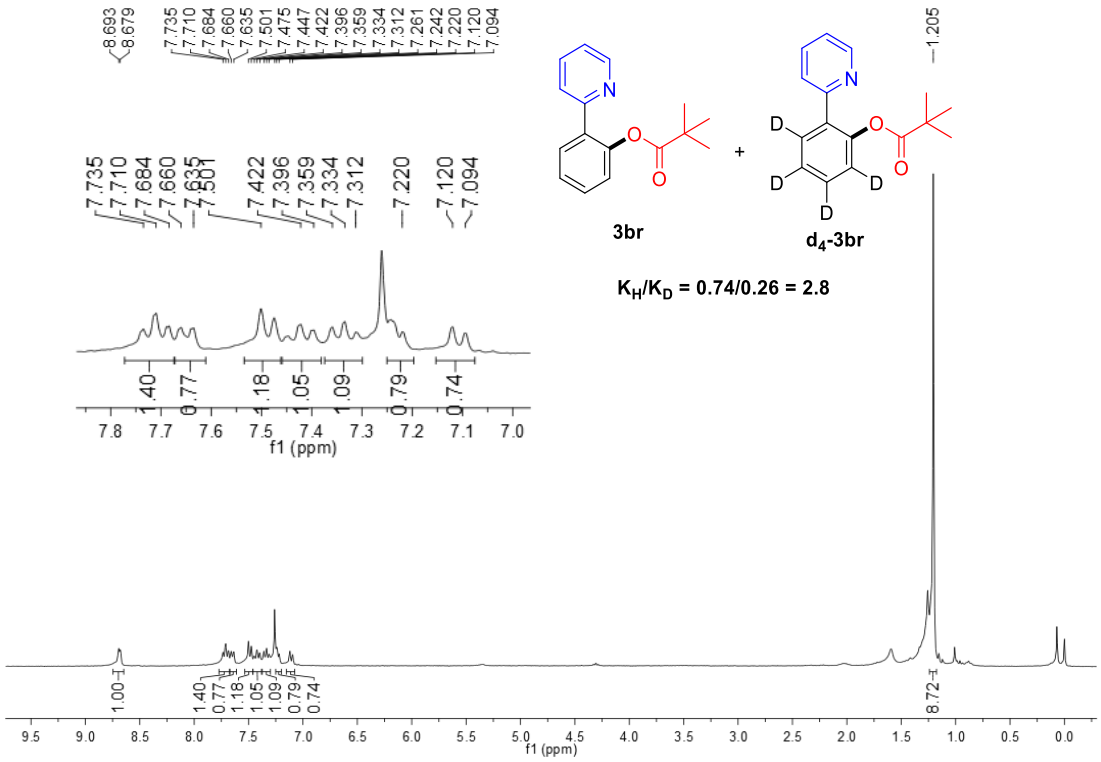


Figure S2

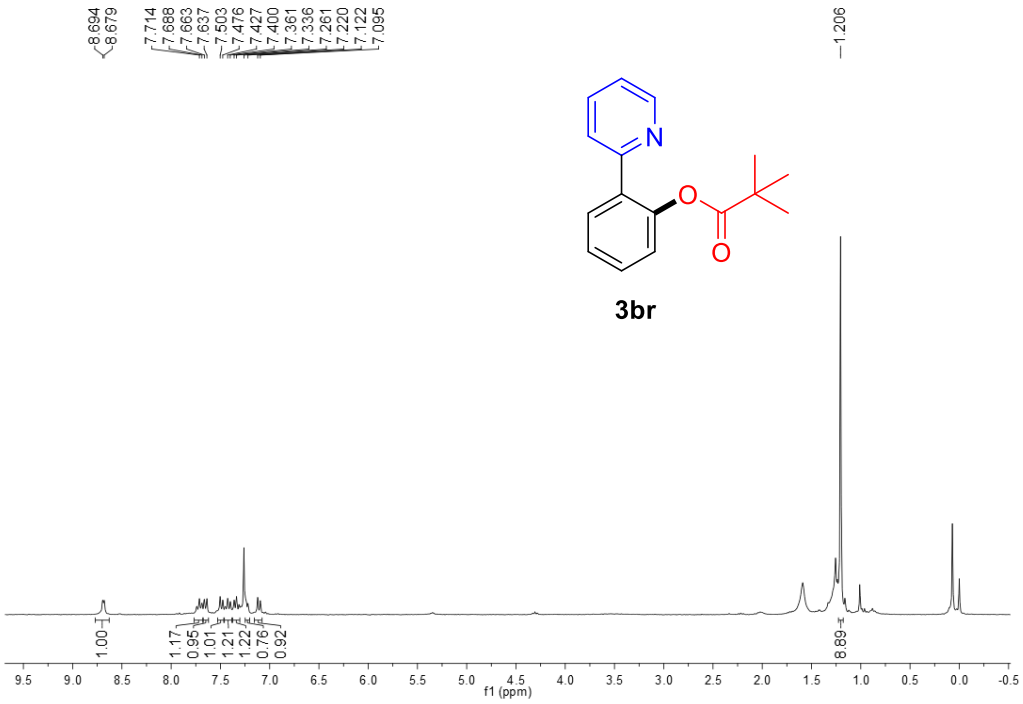
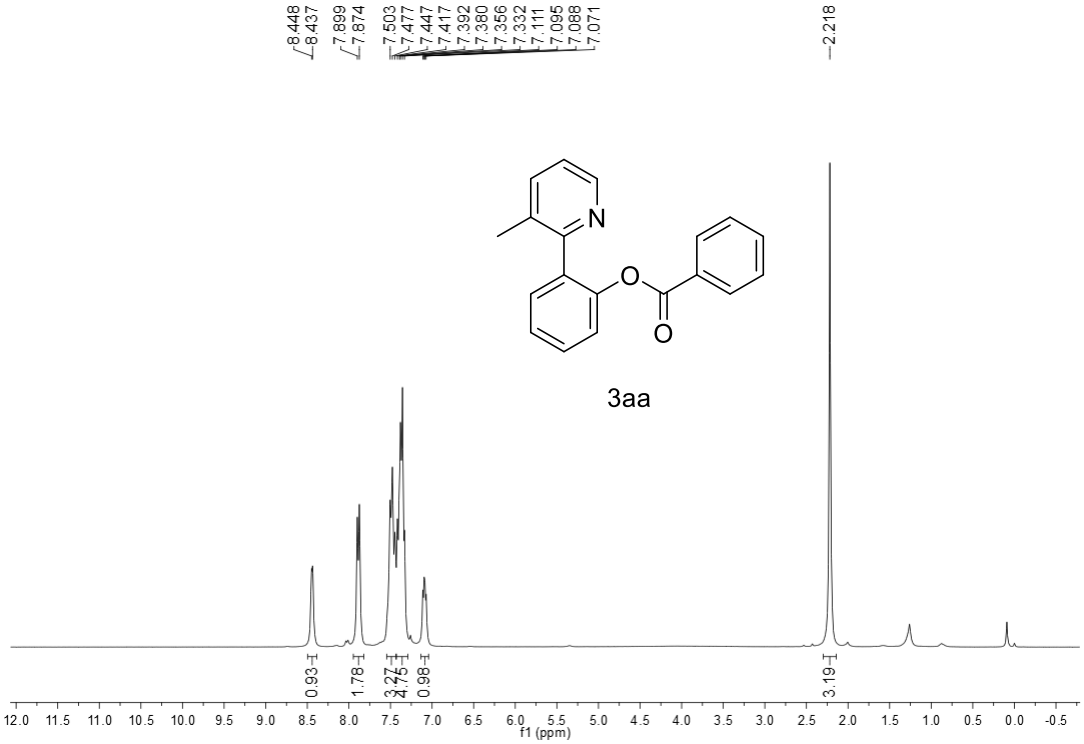
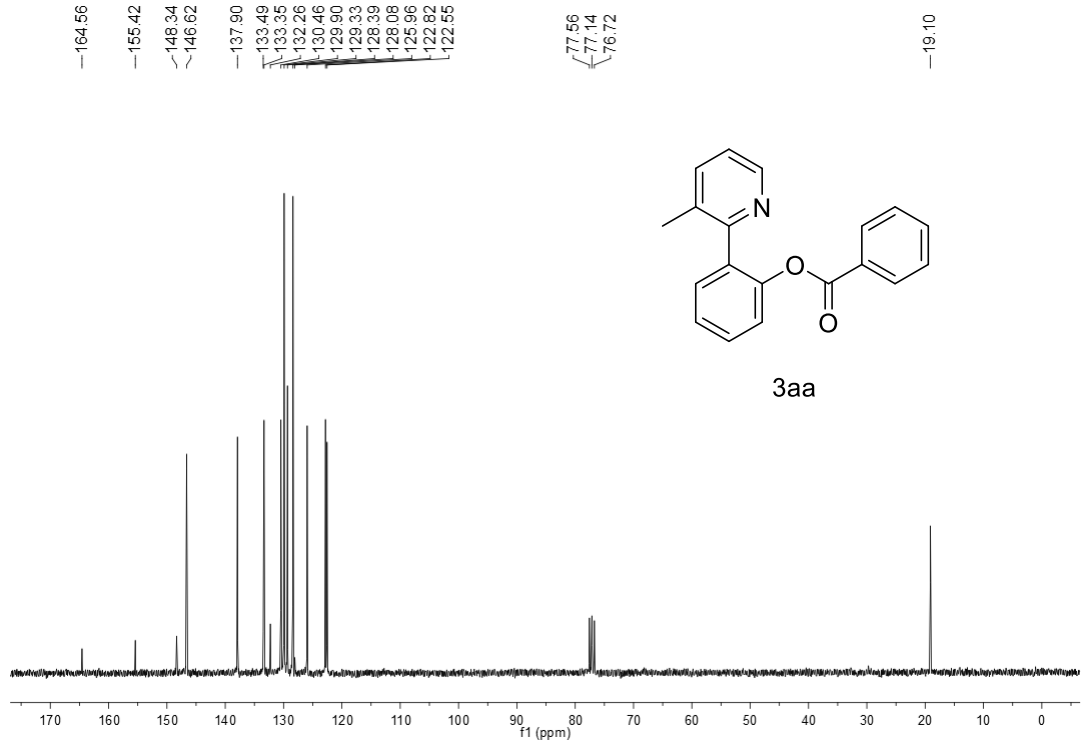
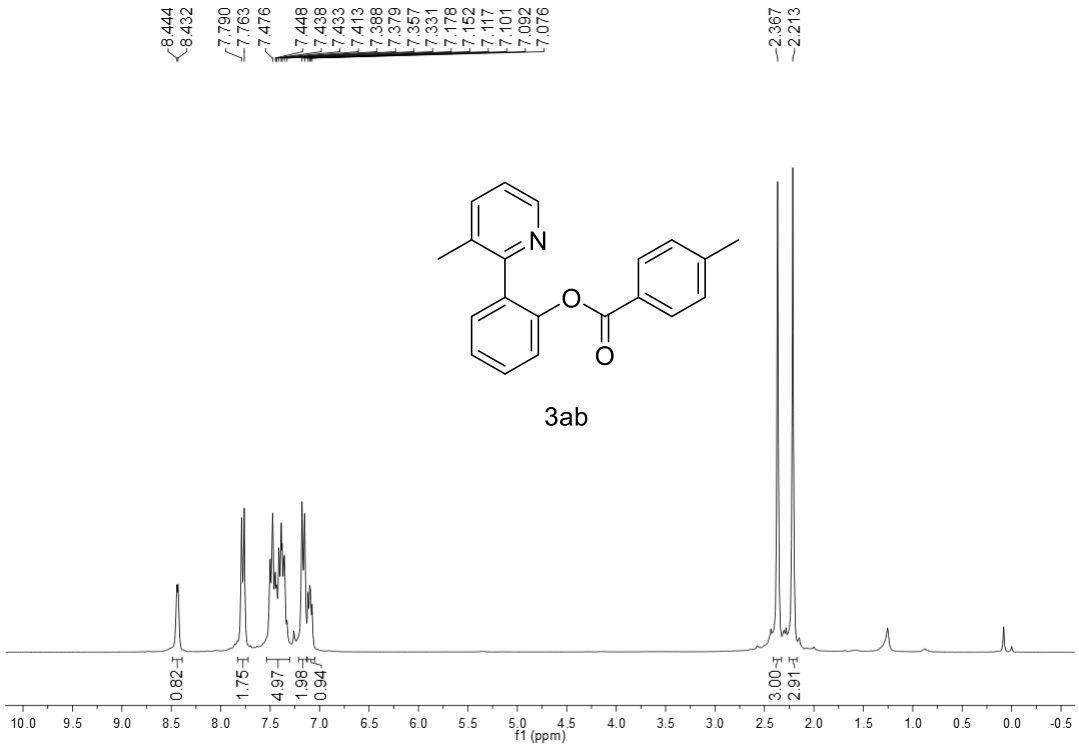


Figure S3

Copies of ^{1}H and ^{13}C NMR Spectra



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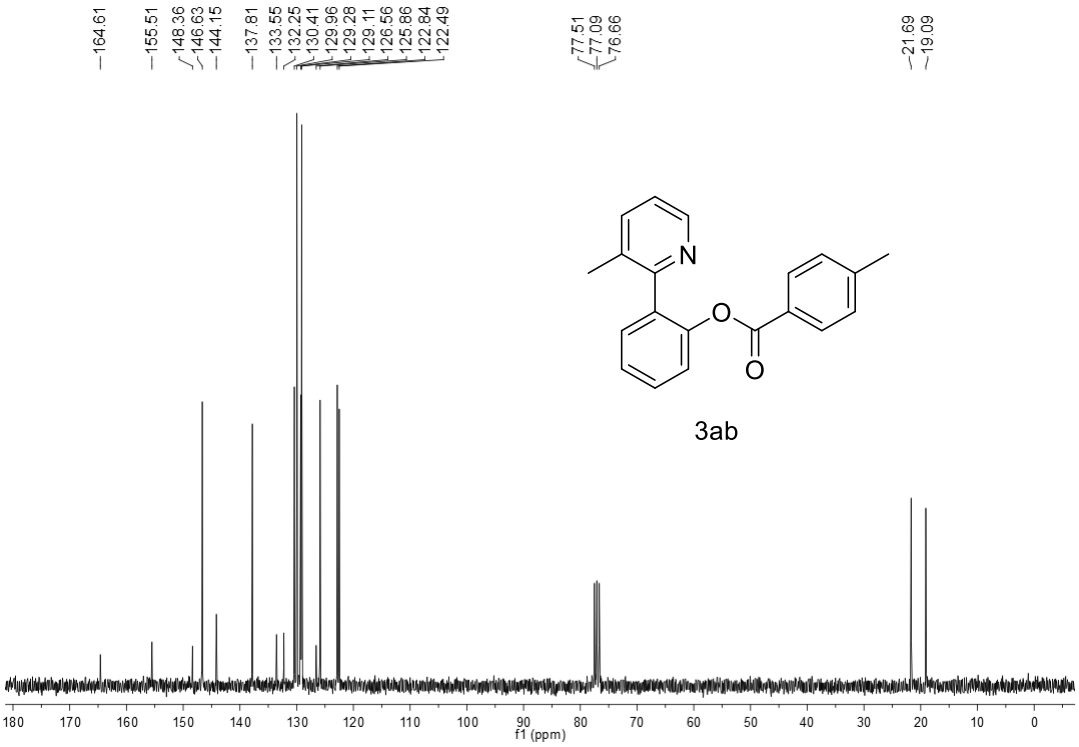
7.763
7.476
7.448
7.438
7.433
7.413
7.388
7.379
7.357
7.331
7.178
7.152
7.117
7.101
7.092
7.076
2.367
2.213
N
O
O
3ab
0.82
1.75
4.97
1.98
0.94
3.00
2.91
f1 (ppm)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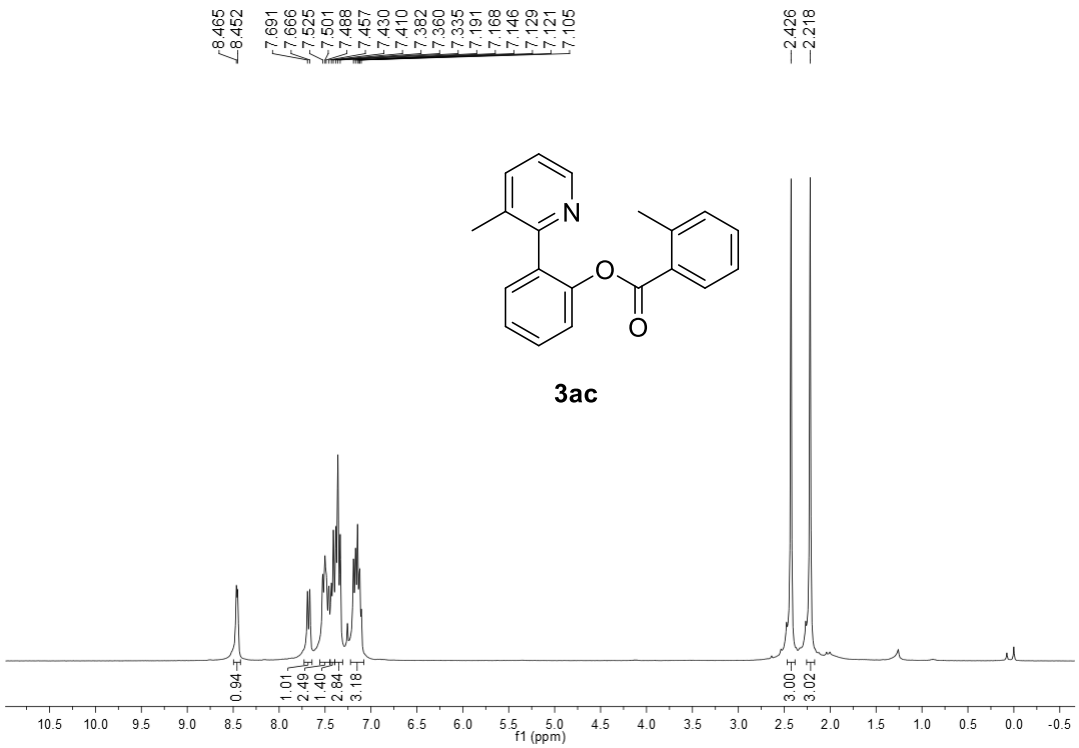
155.51
148.36
146.63
144.15
137.81
133.55
132.25
130.41
129.96
129.28
129.11
126.56
125.86
122.84
122.49
77.51
77.09
76.66
21.69
19.09
N
O
O
3ab
f1 (ppm)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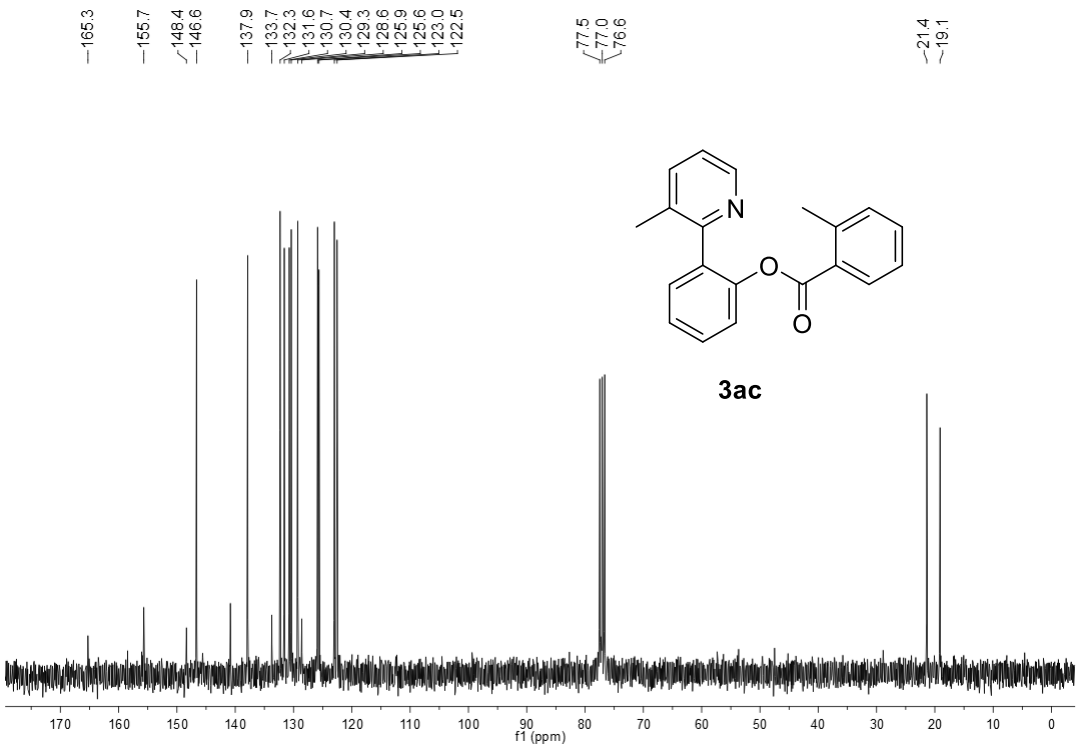
7.691
7.666
7.525
7.501
7.488
7.457
7.430
7.410
7.382
7.360
7.335
7.191
7.168
7.146
7.129
7.121
7.105
2.426
2.218
N
O
O
3ac
0.94
1.01
2.49
1.40
2.84
3.18
3.00
3.02
f1 (ppm)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155.7
148.4
146.6
137.9
133.7
132.3
131.6
130.7
130.4
129.3
128.6
125.9
125.6
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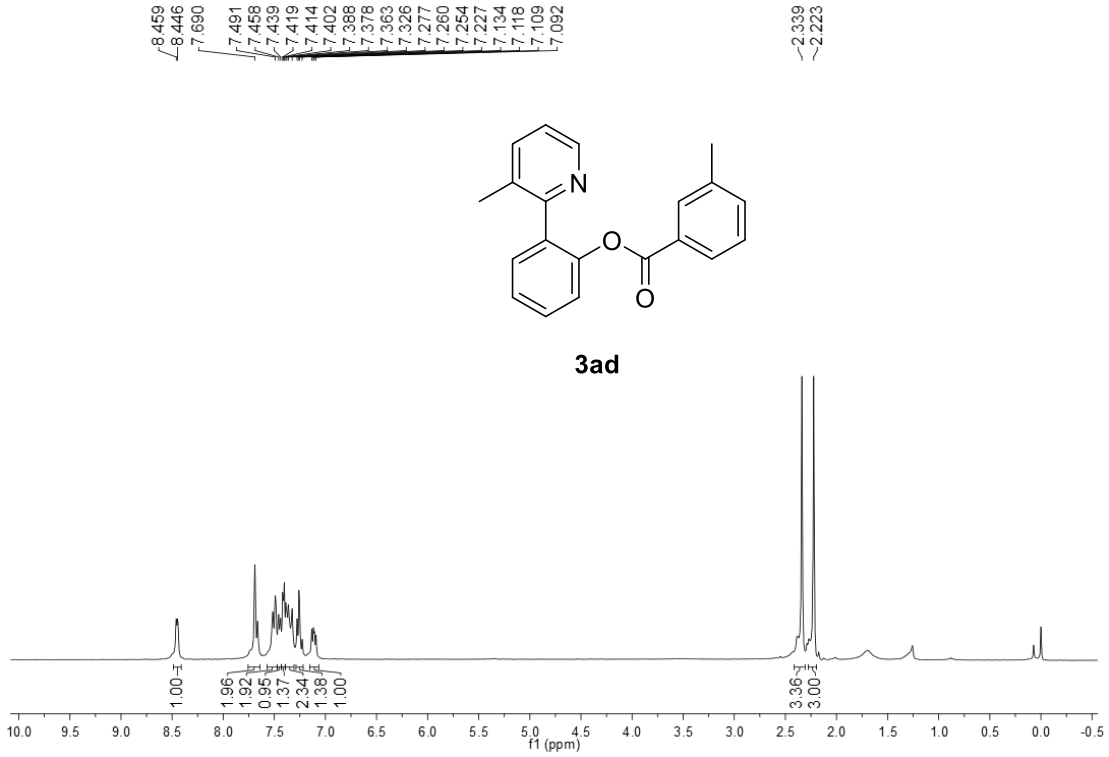
77.5
77.0
76.6
21.4
19.1
N
O
O
3ac
f1 (ppm)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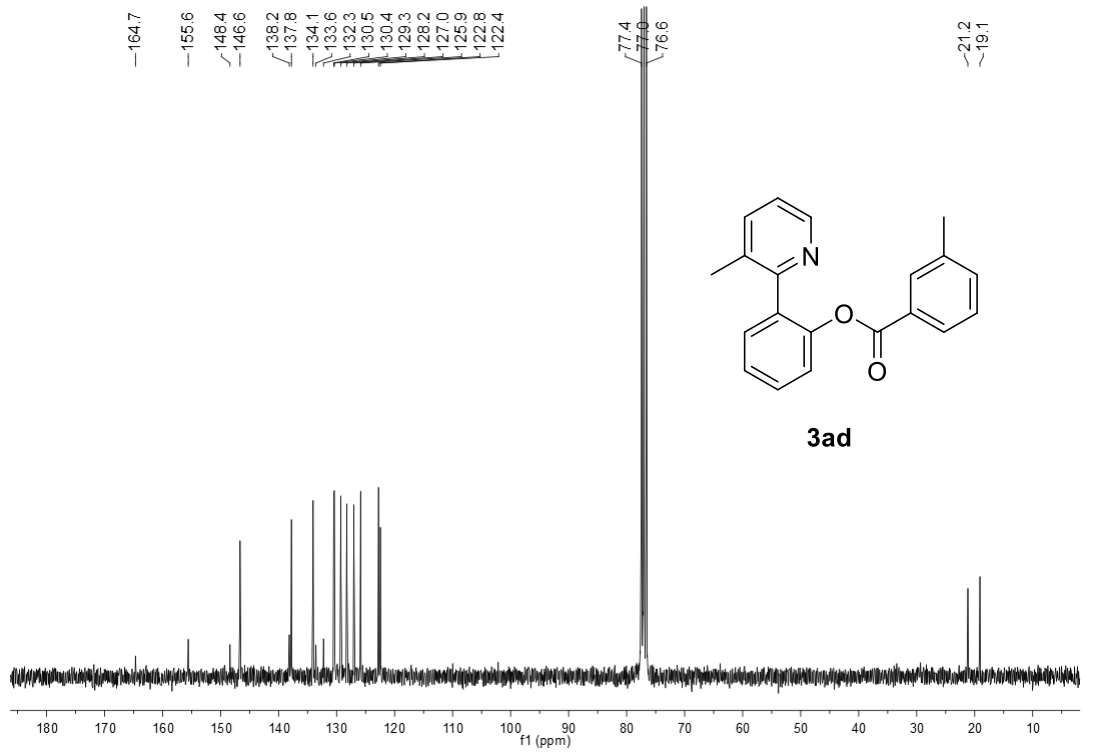
8.446
7.690
7.491
7.458
7.439
7.419
7.414
7.402
7.388
7.378
7.363
7.326
7.277
7.260
7.254
7.227
7.134
7.118
7.109
7.092
2.339
2.223
N
O
O
3ad
1.00
1.96
1.92
0.95
1.37
2.34
1.38
1.00
3.36
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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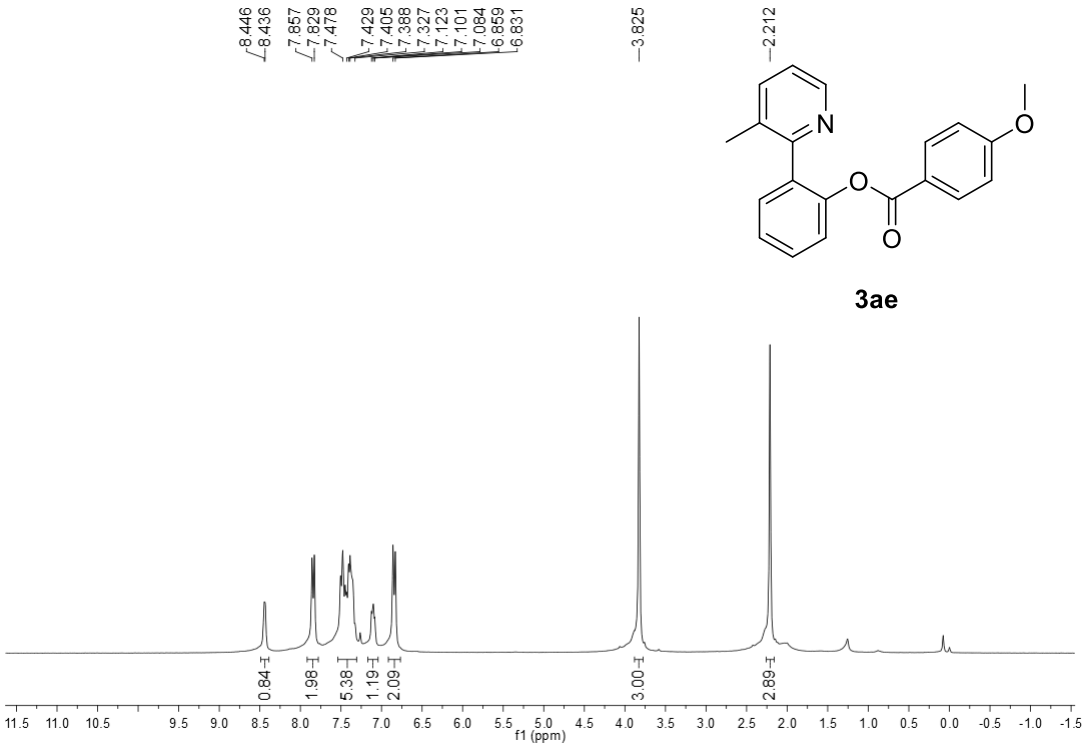
148.4
146.6
138.2
137.8
134.1
133.6
132.3
130.5
130.4
129.3
128.2
127.0
125.9
122.8
122.4
77.4
77.0
76.6
21.2
19.1
N
O
O
3ad
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.436
7.857
7.829
7.478
7.429
7.405
7.388
7.327
7.123
7.101
7.084
6.859
6.831
3.825
2.212
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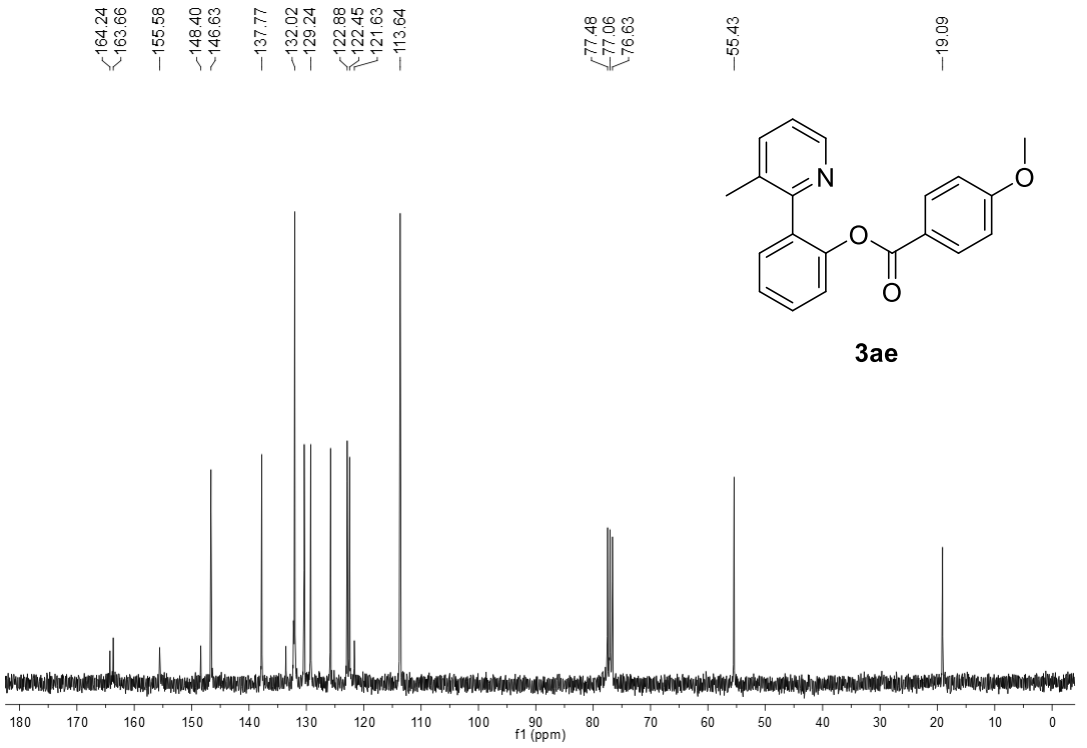
O
O
O
3ae
0.84
1.98
5.38
1.19
2.09
3.00
2.89
f1 (ppm)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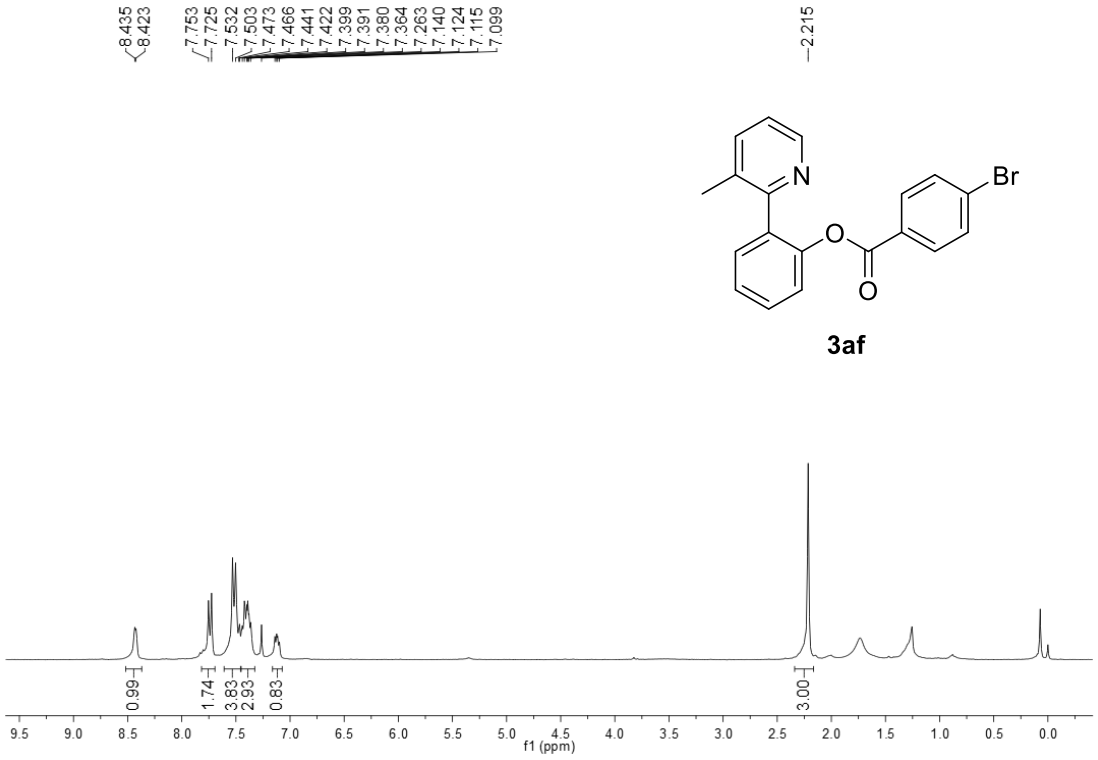
163.66
155.58
148.40
146.63
137.77
132.02
129.24
122.88
122.45
121.63
113.64
77.48
77.06
76.63
55.43
19.09
N
O
O
O
3ae
f1 (ppm)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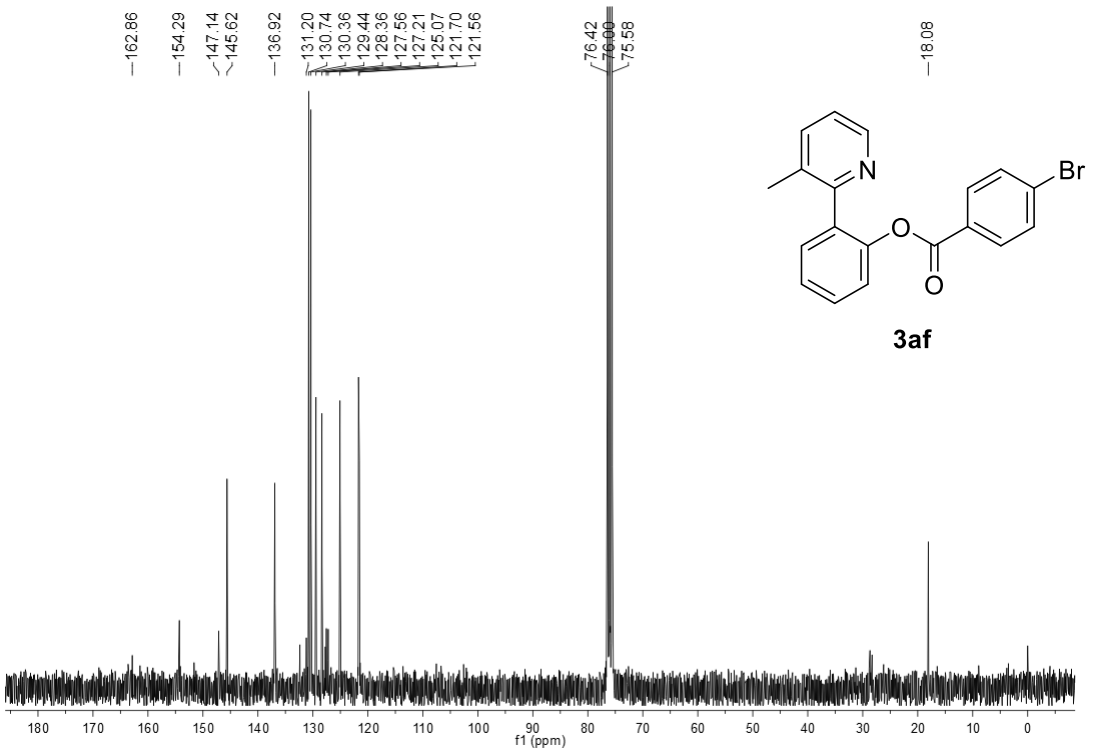
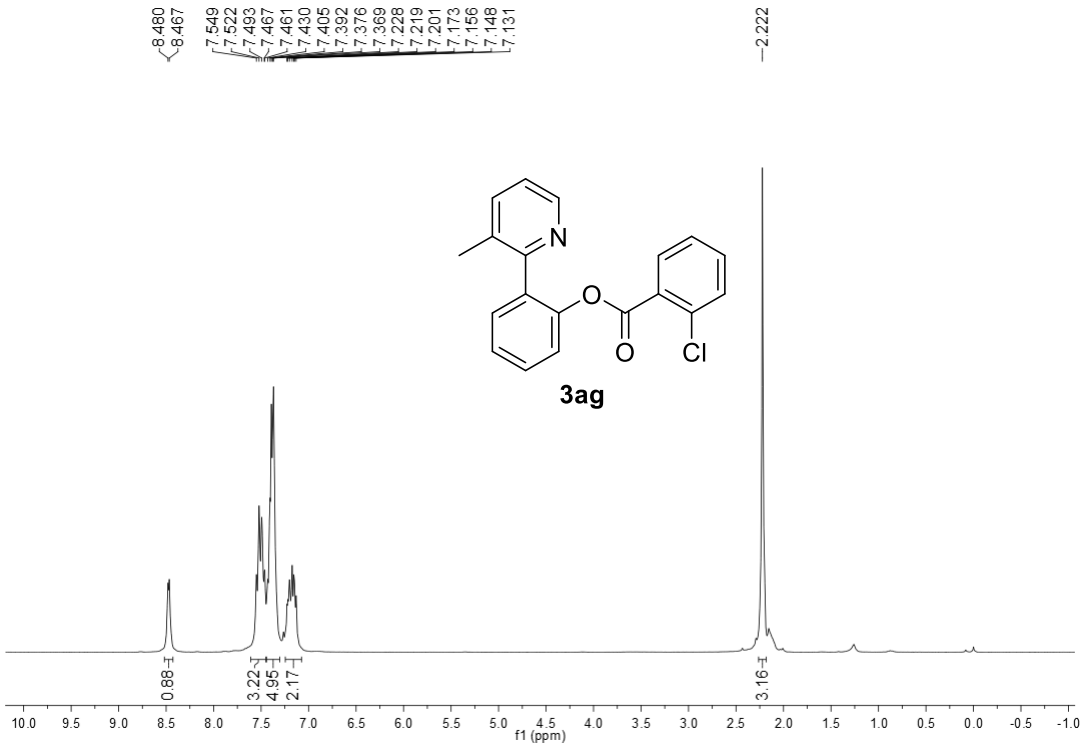
7.503
7.473
7.466
7.441
7.422
7.399
7.391
7.380
7.364
7.263
7.140
7.124
7.115
7.099
2.215
N
Br
O
O
3af
0.99
1.74
3.83
2.93
0.83
3.00
f1 (ppm)


162.86
154.29
147.14
145.62
136.92
131.20
130.74
130.36
129.44
128.36
127.56
127.21
125.07
121.70
121.56
76.42
76.00
75.58
18.08
N
Br
O
O
3af
f1 (ppm)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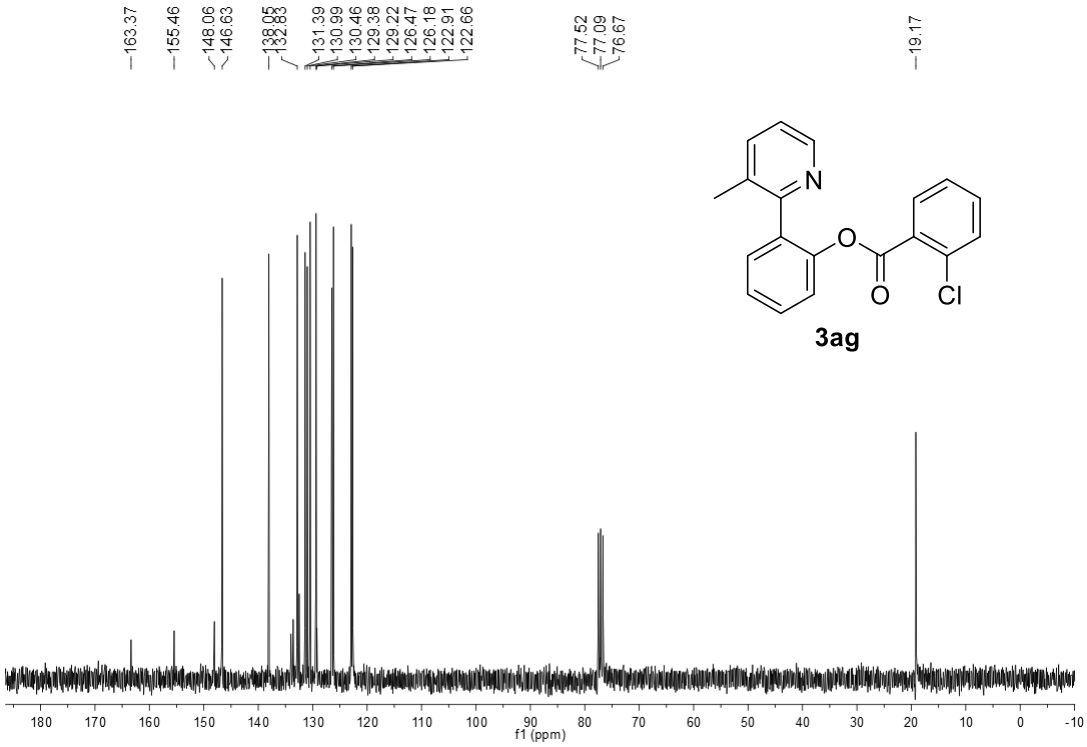
7.522
7.493
7.467
7.461
7.430
7.405
7.392
7.376
7.369
7.228
7.219
7.201
7.173
7.156
7.148
7.131
2.222
N
O
O
Cl
3ag
0.88
3.22
4.95
2.17
3.16
f1 (ppm)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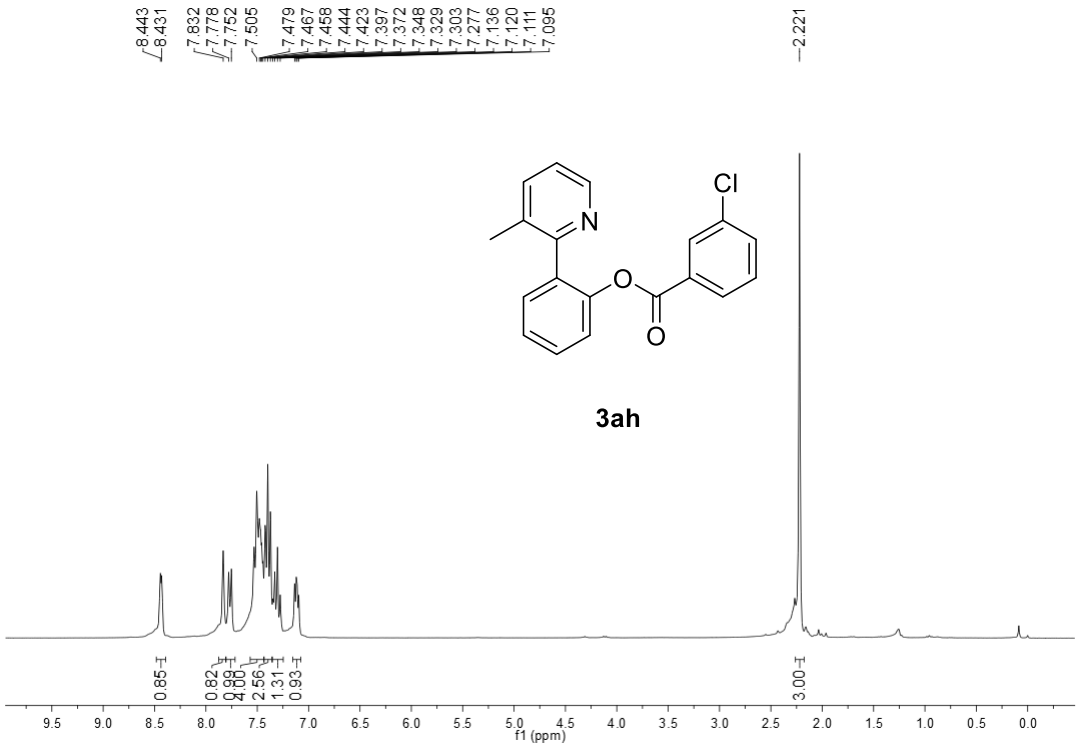
146.63
138.05
132.83
131.39
130.99
130.46
129.38
129.22
126.47
126.18
122.91
122.66
77.52
77.09
76.67
19.17
N
O
O
Cl
3ag
f1 (ppm)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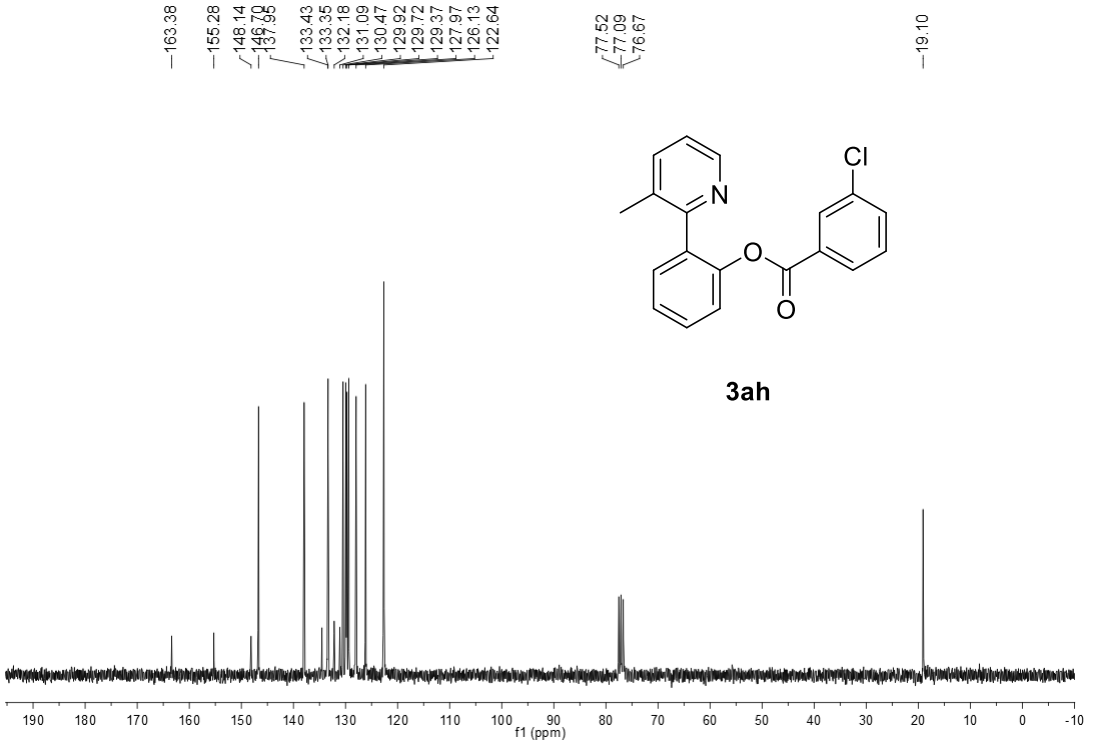
7.752
7.505
7.479
7.467
7.458
7.444
7.423
7.397
7.372
7.348
7.329
7.303
7.277
7.136
7.120
7.111
7.095
2.221
Cl
N
O
O
3ah
0.85
0.82
0.99
4.00
2.56
1.31
0.93
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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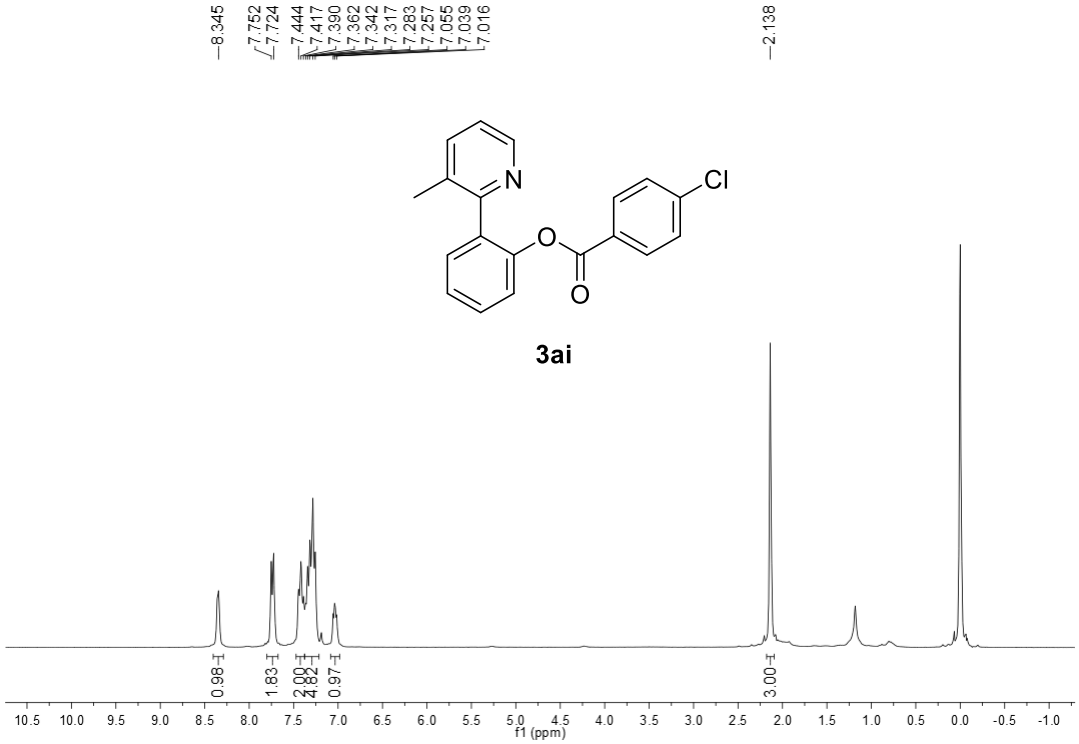
146.70
137.95
133.43
133.35
132.18
131.09
130.47
129.92
129.72
129.37
127.97
126.13
122.64
77.52
77.09
76.67
19.10
Cl
N
O
O
3ah
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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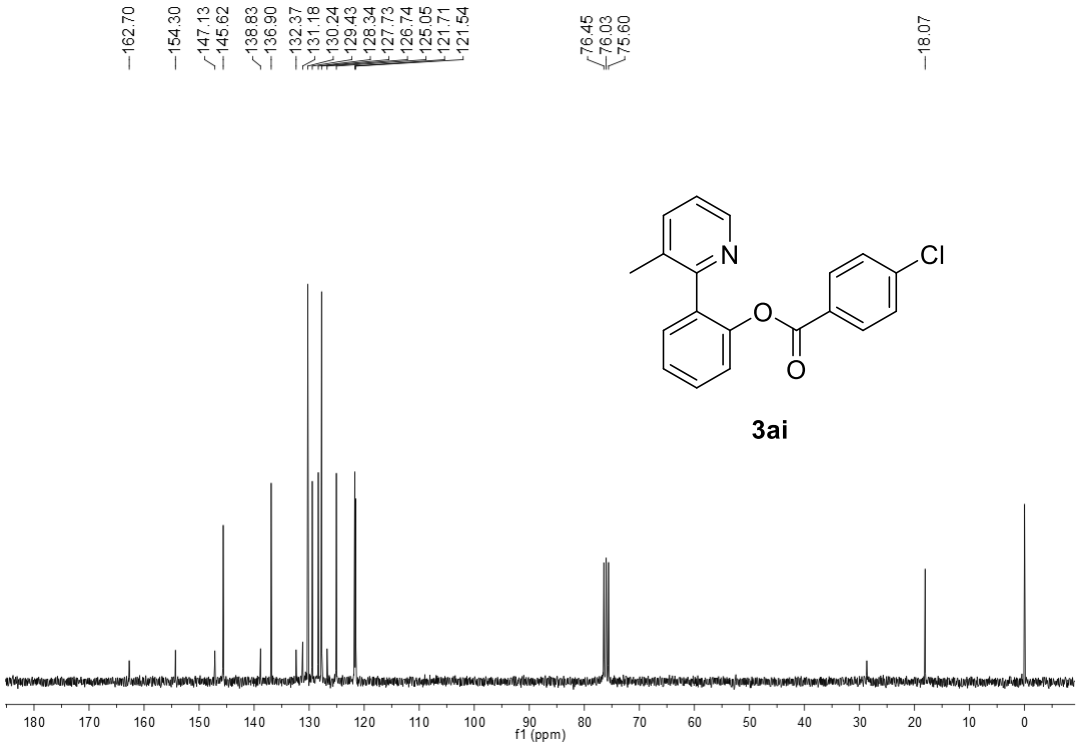
7.724
7.444
7.417
7.390
7.362
7.342
7.317
7.283
7.257
7.055
7.039
7.016
2.138
N
O
O
Cl
0.98
1.83
2.00
2.82
0.97
3.00
f1 (ppm)

3ai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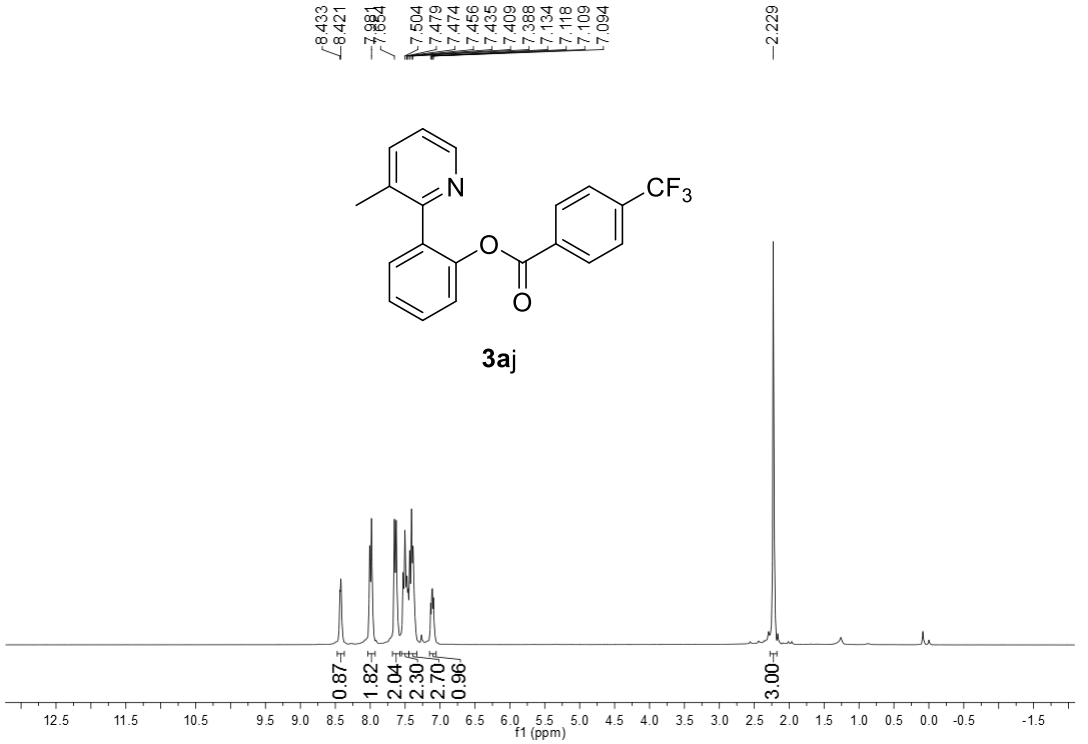
154.30
147.13
145.62
138.83
136.90
132.37
131.18
130.24
129.43
128.34
127.73
126.74
125.05
121.71
121.54
76.45
76.03
75.60
18.07
N
O
O
Cl
f1 (ppm)

3ai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7.388
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7.109
7.094
2.229
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CF3
3aj
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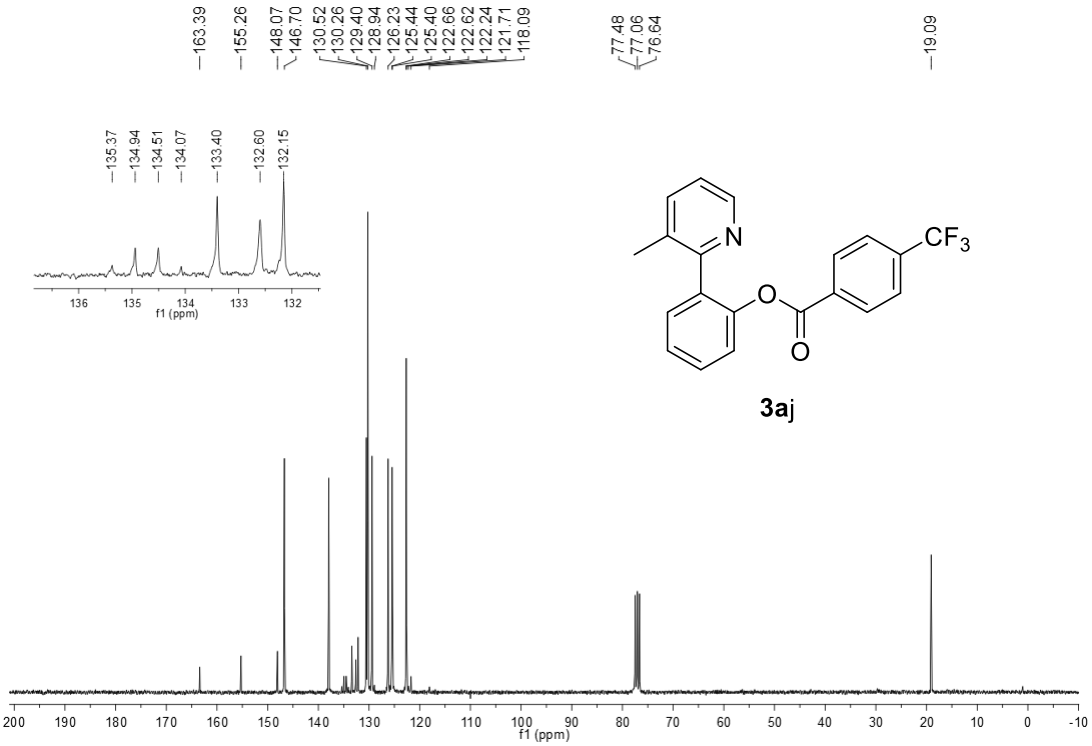
1.82
2.04
2.30
2.70
0.96
3.00
f1 (ppm)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146.70
130.52
130.26
129.40
128.94
126.23
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125.40
122.66
122.62
122.24
121.71
118.09
77.48
77.06
76.64
19.09
135.37
134.94
134.51
134.07
133.40
132.60
132.15
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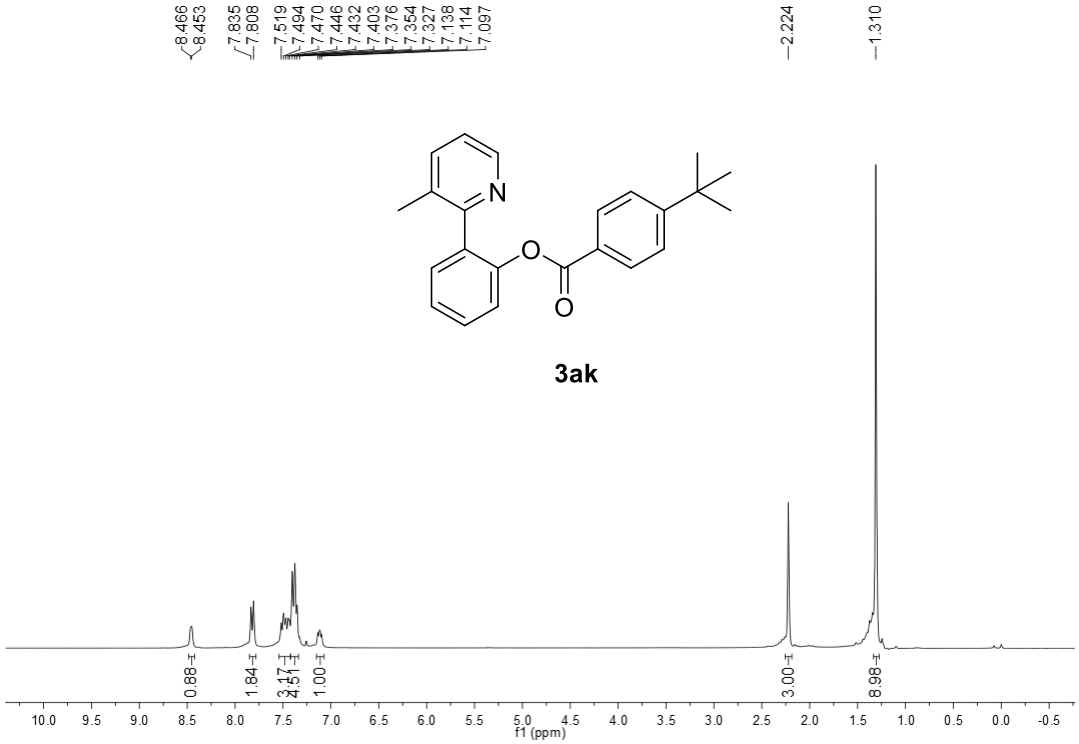
N
O
O
CF3
3aj
f1 (ppm)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7.494
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7.446
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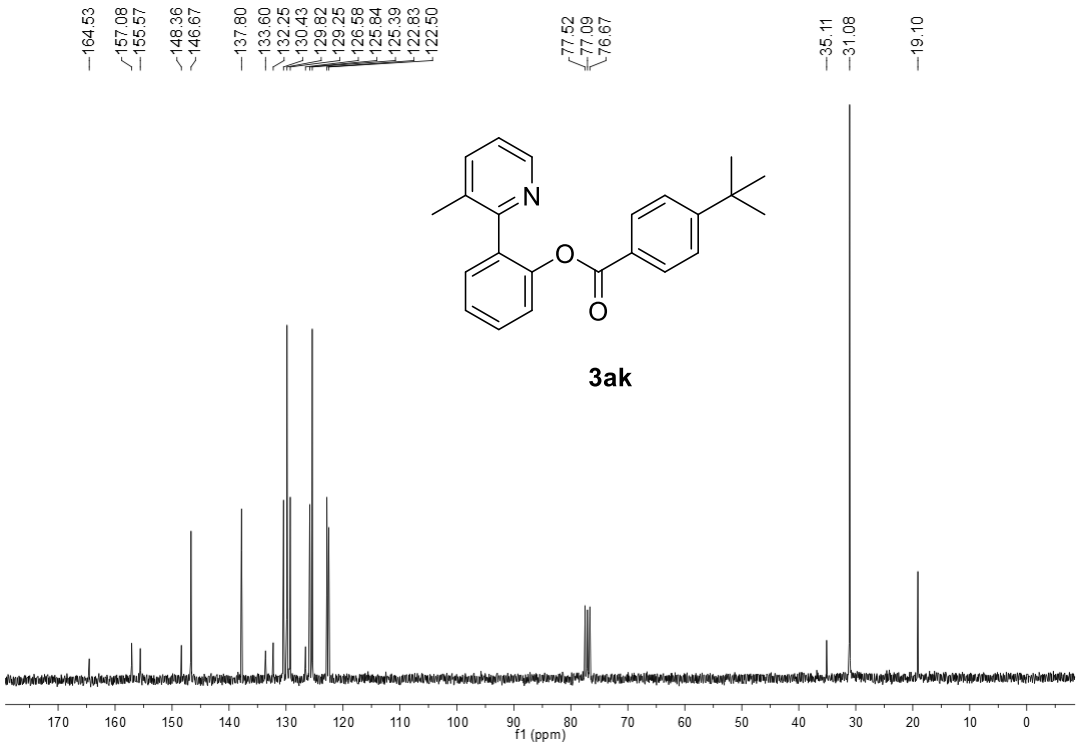
7.403
7.376
7.354
7.327
7.138
7.114
7.097
2.224
1.310
N
O
O
0.88
1.84
3.17
4.51
1.00
3.00
8.98
f1 (ppm)

3ak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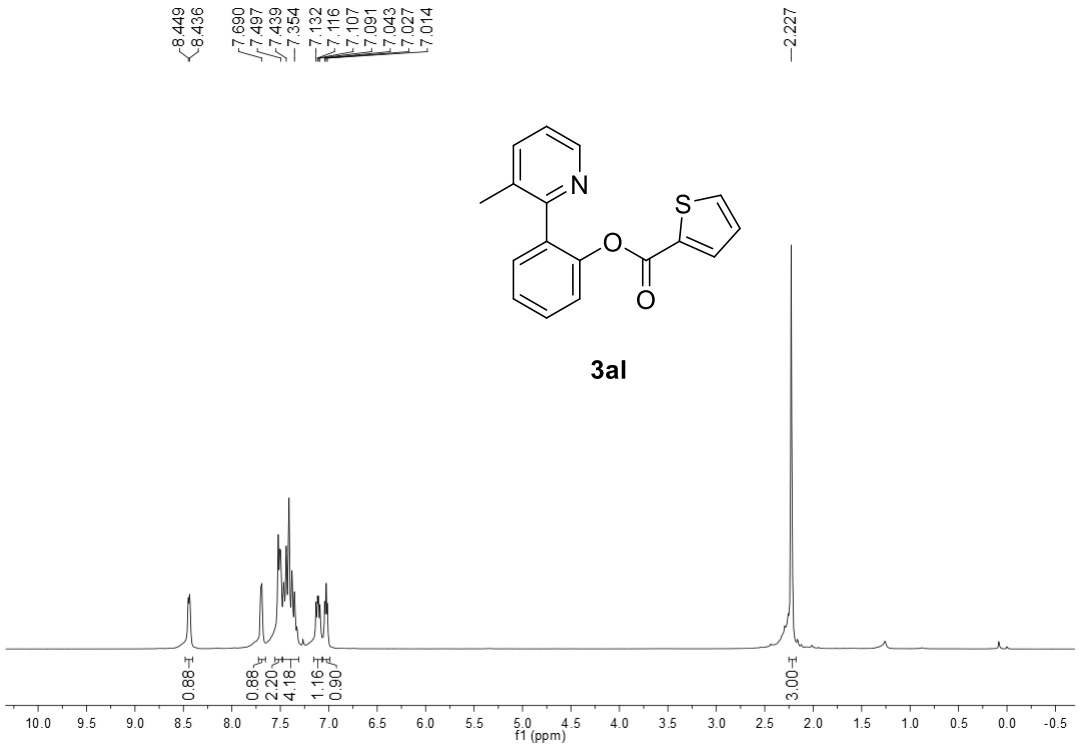
157.08
155.57
148.36
146.67
137.80
133.60
132.25
130.43
129.82
129.25
126.58
125.84
125.39
122.83
122.50
77.52
77.09
76.67
35.11
31.08
19.10
N
O
O
f1 (ppm)

3ak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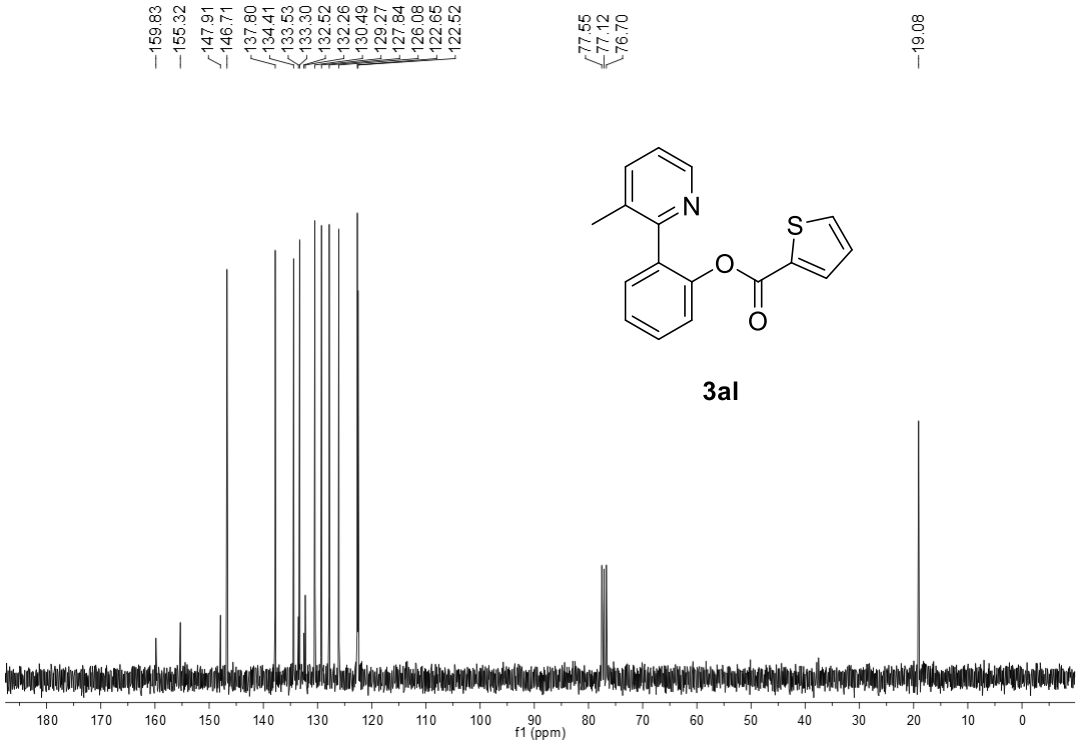
7.354
7.132
7.116
7.107
7.091
7.043
7.027
7.014
2.227
N
S
O
O
3al
0.88
0.88
2.20
4.18
1.16
0.90
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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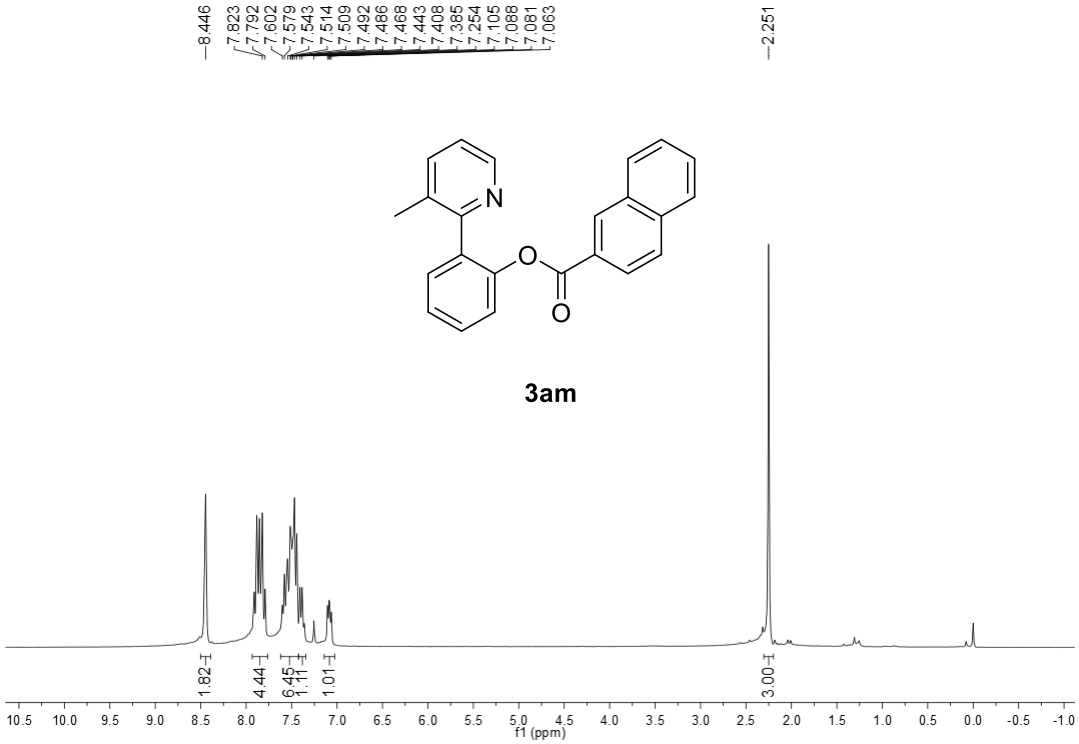
146.71
137.80
134.41
133.53
133.30
132.52
132.26
130.49
129.27
127.84
126.08
122.65
122.52
77.55
77.12
76.70
19.08
N
S
O
O
3al
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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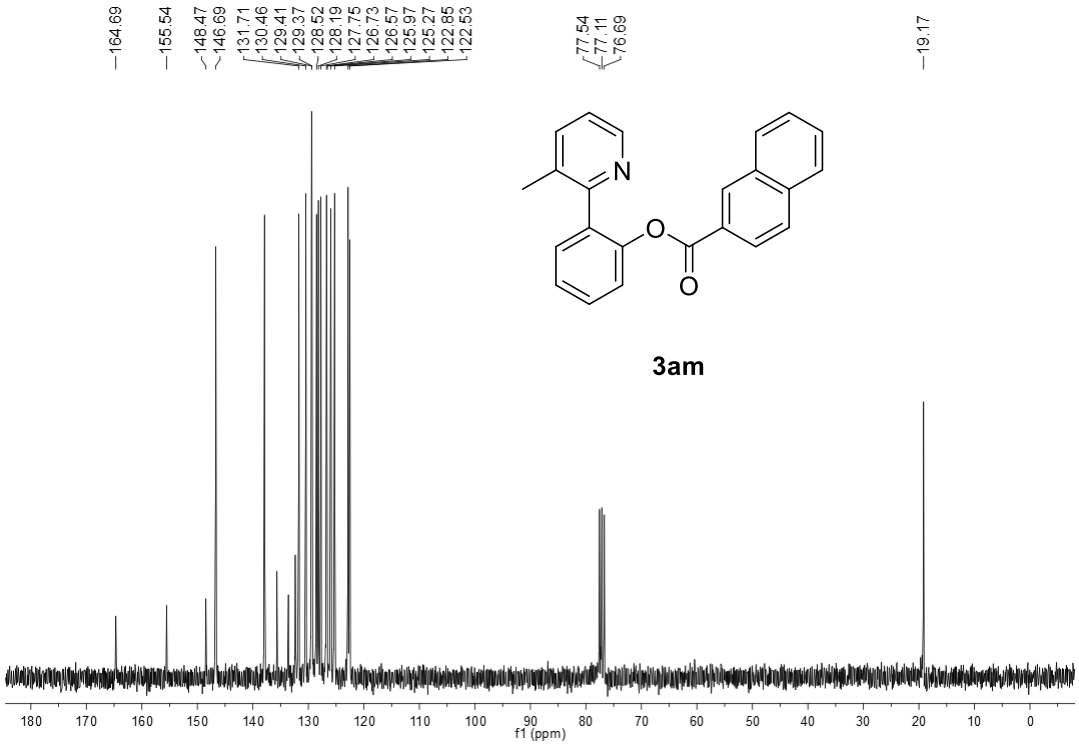
7.792
7.602
7.579
7.543
7.514
7.509
7.492
7.486
7.468
7.443
7.408
7.385
7.254
7.105
7.088
7.081
7.063
2.251
N
O
O
1.82
4.44
6.45
1.11
1.01
3.00
f1 (ppm)

3am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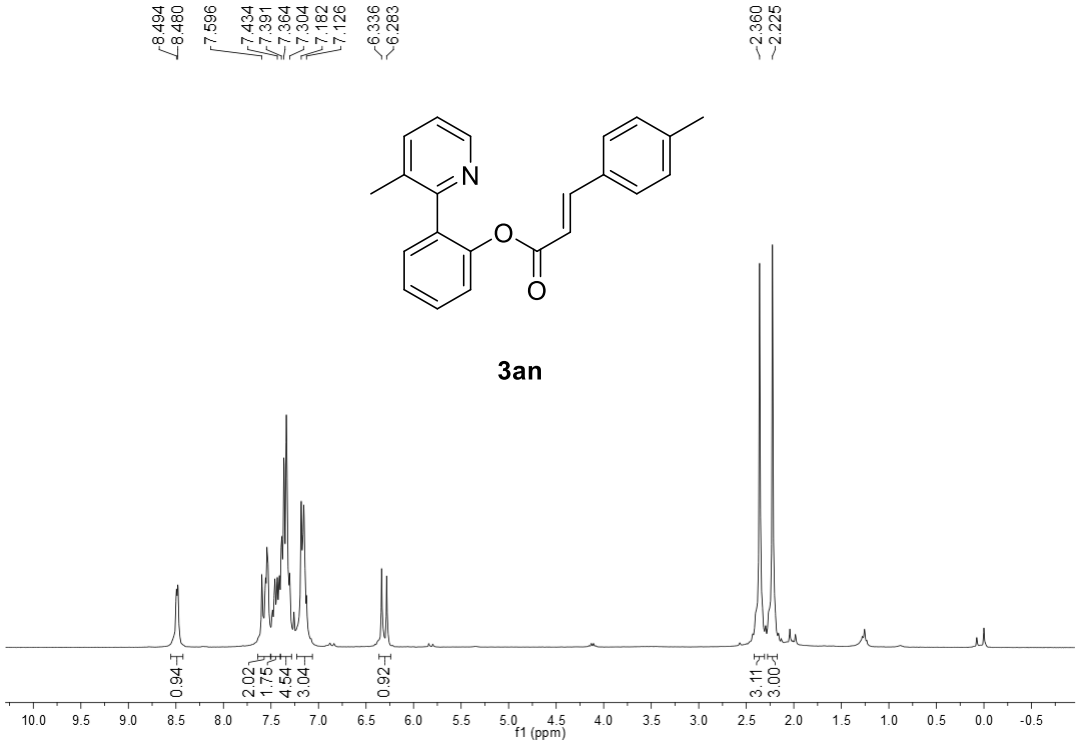
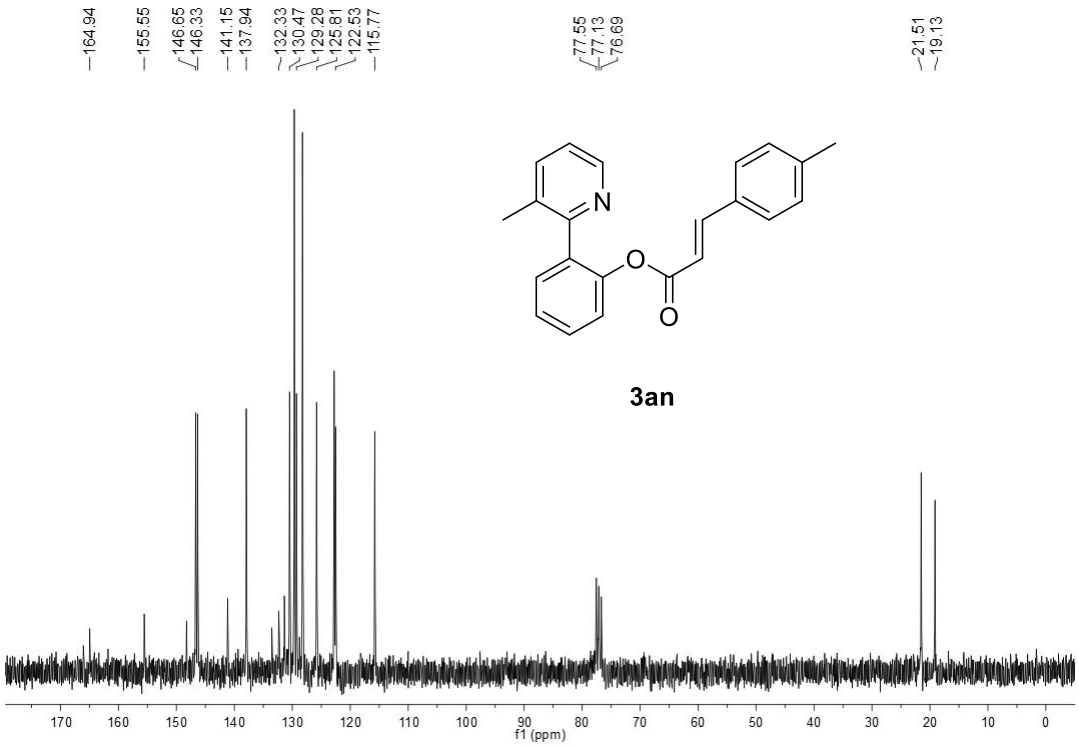
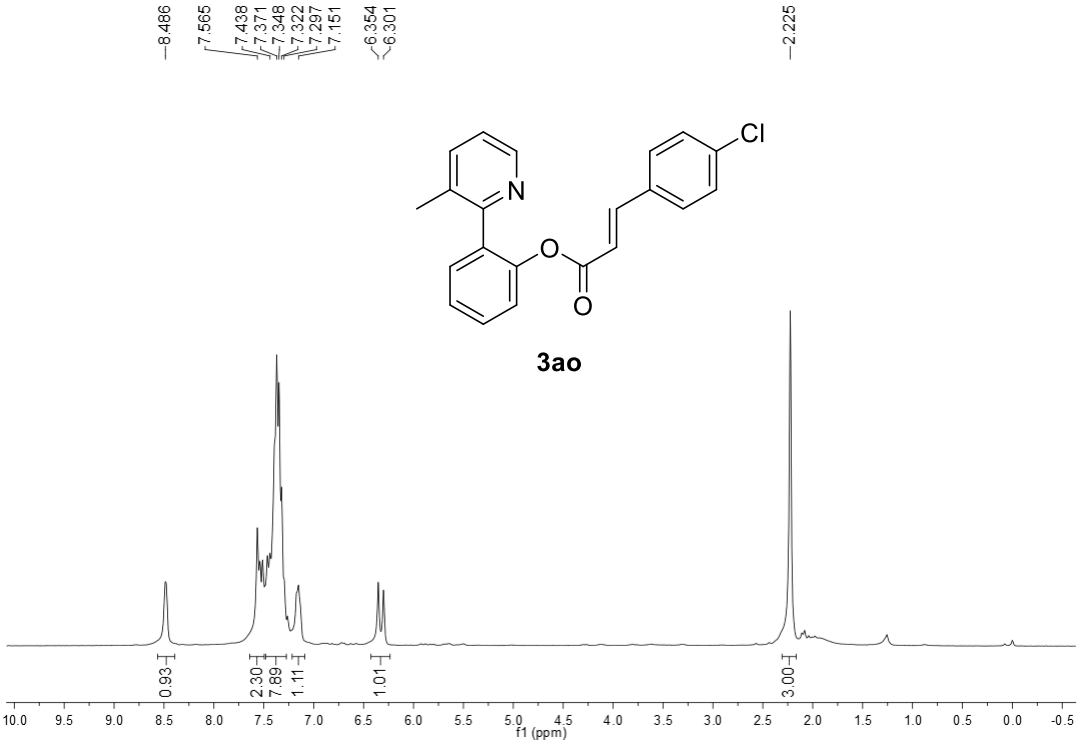
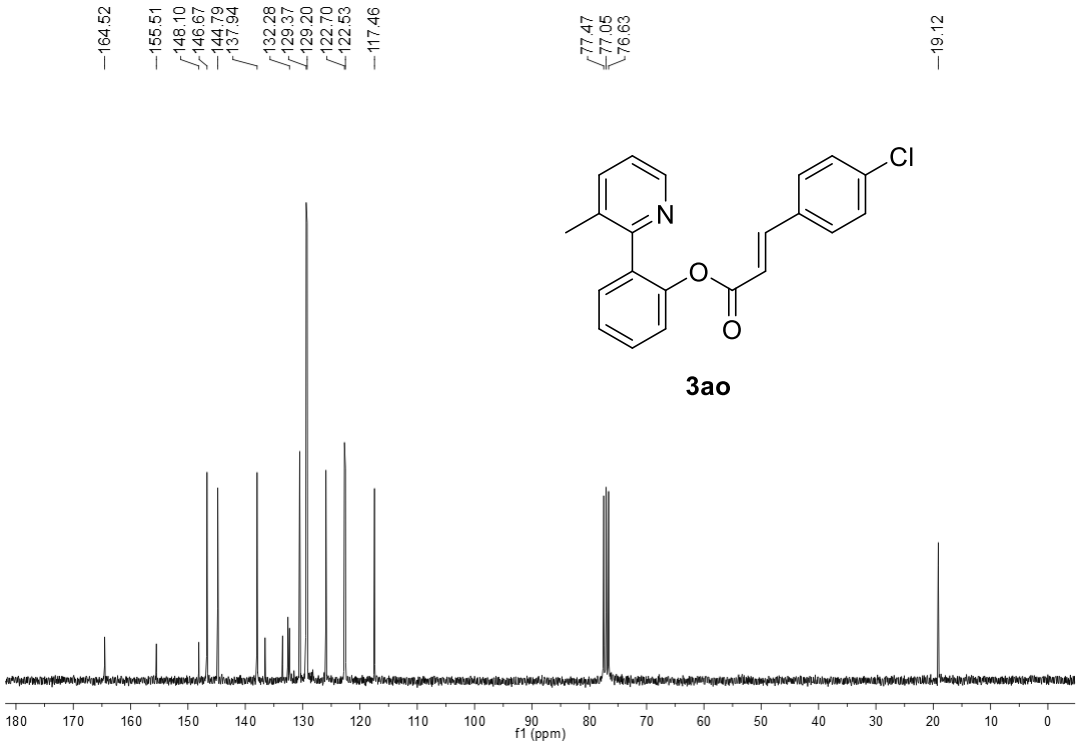
155.54
148.47
146.69
131.71
130.46
129.41
129.37
128.52
128.19
127.75
126.73
126.57
125.97
125.27
122.85
122.53
77.54
77.11
76.69
19.17
N
O
O
f1 (ppm)

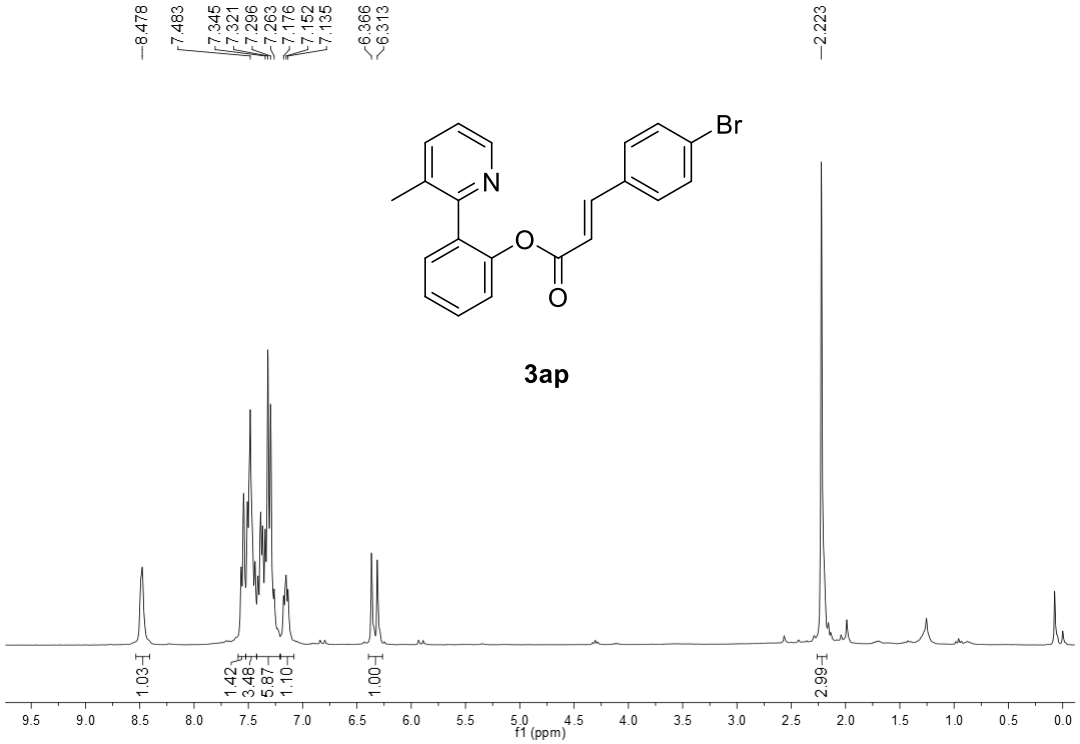
3am


8.494
8.480
7.596
7.434
7.391
7.364
7.304
7.182
7.126
6.336
6.283
2.360
2.225
N
O
O
3an
0.94
2.02
1.75
4.54
3.04
0.92
3.11
3.00
f1 (ppm)

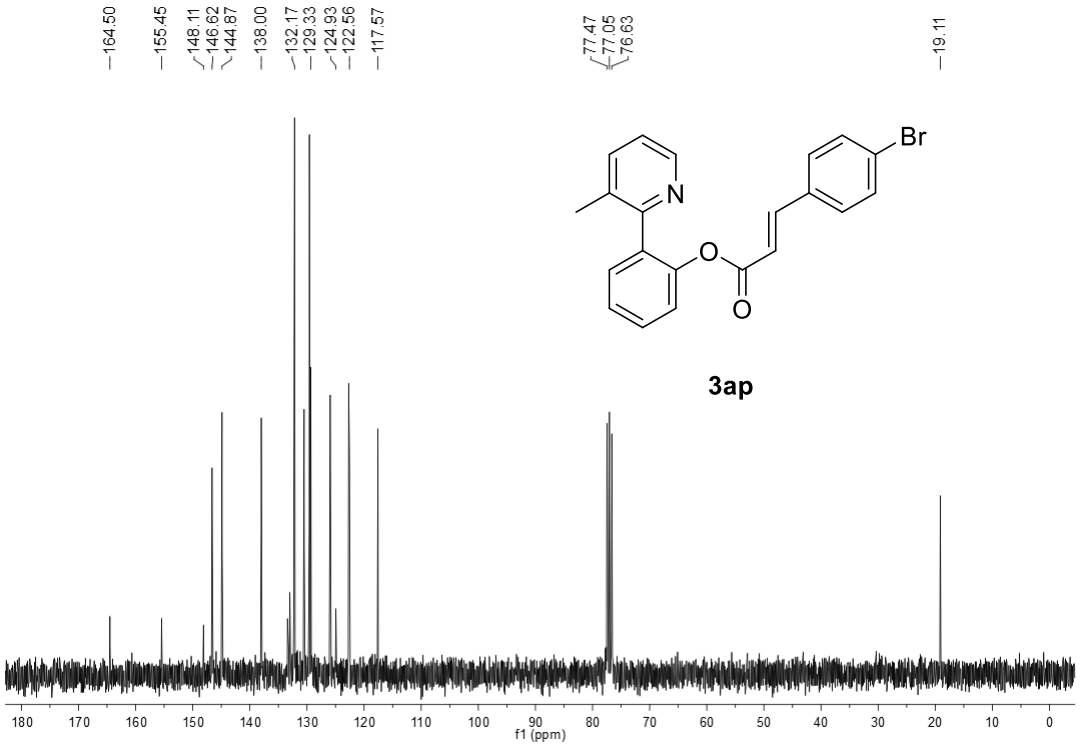

164.94
155.55
146.65
146.33
141.15
137.94
132.33
130.47
129.28
125.81
122.53
115.77
77.55
77.13
76.69
21.51
19.13
N
O
O
3an
f1 (ppm)


8.486
7.565
7.438
7.371
7.348
7.322
7.297
7.151
6.354
6.301
2.225
Cl
N
O
O
3ao
0.93
2.30
7.89
1.11
1.01
3.00
f1 (ppm)

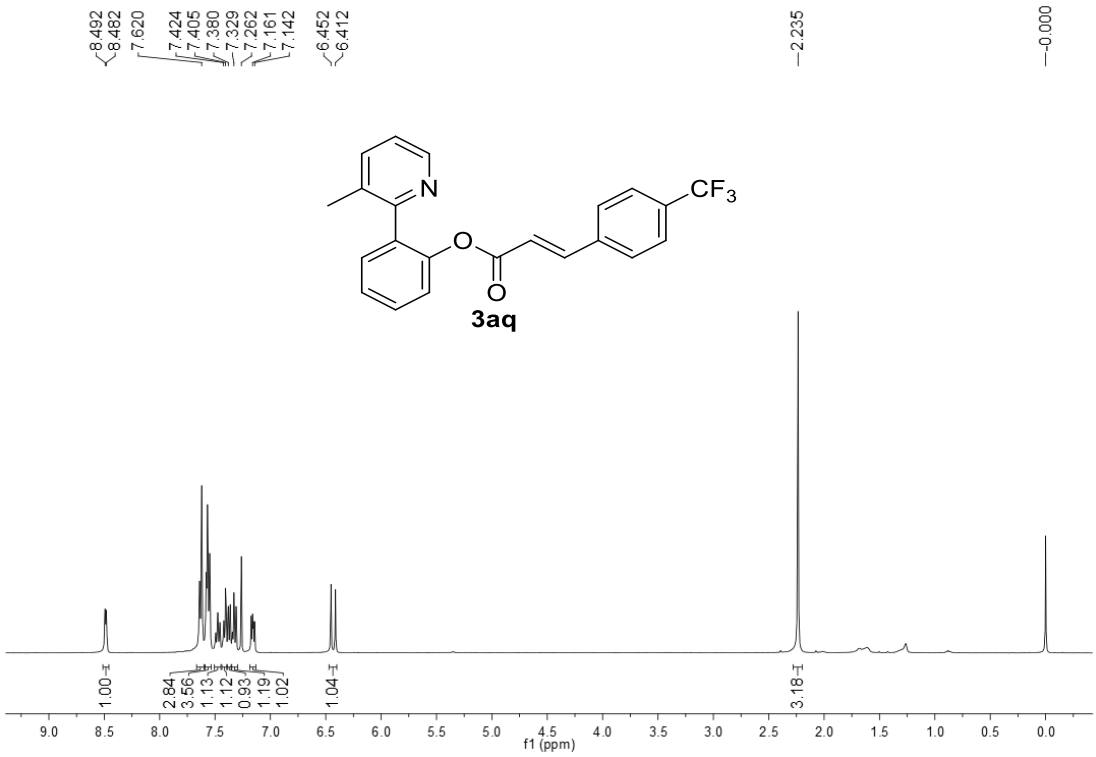

164.52
155.51
148.10
146.67
144.79
137.94
132.28
129.37
129.20
122.70
122.53
117.46
77.47
77.05
76.63
19.12
Cl
N
O
O
3ao
f1 (ppm)

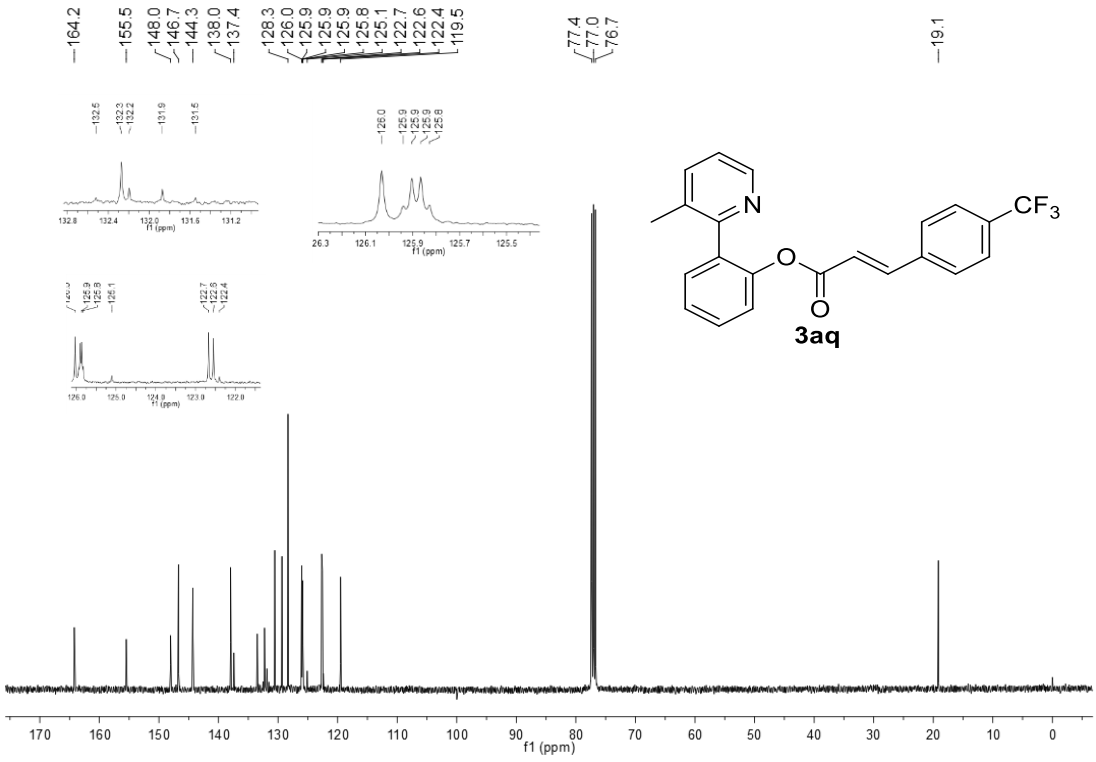

8.478
7.483
7.345
7.321
7.296
7.263
7.176
7.152
7.135
6.366
6.313
2.223
Br
N
O
O
1.03
1.42
3.48
5.87
1.10
1.00
2.99
f1 (ppm)

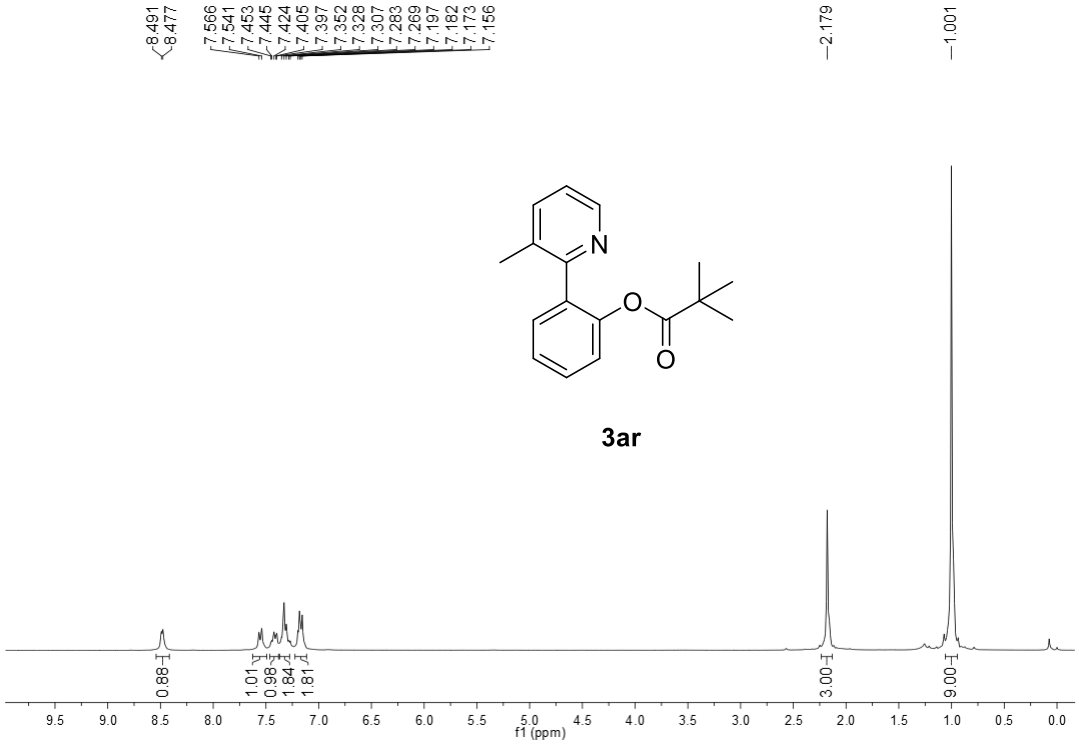
3ap

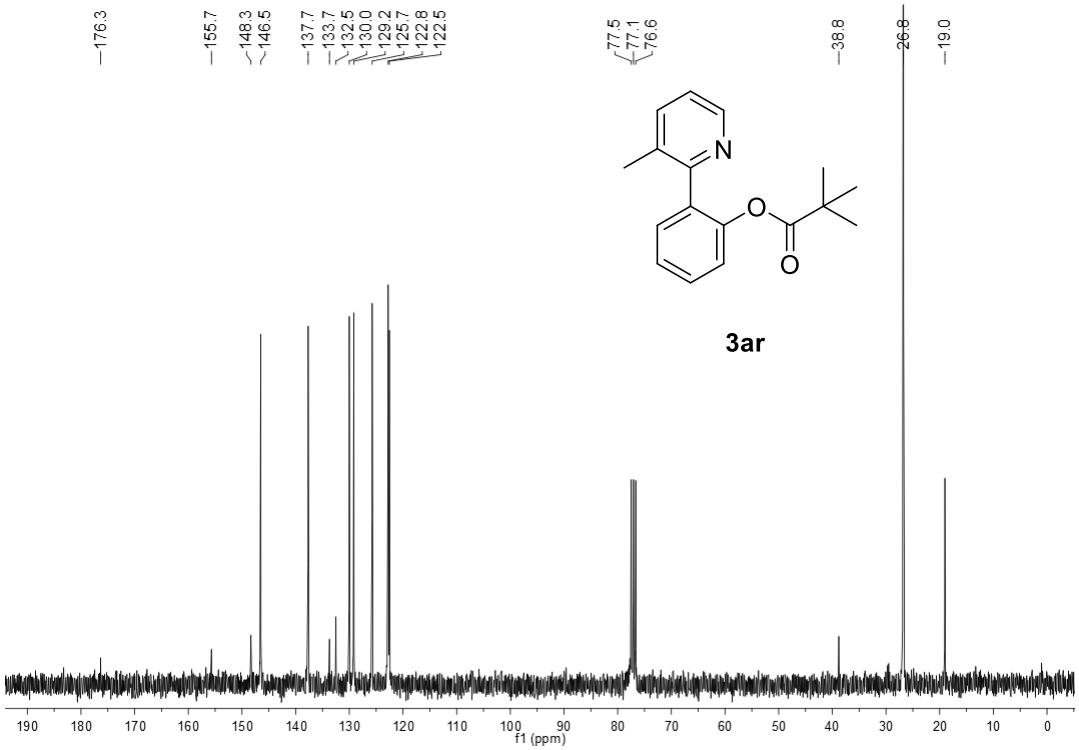

164.50
155.45
148.11
146.62
144.87
138.00
132.17
129.33
124.93
122.56
117.57
77.47
77.05
76.63
19.11
Br
N
O
O
f1 (ppm)

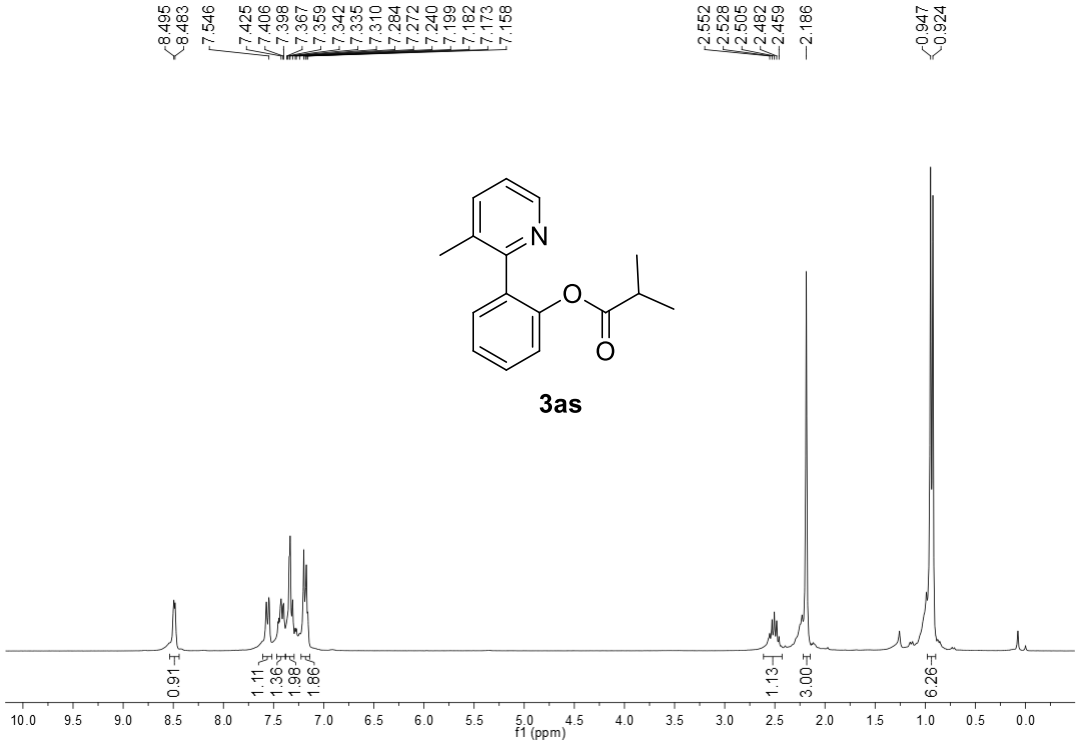
3ap


8.492
8.482
7.620
7.424
7.405
7.380
7.329
7.262
7.161
7.142
6.452
6.412
2.235
0.000
N
O
O
CF3
3aq
1.00
2.84
3.56
1.13
1.12
0.93
1.19
1.02
1.04
3.18
f1 (ppm)

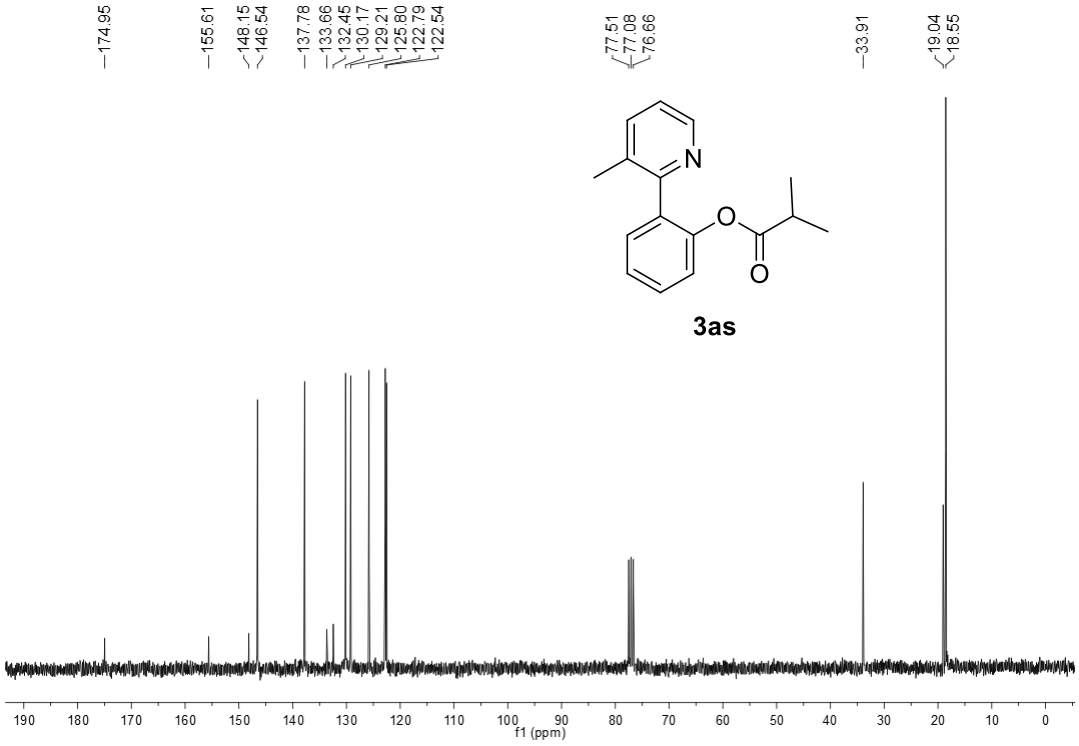

164.2
155.5
148.0
146.7
144.3
138.0
137.4
128.3
126.0
125.9
125.9
125.9
125.8
125.1
122.7
122.6
122.4
119.5
77.4
77.0
76.7
19.1
N
O
O
CF3
3aq
f1 (ppm)


8.491
8.477
7.566
7.541
7.453
7.445
7.424
7.405
7.397
7.352
7.328
7.307
7.283
7.269
7.197
7.182
7.173
7.156
2.179
1.001
N
O
O
3ar
0.88
1.01
0.98
1.84
1.81
3.00
9.00
f1 (ppm)

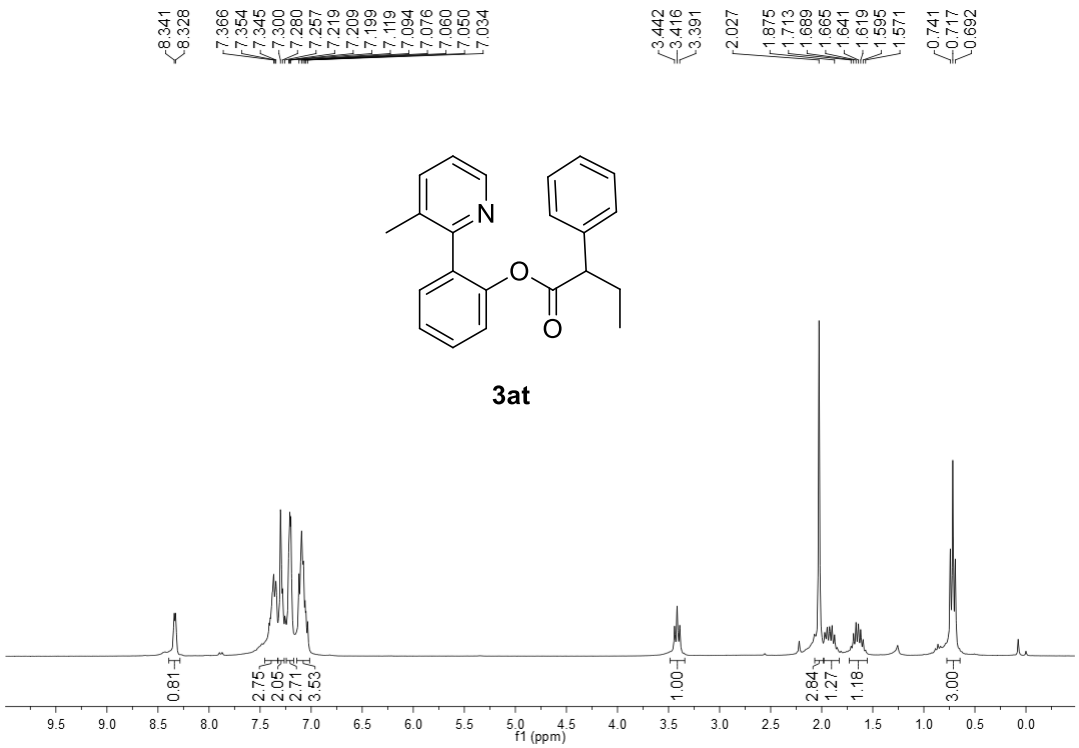

176.3
155.7
148.3
146.5
137.7
133.7
132.5
130.0
129.2
125.7
122.8
122.5
77.5
77.1
76.6
38.8
26.8
19.0
N
O
O
3ar
f1 (ppm)


8.495
8.483
7.546
7.425
7.406
7.398
7.367
7.359
7.342
7.335
7.310
7.284
7.272
7.240
7.199
7.182
7.173
7.158
2.552
2.528
2.505
2.482
2.459
2.186
0.947
0.924
N
O
O
0.91
1.11
1.36
1.98
1.86
1.13
3.00
6.26
f1 (ppm)

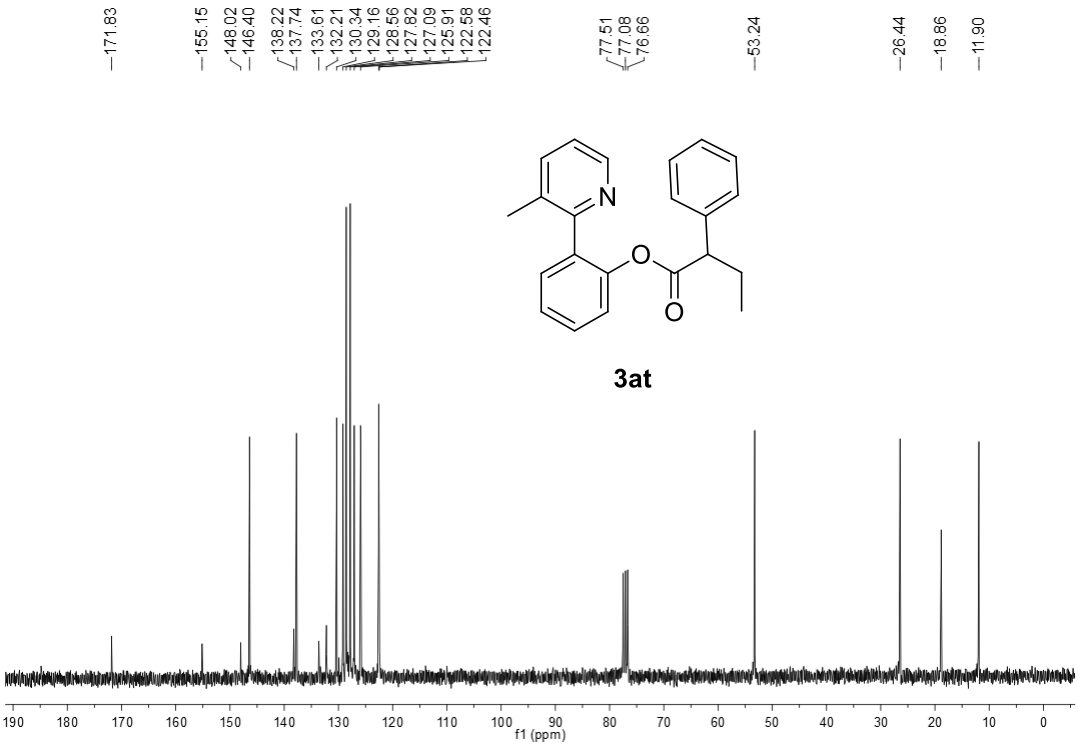
3as


174.95
155.61
148.15
146.54
137.78
133.66
132.45
130.17
129.21
125.80
122.79
122.54
77.51
77.08
76.66
33.91
19.04
18.55
N
O
O
f1 (ppm)

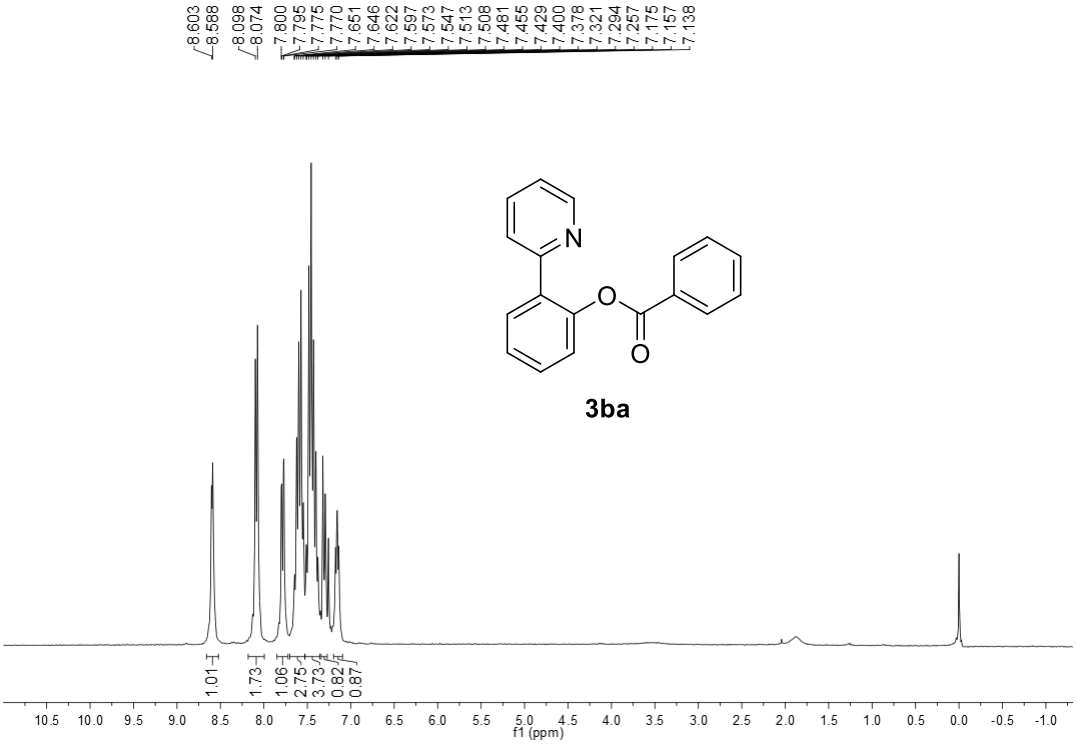
3as

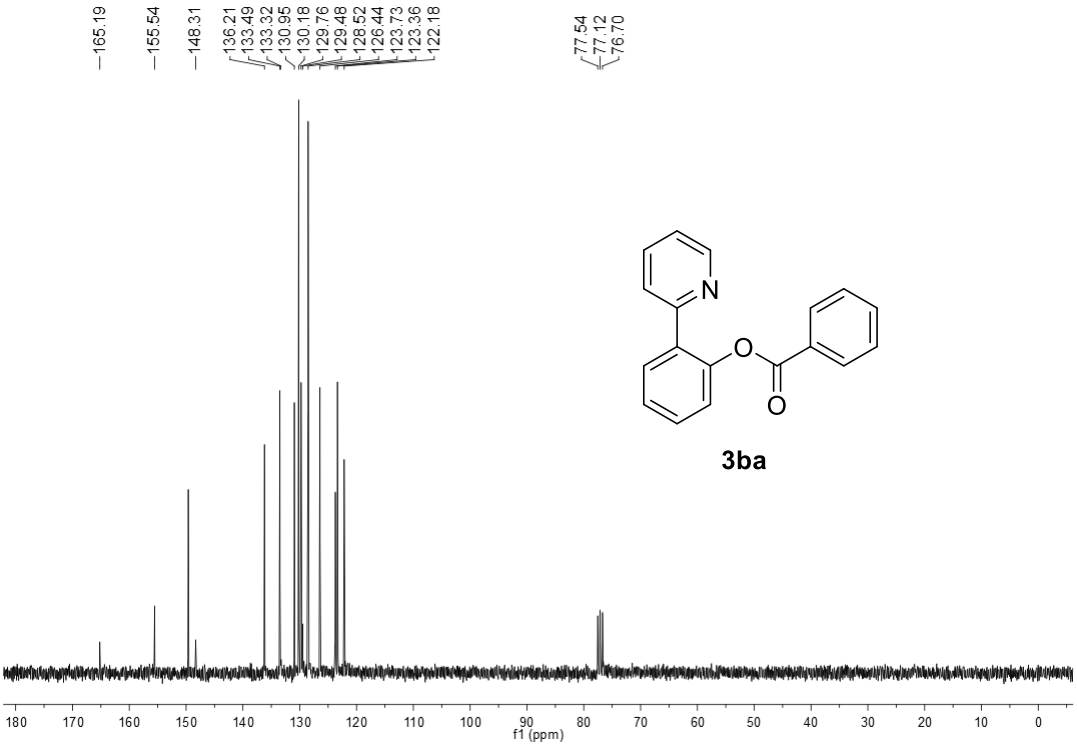

8.341
8.328
7.366
7.354
7.345
7.300
7.280
7.257
7.219
7.209
7.199
7.119
7.094
7.076
7.060
7.050
7.034
3.442
3.416
3.391
2.027
1.875
1.713
1.689
1.665
1.641
1.619
1.595
1.571
0.741
0.717
0.692
N
O
O
0.81
2.75
2.05
2.71
3.53
1.00
2.84
1.27
1.18
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

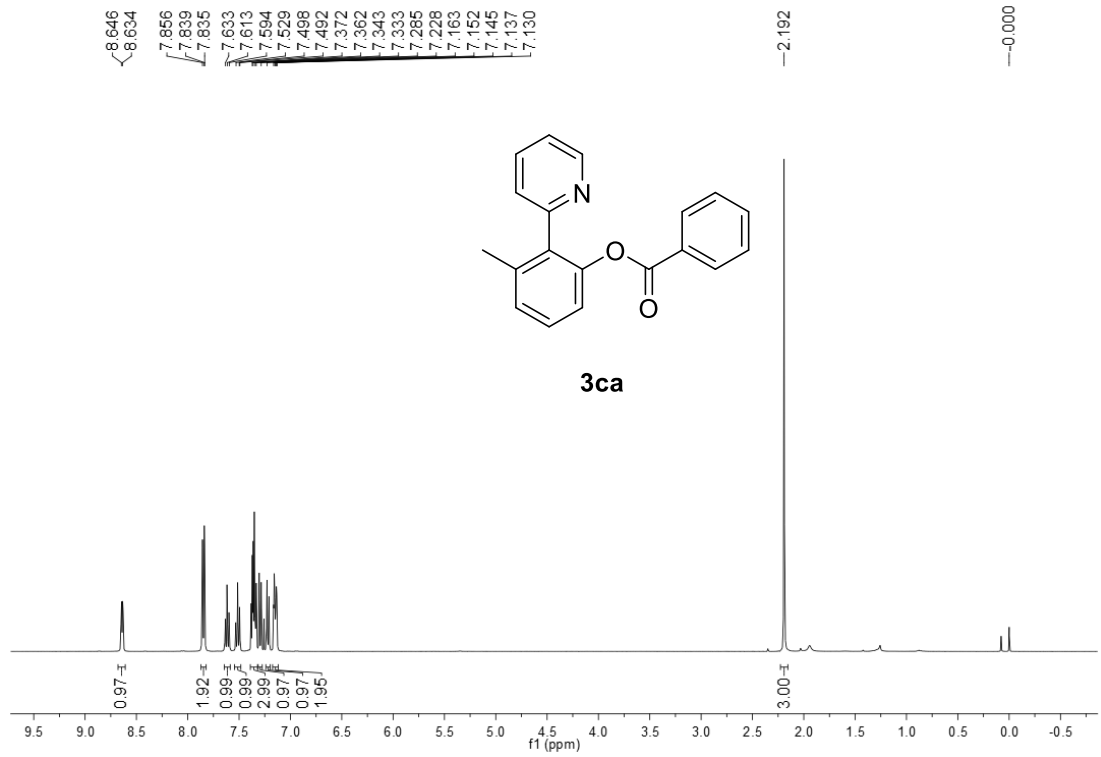
3at


171.83
155.15
148.02
146.40
138.22
137.74
133.61
132.21
130.34
129.16
128.56
127.82
127.09
125.91
122.58
122.46
77.51
77.08
76.66
53.24
26.44
18.86
11.90
N
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

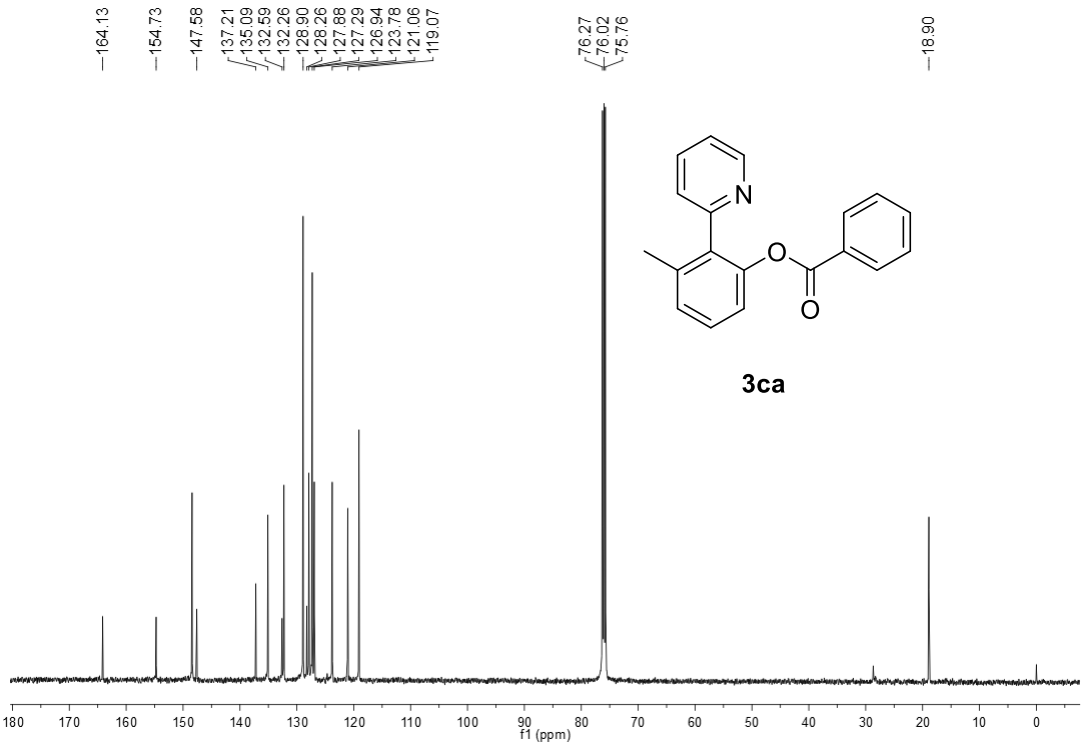
3at


8.603
8.588
8.098
8.074
7.800
7.795
7.775
7.770
7.651
7.646
7.622
7.597
7.573
7.547
7.513
7.508
7.481
7.455
7.429
7.400
7.378
7.321
7.294
7.257
7.175
7.157
7.138
1.01
1.73
1.06
2.75
3.73
0.82
0.87
f1 (ppm)
N
O
O
3ba

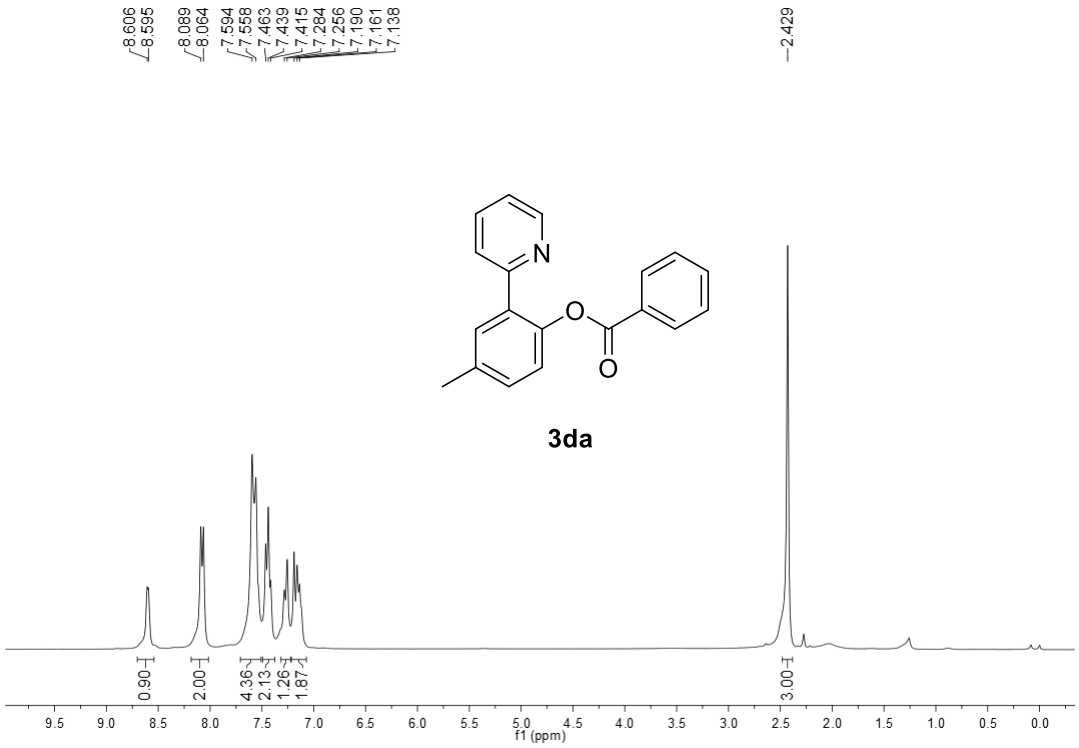

165.19
155.54
148.31
136.21
133.49
133.32
130.95
130.18
129.76
129.48
128.52
126.44
123.73
123.36
122.18
77.54
77.12
76.70
f1 (ppm)
N
O
O
3ba

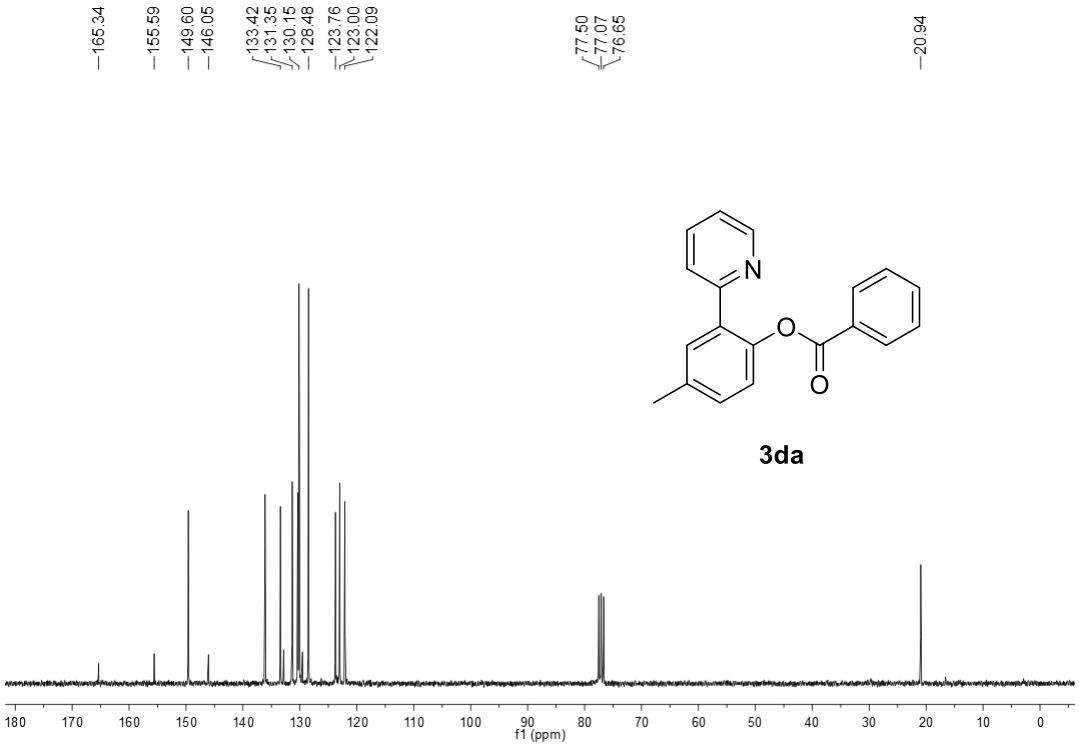

8.646
8.634
7.856
7.839
7.835
7.633
7.613
7.594
7.529
7.498
7.492
7.372
7.362
7.343
7.333
7.285
7.228
7.163
7.152
7.145
7.137
7.130
2.192
0.000
0.97
1.92
0.99
0.99
2.99
0.97
0.97
1.95
3.00
f1 (ppm)

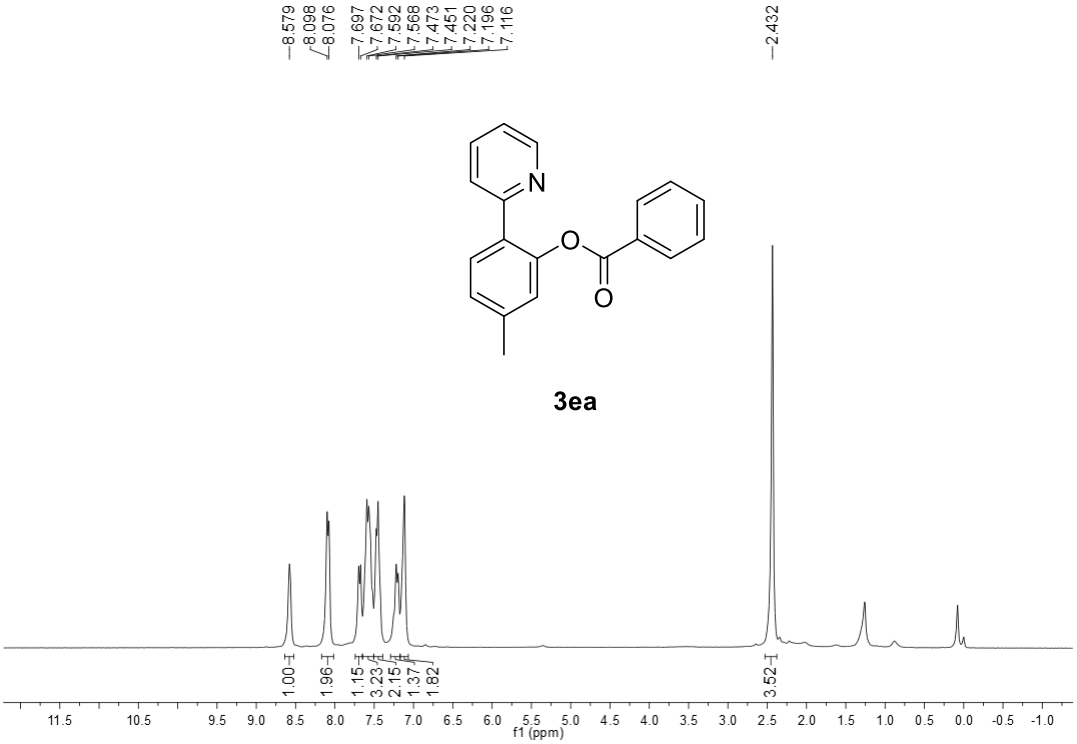
3ca


164.13
154.73
147.58
137.21
135.09
132.59
132.26
128.90
128.26
127.88
127.29
126.94
123.78
121.06
119.07
76.27
76.02
75.76
18.90
f1 (ppm)

3ca


8.606
8.595
8.089
8.064
7.594
7.558
7.463
7.439
7.415
7.284
7.256
7.190
7.161
7.138
2.429
N
O
O
3da
0.90
2.00
4.36
2.13
1.26
1.87
3.00
f1 (ppm)


165.34
155.59
149.60
146.05
133.42
131.35
130.15
128.48
123.76
123.00
122.09
77.50
77.07
76.65
20.94
N
O
O
3da
f1 (ppm)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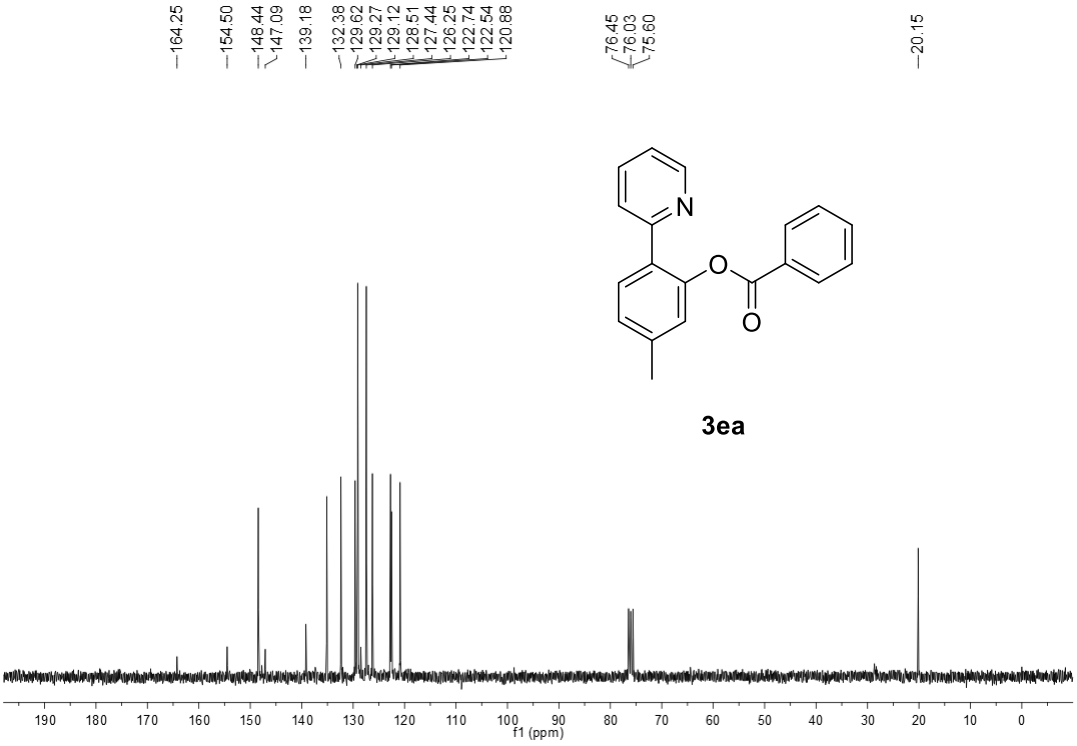
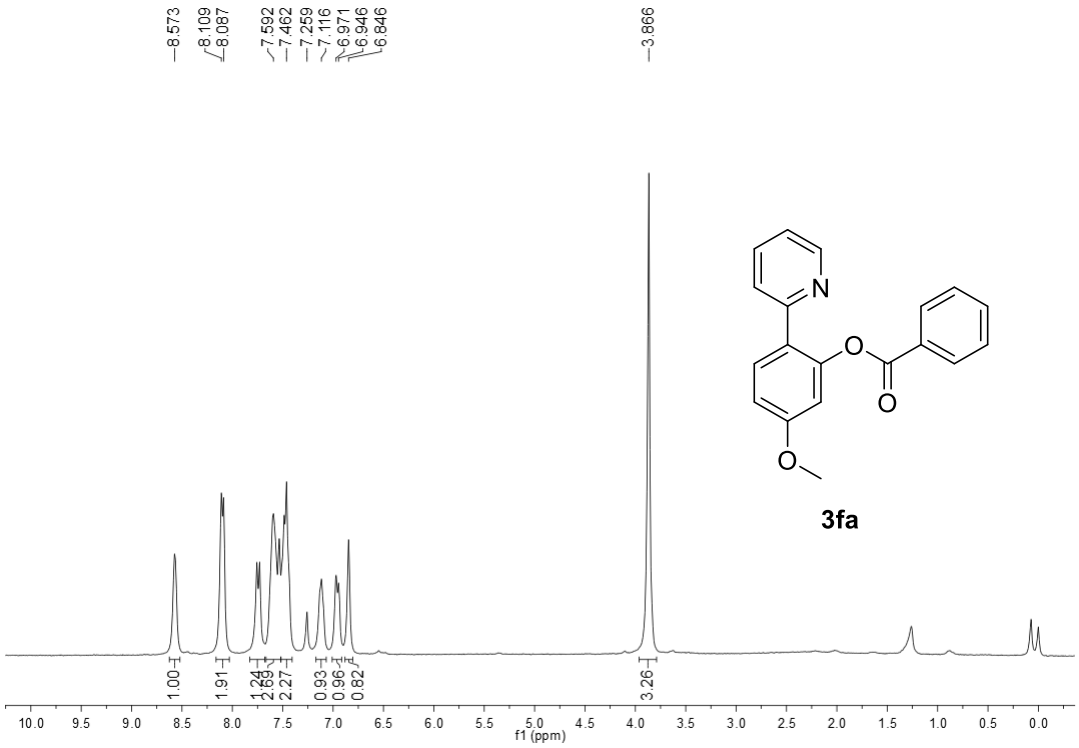
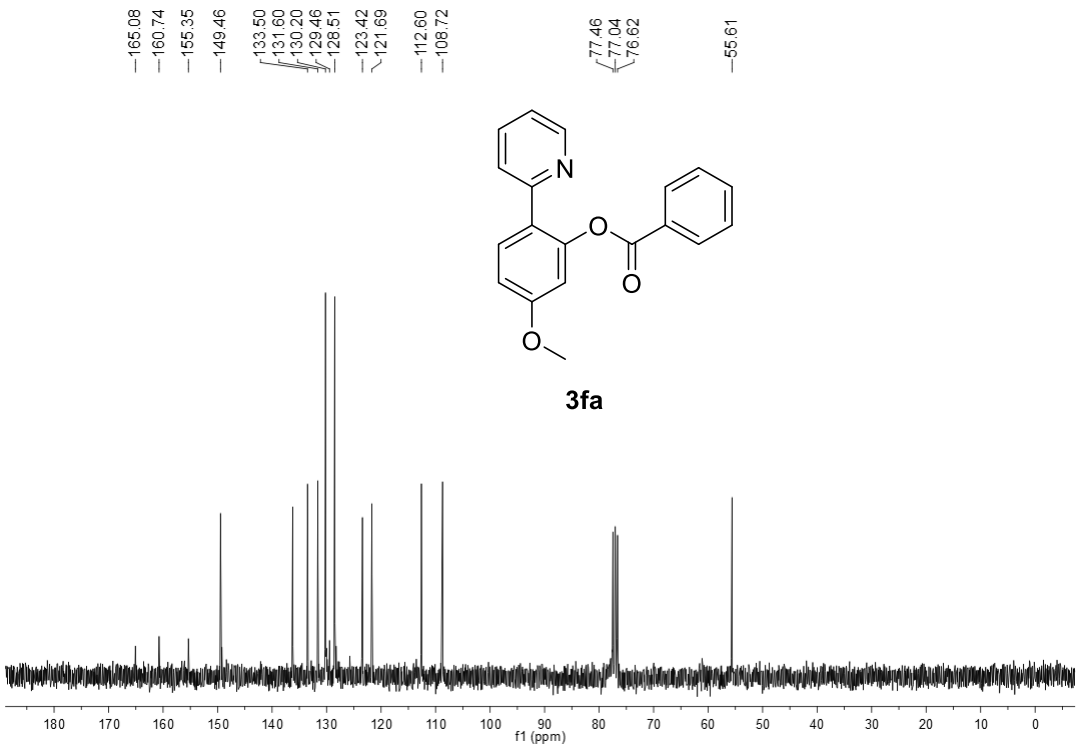
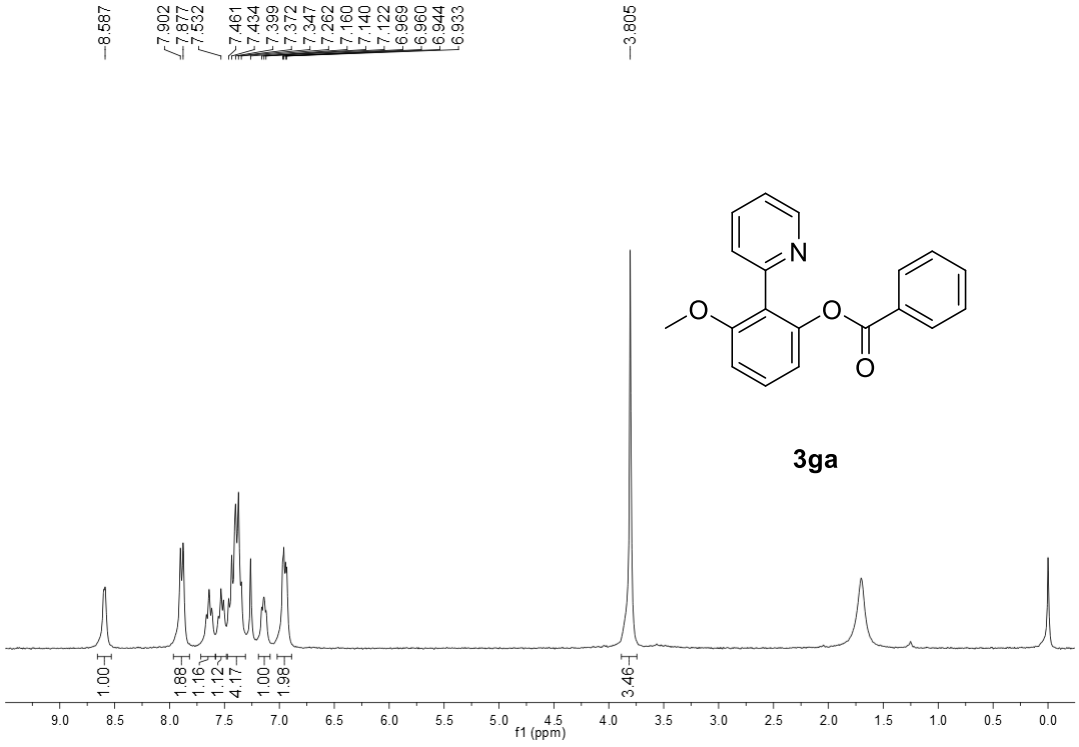
8.076
7.697
7.672
7.592
7.568
7.473
7.451
7.220
7.196
7.116
2.432
N
O
O
3ea
1.00
1.96
1.15
3.23
2.15
1.37
1.82
3.52
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

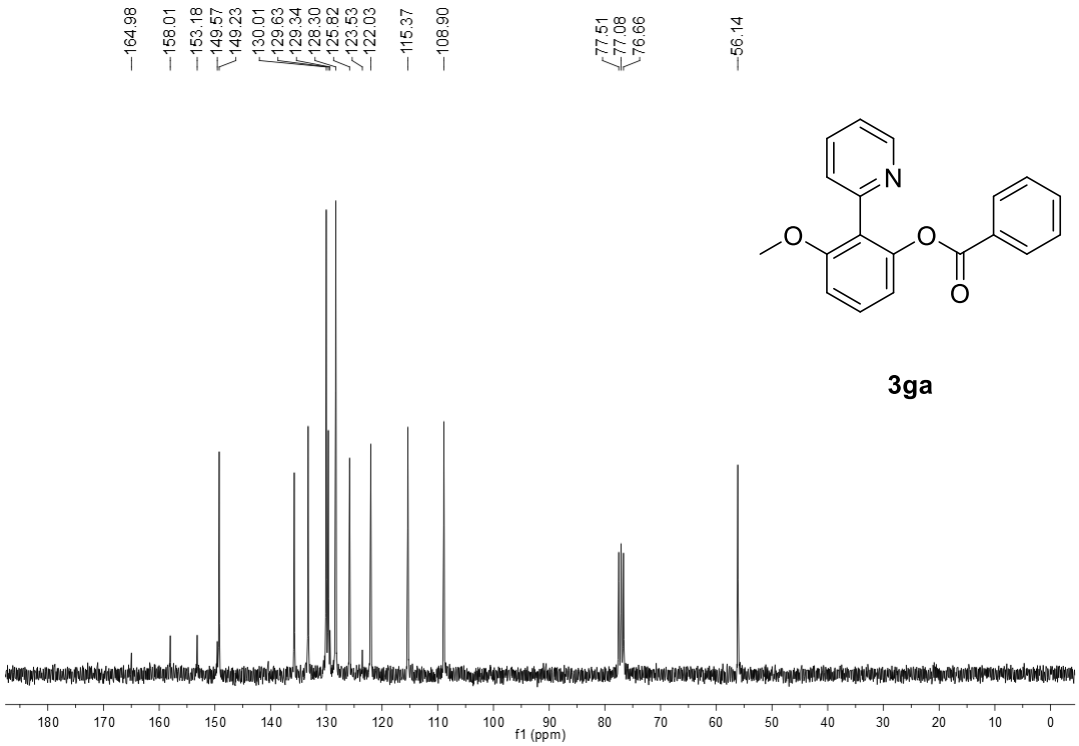

164.25
154.50
148.44
147.09
139.18
132.38
129.62
129.27
129.12
128.51
127.44
126.25
122.74
122.54
120.88
76.45
76.03
75.60
20.15
N
O
O
3ea
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.573
8.109
8.087
7.592
7.462
7.259
7.116
6.971
6.946
6.846
3.866
1.00
1.91
1.24
2.69
2.27
0.93
0.96
0.82
3.26
f1 (ppm)
3fa

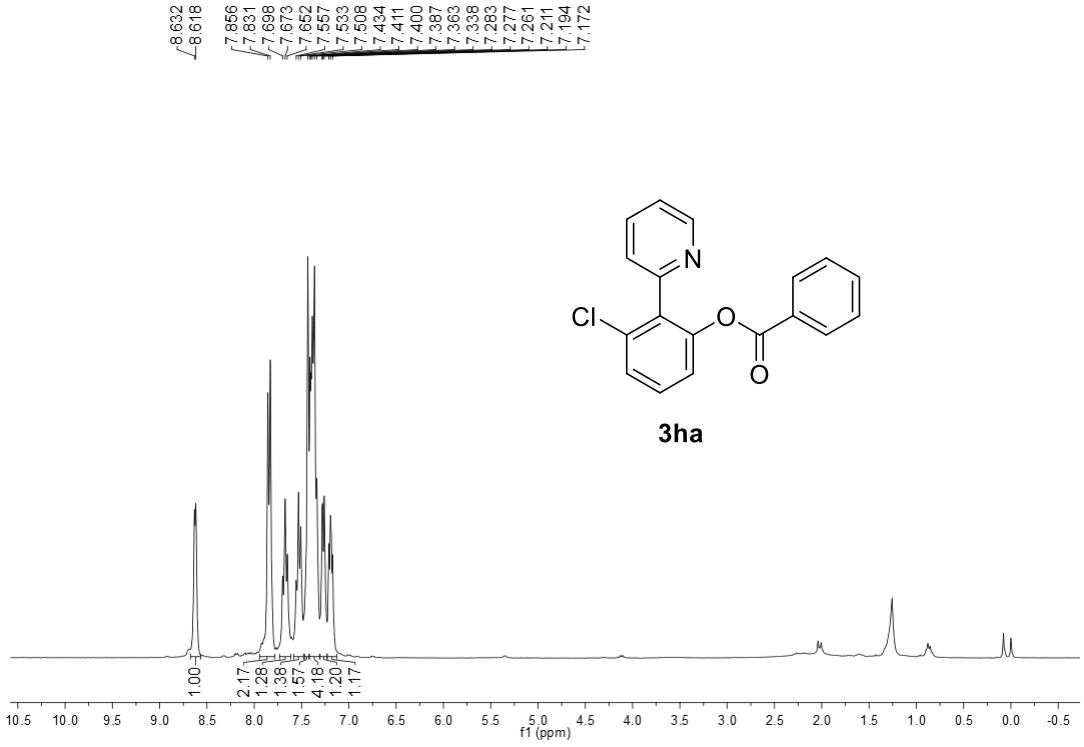

165.08
160.74
155.35
149.46
133.50
131.60
130.20
129.46
128.51
123.42
121.69
112.60
108.72
77.46
77.04
76.62
55.61
f1 (ppm)
3fa


8.587
7.902
7.877
7.532
7.461
7.434
7.399
7.372
7.347
7.262
7.160
7.140
7.122
6.969
6.960
6.944
6.933
3.805
N
O
O
O
1.00
1.88
1.16
1.12
4.17
1.00
1.98
3.46
f1 (ppm)

3ga


164.98
158.01
153.18
149.57
149.23
130.01
129.63
129.34
128.30
125.82
123.53
122.03
115.37
108.90
77.51
77.08
76.66
56.14
N
O
O
O
f1 (ppm)

3ga


8.632
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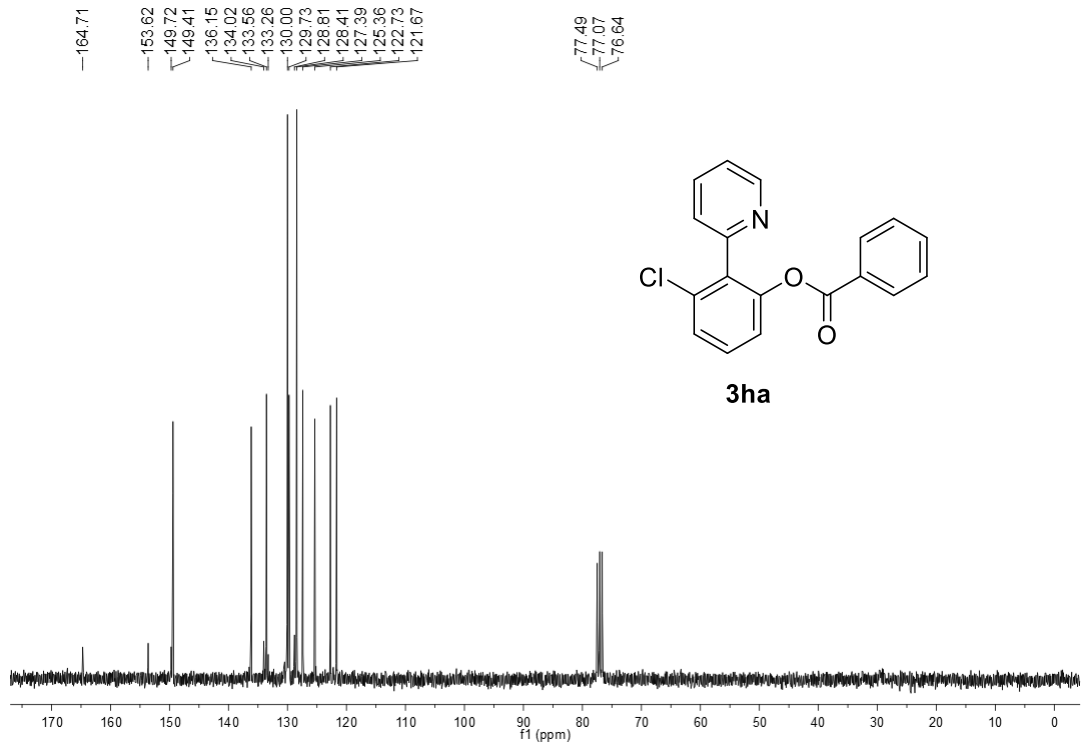
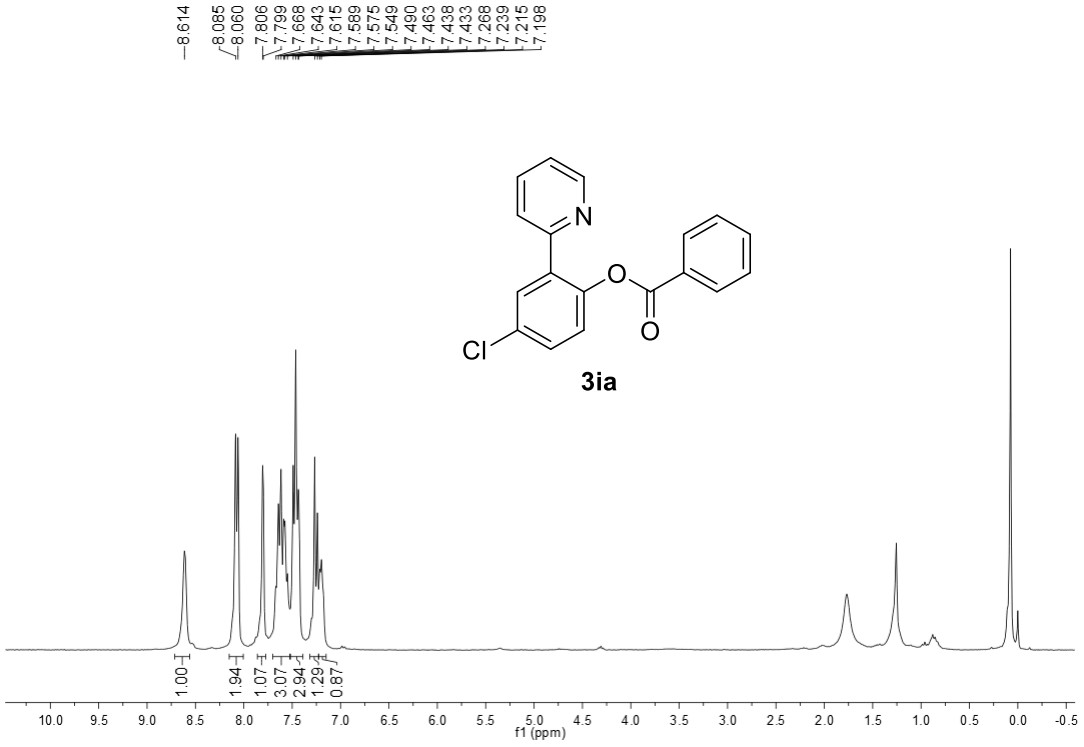
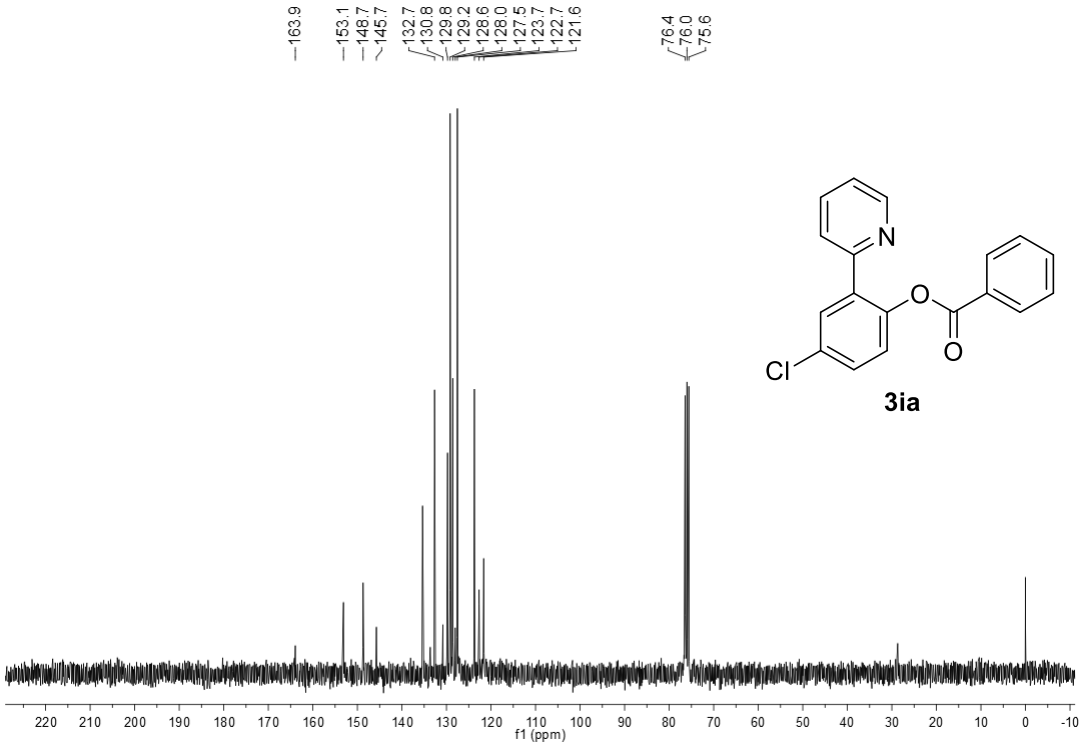
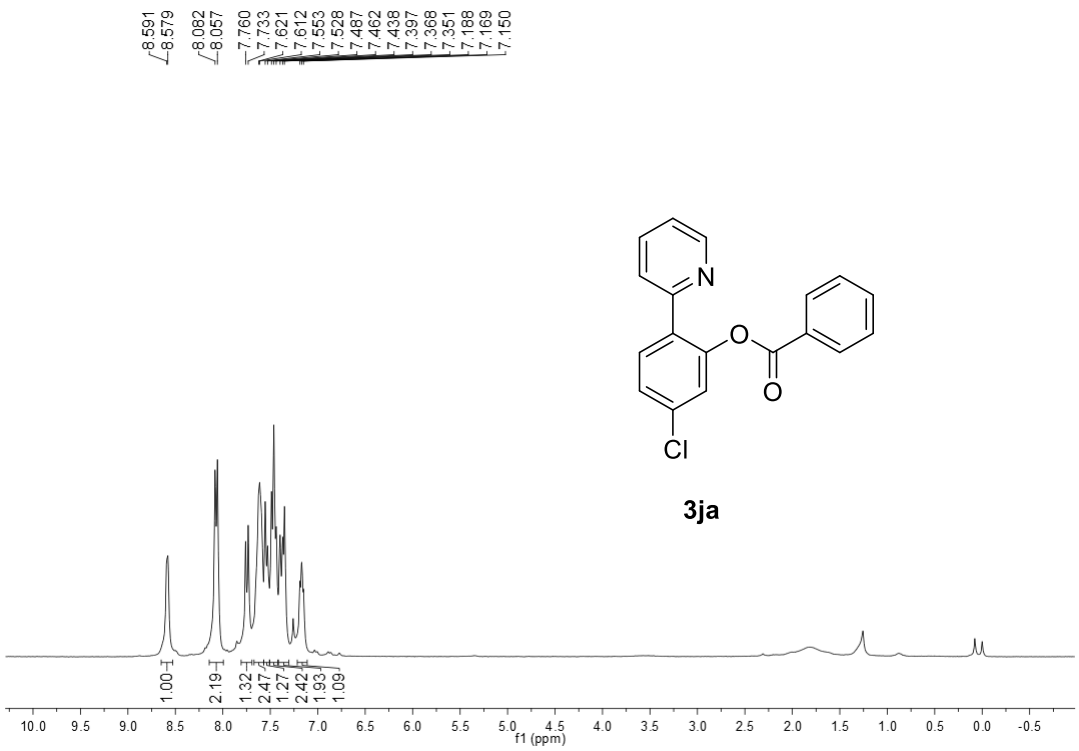
7.673
7.652
7.557
7.533
7.508
7.434
7.411
7.400
7.387
7.363
7.338
7.283
7.277
7.261
7.211
7.194
7.172
N
Cl
O
O
3ha
1.00
2.17
1.28
1.38
1.57
4.18
1.20
1.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

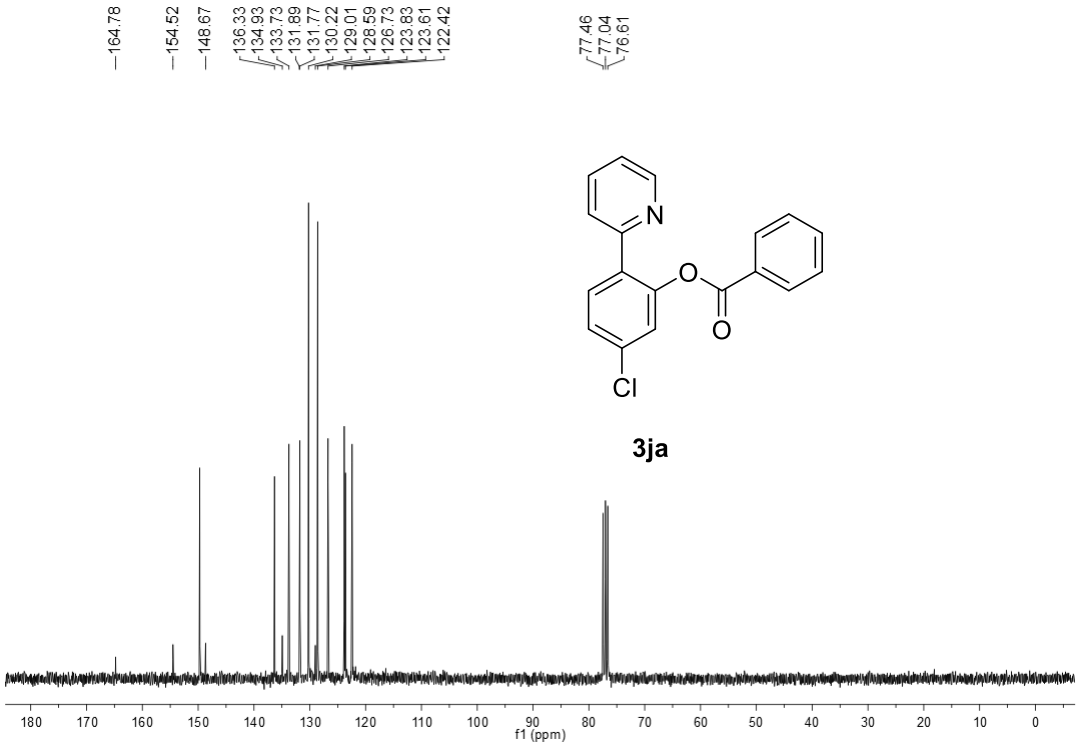

164.71
153.62
149.72
149.41
136.15
134.02
133.56
133.26
130.00
129.73
128.81
128.41
127.39
125.36
122.73
121.67
77.49
77.07
76.64
N
Cl
O
O
3ha
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.614
8.085
8.060
7.806
7.799
7.668
7.643
7.615
7.589
7.575
7.549
7.490
7.463
7.438
7.433
7.268
7.239
7.215
7.198
N
O
O
Cl
3ia
1.00
1.94
1.07
3.07
2.94
1.29
0.87
f1 (ppm)

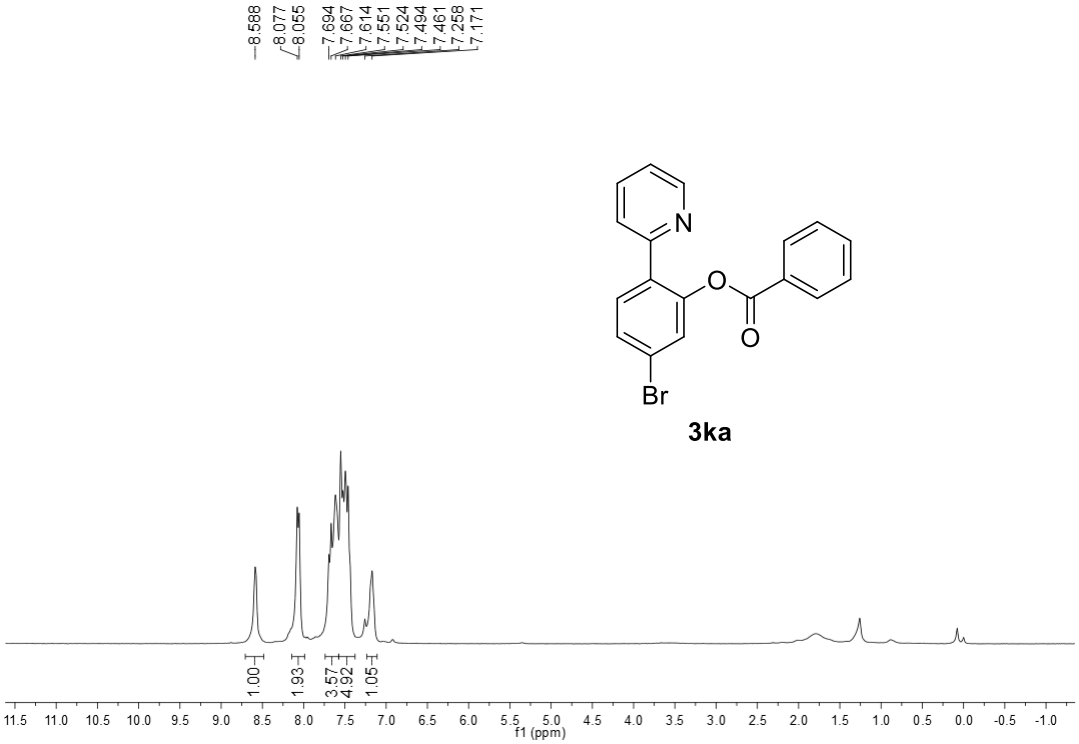

163.9
153.1
148.7
145.7
132.7
130.8
129.8
129.2
128.6
128.0
127.5
123.7
122.7
121.6
76.4
76.0
75.6
N
O
O
Cl
3ia
f1 (ppm)

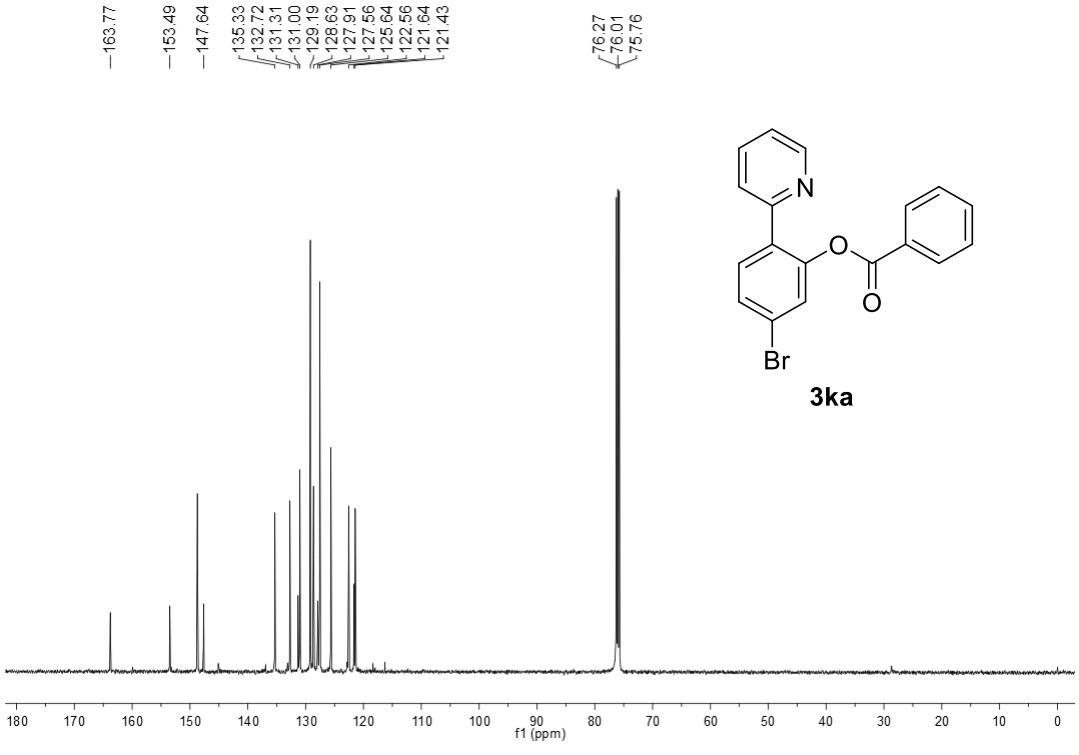

8.591
8.579
8.082
8.057
7.760
7.733
7.621
7.612
7.553
7.528
7.487
7.462
7.438
7.397
7.368
7.351
7.188
7.169
7.150
N
O
O
Cl
1.00
2.19
1.32
2.47
1.27
2.42
1.93
1.09
f1 (ppm)

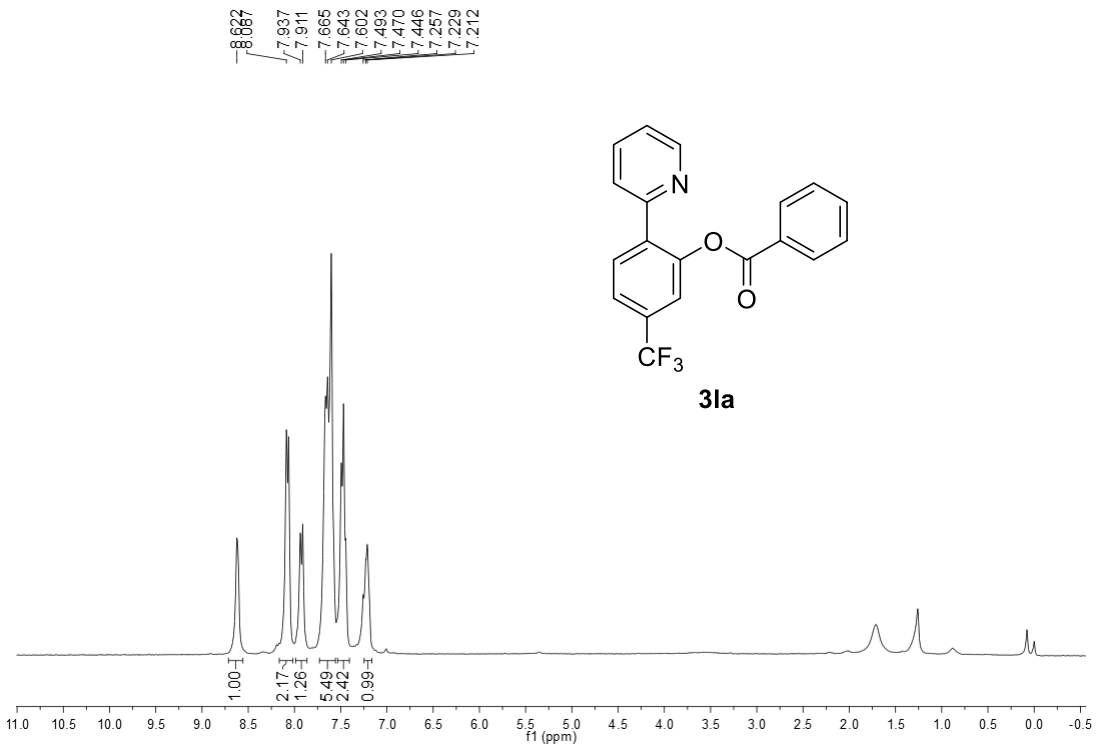
3ja

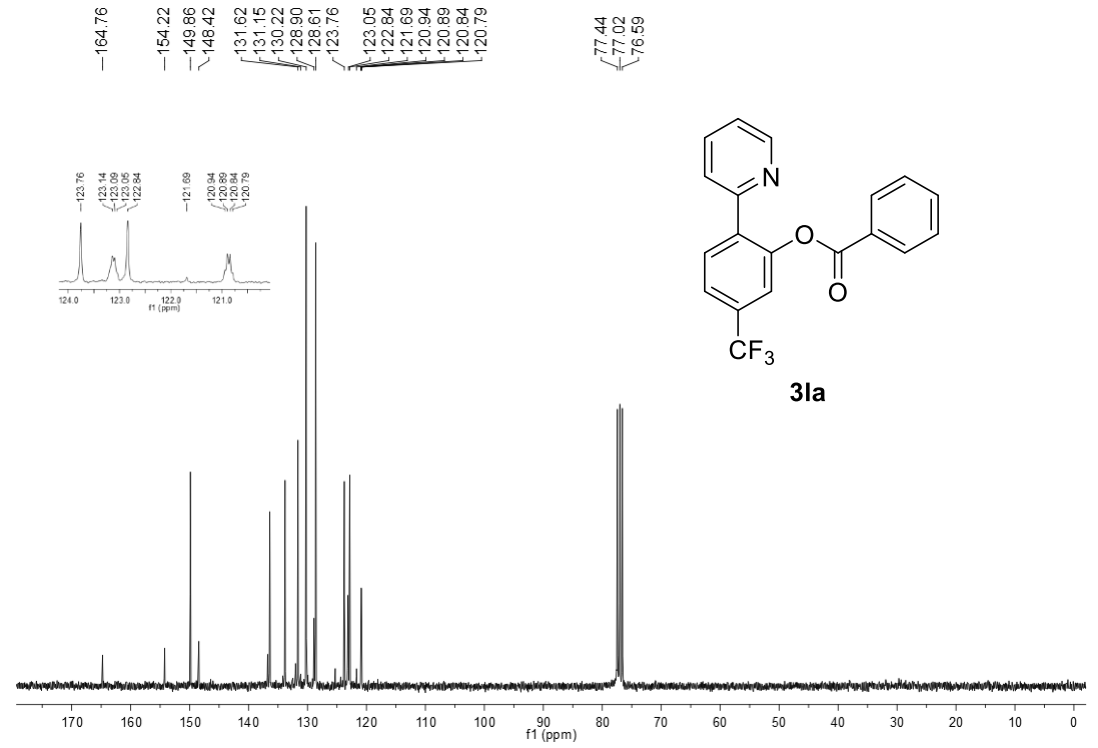

164.78
154.52
148.67
136.33
134.93
133.73
131.89
131.77
130.22
129.01
128.59
126.73
123.83
123.61
122.42
77.46
77.04
76.61
N
O
O
Cl
f1 (ppm)

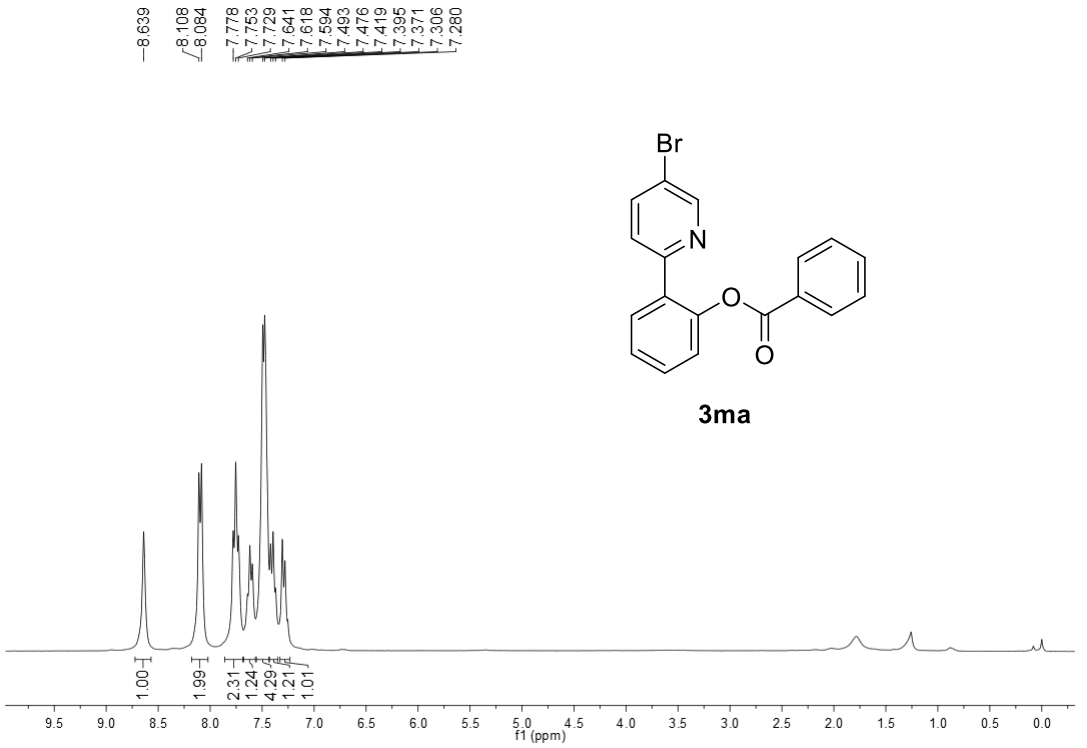
3ja

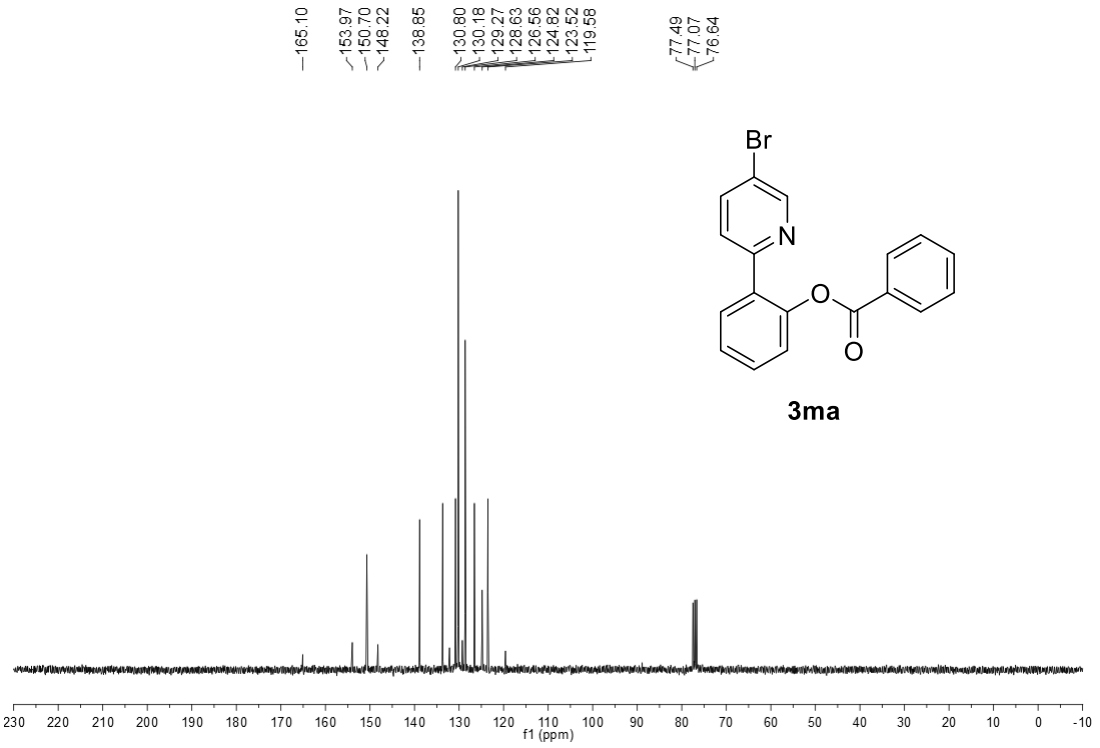

8.588
8.077
8.055
7.694
7.667
7.614
7.551
7.524
7.494
7.461
7.258
7.171
N
O
O
Br
3ka
1.00
1.93
3.57
4.92
1.05
f1 (ppm)

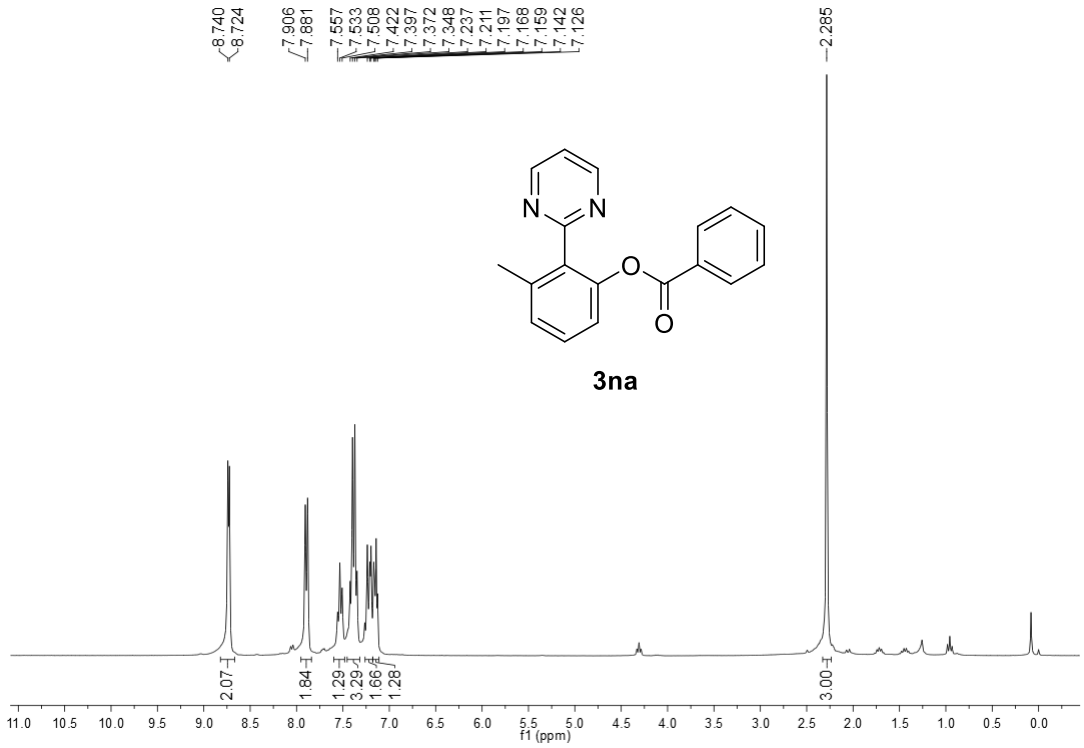

163.77
153.49
147.64
135.33
132.72
131.31
131.00
129.19
128.63
127.91
127.56
125.64
122.56
121.64
121.43
76.27
76.01
75.76
N
O
O
Br
3ka
f1 (ppm)


8.622
8.087
7.937
7.911
7.665
7.643
7.602
7.493
7.470
7.446
7.257
7.229
7.212
N
O
O
CF3
3la
1.00
2.17
1.26
5.49
2.42
0.99
f1 (ppm)

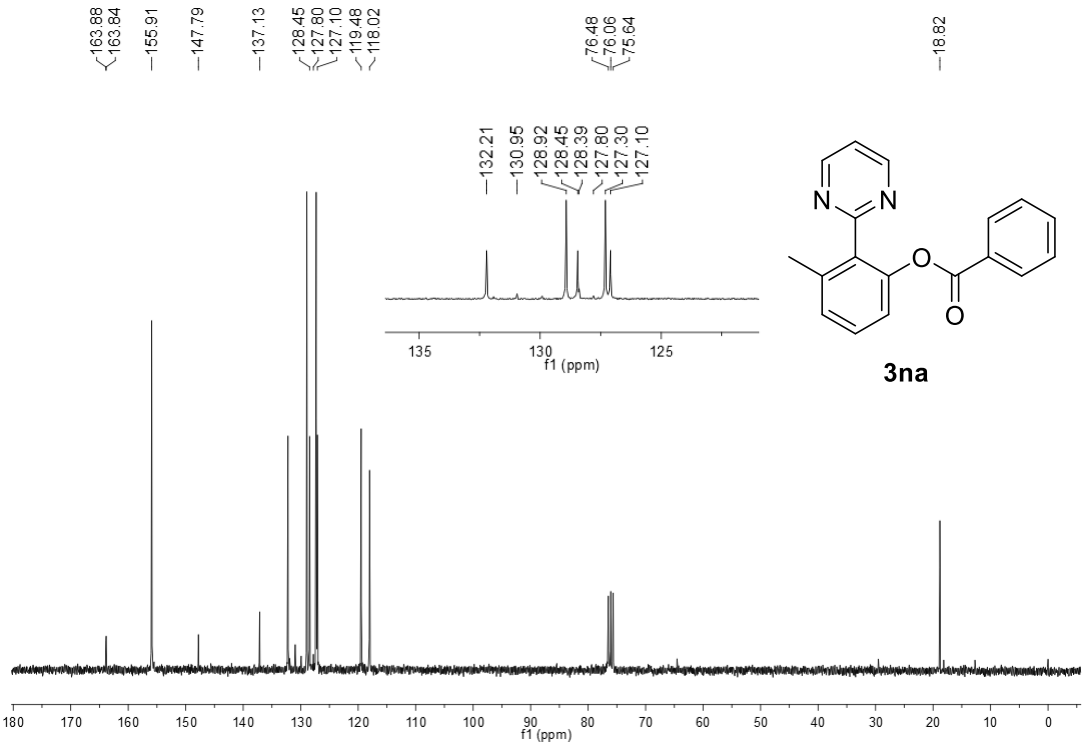

164.76
154.22
149.86
148.42
131.62
131.15
130.22
128.90
128.61
123.76
123.05
122.84
121.69
120.94
120.89
120.84
120.79
77.44
77.02
76.59
123.76
123.14
123.09
123.05
122.84
121.69
120.94
120.89
120.84
120.79
N
O
O
CF3
3la
f1 (ppm)


8.639
8.108
8.084
7.778
7.753
7.729
7.641
7.618
7.594
7.493
7.476
7.419
7.395
7.371
7.306
7.280
Br
N
O
O
3ma
1.00
1.99
2.31
1.24
4.29
1.21
1.01
f1 (ppm)

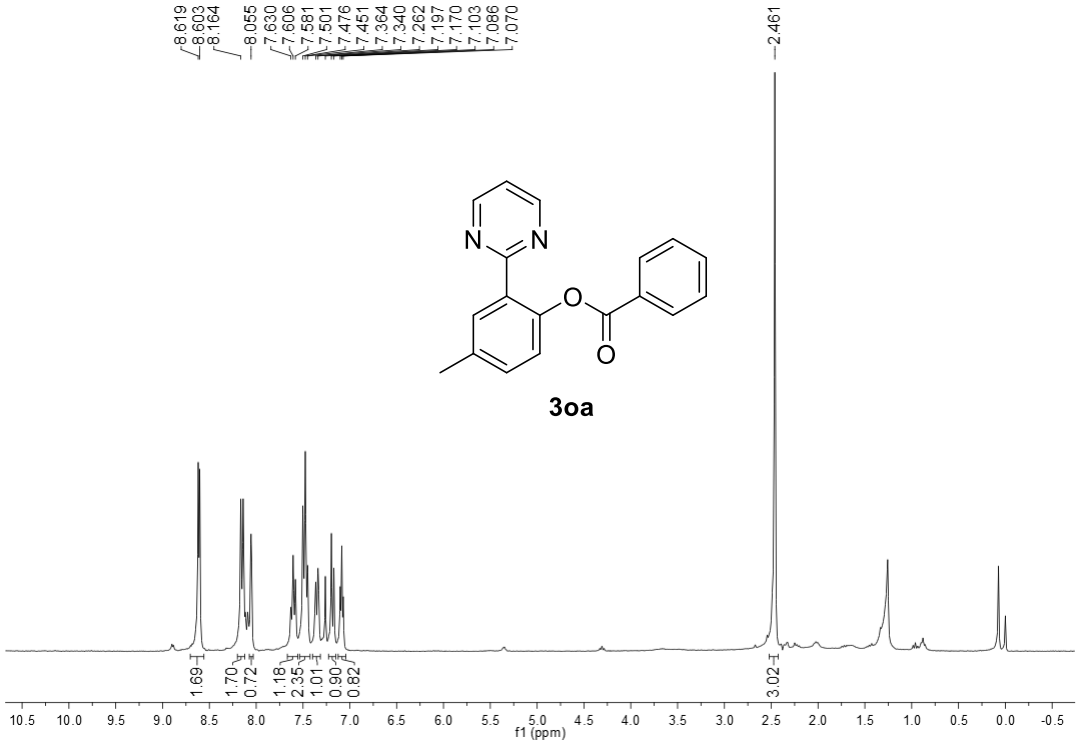

165.10
153.97
150.70
148.22
138.85
130.80
130.18
129.27
128.63
126.56
124.82
123.52
119.58
77.49
77.07
76.64
Br
N
O
O
3ma
f1 (ppm)

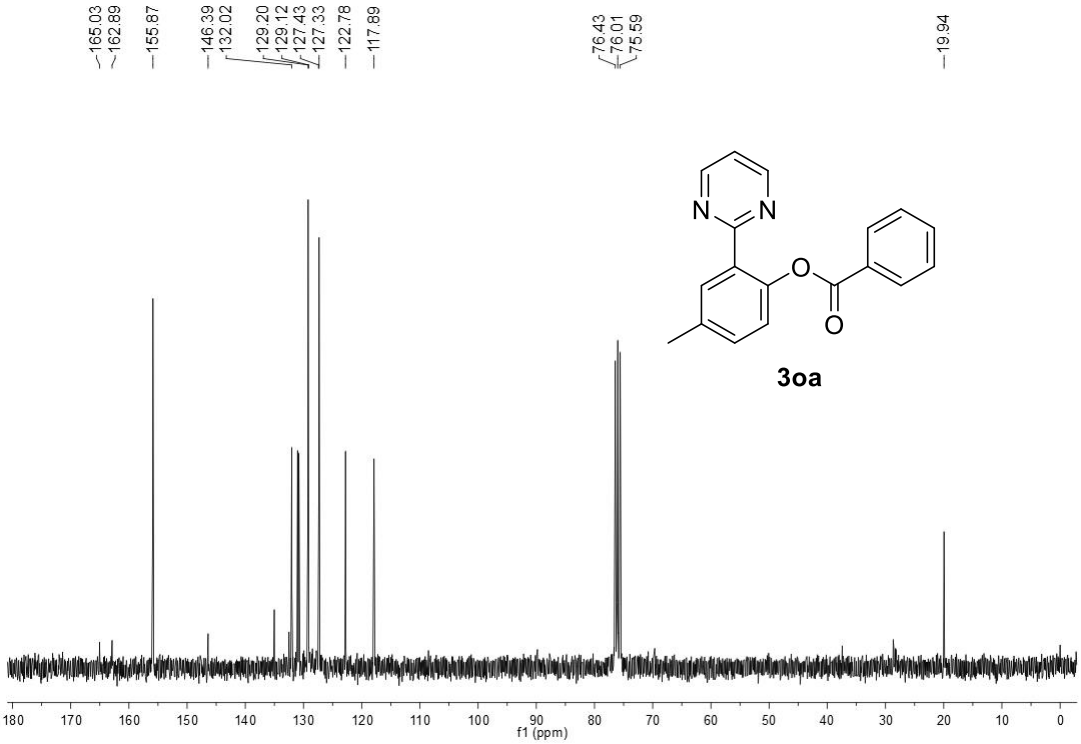

8.740
8.724
7.906
7.881
7.557
7.533
7.508
7.422
7.397
7.372
7.348
7.237
7.211
7.197
7.168
7.159
7.142
7.126
2.285
2.07
1.84
1.29
3.29
1.66
1.28
3.00
f1 (ppm)

3na


163.88
163.84
155.91
147.79
137.13
128.45
127.80
127.10
119.48
118.02
76.48
76.06
75.64
18.82
132.21
130.95
128.92
128.45
128.39
127.80
127.30
127.10
f1 (ppm)

3na


8.619
8.603
8.164
8.055
7.630
7.606
7.581
7.501
7.476
7.451
7.364
7.340
7.262
7.197
7.170
7.103
7.086
7.070
2.461
N
N
O
O
3oa
1.69
1.70
0.72
1.18
2.35
1.01
0.90
0.82
3.02
f1 (ppm)


165.03
162.89
155.87
146.39
132.02
129.20
129.12
127.43
127.33
122.78
117.89
76.43
76.01
75.59
19.94
N
N
O
O
3oa
f1 (ppm)