Electronic Supporting Information

Palladium Catalyzed Oxidative Suzuki Coupling Reaction of Indolizine at 3-position using Oxygen Gas as the Solo Oxidant

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General Methods and materials:

Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker 400 MHz spectrometers. Chemical shifts were reported relative to internal tetramethylsilane (δ 0.00 ppm) or $CDCl_3$ (δ 7.26 ppm) for ^{1}H NMR and $CDCl_3$ (δ 77.0 ppm) for ^{13}C NMR. Flash column chromatography was performed on 300-400 mesh silica gels. Analytical thin layer chromatography was performed with pre-coated glass baked plates (250μ) and visualized by fluorescence. HRMS were recorded on Bruker micrOTOF-Q spectrometer. IR spectra were recorded by Nicolet Avatar 360 spectrometer.

Substrates were synthesized according to the literature as below:

1. N. P. Buu-Hoi, P. Jacquignon, N. D. Xuong, D. Lavit, *J. Org. Chem.* **1954**, *19*, 1370-1375. (**1n** and **1o)**
2. L. Zhang, F. Liang, L. Sun, Y. Hu, H. Hu, *Synthesis*, **2000**, 1733-1737. (Other indolizines)

Characteristic data of new compounds

Compound ***3aa*** (N,N-dimethyl-3-phenylindolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.23 (d, J = 7.1 Hz, 1H), 7.96 (d, J = 9.0 Hz, 1H), 7.54 (d, J = 7.2 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.2 Hz, 1H), 6.97 (s, 1H), 6.91 (dd, J = 8.8, 6.7 Hz, 1H), 6.61 (t, J = 6.6 Hz, 1H), 3.20 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.8, 135.1, 131.6, 129.1, 128.5, 127.8, 125.1, 122.6, 120.3, 120.2, 114.6, 112.1, 107.5; IR (NaCl): 2958, 2924, 2853, 1600, 1541, 1494, 1511, 1456, 1411; HRMS (ESI): m/z calcd for $C_{17}H_{16}N_2O$: 265.1341 $[M+H]^+$; found: 265.1341.

Compound ***3ab*** (N,N-dimethyl-3-(4-(trifluoromethyl)phenyl)indolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.27 (d, J = 7.1 Hz, 1H), 7.98 (d, J = 9.1 Hz, 1H), 7.76 (d, J = 8.2 Hz, 2H), 7.68 (d, J = 8.2 Hz, 2H), 7.05 (s, 4H), 6.98 (dd, J = 8.8, 7.0 Hz, 1H), 6.69 (t, J = 6.6 Hz, 1H), 3.23 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.5, 135.7, 135.2 (q, J = 5.1 Hz), 129.5 (q, J = 129.7 Hz), 128.3, 126.1 (q, J = 15.0 Hz), 123.6, 122.7, 122.4, 120.9, 120.4, 115.5, 112.7, 108.0; IR (NaCl): 2933, 1612, 1514, 1492, 1452; HRMS (ESI): m/z calcd for $C_{18}H_{15}F_3N_2O$: 333.1215 $[M+H]^+$; found: 333.1218.

Compound ***3ac*** (3-(4-chlorophenyl)-N,N-dimethylindolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.20 (d, J = 7.1 Hz, 1H), 7.98 (d, J = 9.1 Hz, 1H), 7.49 (s, 4H), 6.99 (s, 1H), 6.96 (dd, J = 8.6, 7.0 Hz, 1H), 6.66 (t, J = 6.7 Hz, 1H), 3.23 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.6, 135.2, 133.6, 130.0, 129.7, 129.4, 123.8, 122.4, 120.5, 120.3, 114.8, 112.4, 107.7; IR (NaCl): 2927, 1609, 1538, 1509, 1477, 1450, 1411; HRMS (ESI): m/z calcd for $C_{17}H_{15}ClN_2O$: 299.0951 $[M+H]^+$; found: 299.0952.

Compound ***3ad*** (N,N-dimethyl-3-(m-tolyl)indolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.22 (d, J = 7.1 Hz, 1H), 7.96 (d, J = 9.1 Hz, 1H), 7.39 – 7.30 (m, 3H), 7.18 (d, J = 7.0 Hz, 1H), 6.95 (s, 1H), 6.89 (dd, J = 8.8, 6.8 Hz, 1H), 6.59 (t, J = 6.8 Hz, 1H), 3.19 (s, 6H), 2.41 (s, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz): 167.8, 138.8, 135.1, 131.5, 129.2, 129.0, 128.6, 125.5, 125.3, 122.8, 120.2, 120.2, 114.6, 112.0, 107.3, 21.5; IR (NaCl): 2924, 1605, 1510, 1449, 1400; HRMS (ESI): m/z calcd for $C_{18}H_{18}N_2O$: 279.1497 $[M+H]^+$; found: 279.1492.

Compound ***3ae*** (N,N-dimethyl-3-(p-tolyl)indolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.23 (d, J = 7.1 Hz, 1H), 7.98 (d, J = 9.1 Hz, 1H), 7.45 (d, J = 7.9 Hz, 2H), 7.32 (d, J = 7.8 Hz, 2H), 6.97 (s, 1H), 6.96 (dd, J = 8.5, 6.9 Hz, 1H), 6.62 (t, J = 6.6 Hz, 1H), 3.23 (s, 6H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.8, 137.7, 135.0, 129.8, 128.7, 128.5, 125.2, 122.7, 120.2, 120.1, 114.4, 111.9, 107.3, 21.3; IR (NaCl): 2923, 1606, 1546, 1511, 1450, 1405; HRMS (ESI): m/z calcd for $C_{18}H_{18}N_2O$: 279.1497 $[M+H]^+$; found: 279.1498.

Compound ***3af*** (N,N-dimethyl-3-(o-tolyl)indolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.04 (d, J = 9.0 Hz, 1H), 7.59 (d, J = 7.0 Hz, 1H), 7.43 – 7.30 (m, 4H), 6.95 (dd, J = 8.6, 7.2 Hz, 1H), 6.93 (s, 1H), 6.61 (t, J = 6.7 Hz, 1H), 3.25 (s, 6H) , 2.15 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.9, 138.5, 134.7, 131.4, 130.6, 130.6, 128.9, 126.2, 124.1, 123.0, 120.2, 120.1, 114.8, 111.9, 106.4, 19.7; IR (NaCl): 3057, 3015, 2925, 1745, 1608, 1543, 1510, 1451, 1407; HRMS (ESI): m/z calcd for $C_{18}H_{18}N_2O_2$: 279.1497 $[M+H]^+$; found: 279.1497.

Compound ***3ag*** (3-(4-methoxyphenyl)-N,N-dimethylindolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.16 (d, J = 7.0 Hz, 1H), 7.96 (d, J = 9.1 Hz, 1H), 7.46 (d, J = 8.6 Hz, 2H), 7.04 (d, J = 8.6 Hz, 2H), 6.96 – 6.87 (m, 2H), 6.61 (t, J = 6.7 Hz, 1H), 3.89 (s, 3H), 3.22 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.8, 159.4, 134.8, 130.1, 124.9, 124.0, 122.6, 120.2, 120.0, 114.5, 114.2, 111.9, 107.2, 55.4; IR (NaCl): 3047, 2933, 1711, 1609, 1546, 1490, 1453, 1408; HRMS (ESI): m/z calcd for $C_{18}H_{18}N_2O_2$: 295.1447 $[M+H]^+$; found: 295.1447.

Compound ***3ah*** (3-(3,5-dimethylphenyl)-N,N-dimethylindolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.26 (d, J = 7.1 Hz, 1H), 7.99 (d, J = 9.1 Hz, 1H), 7.18 (s, 2H), 7.05 (s, 1H), 6.97 (s, 1H), 6.93 (dd, J = 8.8, 7.0 Hz, 1H), 6.63 (t, J = 6.7 Hz, 1H), 3.23 (s, 6H), 2.41 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.8, 138.7, 135.1, 131.5, 129.5, 126.2, 125.4, 122.9, 120.2, 120.1, 114.5, 111.9, 107.2, 21.4; IR (NaCl): 2920, 1602, 1540, 1510, 1451, 1404; HRMS (ESI): m/z calcd for $C_{19}H_{20}N_2O$: 293.1654 $[M+H]^+$; found: 293.1651.

Compound ***3ai*** (3-(4-fluorophenyl)-N,N-dimethylindolizine-1-carboxamide): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.16 (d, J = 7.0 Hz, 1H), 7.96 (d, J = 9.1 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.22 (t, J = 8.6 Hz, 2H), 6.98 (s, 1H), 6.96 (d, J = 8.1 Hz, 1H), 6.66 (t, J = 6.7 Hz, 1H), 3.25 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): 167.6, 162.3 (d, J = 246.4 Hz), 135.0, 130.4 (d, J = 8.1 Hz), 127.7 (d, J = 3.4 Hz), 124.0, 122.4, 120.28, 120.25, 116.1 (d, J = 21.5 Hz), 114.6, 112.2, 107.5; IR (NaCl): 2924, 2854, 1608, 1545, 1511, 1487, 1452, 1404; HRMS (ESI): m/z calcd for $C_{17}H_{15}FN_2O$: 283.1247 $[M+H]^+$; found: 283.1247.

Compound ***3ga*** (tert-butyl 3-phenylindolizine-1-carboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.26 (d, J = 7.1 Hz, 1H), 8.22 (d, J = 9.1 Hz, 1H), 7.53 (d, J = 7.2 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.2 Hz, 1H), 7.26 (s, 1H), 7.03 (dd, J = 8.6, 6.8 Hz, 1H), 6.66 (t, J = 6.4 Hz, 1H), 1.64 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): 164.6, 135.9, 131.4, 129.1, 302.8, 128.7, 127.9, 126.1, 123.3, 121.8, 120.3, 116.4, 112.4, 106.0, 79.6, 28.6; IR (NaCl): 2973, 2926, 1687, 1543, 1511,

1449, 1420; HRMS (ESI): m/z calcd for $C_{19}H_{19}NO_2$: 294.1494 $[M+H]^+$; found: 294.1495.

Compound ***3ha*** (ethyl 3-phenylpyrrolo[2,1-a]isoquinoline-1-carboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 9.84 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 8.3 Hz, 2H), 7.57 – 7.47 (m, 5H), 7.43 (t, *J* = 7.1 Hz, 1H), 7.31 (s, 1H), 6.92 (d, *J* = 7.4 Hz, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.44 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 165.5, 132.6, 131.3, 129.3, 129.0, 128.9, 128.2, 128.0, 127.6, 127.5, 127.3, 126.6, 126.1, 121.9, 116.5, 113.5, 109.1, 60.1, 14.6; IR (NaCl): 3065, 2979, 2930, 1698, 1644, 1604, 1551, 1506, 1459; HRMS (ESI): m/z calcd for $C_{21}H_{17}NO_2$: 316.1338 $[M+H]^+$; found: 316.1335.

Compound ***3ia*** (3-phenylpyrrolo[2,1-a]isoquinoline-1-carbonitrile): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.89 (d, *J* = 8.1 Hz, 1H), 8.01 (d, *J* = 7.4 Hz, 1H), 7.72 – 7.61 (m, 2H), 7.61 – 7.44 (m, 6H), 7.01 (s, 1H), 6.97 (d, *J* = 7.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): 134.3, 130.2, 129.2, 129.1, 128.8, 128.7, 128.5, 128.1, 128.1, 127.2, 127.1, 125.1, 123.2, 121.8, 118.5, 115.4, 113.7; IR (NaCl): 3057, 2928, 2212, 1724, 1603, 1548, 1520, 1486, 1457; HRMS (ESI): m/z calcd for $C_{19}H_{12}N_2$: 269.1079 $[M+H]^+$; found: 269.1082.

Compound ***3jb*** (dimethyl 3-(4-(trifluoromethyl)phenyl)indolizine-1,2-dicarboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.26 (d, *J* = 9.1 Hz, 1H), 8.04 (d, *J* = 7.0 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.19 (dd, *J* = 8.7, 7.0 Hz, 1H), 6.80 (t, *J* = 6.8 Hz, 1H), 3.94 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 166.9, 164.4, 159.3 (q, *J* = 1.2 Hz), 135.7, 132.5 (q, *J* = 1.2 Hz), 131.0 (q, *J* = 32.7 Hz), 130.3, 126.9 (q, *J* = 3.8 Hz), 126.2 (q, *J* = 3.7 Hz), 125.9, 123.8 (q, *J* = 95.5 Hz), 123.5, 122.7, 120.5, 115.5, 114.1, 102.4, 52.7, 51.6; IR (NaCl): 3133, 2954, 2850, 1734, 1696, 1608, 1545, 1519, 1449; HRMS (ESI): m/z calcd for $C_{19}H_{14}F_3NO_4$: 378.0953 $[M+H]^+$; found: 378.0959.

Compound ***3jc*** (dimethyl 3-(4-chlorophenyl)indolizine-1,2-dicarboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.22 (d, *J* = 9.1 Hz, 1H), 7.98 (d, *J* = 7.0 Hz, 1H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.12 (dd, *J* = 8.4, 7.3 Hz, 1H), 6.73 (t, *J* = 6.8 Hz, 1H), 3.89 (s, 3H), 3.80 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 166.6, 164.1, 135.4, 135.2, 131.4, 129.5, 127.3, 123.7, 123.7, 123.3, 122.3, 120.5, 113.8, 102.2, 52.5, 51.4; IR (NaCl): 2950, 1730, 1699, 1589, 1511, 1493, 1451; HRMS (ESI): m/z calcd for $C_{18}H_{14}ClNO_4$: 344.0690 $[M+H]^+$; found: 344.0693.

Compound ***3je*** (dimethyl 3-(3-fluorophenyl)indolizine-1,2-dicarboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.25 (d, *J* = 9.1 Hz, 1H), 8.07 (d, *J* = 7.1 Hz, 1H), 7.50 (dd, *J* = 14.0, 7.8 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.25 (d, *J* = 9.4 Hz, 1H), 7.21 – 7.13 (m, 2H), 6.78 (t, *J* = 6.7 Hz, 1H), 3.93 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 165.4 (d, *J* = 251.5 Hz), 164.2, 161.7, 135.4, 130.9 (d, *J* = 8.3 Hz), 130.8 (d, *J* = 8.5 Hz), 125.7 (d, *J* = 3.1 Hz), 123.8, 123.45 (d, *J* = 2.4 Hz), 123.39, 122.5, 120.5, 116.9 (d, *J* = 22.0 Hz), 116.1 (d, *J* = 20.9 Hz), 113.8, 102.2, 52.6, 51.4; IR (NaCl): 2951, 2853, 1733, 1698, 1637, 1612, 1583, 1511, 1449; HRMS (ESI): m/z calcd for $C_{18}H_{14}FNO_4$: 328.0985 $[M+H]^+$; found: 328.0988.

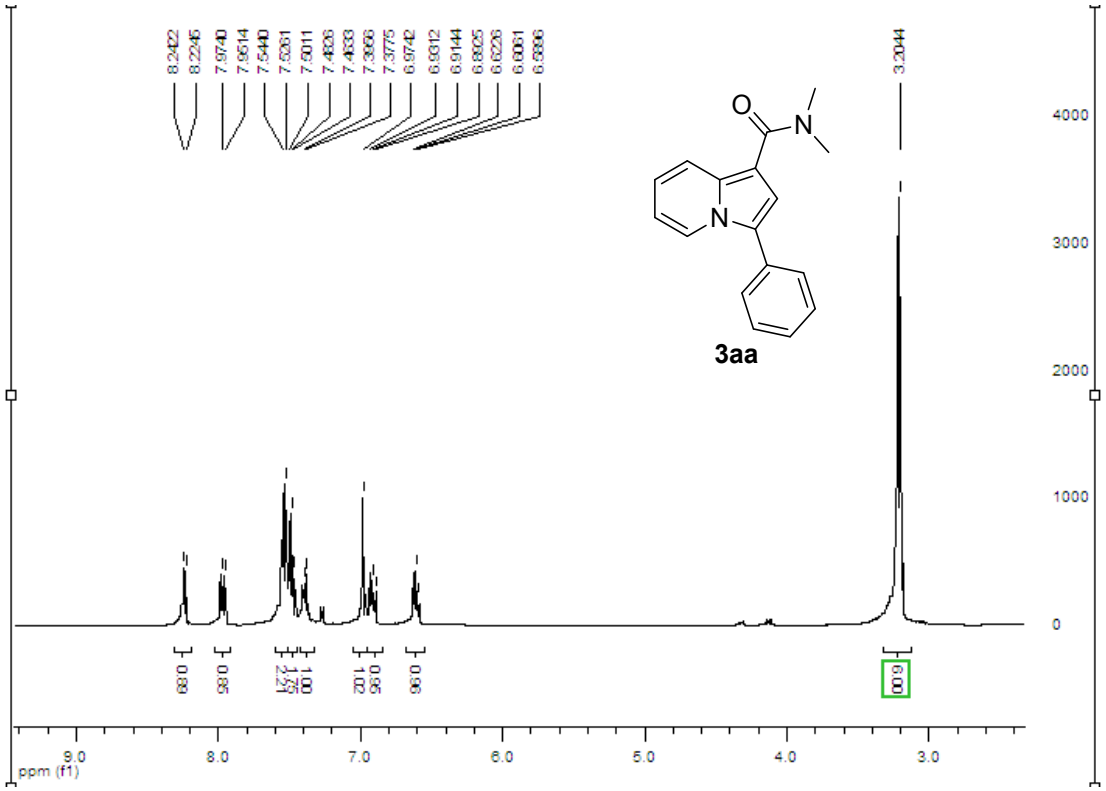
Compound ***3jf*** (dimethyl 3-(4-fluorophenyl)indolizine-1,2-dicarboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.24 (d, *J* = 9.1 Hz, 1H), 7.98 (d, *J* = 7.0 Hz, 1H), 7.51 (dd, *J* = 8.4, 5.4 Hz, 2H), 7.22 (app

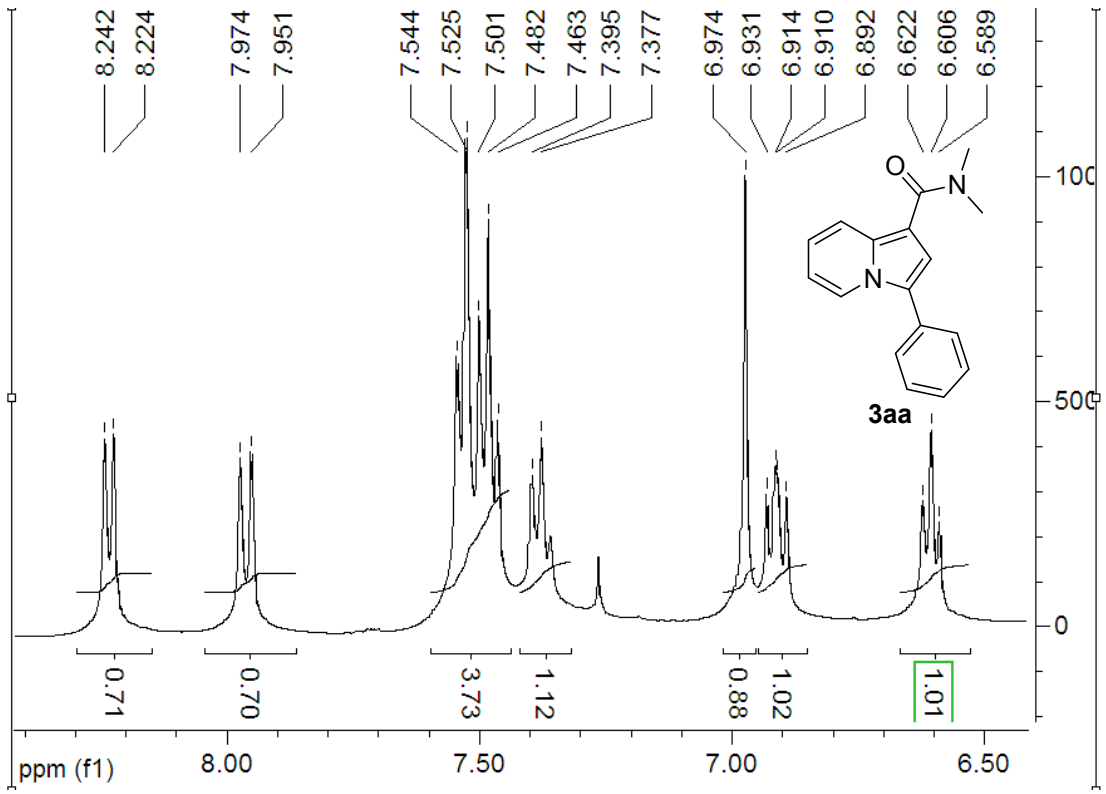
t, *J* = 8.5 Hz, 2H), 7.14 (dd, *J* = 8.7, 7.0 Hz, 1H), 6.75 (t, *J* = 6.7 Hz, 1H), 3.92 (s, 3H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 165.5 (d, *J* = 252.2 Hz), 164.3, 161.8, 135.2, 132.1 (d, *J* = 8.3 Hz), 124.8 (d, *J* = 3.4 Hz), 124.0, 123.7, 123.4, 122.2, 120.4, 116.3 (d, *J* = 21.6 Hz), 113.7, 102.0, 52.5, 51.4; IR (NaCl): 2957, 2823, 2853, 1723, 1702, 1636, 1597, 1546, 1513, 1449; HRMS (ESI): m/z calcd for $C_{18}H_{14}FNO_4$: 328.0985 $[M+H]^+$; found: 328.0989.

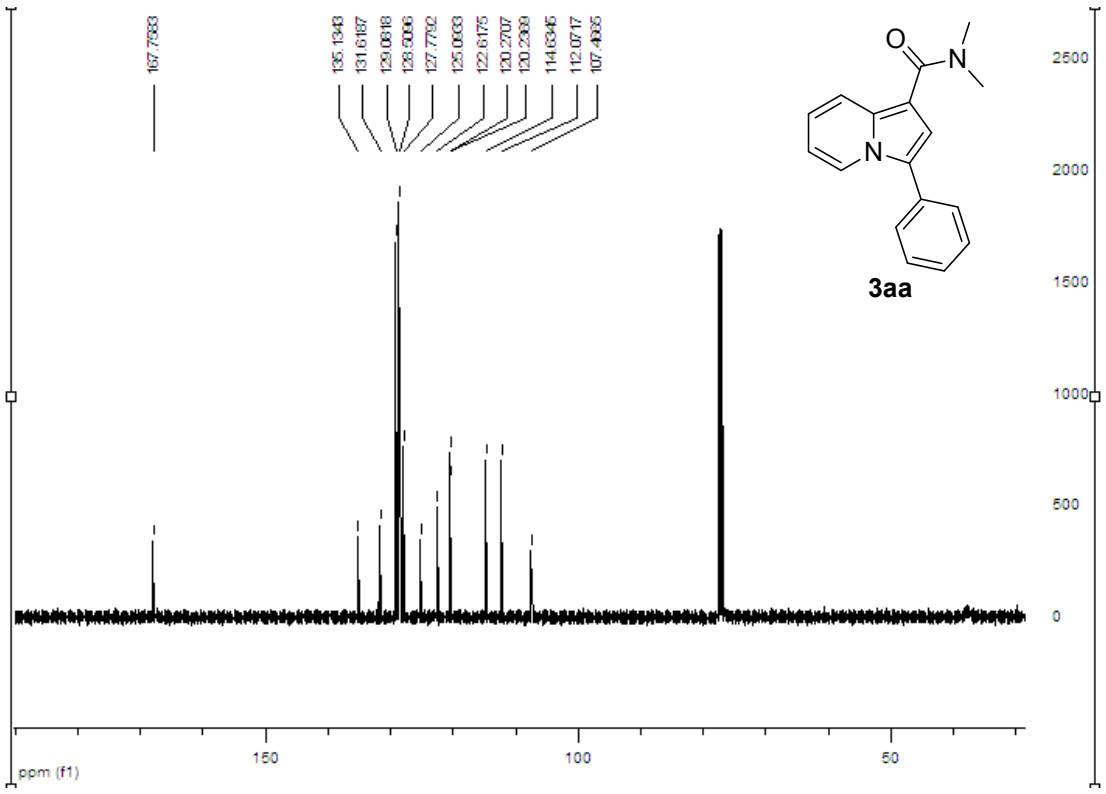
Compound ***3jg*** (dimethyl 3-(4-acetylphenyl)indolizine-1,2-dicarboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.24 (d, *J* = 9.1 Hz, 1H), 8.10 – 8.05 (m, 3H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.15 (dd, *J* = 8.7, 7.1 Hz, 1H), 6.76 (t, *J* = 6.8 Hz, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 2.65 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 197.3, 166.6, 164.0, 137.1, 135.7, 133.7, 129.9, 129.1, 124.0, 123.7, 123.4, 122.8, 120.6, 114.0, 102.6, 52.6, 51.4, 29.7; IR (NaCl): 2924, 2853, 1733, 1688, 1606, 1511, 1453; HRMS (ESI): m/z calcd for $C_{20}H_{17}NO_5$: 352.1185 $[M+H]^+$; found: 352.1183.

Compound ***3ma*** (dibutyl 3-phenylindolizine-1,2-dicarboxylate): ^{1}H NMR ($CDCl_3$, 400 MHz): 8.23 (d, *J* = 9.1 Hz, 1H), 8.01 (d, *J* = 7.1 Hz, 1H), 7.53- 7.40 (m, 5H), 7.09 (d, *J* = 8.3, 6.8 Hz, 1H), 6.69 (t, *J* = 6.6 Hz, 1H), 4.31 (t, *J* = 6.6 Hz, 2H), 4.18 (t, *J* = 6.6 Hz, 2H), 1.73 (quintet, *J* = 7.1 Hz, 2H), 1.57 – 1.41 (m, 4H), 1.19 (quintet, *J* = 7.5 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H), 0.81 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 166.4, 163.9, 135.3, 130.0, 129.1, 129.1, 129.0, 124.8, 123.5, 123.4, 122.5, 120.4, 113.4, 102.1, 65.2, 63.9, 31.0, 30.5, 19.3, 19.0, 13.8, 13.6; IR (NaCl): 2959, 2872, 1732, 1693, 1512, 1440, 1404; HRMS (ESI): m/z calcd for $C_{24}H_{27}NO_4$: 394.2018 $[M+H]^+$; found: 394.2016.

Copies of Compounds' NMR spectra



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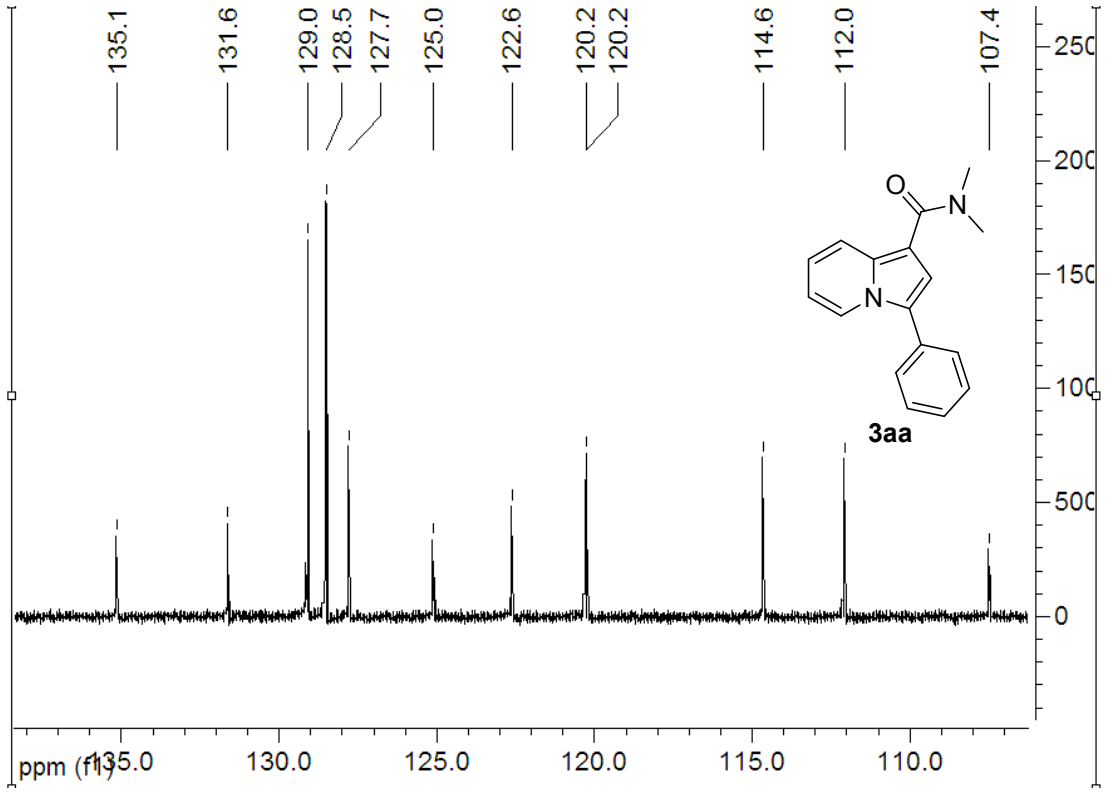
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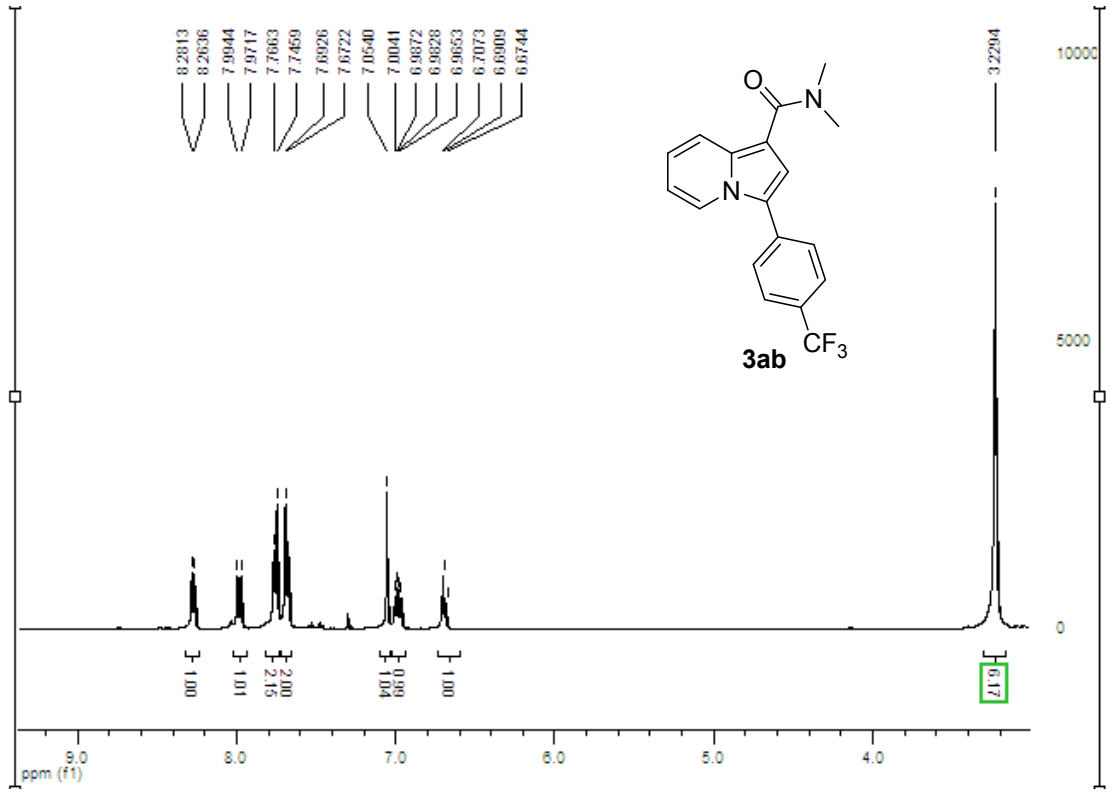
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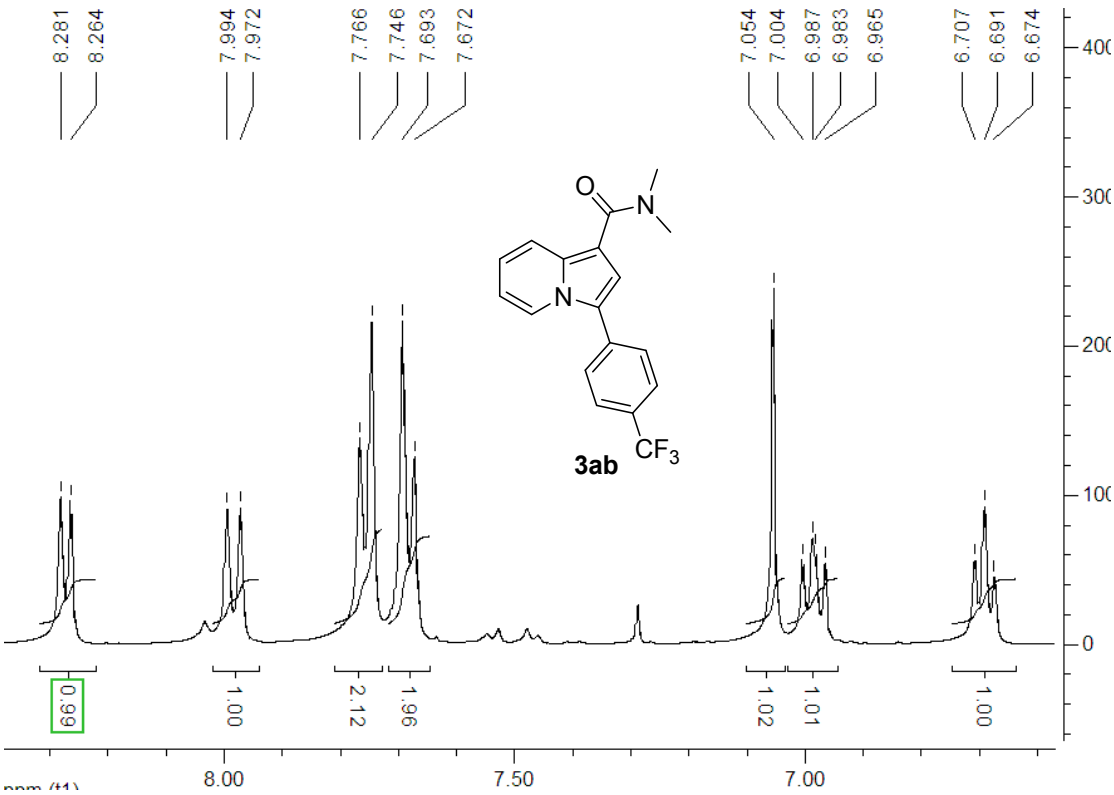
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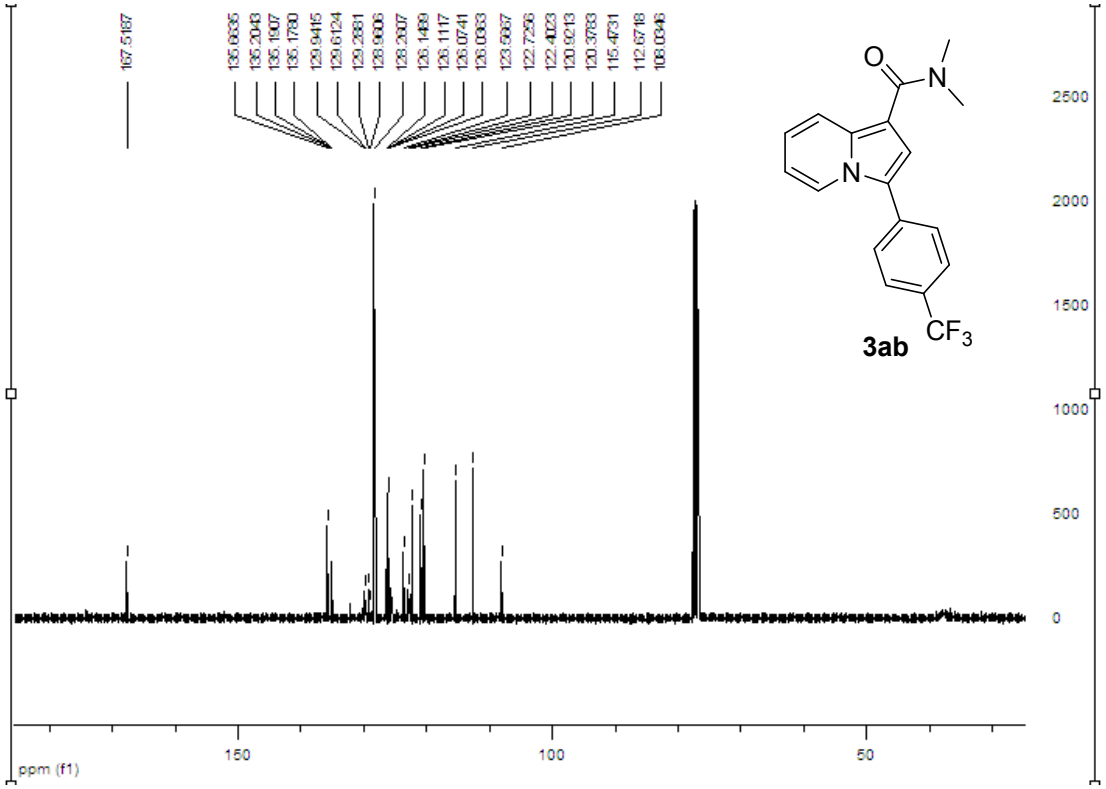
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128.9606
128.2907
126.1489
126.1117
126.0741
126.0363
123.5957
122.7256
122.4023
120.9213
120.3783
115.4731
112.6718
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N
N
CF3
3ab
2500
2000
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1000
500
0
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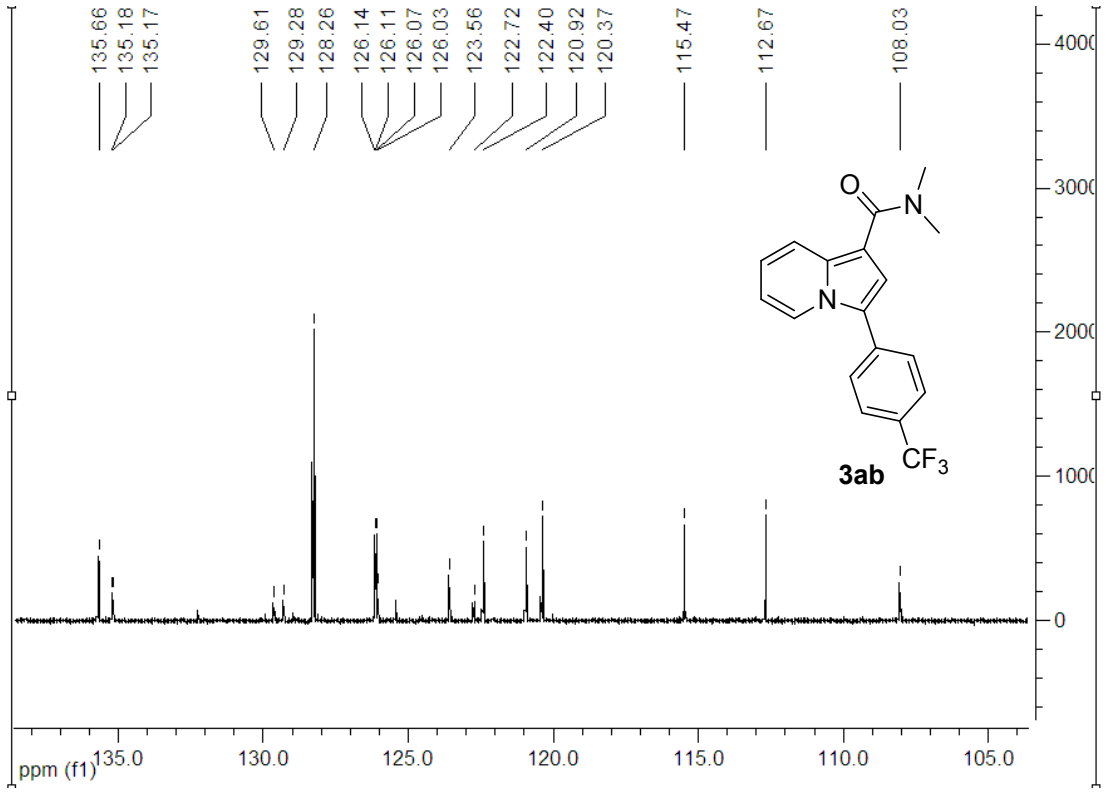
100
50
ppm (f1)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135.17
129.61
129.28
128.26
126.14
126.11
126.07
126.03
123.56
122.72
122.40
120.92
120.37
115.47
112.67
108.03
O
N
N
CF3
3ab
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1000
0
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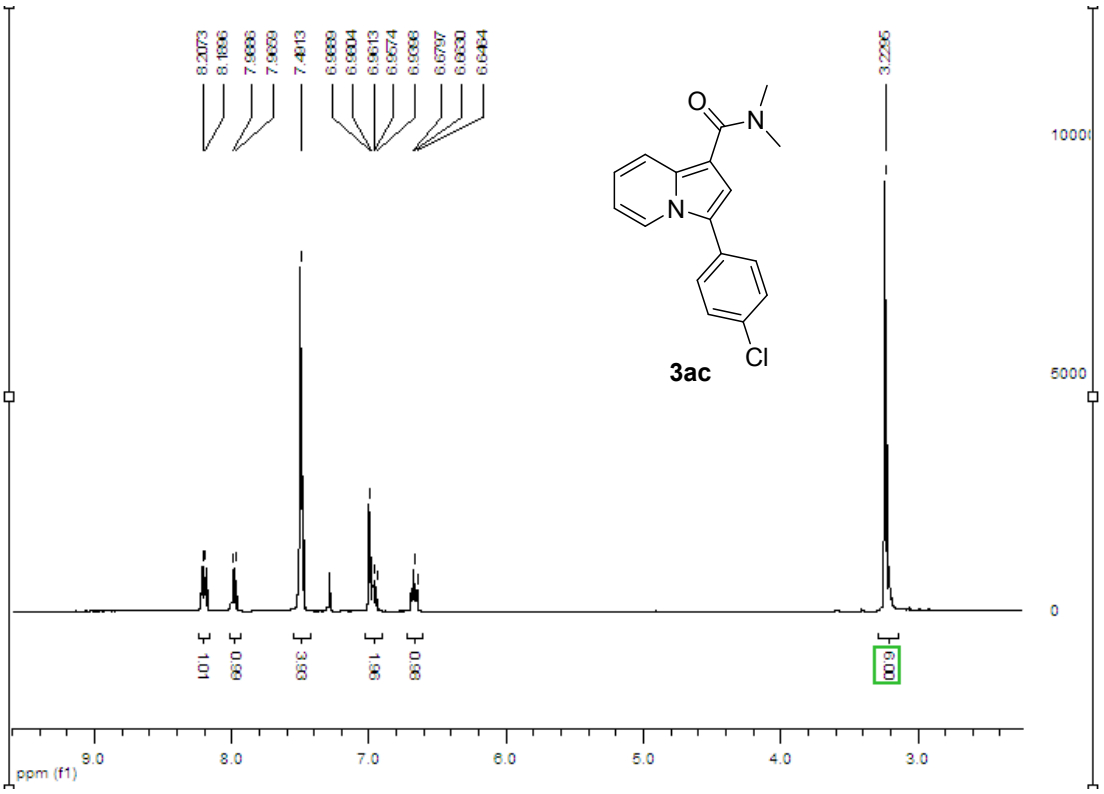
130.0
125.0
120.0
115.0
110.0
105.0
ppm (f1)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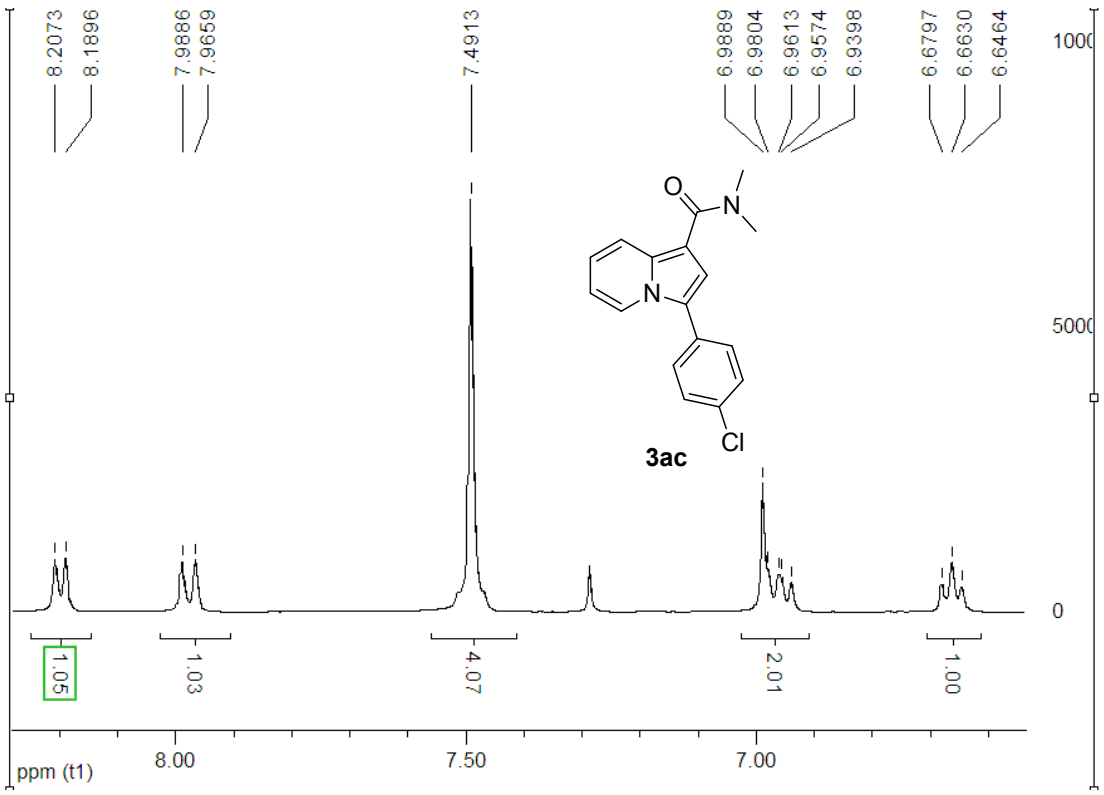
8.1896
7.9886
7.9659
7.4913
6.9889
6.9804
6.9613
6.9574
6.9398
6.6797
6.6630
6.6464
3.2295
O
N
N
Cl
3ac
1.01
0.99
3.93
1.96
0.98
1.00
10000
5000
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm (f1)


8.2073
8.1896
7.9886
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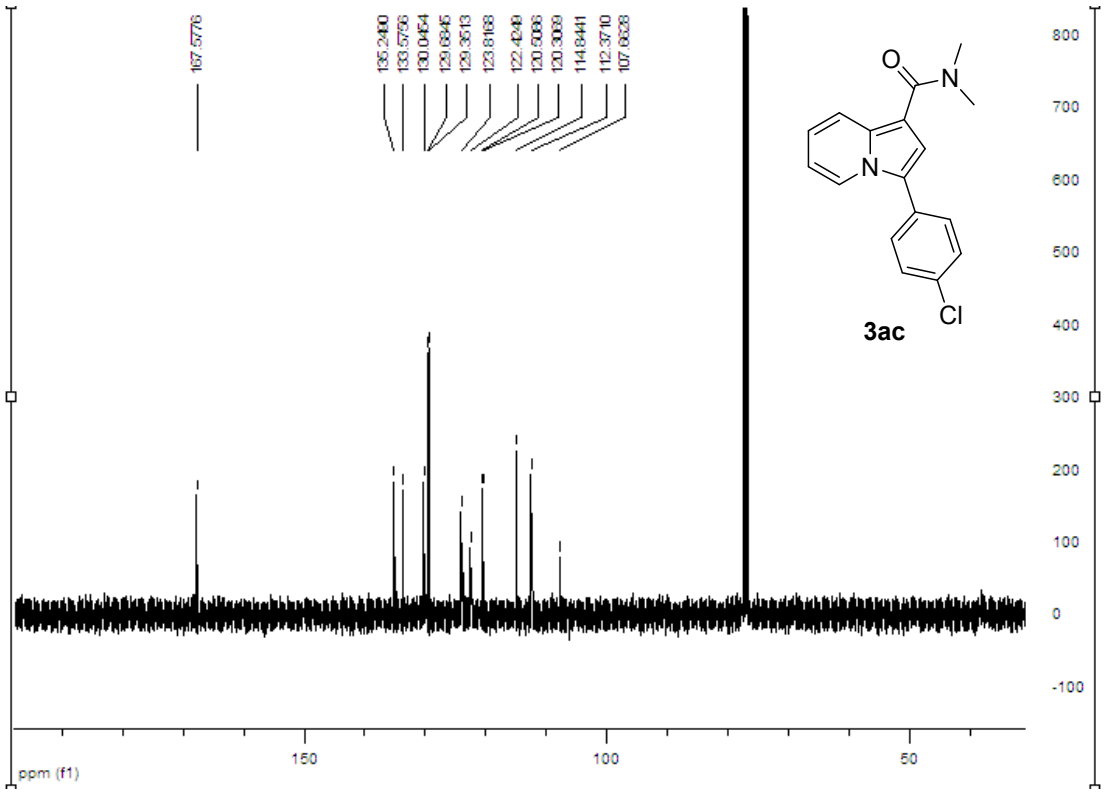
7.4913
6.9889
6.9804
6.9613
6.9574
6.9398
6.6797
6.6630
6.6464
O
N
N
Cl
3ac
1.05
1.03
4.07
2.01
1.00
10000
5000
0
8.00
7.50
7.00
ppm (t1)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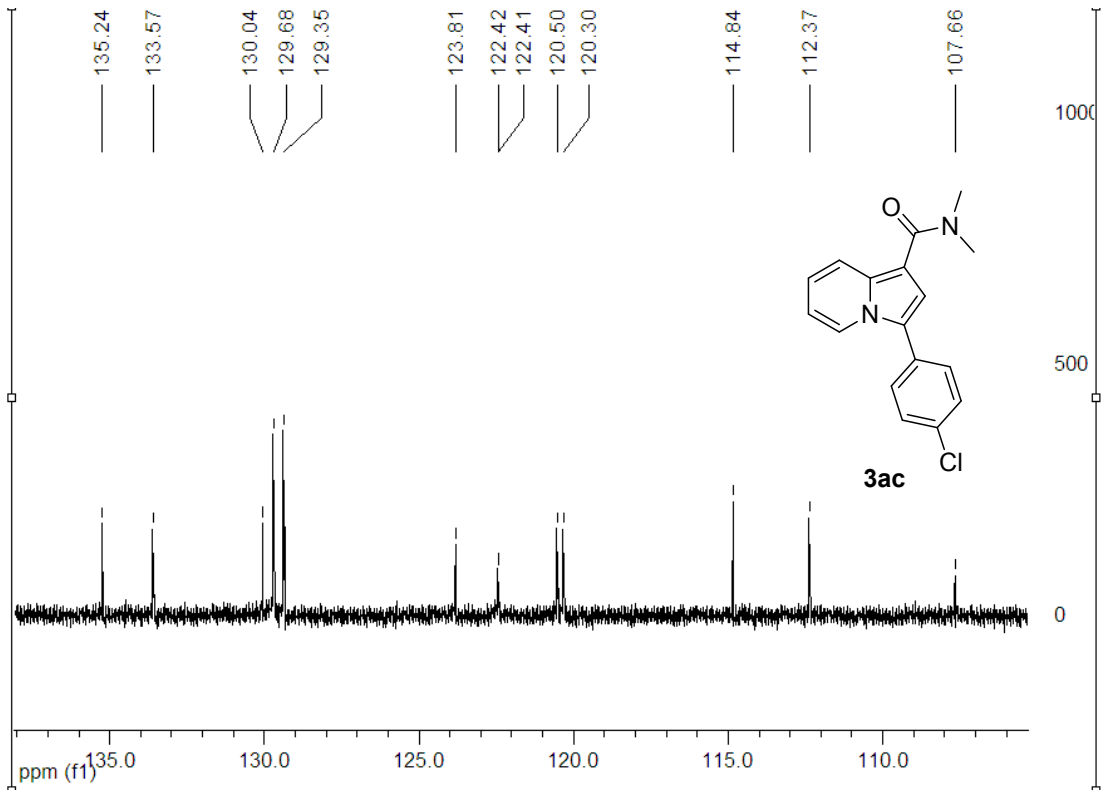
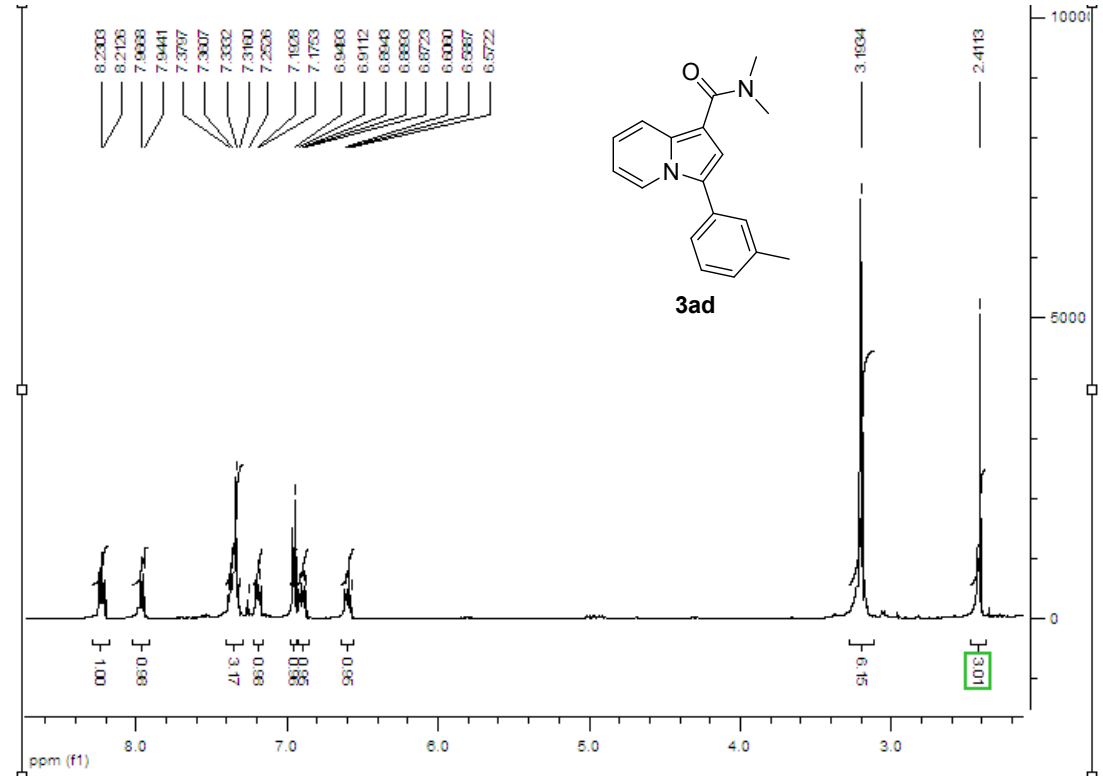
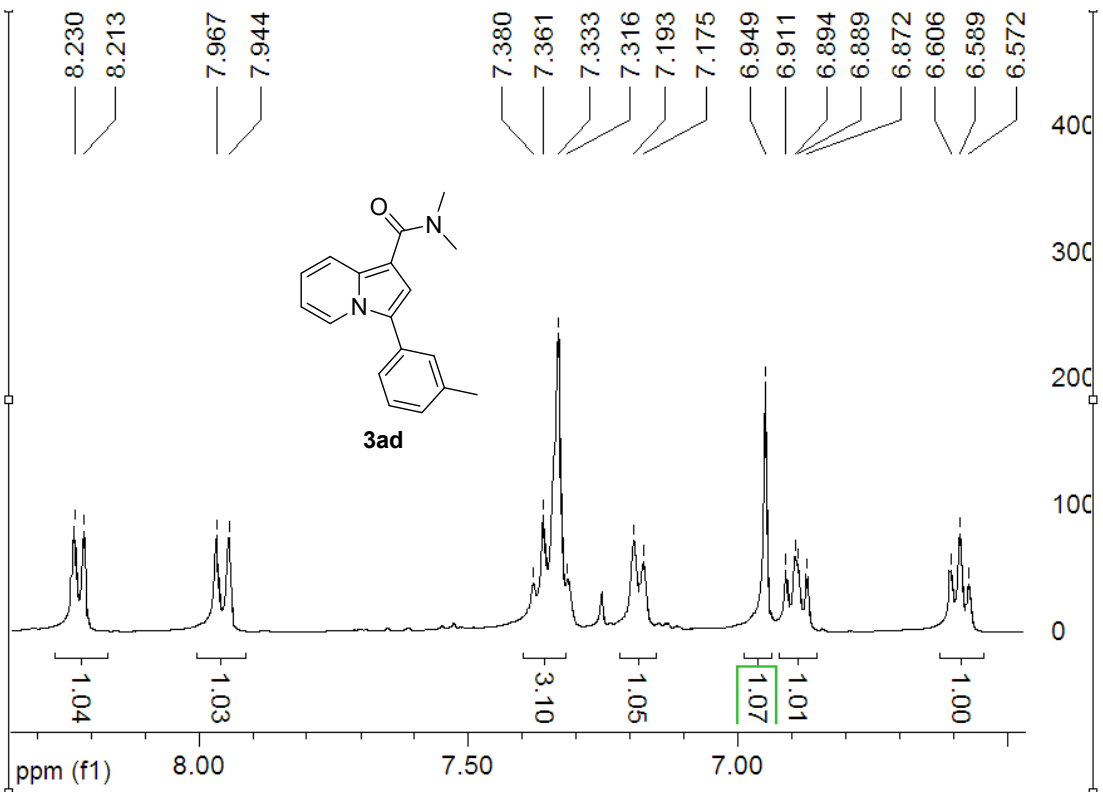
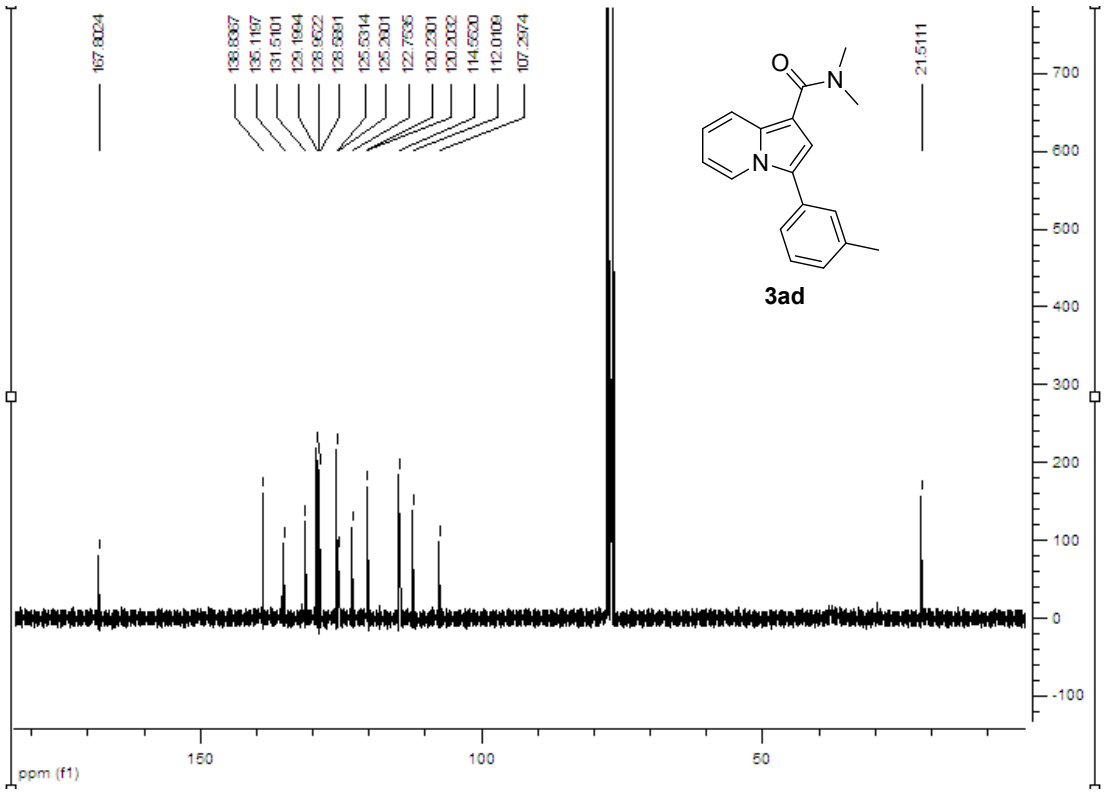
133.5756
130.0454
129.6845
129.3513
123.8168
122.4249
120.5066
120.3069
114.8441
112.3710
107.6628
O
N
N
Cl
3ac
800
700
600
500
400
300
200
100
0
-100
150
100
50
ppm (f1)


135.24
133.57
130.04
129.68
129.35
123.81
122.42
122.41
120.50
120.30
114.84
112.37
107.66
O
N
N
Cl
3ac
1000
500
0
135.0
130.0
125.0
120.0
115.0
110.0
ppm (f1)


8.2303
8.2126
7.9638
7.9441
7.3797
7.3607
7.3332
7.3160
7.2526
7.1928
7.1753
6.9403
6.9112
6.8943
6.8803
6.8723
6.6000
6.5887
6.5722
3.1934
2.4113
O
N
N
3ad
10000
5000
0
1.00
0.98
3.17
0.98
8.88
0.96
6.15
3.01
8.0
7.0
6.0
5.0
4.0
3.0
ppm (f1)


8.230
8.213
7.967
7.944
7.380
7.361
7.333
7.316
7.193
7.175
6.949
6.911
6.894
6.889
6.872
6.606
6.589
6.572
O
N
N
3ad
400
300
200
100
0
1.04
1.03
3.10
1.05
1.07
1.01
1.00
ppm (f1)
8.00
7.50
7.00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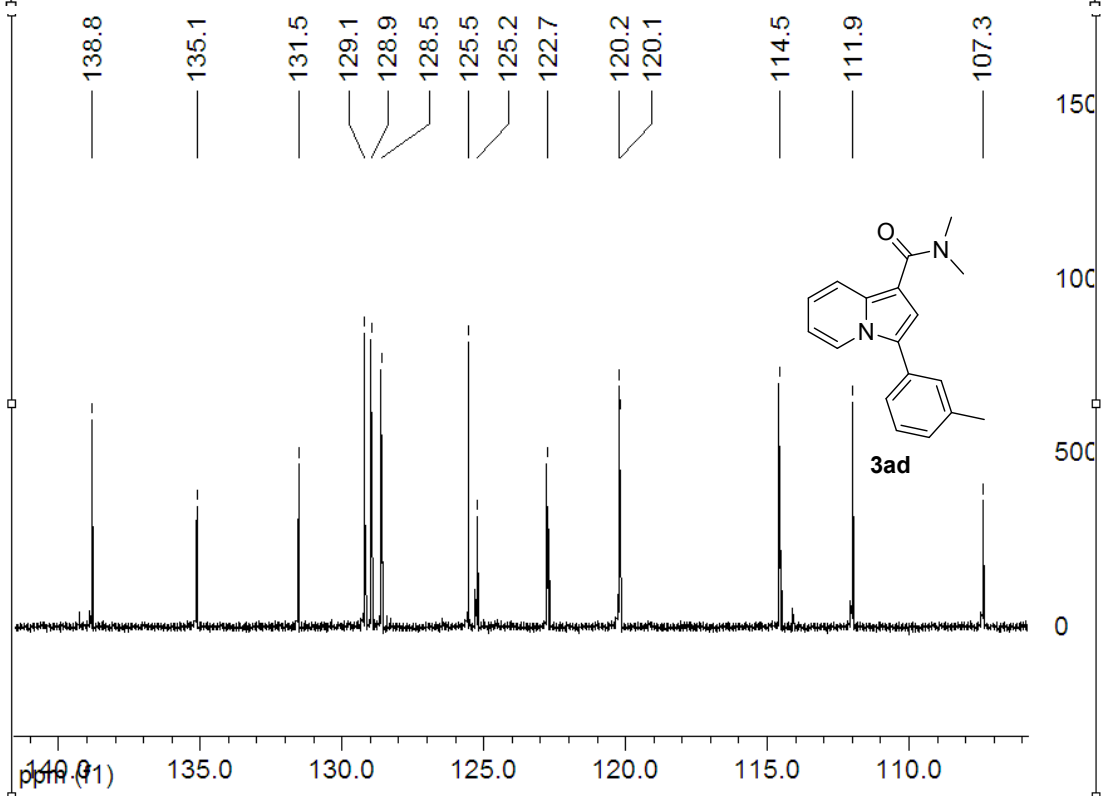
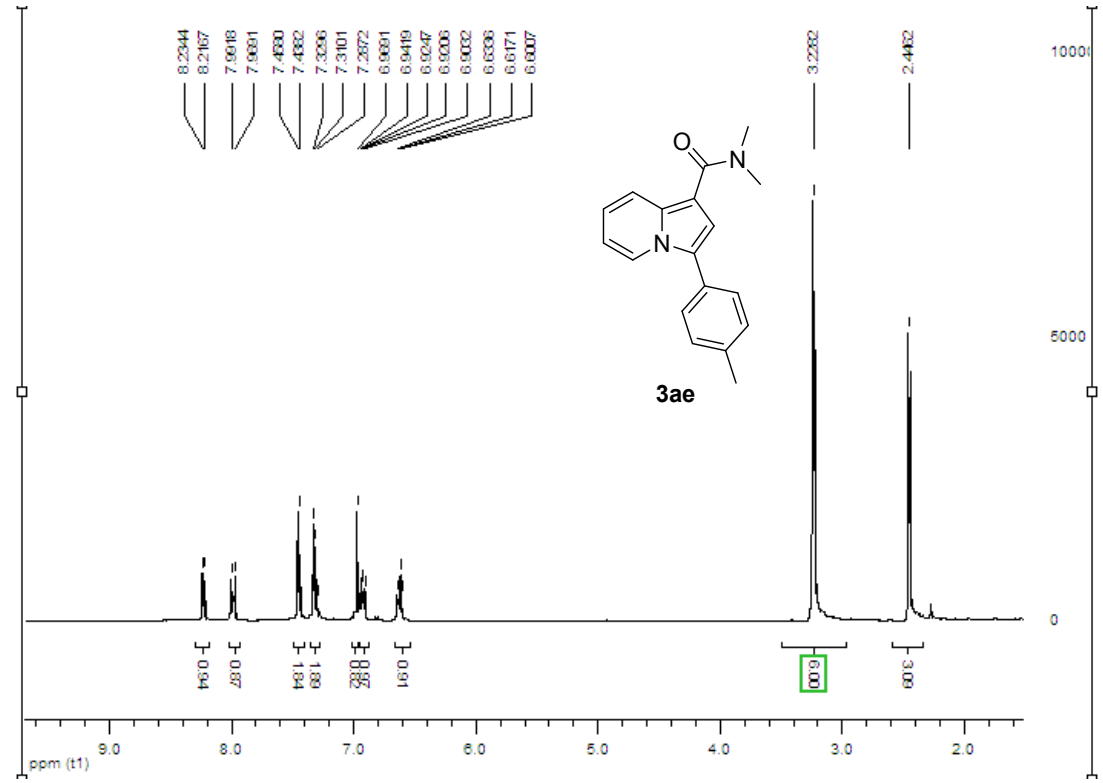
138.8367
135.1197
131.5101
129.1994
128.9622
128.8991
125.5314
125.2001
122.7535
120.2301
120.2032
114.5620
112.0109
107.2974
21.5111
O
N
N
3ad
700
600
500
400
300
200
100
0
-100
150
100
50
ppm (f1)


138.8
135.1
131.5
129.1
128.9
128.5
125.5
125.2
122.7
120.2
120.1
114.5
111.9
107.3
O
N
N
3ad
150
100
500
0
140.0
135.0
130.0
125.0
120.0
115.0
110.0
ppm (f1)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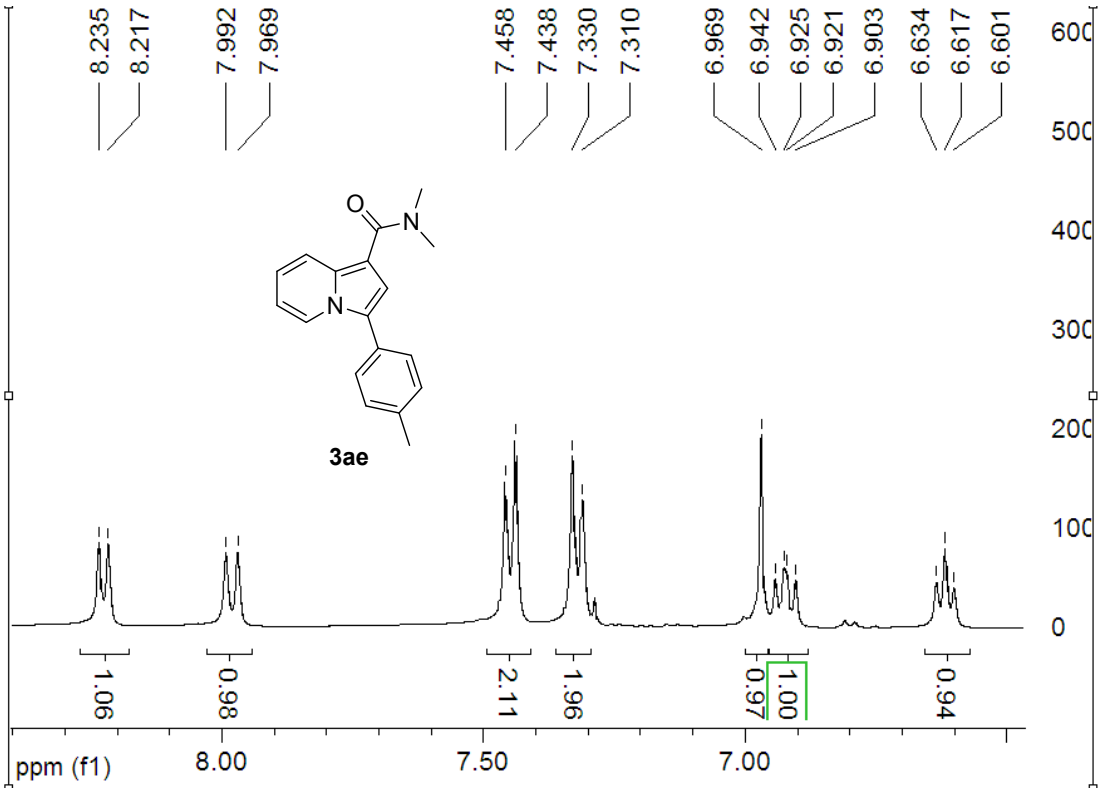
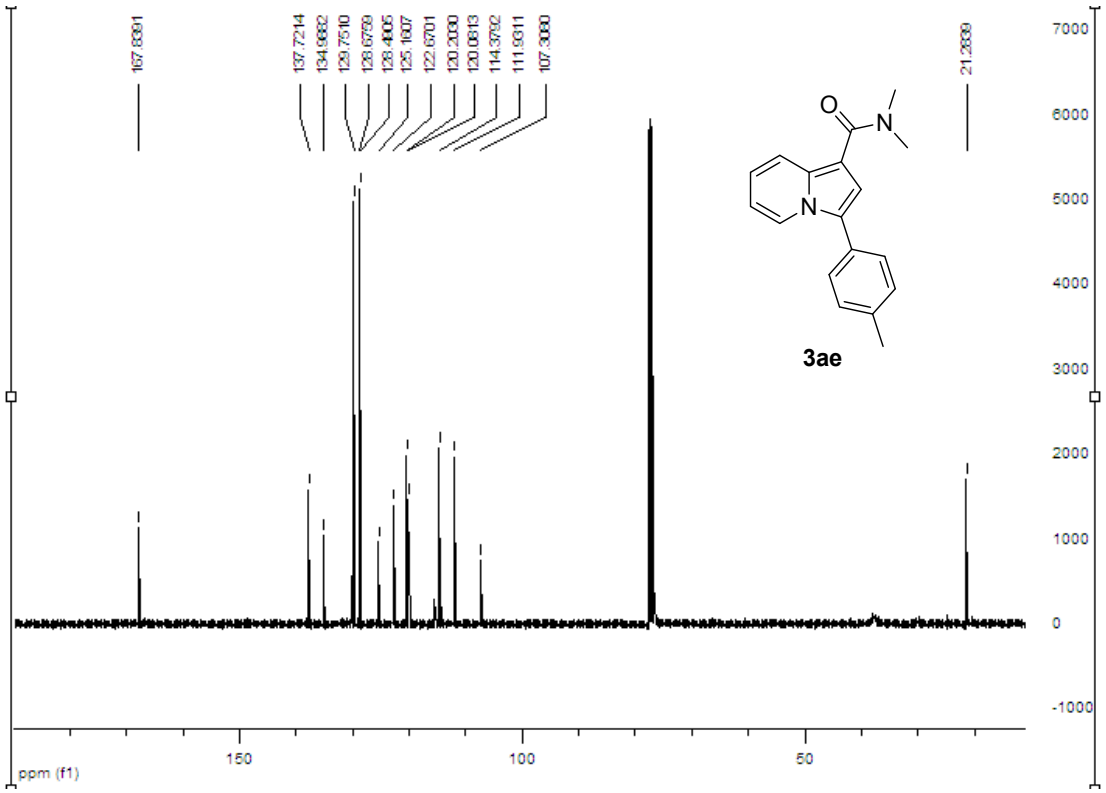
8.2167
7.9918
7.9691
7.4330
7.4132
7.3336
7.3101
7.2872
6.9691
6.9419
6.9247
6.9006
6.9032
6.6336
6.6171
6.6007
3.2282
2.4432
O
N
N
3ae
10000
5000
0
0.94
0.87
1.84
1.89
2.88
2.55
1.91
6.00
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)


8.235
8.217
7.992
7.969
7.458
7.438
7.330
7.310
6.969
6.942
6.925
6.921
6.903
6.634
6.617
6.601
O
N
N
3ae
600
500
400
300
200
100
0
1.06
0.98
2.11
1.96
0.97
1.00
0.94
ppm (f1)
8.00
7.50
7.00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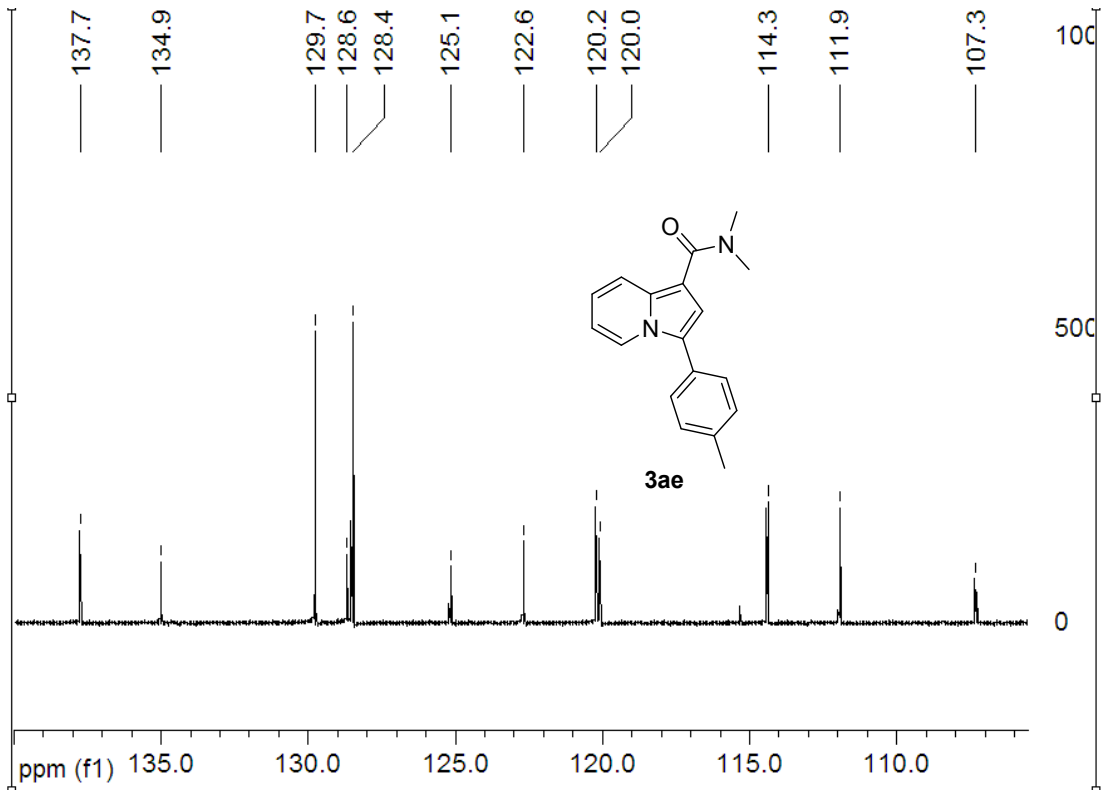
134.9682
129.7510
128.6759
128.4405
125.1007
122.6701
120.2000
120.0613
114.3792
111.9311
107.3000
21.2839
7000
6000
5000
4000
3000
2000
1000
0
-1000
150
100
50
ppm (f1)
O
N
N
3ae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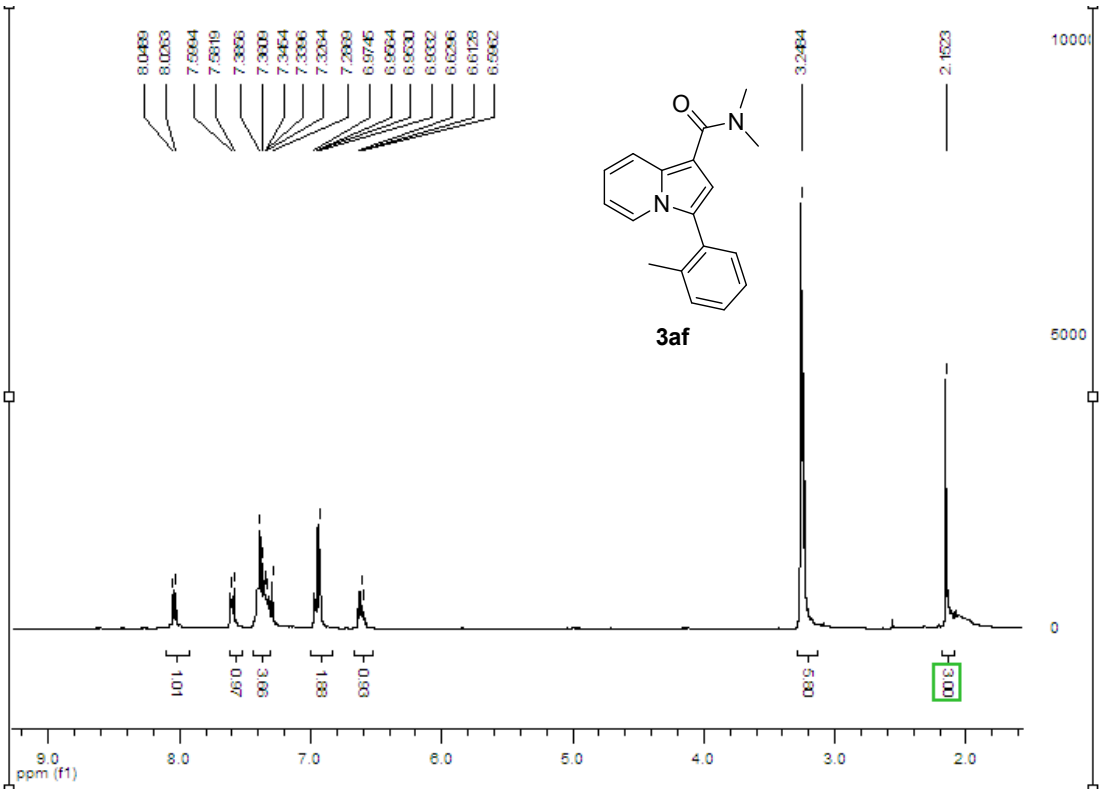
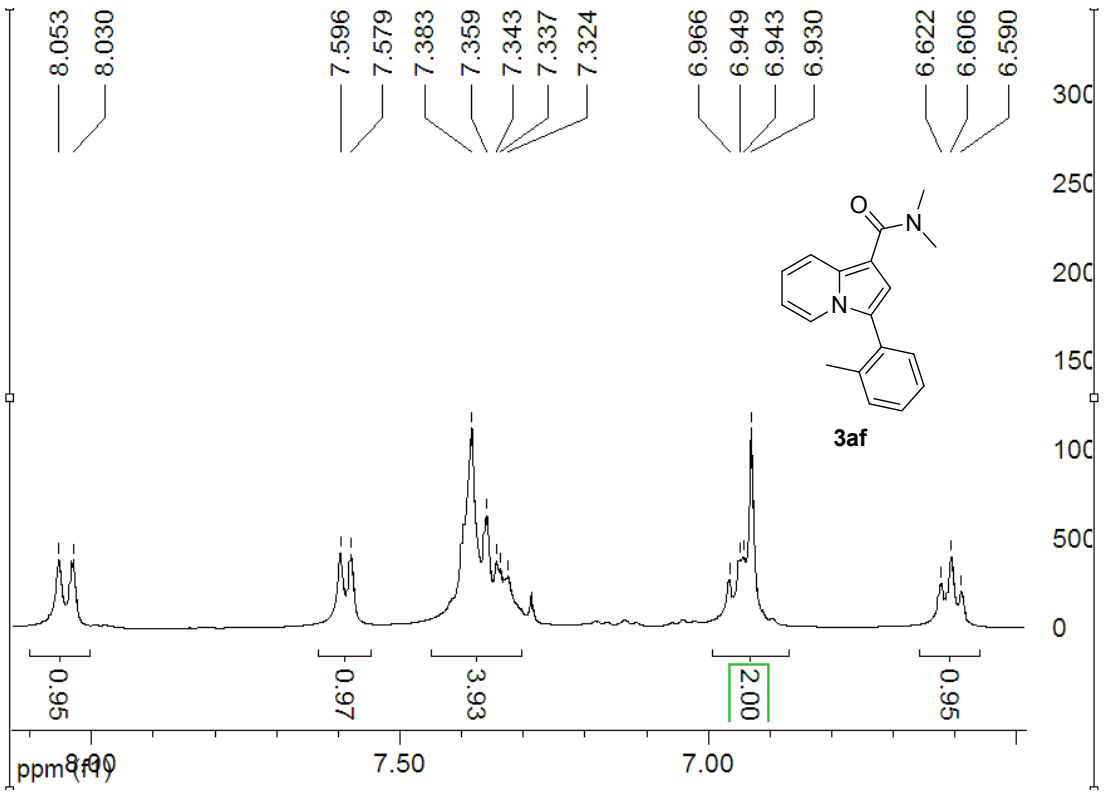
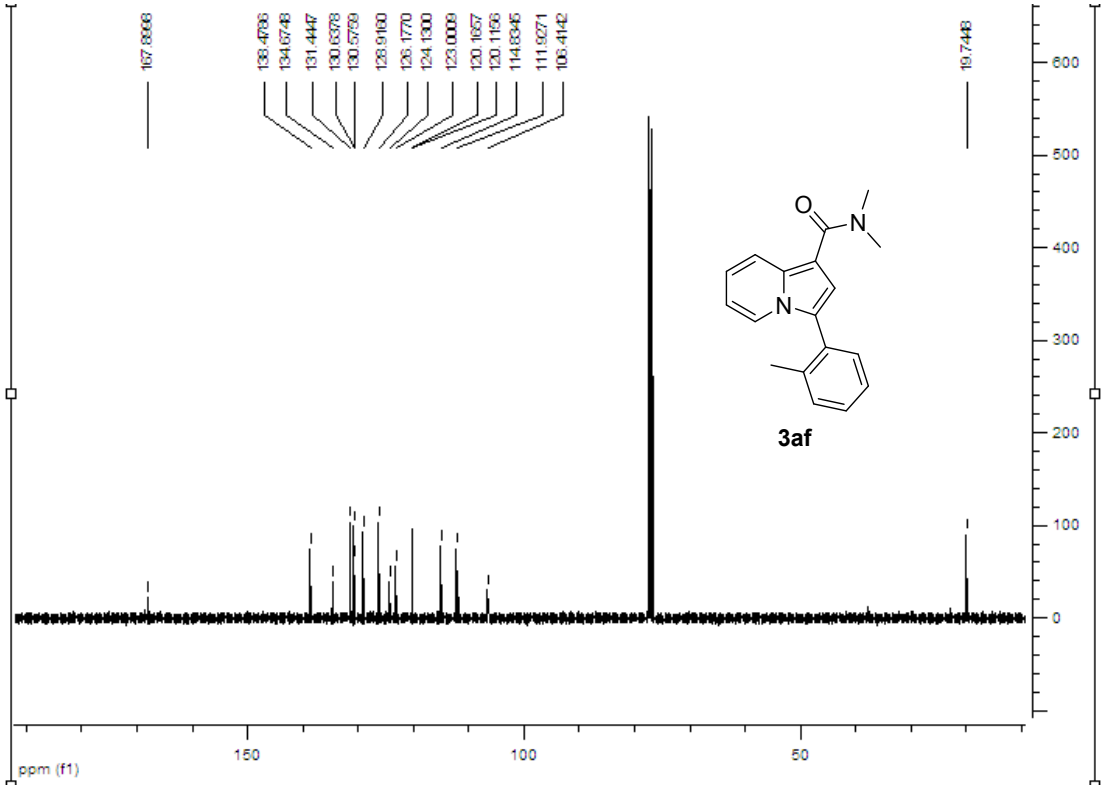
134.9
129.7
128.6
128.4
125.1
122.6
120.2
120.0
114.3
111.9
107.3
100
500
0
ppm (f1)
135.0
130.0
125.0
120.0
115.0
110.0
O
N
N
3ae


8.0489
8.0353
7.5994
7.5819
7.3956
7.3009
7.3454
7.3306
7.3264
7.2939
6.9745
6.9664
6.9530
6.9332
6.6256
6.6128
6.5982
3.2484
2.1523
O
N
N
3af
10000
5000
0
1.01
0.97
3.66
1.88
0.93
5.80
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (f1)


8.053
8.030
7.596
7.579
7.383
7.359
7.343
7.337
7.324
6.966
6.949
6.943
6.930
6.622
6.606
6.590
O
N
N
3af
300
250
200
150
100
500
0
0.95
0.97
3.93
2.00
0.95
8.00
7.50
7.00
ppm (f1)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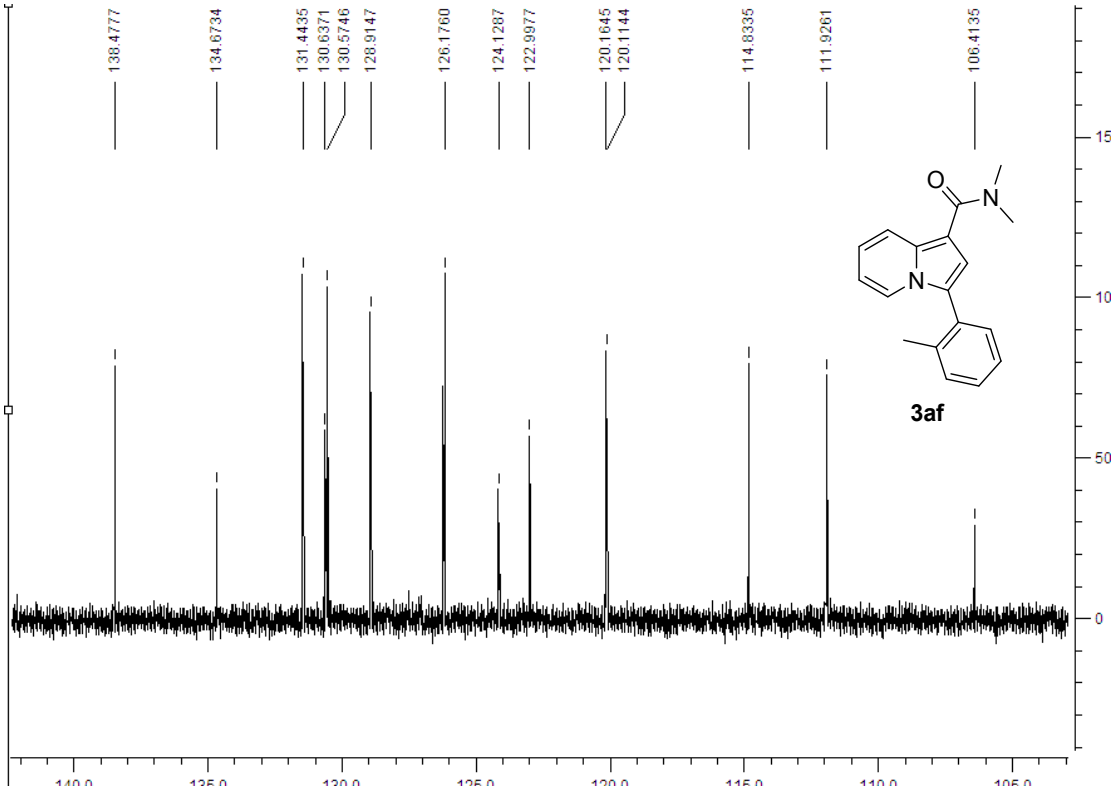
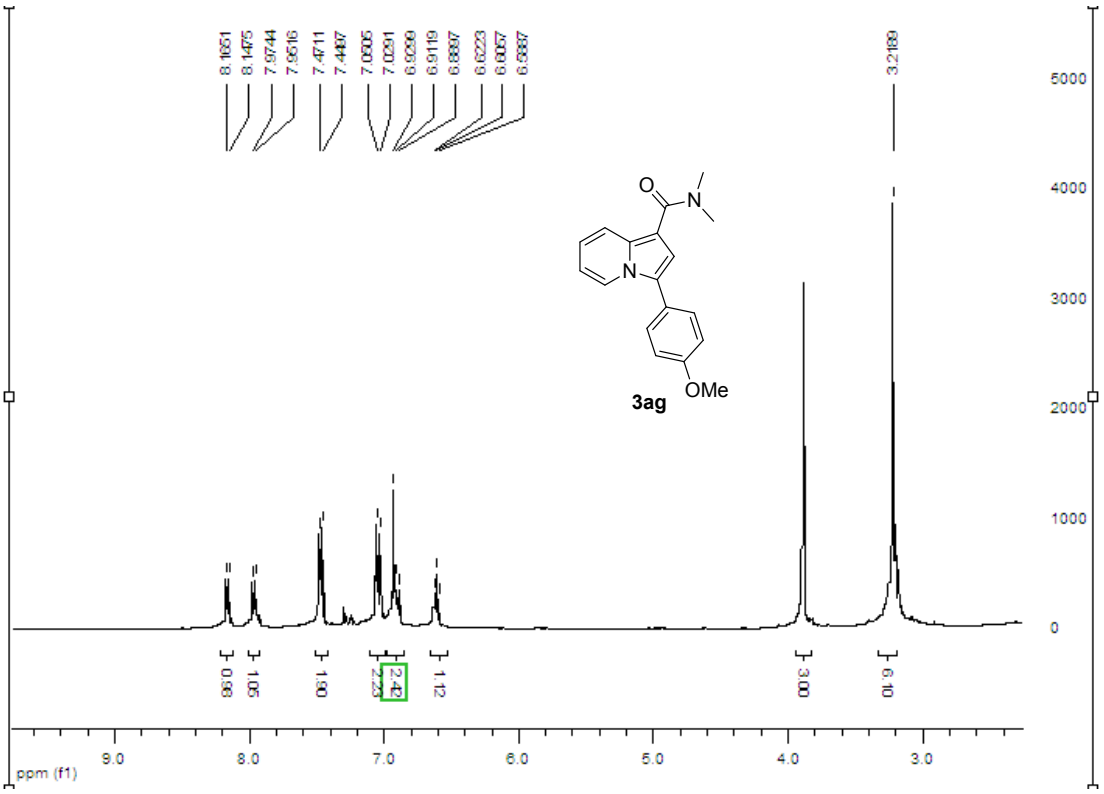
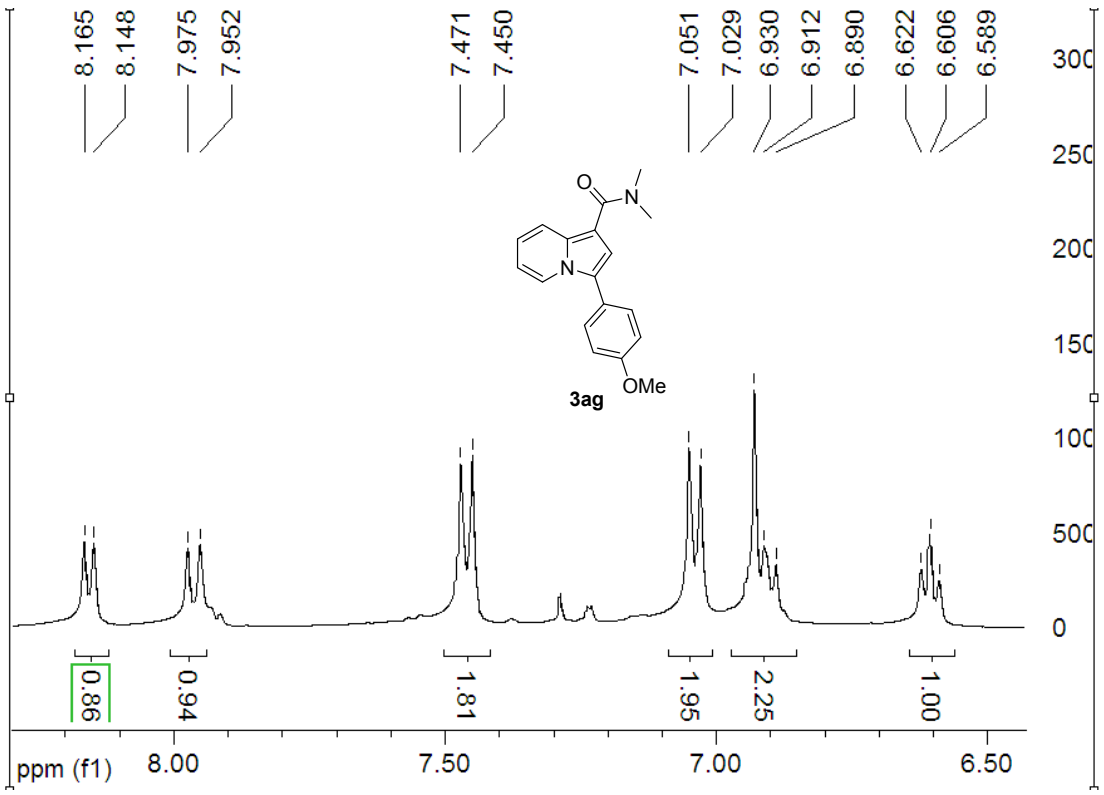
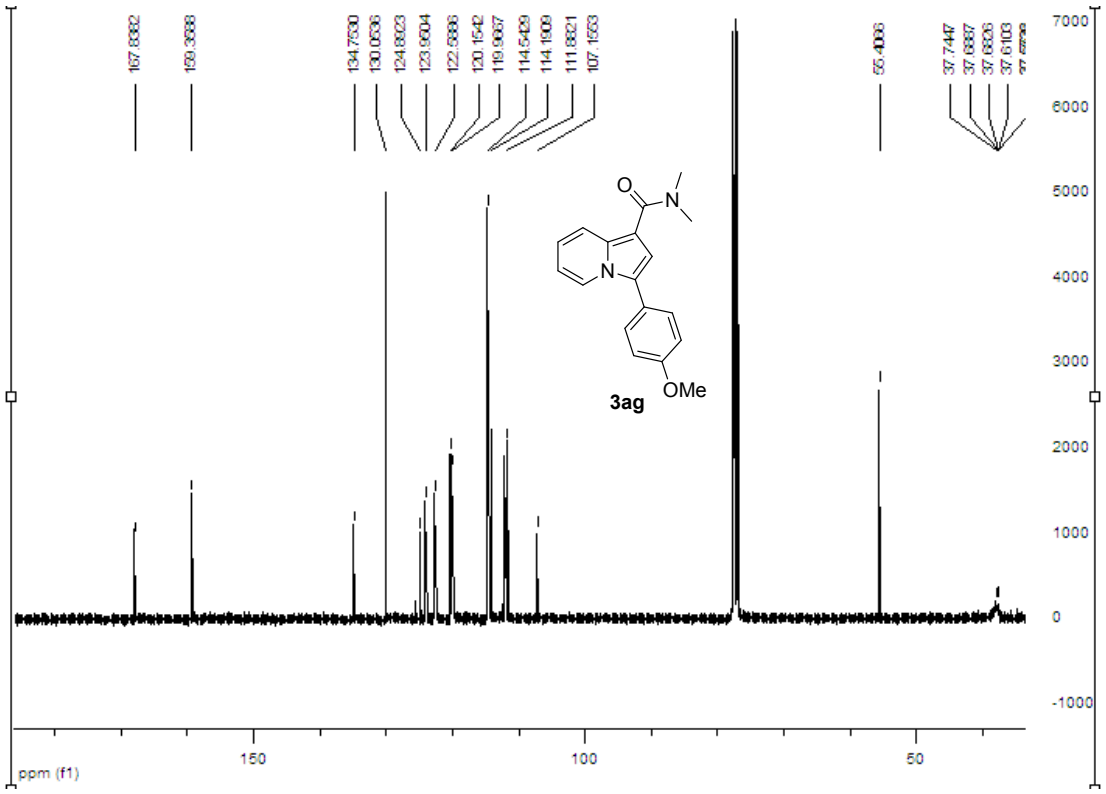
134.6748
131.4447
130.6378
130.5759
128.9160
126.1770
124.1300
123.0009
120.1657
120.1156
114.8345
111.9271
106.4142
19.7448
O
N
N
3af
600
500
400
300
200
100
0
150
100
50
ppm (f1)


138.4777
134.6734
131.4435
130.6371
130.5746
128.9147
126.1760
124.1287
122.9977
120.1645
120.1144
114.8335
111.9261
106.4135
O
N
N
3af
15
10
50
0


8.1651
8.1475
7.9744
7.9516
7.4711
7.4497
7.0005
7.0291
6.9299
6.9119
6.8397
6.6223
6.6057
6.5897
3.2189
O
N
N
OMe
3ag
0.98
1.05
1.90
2.23
2.42
1.12
3.00
6.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm (f1)
5000
4000
3000
2000
1000
0


8.165
8.148
7.975
7.952
7.471
7.450
7.051
7.029
6.930
6.912
6.890
6.622
6.606
6.589
O
N
N
OMe
3ag
0.86
0.94
1.81
1.95
2.25
1.00
8.00
7.50
7.00
6.50
ppm (f1)
300
250
200
150
100
500
0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130.0536
124.8023
123.9904
122.5986
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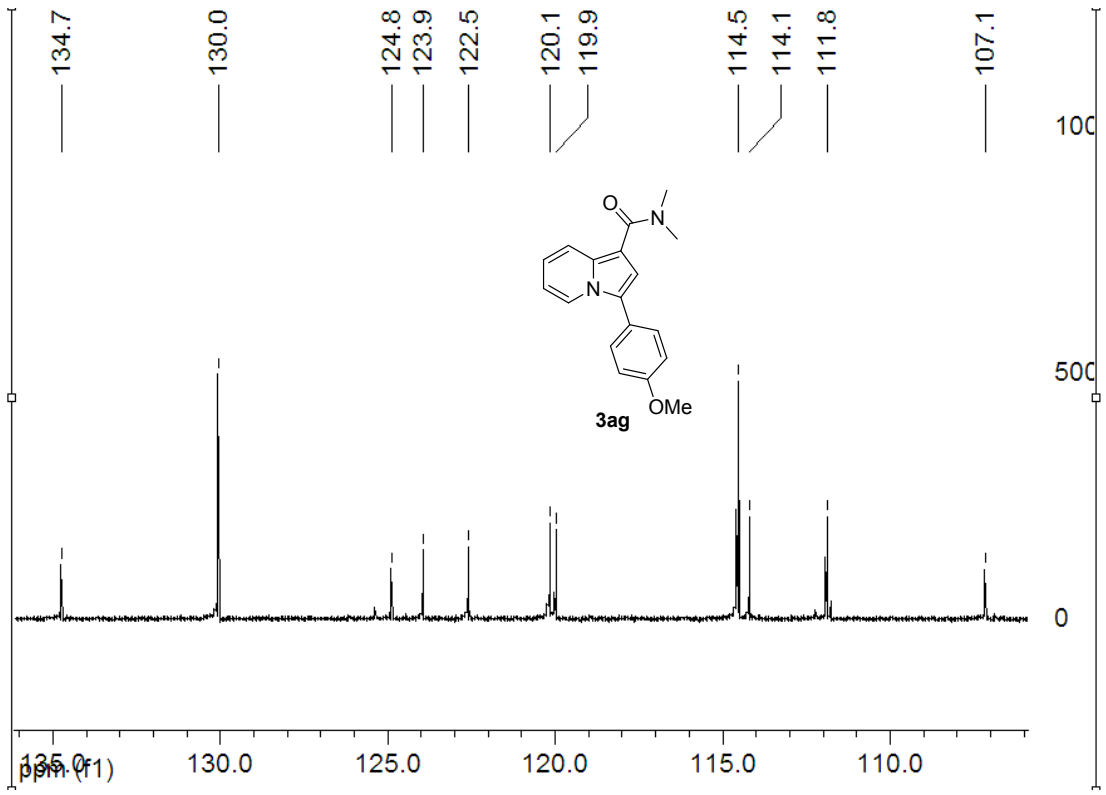
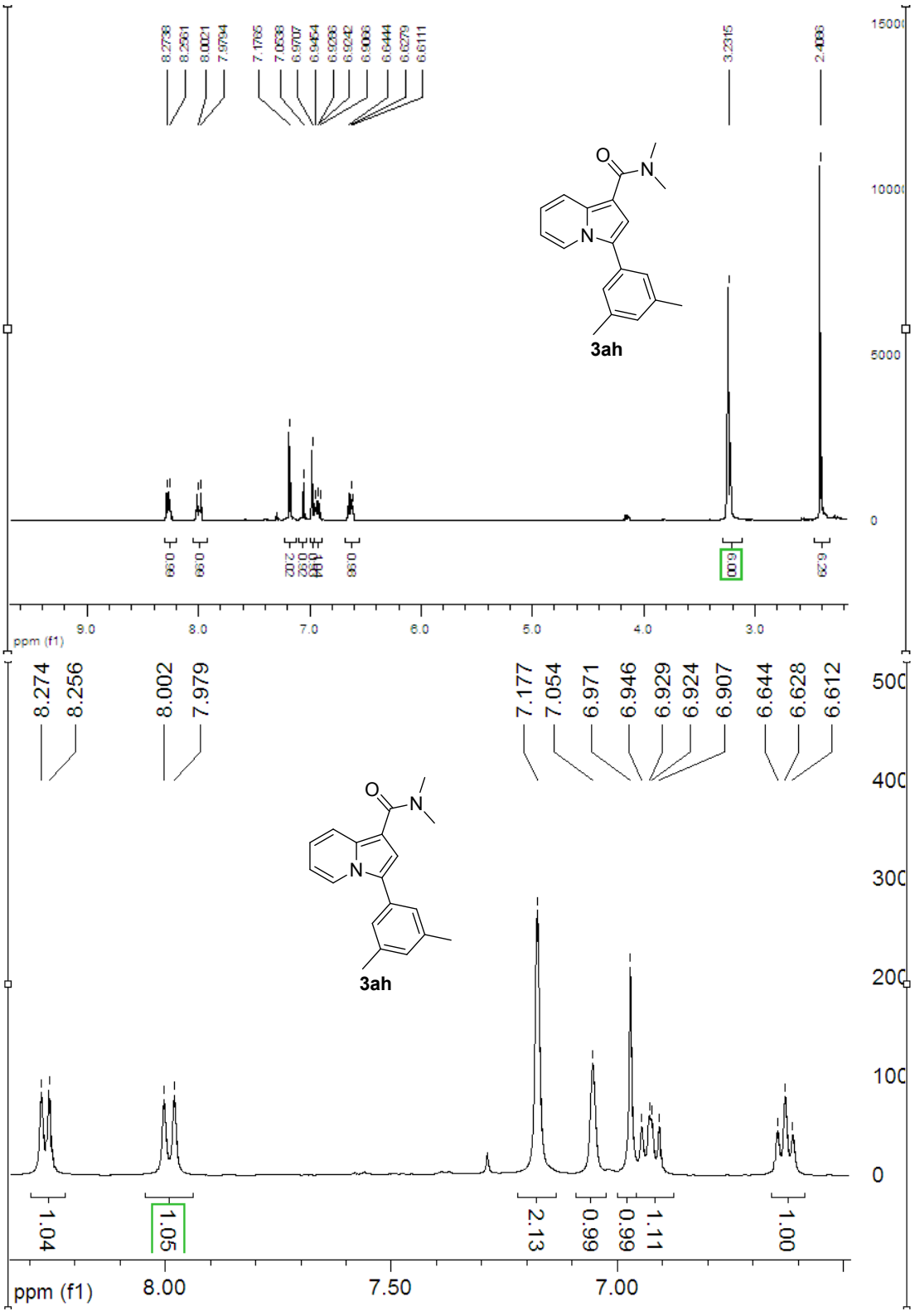
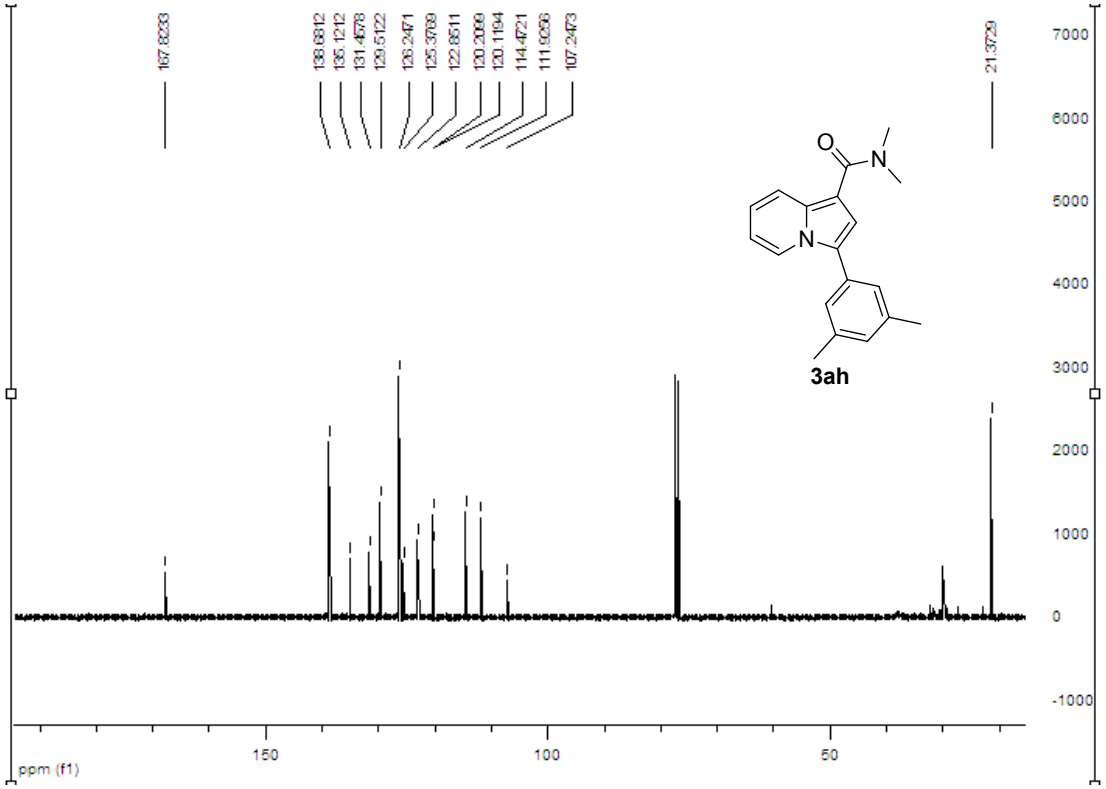
119.9967
114.5429
114.1909
111.8321
107.1553
55.4036
37.7447
37.6887
37.6326
37.6103
7000
6000
5000
4000
3000
2000
1000
0
-1000
150
100
50
ppm (f1)
O
N
N
OMe
3ag


134.7
130.0
124.8
123.9
122.5
120.1
119.9
114.5
114.1
111.8
107.1
100
500
0
135.0
130.0
125.0
120.0
115.0
110.0
ppm (f1)
O
N
N
OMe
3ag


3ah
ppm (f1)
3ah
ppm (f1)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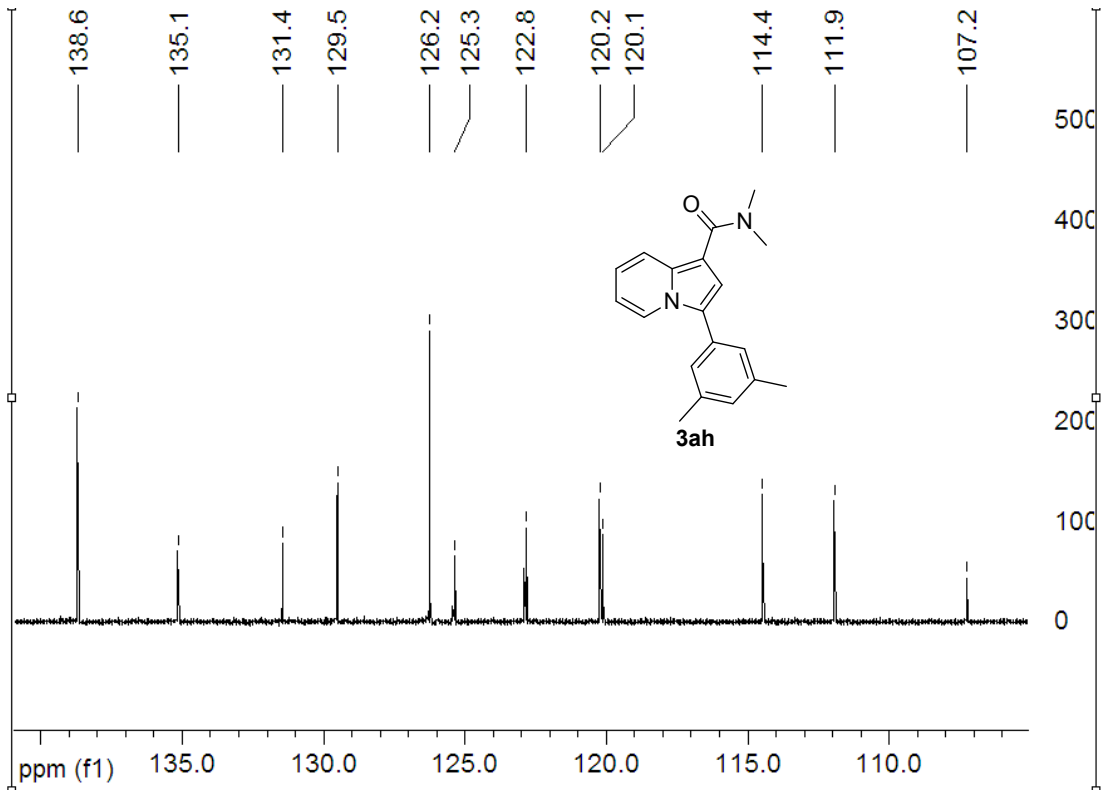
135.1212
131.4578
129.5122
126.2471
125.3769
122.8511
120.2066
120.1194
114.4721
111.9256
107.2473
21.3729
O
N
N
3ah
7000
6000
5000
4000
3000
2000
1000
0
-1000
150
100
50
ppm (f1)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135.1
131.4
129.5
126.2
125.3
122.8
120.2
120.1
114.4
111.9
107.2
O
N
N
3ah
500
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300
200
100
0
ppm (f1)
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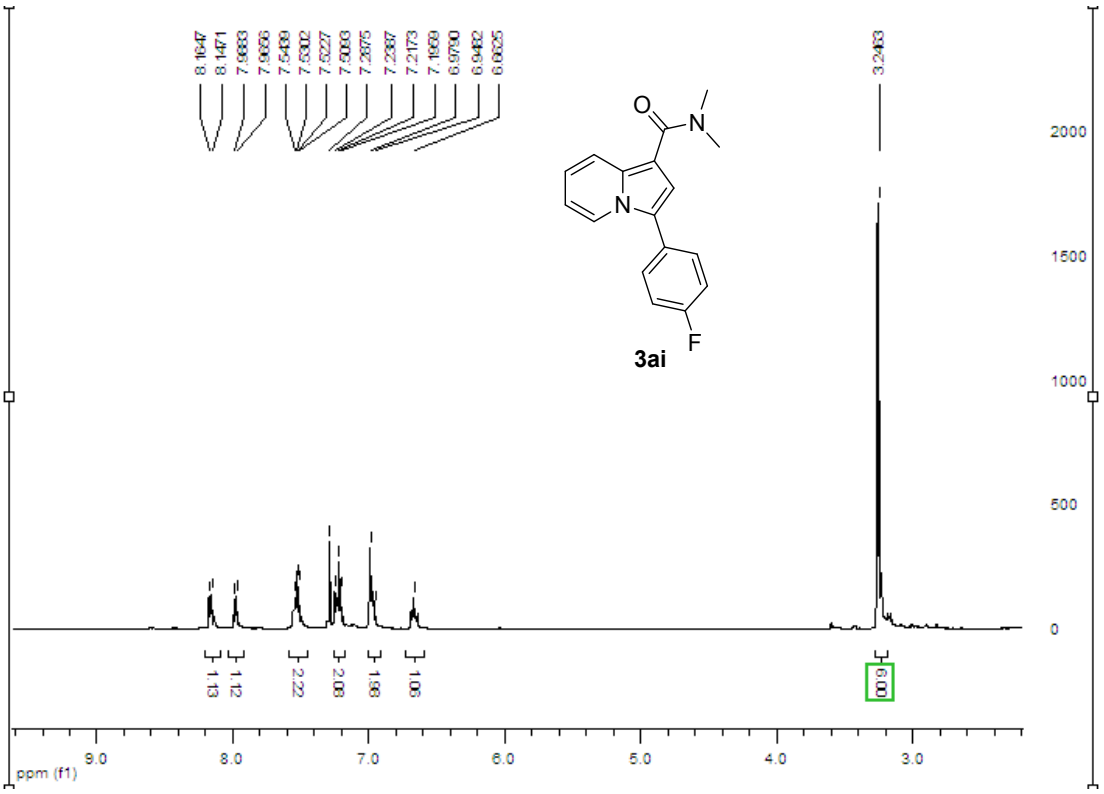
130.0
125.0
120.0
115.0
110.0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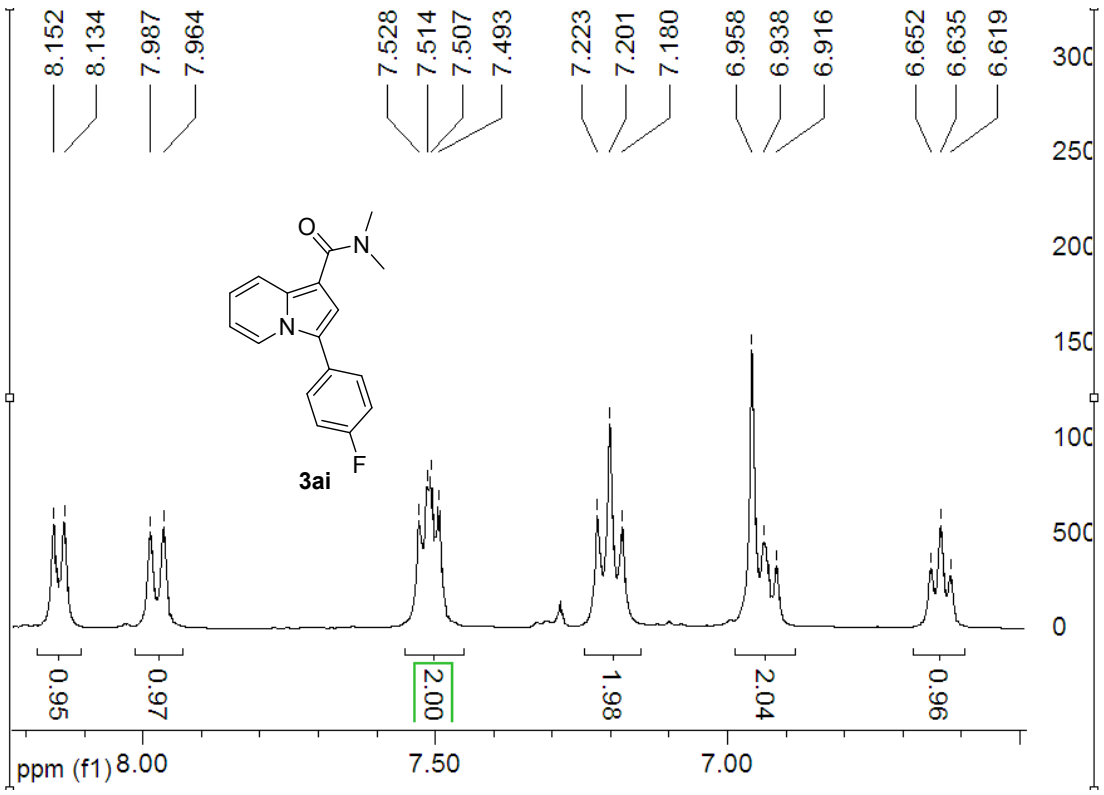
7.9806
7.5439
7.5302
7.5227
7.5093
7.2975
7.2397
7.2173
7.1999
6.9700
6.9482
6.6625
3.2483
O
N
N
F
3ai
1.13
1.12
2.22
2.08
1.98
1.06
6.00
ppm (f1)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2000
1500
1000
500
0


8.152
8.134
7.987
7.964
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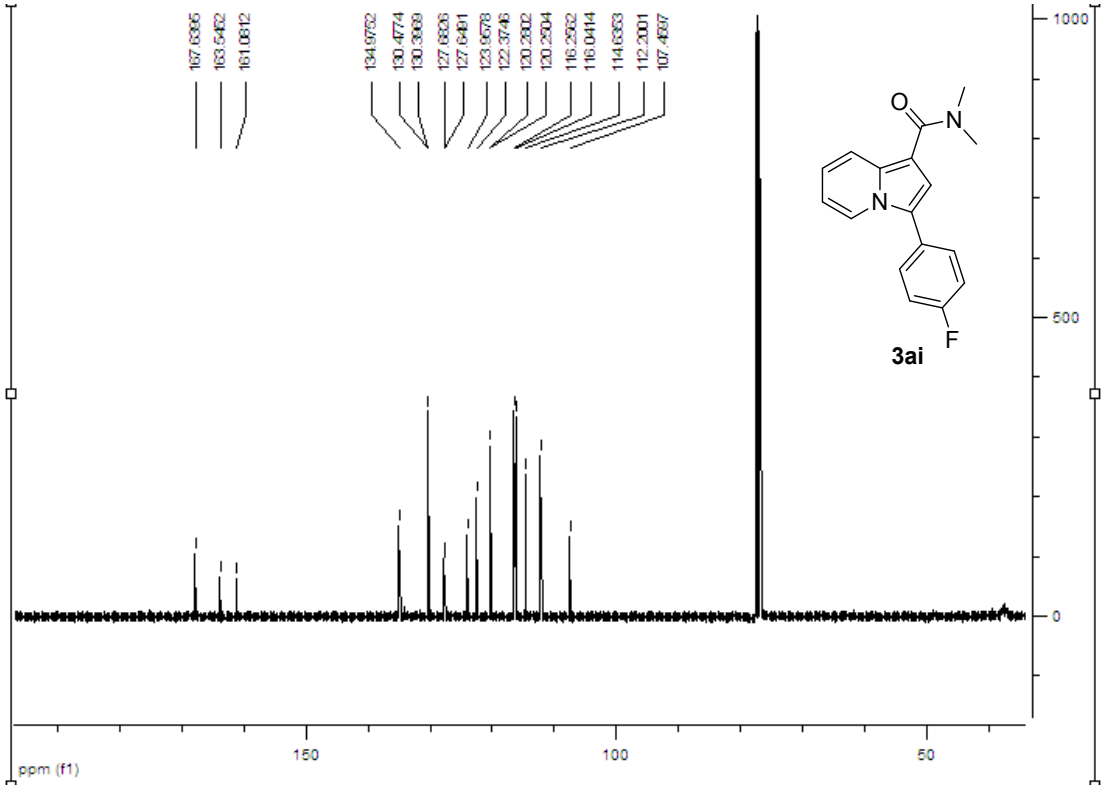
7.514
7.507
7.493
7.223
7.201
7.180
6.958
6.938
6.916
6.652
6.635
6.619
O
N
N
F
3ai
0.95
0.97
2.00
1.98
2.04
0.96
ppm (f1)
8.00
7.50
7.00
300
250
200
150
100
500
0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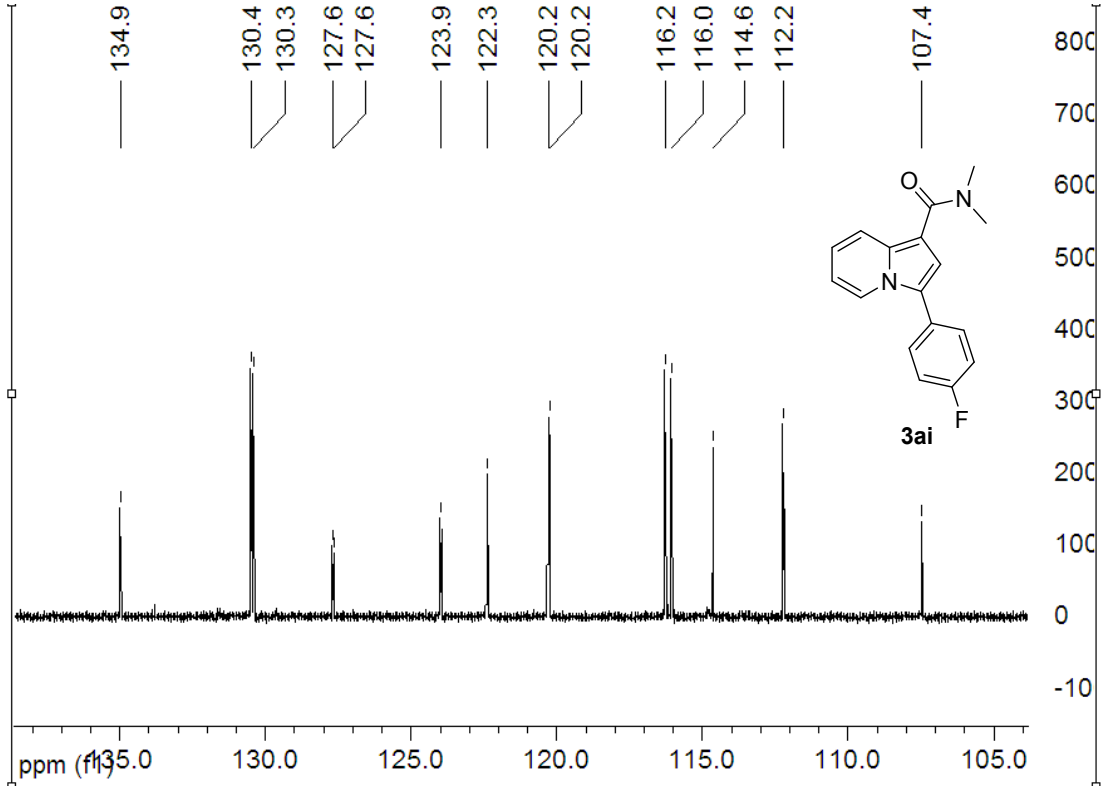
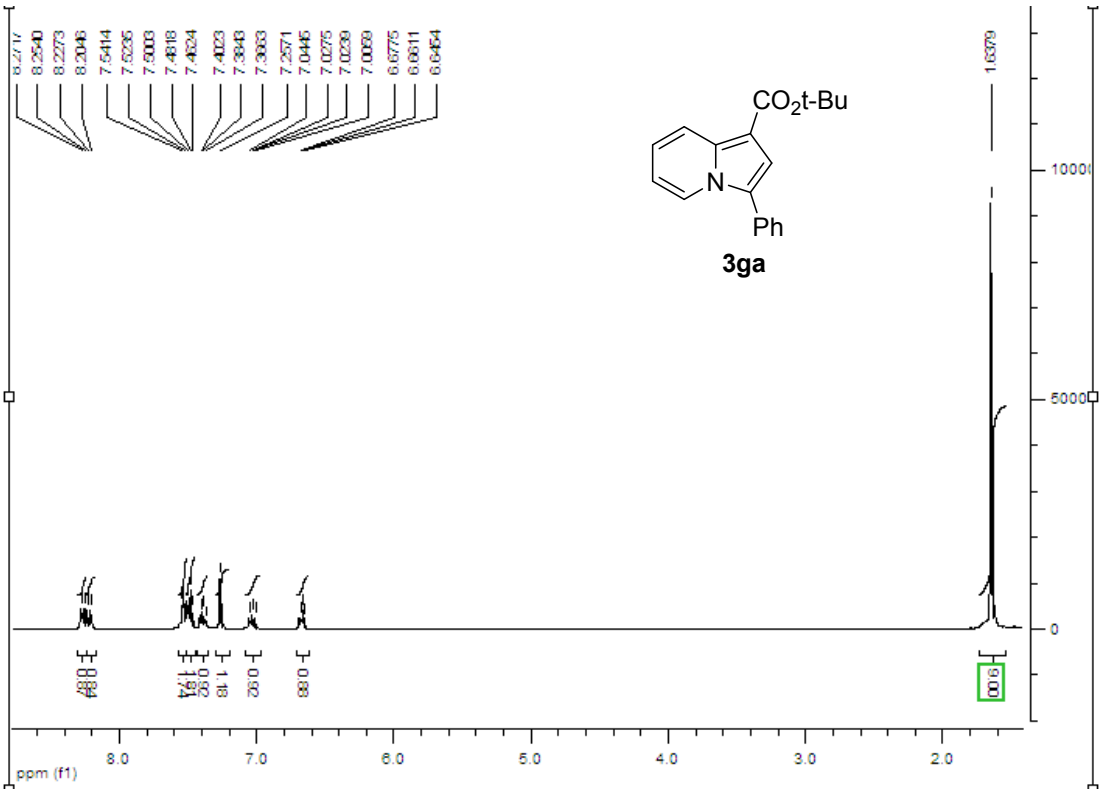
161.0812
134.9752
130.4774
130.3069
127.6826
127.6491
123.9578
122.3746
120.2302
120.2304
116.2962
116.0414
114.6303
112.2001
107.4697
1000
500
0
150
100
50
ppm (f1)
O
N
N
F
3ai


134.9
130.4
130.3
127.6
127.6
123.9
122.3
120.2
120.2
116.2
116.0
114.6
112.2
107.4
800
700
600
500
400
300
200
100
0
-10
135.0
130.0
125.0
120.0
115.0
110.0
105.0
ppm (f1)
O
N
N
F
3ai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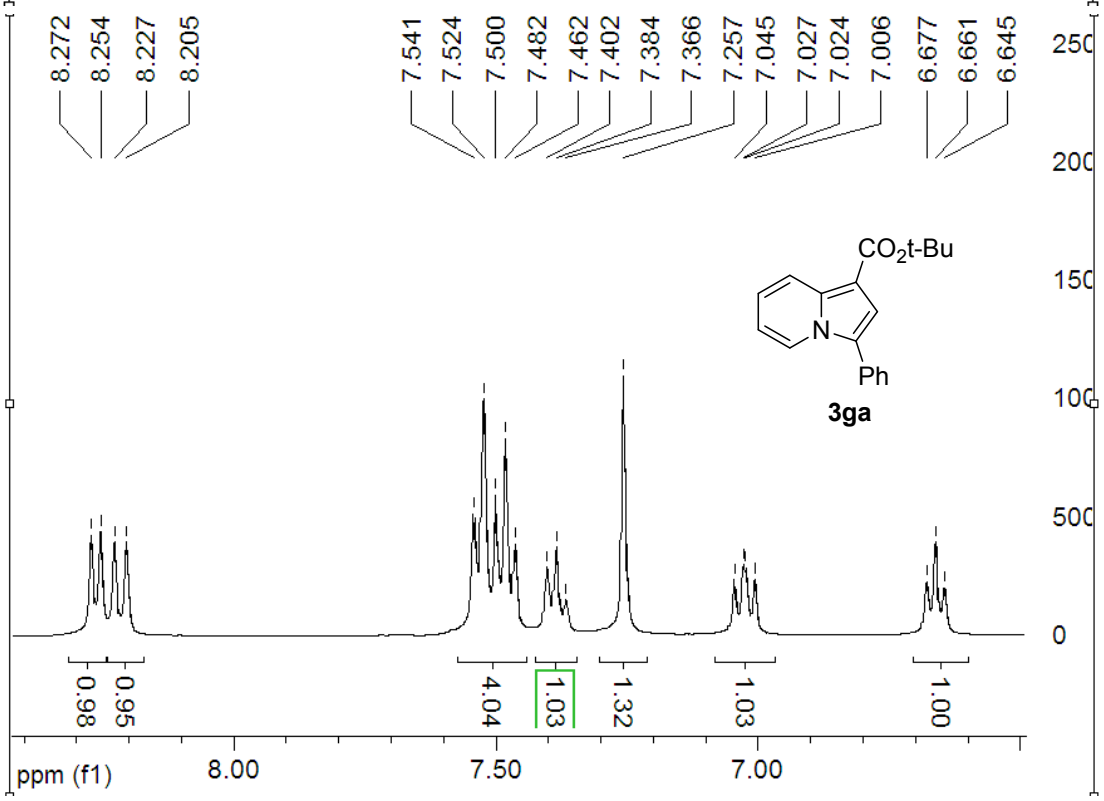
8.254
8.227
8.205
7.541
7.524
7.500
7.482
7.462
7.402
7.384
7.366
7.257
7.045
7.027
7.024
7.006
6.677
6.661
6.645
1.6379
CO2t-Bu
N
Ph
3ga
ppm (f1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0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8.254
8.227
8.205
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7.482
7.462
7.402
7.384
7.366
7.257
7.045
7.027
7.024
7.006
6.677
6.661
6.645
CO2t-Bu
N
Ph
3ga
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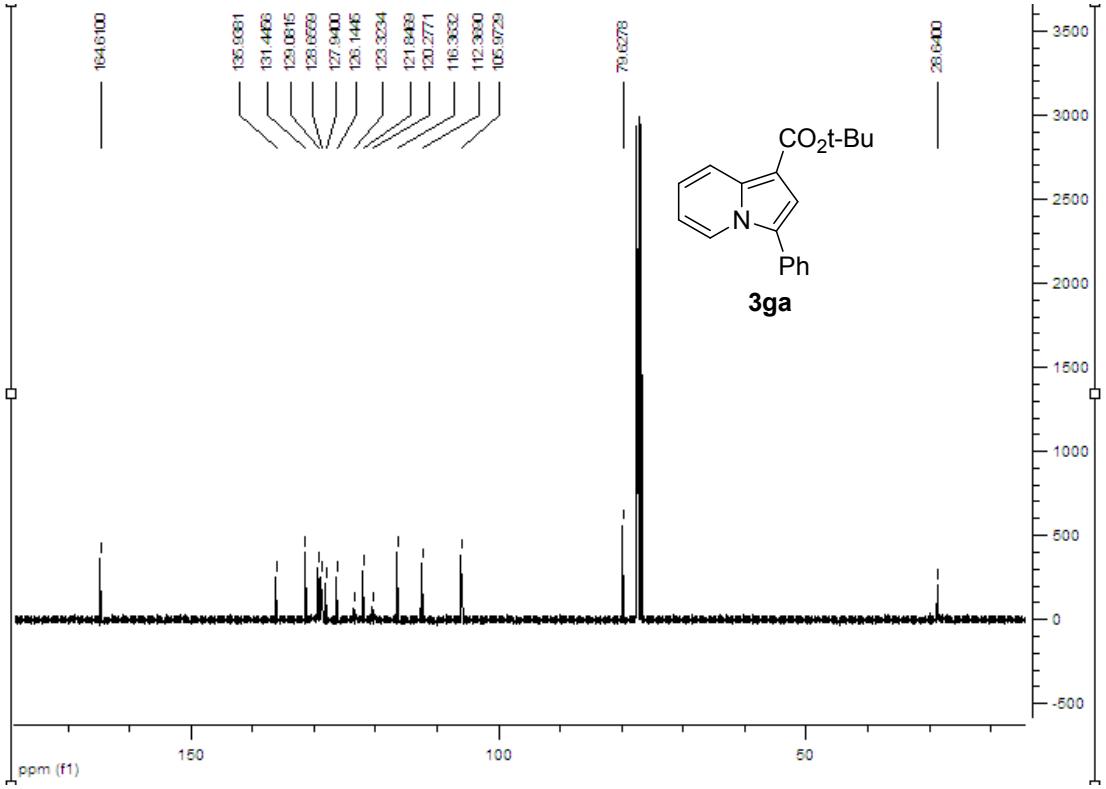
4.04
1.03
1.32
1.03
1.00
ppm (f1)
8.00
7.50
7.00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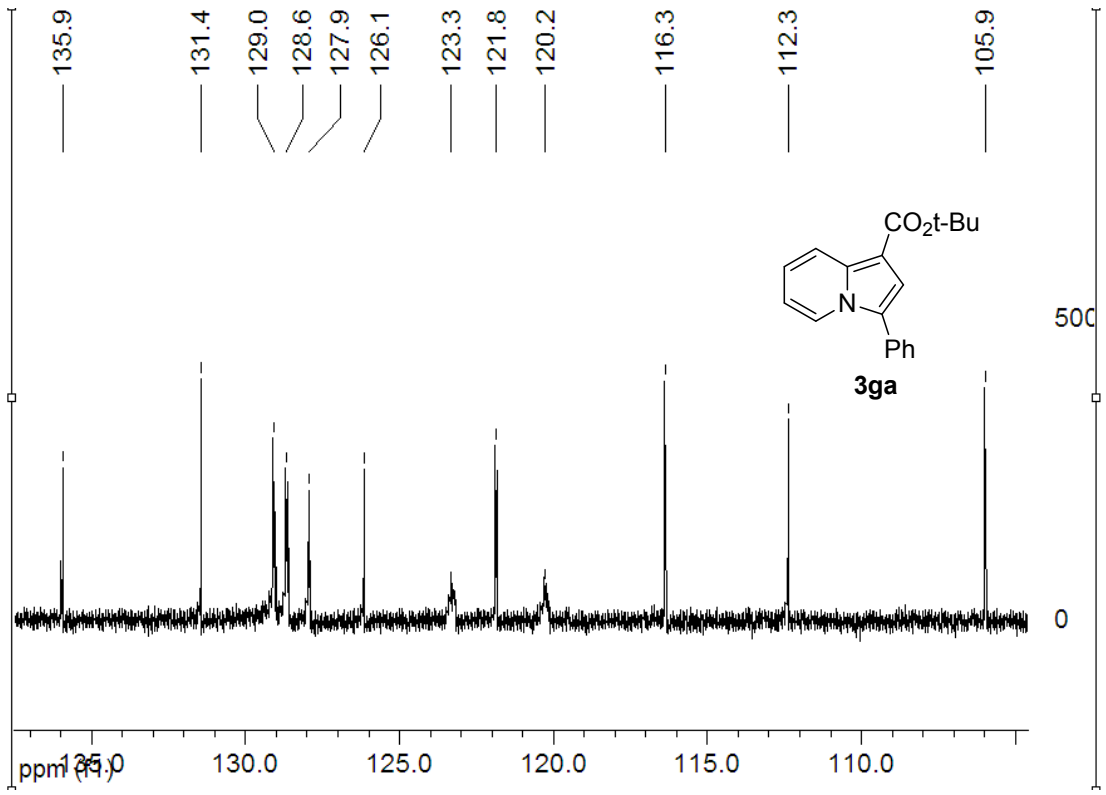
129.0615
128.6699
127.9400
126.1445
123.3234
121.8409
120.2771
116.3632
112.3900
105.9729
79.6278
28.6400
CO2t-Bu
N
Ph
3ga
3500
3000
2500
2000
1500
1000
500
0
-500
150
100
50
ppm (f1)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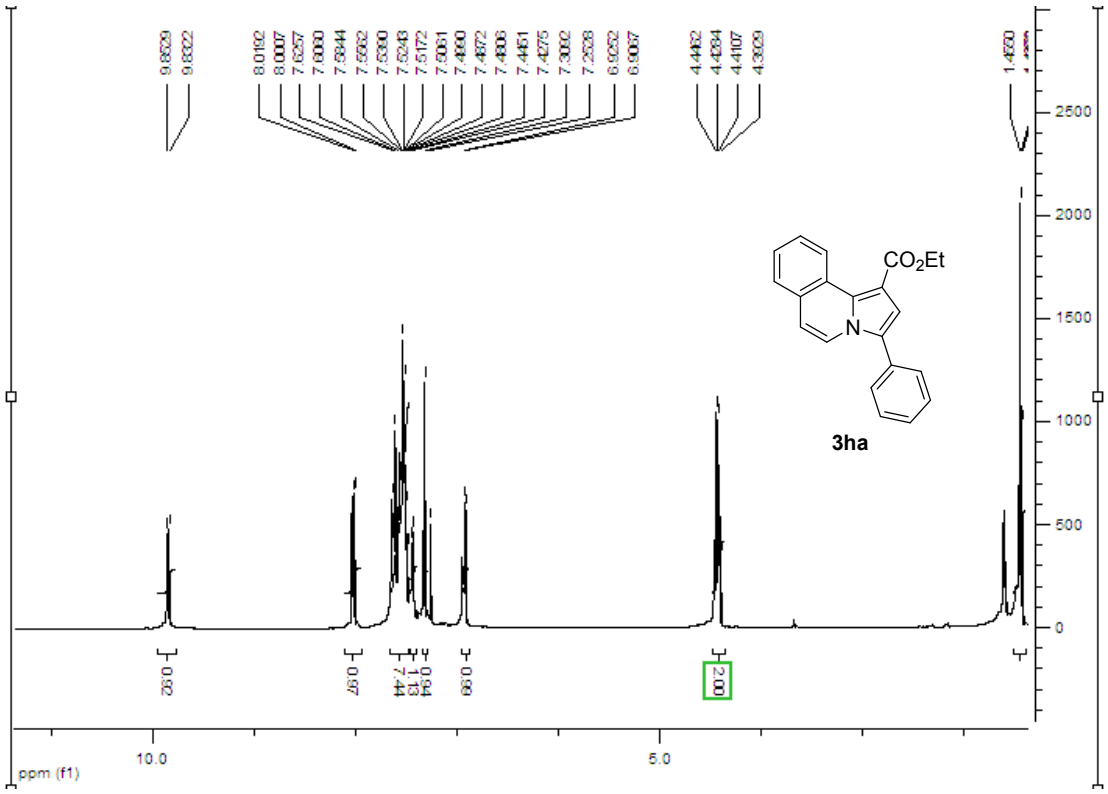
129.0
128.6
127.9
126.1
123.3
121.8
120.2
116.3
112.3
105.9
CO2t-Bu
N
Ph
3ga
500
0
135.0
130.0
125.0
120.0
115.0
110.0
ppm (f1)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8.0007
7.6257
7.6000
7.5944
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7.5248
7.5172
7.5061
7.4900
7.4872
7.4806
7.4451
7.4275
7.3092
7.2528
6.9052
6.9067
4.4482
4.4284
4.4107
4.3929
1.4500
2500
2000
1500
1000
500
0
0.92
0.97
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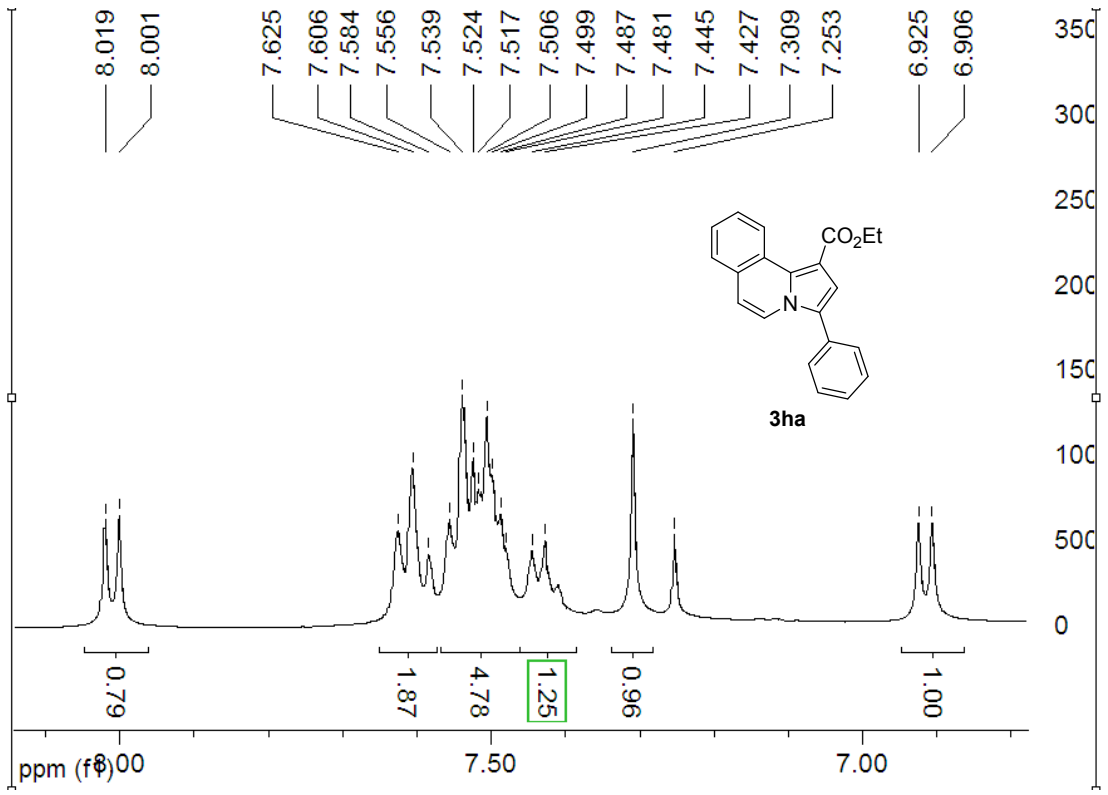
7.44
0.94
0.99
2.00
10.0
5.0
ppm (f1)
CO2Et
N
3ha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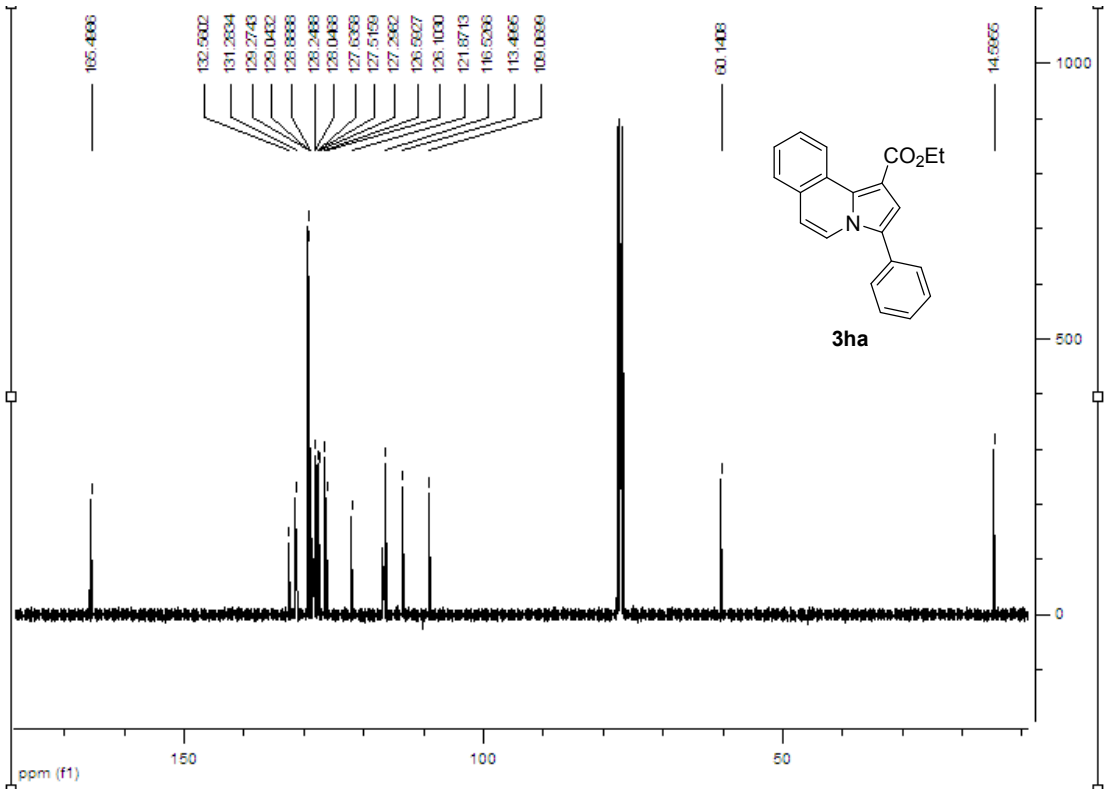
8.001
7.625
7.606
7.584
7.556
7.539
7.524
7.517
7.506
7.499
7.487
7.481
7.445
7.427
7.309
7.253
6.925
6.906
350
300
250
200
150
100
500
0
0.79
1.87
4.78
1.25
0.96
1.00
8.00
7.50
7.00
ppm (f1)
CO2Et
N
3ha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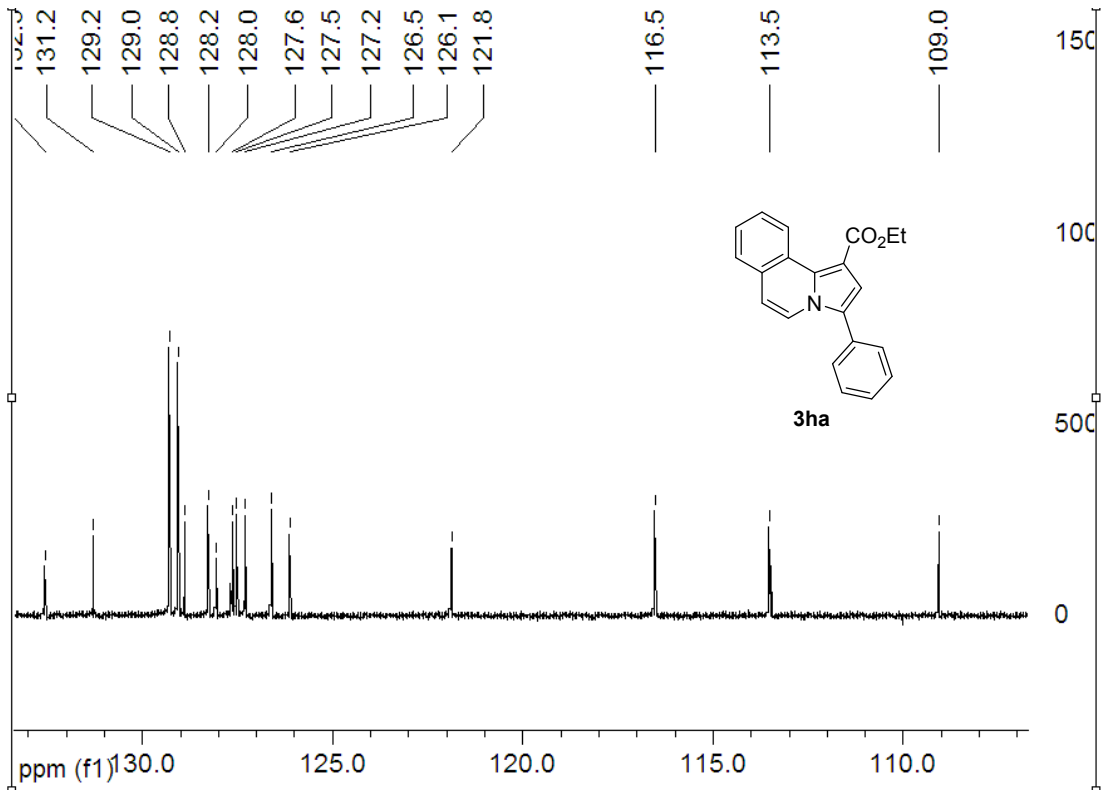
128.2488
128.0468
127.6388
127.5159
127.2962
126.5027
126.1000
121.8713
116.5206
113.4665
109.0999
60.1408
14.3955
1000
500
0
CO2Et
N
3ha
150
100
50
ppm (f1)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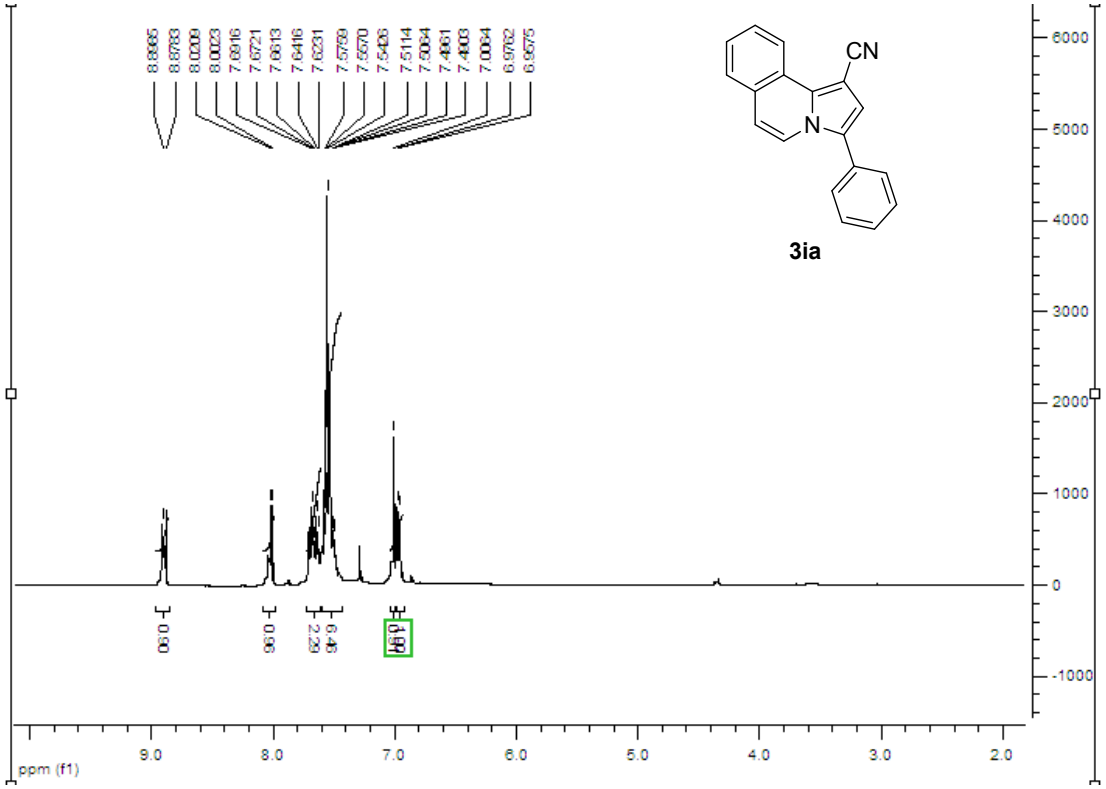
129.2
129.0
128.8
128.2
128.0
127.6
127.5
127.2
126.5
126.1
121.8
116.5
113.5
109.0
150
100
500
0
CO2Et
N
3ha
ppm (f1)
130.0
125.0
120.0
115.0
110.0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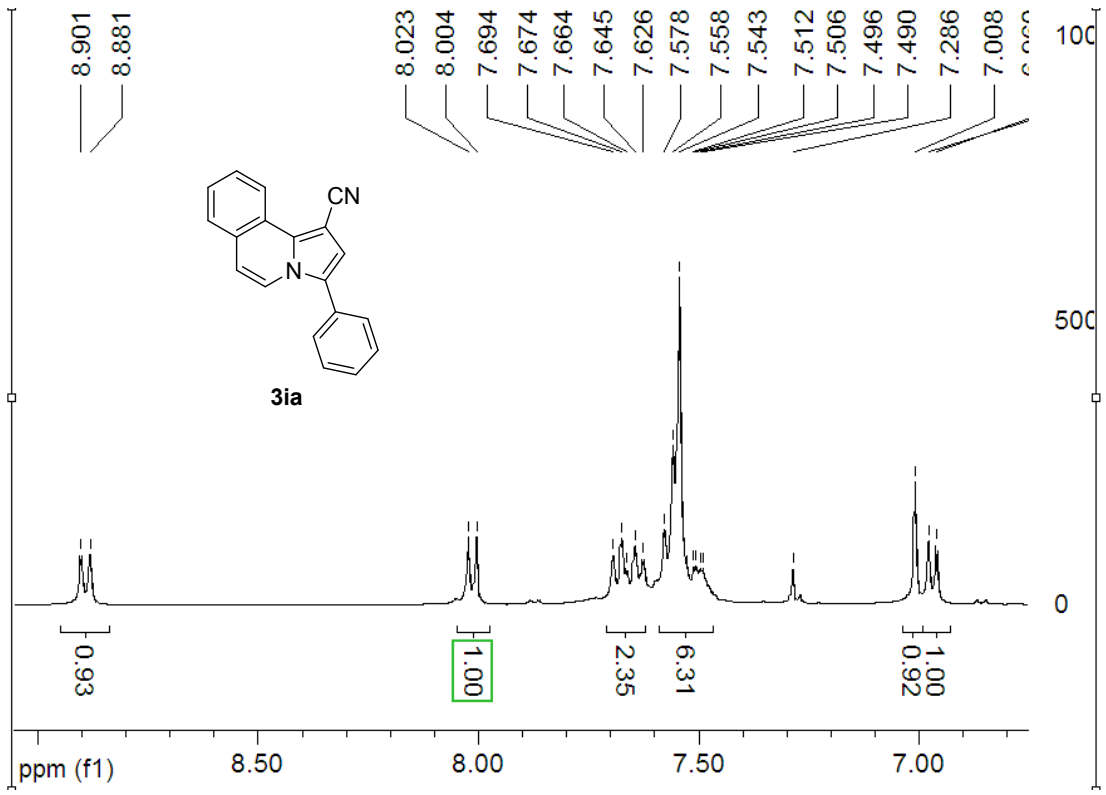
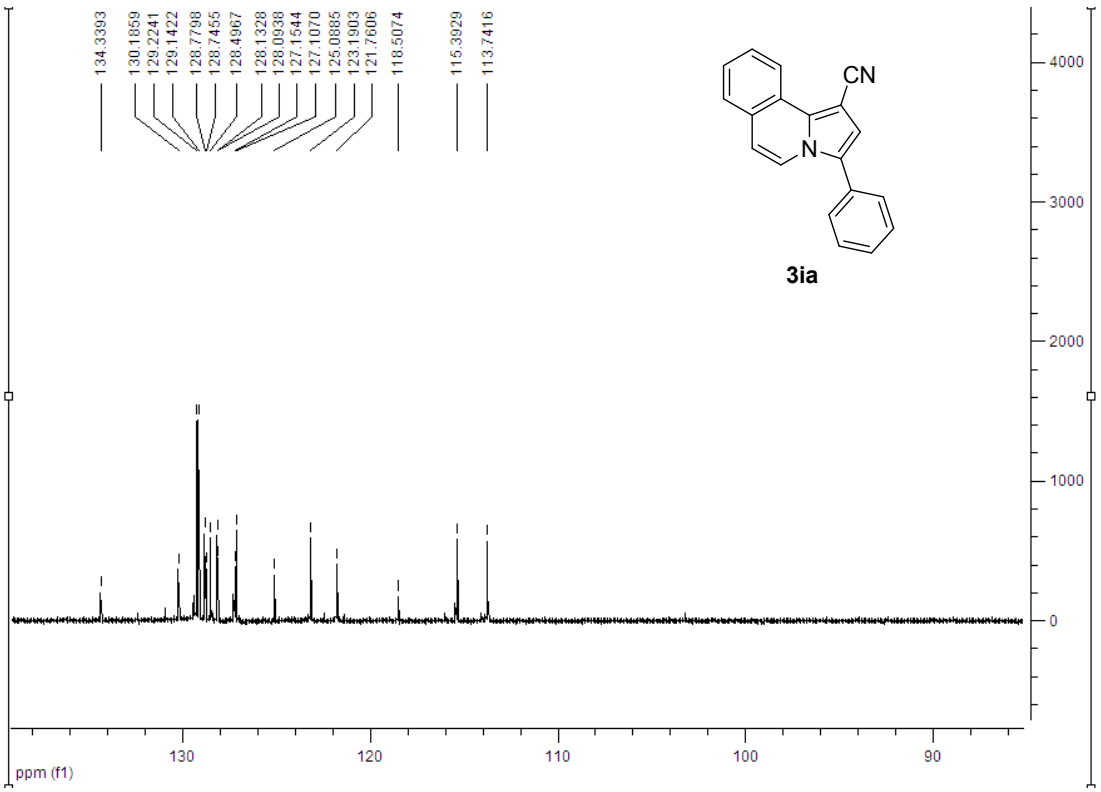
8.8783
8.0009
8.0023
7.9916
7.6721
7.6613
7.6416
7.6231
7.5789
7.5570
7.5406
7.5114
7.4964
7.4961
7.4803
7.0064
6.9762
6.9575
CN
N
3ia
0.90
0.96
2.29
6.46
1.00
6000
5000
4000
3000
2000
1000
0
-1000
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (f1)


8.901
8.881
8.023
8.004
7.694
7.674
7.664
7.645
7.626
7.578
7.558
7.543
7.512
7.506
7.496
7.490
7.286
7.008
CN
N
3ia
0.93
1.00
2.35
6.31
0.92
1.00
100
500
0
ppm (f1)
8.50
8.00
7.50
7.00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130.1859
129.2241
129.1422
128.7798
128.7455
128.4967
128.1328
128.0938
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125.0885
123.1903
121.7606
118.5074
115.3929
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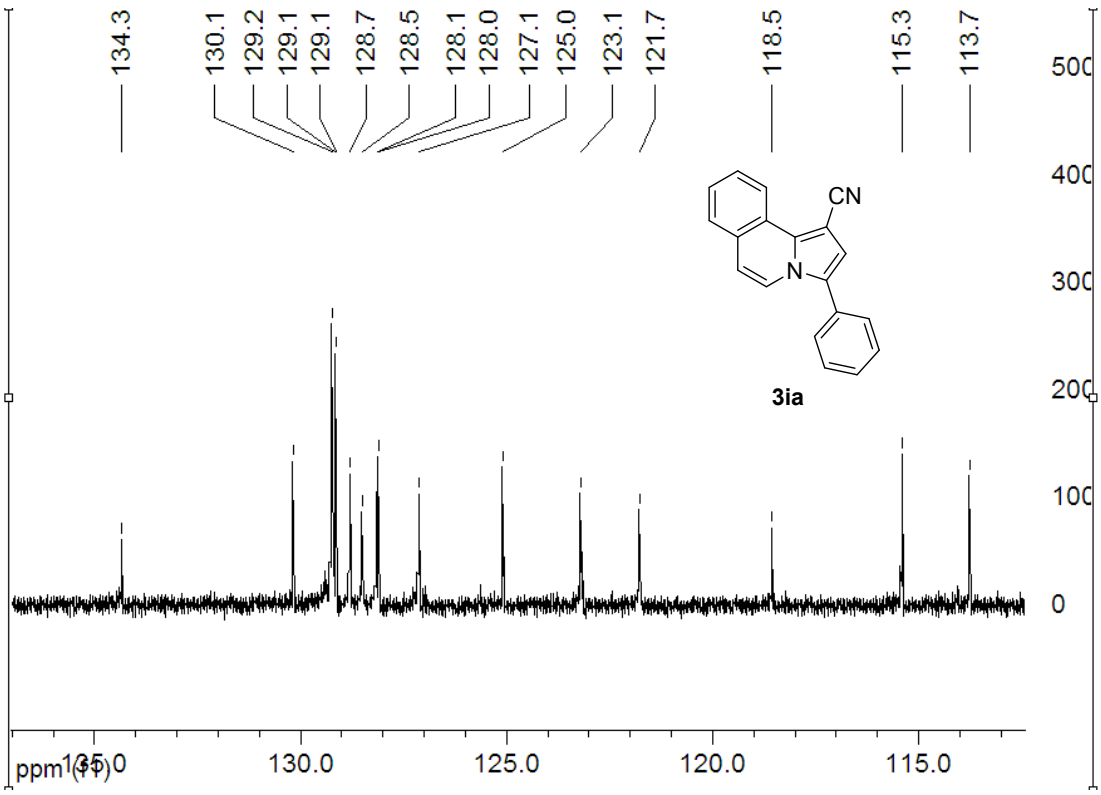
CN
N
3ia
4000
3000
2000
1000
0
130
120
110
100
90
ppm (f1)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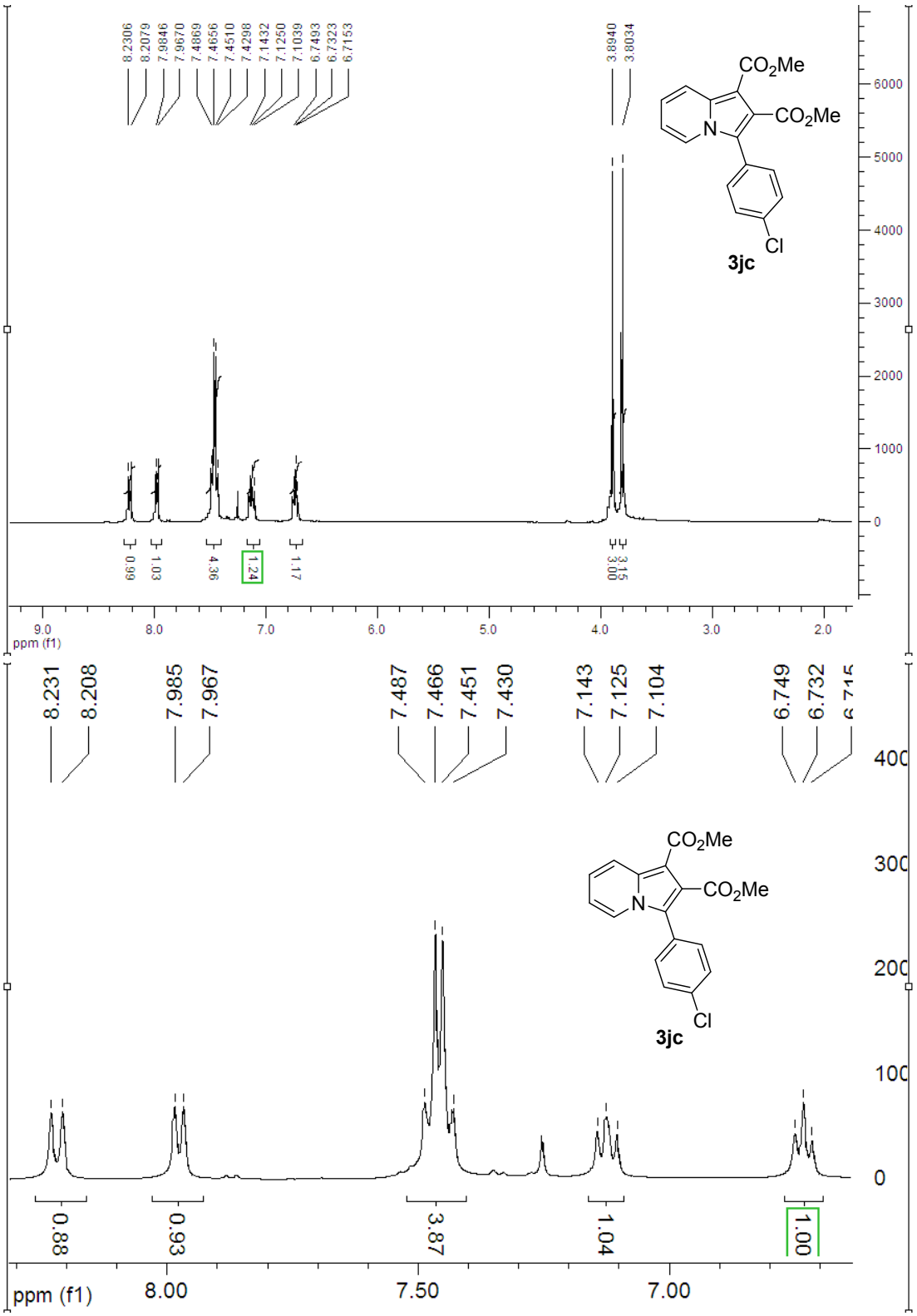
130.1
129.2
129.1
129.1
128.7
128.5
128.1
128.0
127.1
125.0
123.1
121.7
118.5
115.3
113.7
CN
N
3ia
500
400
300
200
100
0
ppm (f1)
135.0
130.0
125.0
120.0
115.0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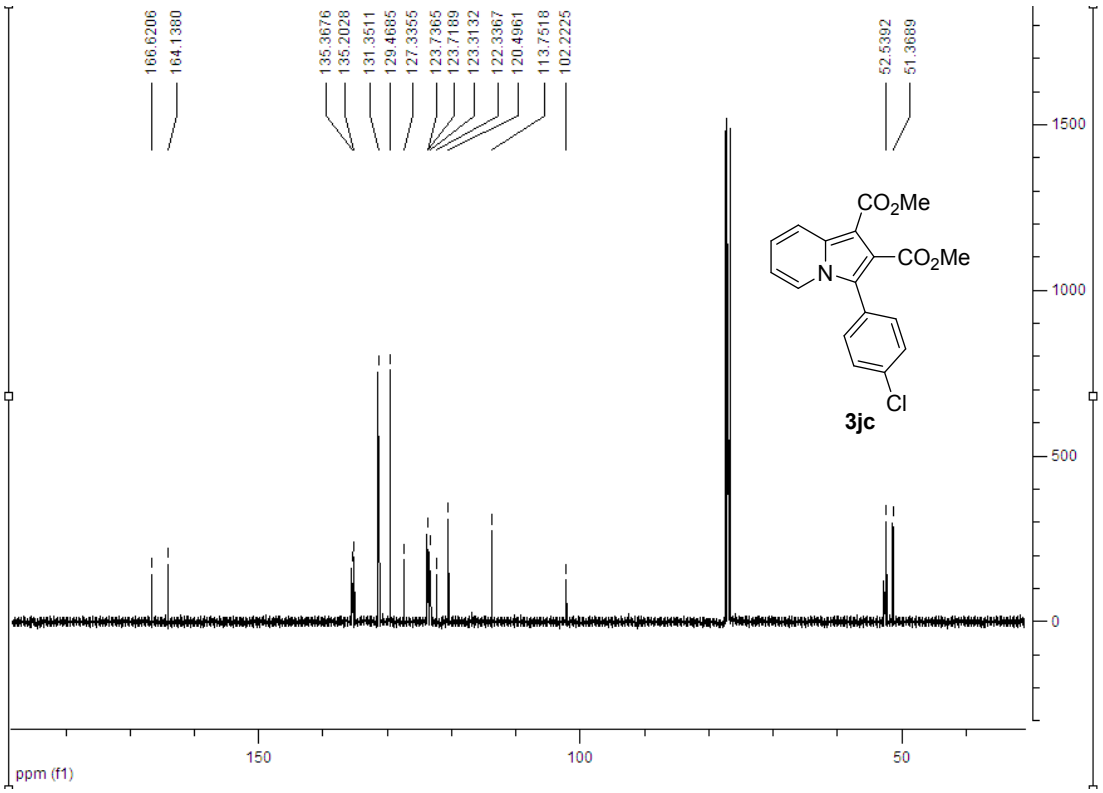
8.2079
7.9846
7.9670
7.4869
7.4656
7.4510
7.4298
7.1432
7.1250
7.1039
6.7493
6.7323
6.7153
3.8940
3.8034
CO2Me
CO2Me
N
Cl
3jc
0.99
1.03
4.36
1.24
1.17
3.15
3.00
ppm (f1)
8.231
8.208
7.985
7.967
7.487
7.466
7.451
7.430
7.143
7.125
7.104
6.749
6.732
0.88
0.93
3.87
1.04
1.00
ppm (f1)
8.00
7.50
7.00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135.3676
135.2028
131.3511
129.4685
127.3355
123.7365
123.7189
123.3132
122.3367
120.4961
113.7518
102.2225
52.5392
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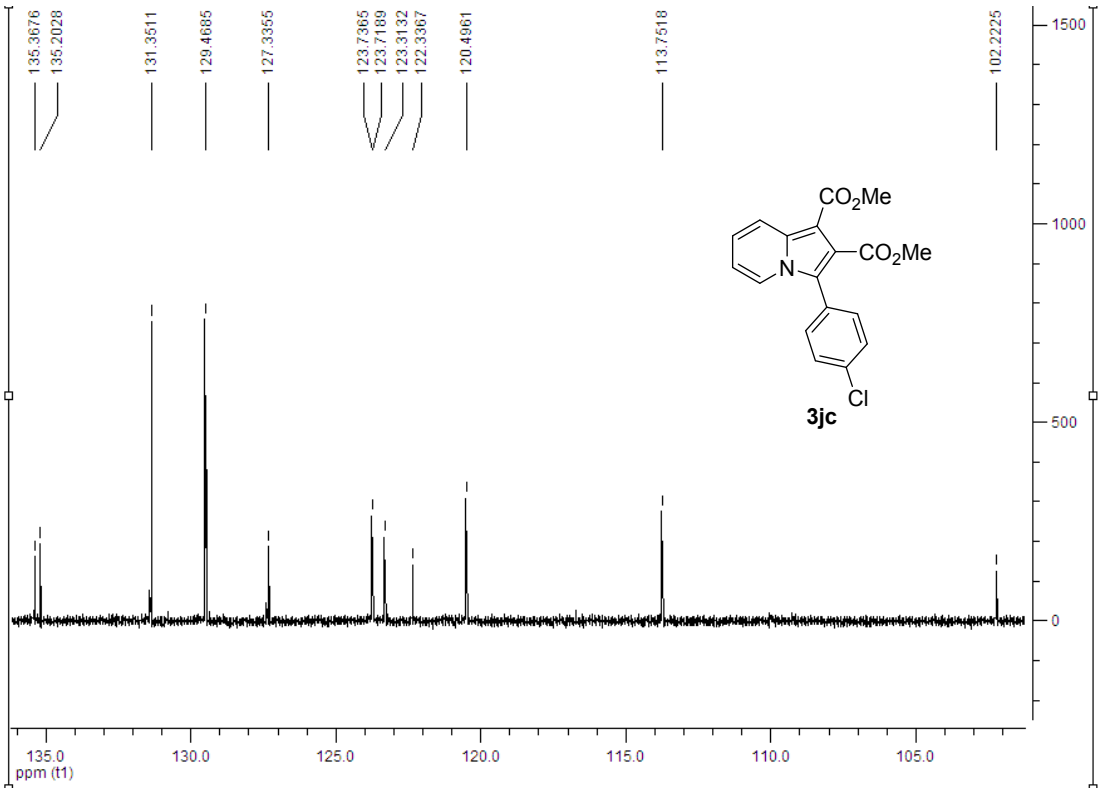
CO2Me
CO2Me
N
Cl
3jc
1500
1000
500
0
150
100
50
ppm (f1)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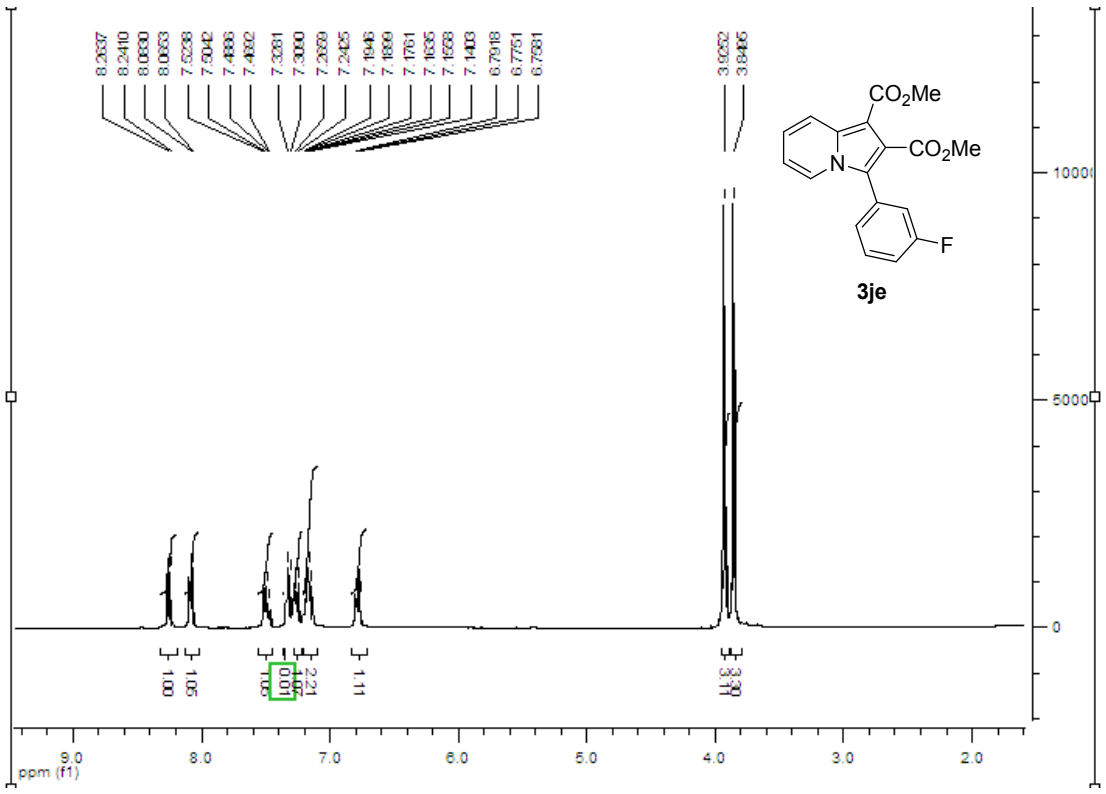
135.2028
131.3511
129.4685
127.3355
123.7365
123.7189
123.3132
122.3367
120.4961
113.7518
102.2225
CO2Me
CO2Me
N
Cl
3jc
1500
1000
500
0
135.0
130.0
125.0
120.0
115.0
110.0
105.0
ppm (t1)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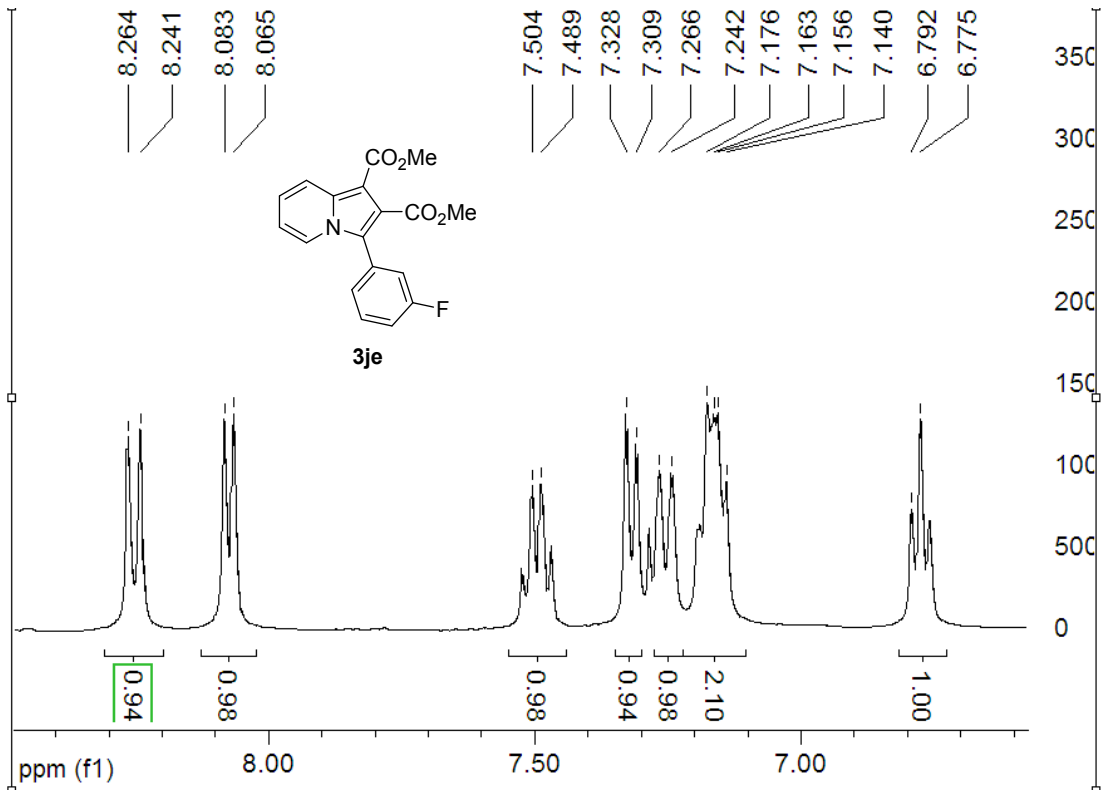
8.2410
8.0830
8.0653
7.5238
7.5042
7.4886
7.4802
7.3381
7.3000
7.2689
7.2425
7.1946
7.1899
7.1761
7.1635
7.1508
7.1403
6.7918
6.7751
6.7581
3.9552
3.8406
CO2Me
CO2Me
N
F
3je
1.00
1.05
1.08
1.00
2.21
1.11
3.39
ppm (f1)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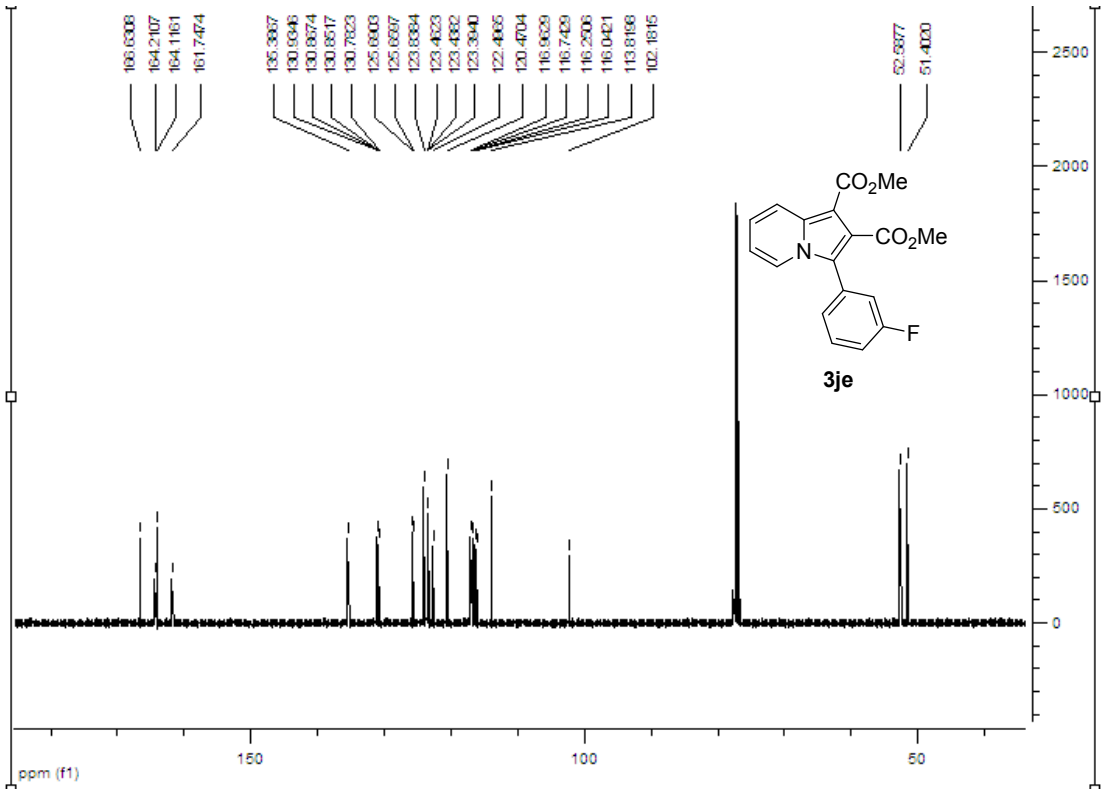
7.328
7.309
7.266
7.242
7.176
7.163
7.156
7.140
6.792
6.775
CO2Me
CO2Me
N
F
3je
0.94
0.98
0.98
0.94
0.98
2.10
1.00
ppm (f1)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130.7823
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125.6597
123.8384
123.4623
123.4382
123.3940
122.4965
120.4704
116.9629
116.7429
116.2506
116.0421
113.8198
102.1815
52.5977
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CO2Me
N
F
3je
2500
2000
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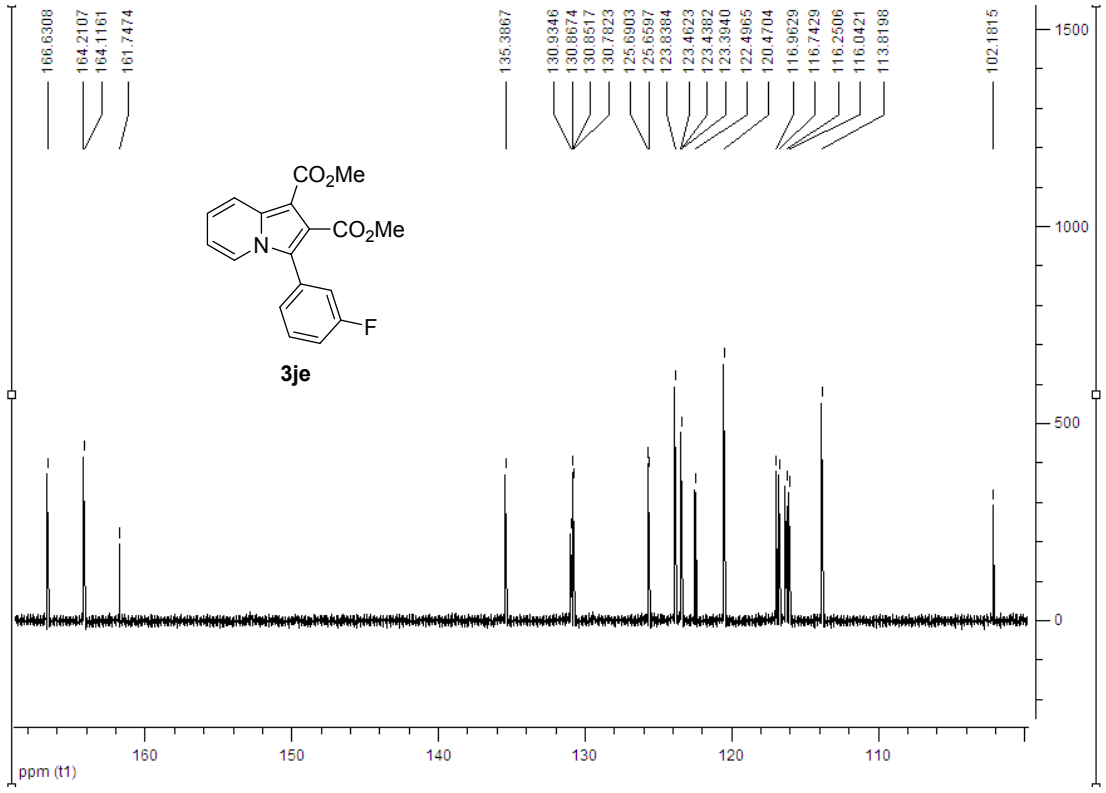
1000
500
0
150
100
50
ppm (f1)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164.2107
164.1161
161.7474
135.3867
130.9346
130.8674
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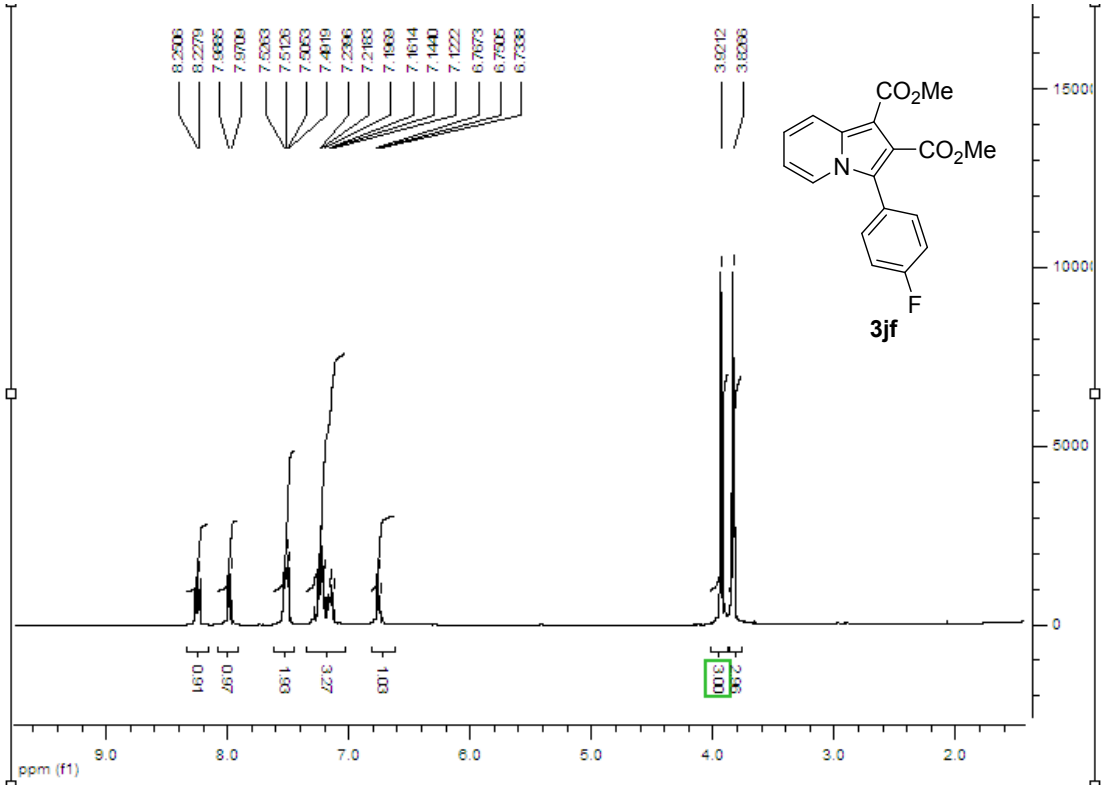
130.7823
125.6903
125.6597
123.8384
123.4623
123.4382
123.3940
122.4965
120.4704
116.9629
116.7429
116.2506
116.0421
113.8198
102.1815
CO2Me
CO2Me
N
F
3je
1500
1000
500
0
160
150
140
130
120
110
ppm (t1)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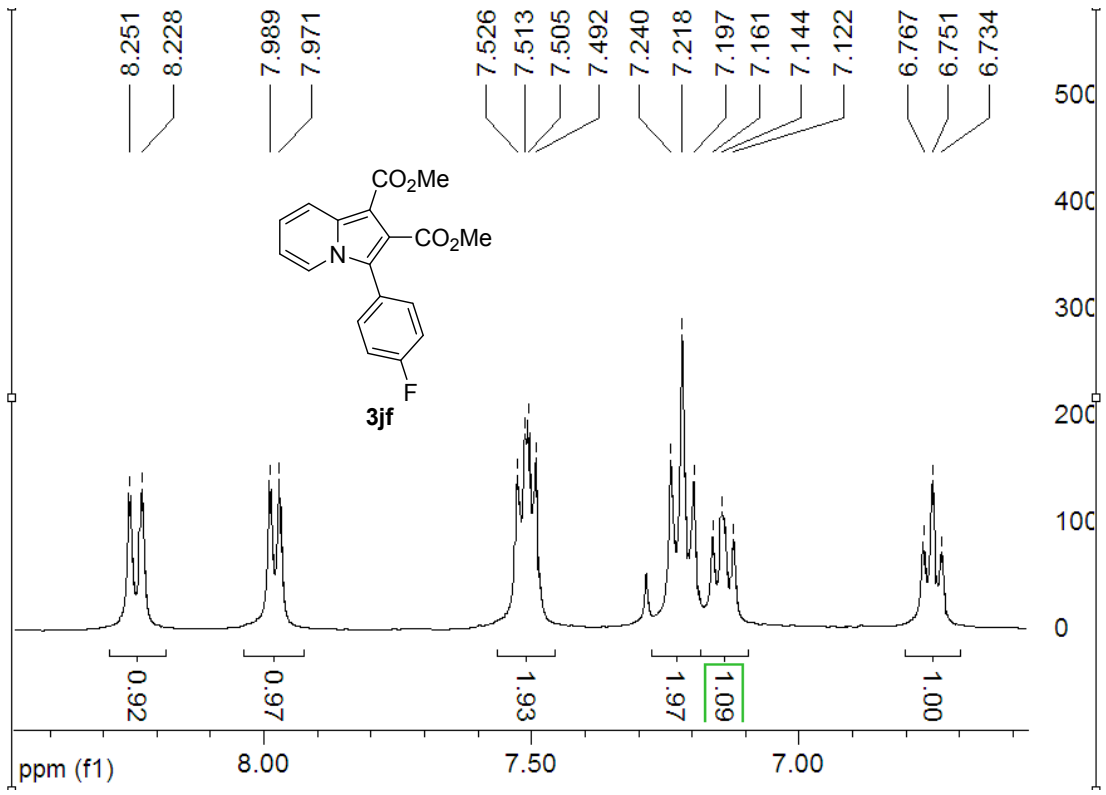
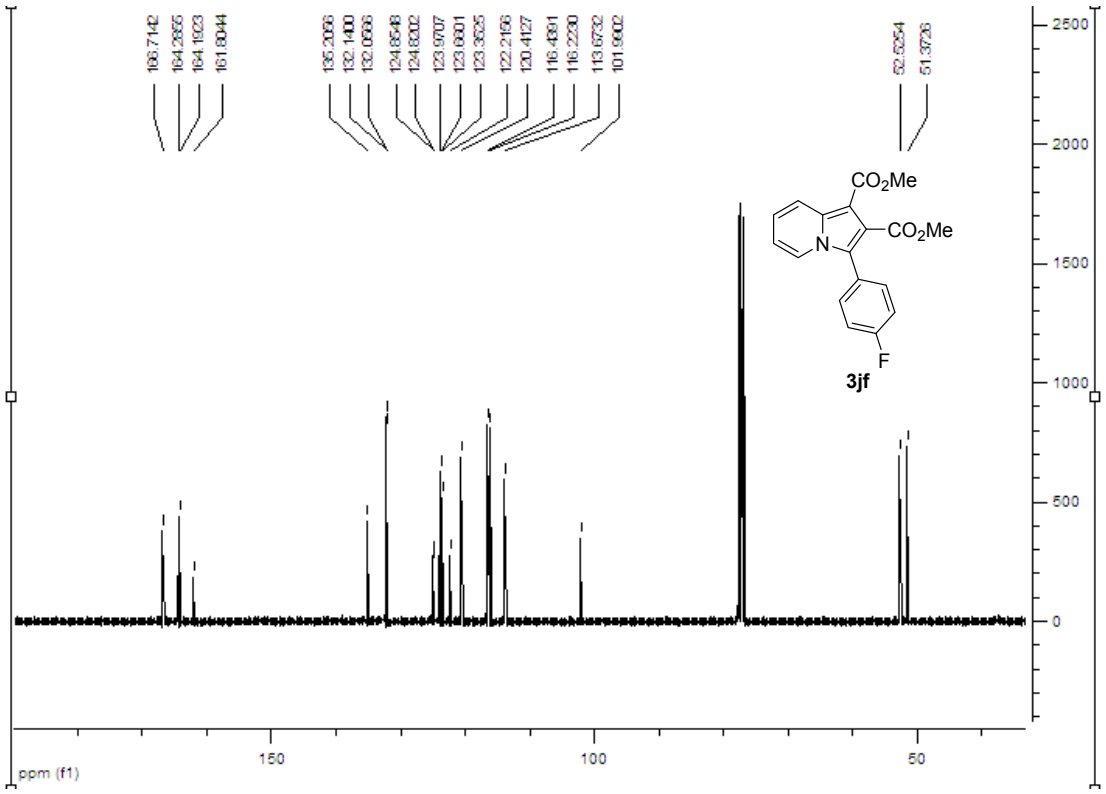
7.9685
7.9709
7.5263
7.5126
7.5053
7.4819
7.2306
7.2183
7.1989
7.1614
7.1440
7.1222
6.7673
6.7505
6.7338
3.9212
3.8298
CO2Me
CO2Me
N
F
3jf
0.91
0.97
1.53
3.27
1.03
3.00
2.95
ppm (f1)


8.251
8.228
7.989
7.971
7.526
7.513
7.505
7.492
7.240
7.218
7.197
7.161
7.144
7.122
6.767
6.751
6.734
CO2Me
CO2Me
N
F
3jf
0.92
0.97
1.93
1.97
1.09
1.00
ppm (f1)
8.00
7.50
7.00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164.1923
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132.0566
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124.8202
123.9707
123.6601
123.3625
122.2156
120.4127
116.4391
116.2230
113.6732
101.9902
52.5254
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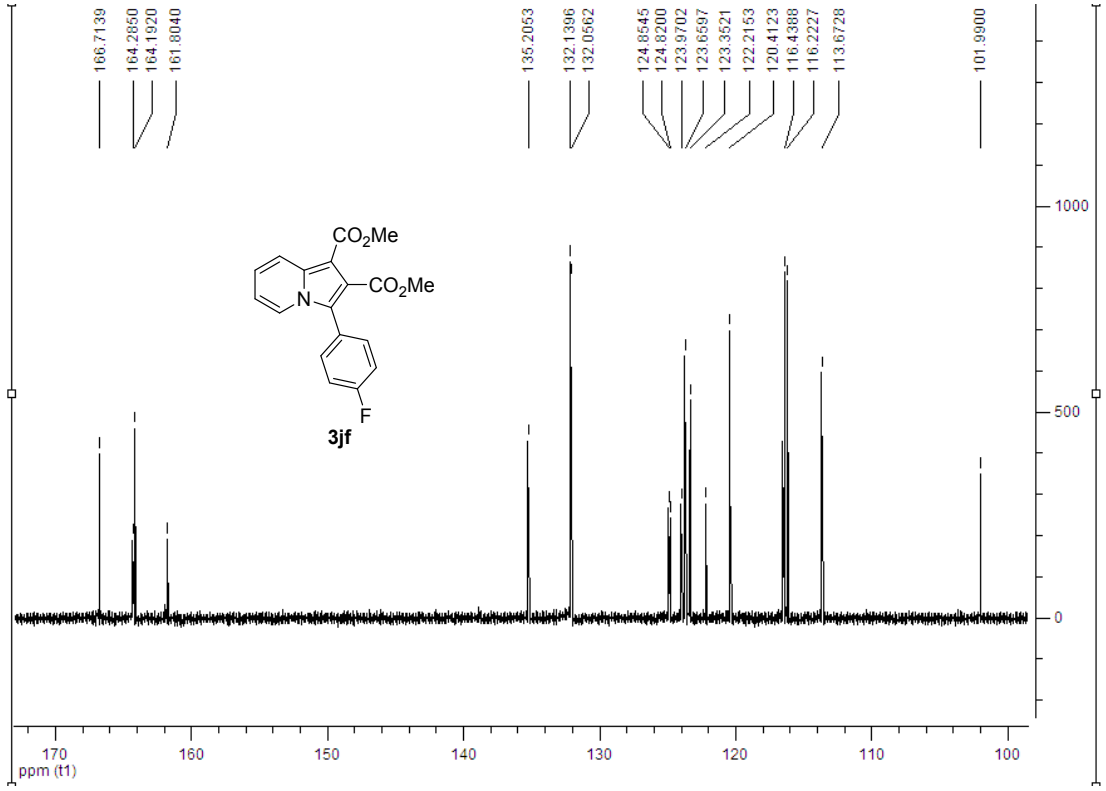
CO2Me
CO2Me
N
F
3jf
2500
2000
1500
1000
500
0
150
100
50
ppm (f1)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164.1920
161.8040
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132.0562
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124.8200
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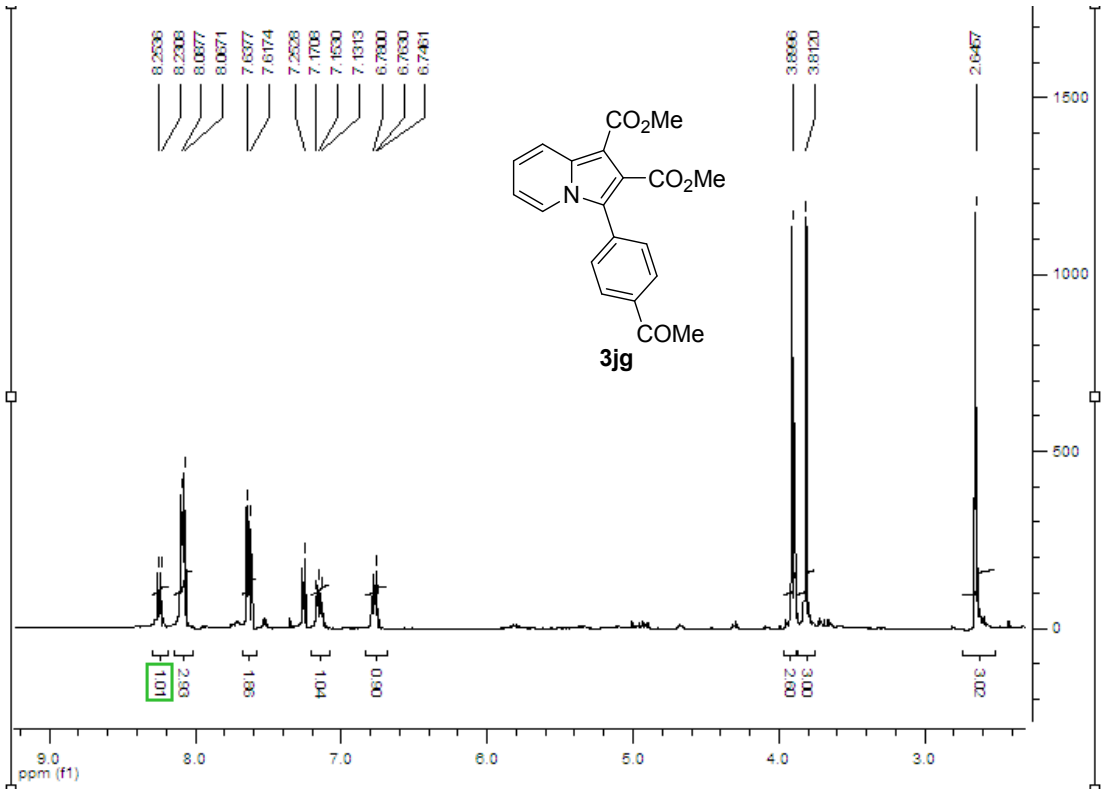
123.6597
123.3521
122.2153
120.4123
116.4388
116.2227
113.6728
101.9900
CO2Me
CO2Me
N
F
3jf
1000
500
0
170
160
150
140
130
120
110
100
ppm (t1)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8.0571
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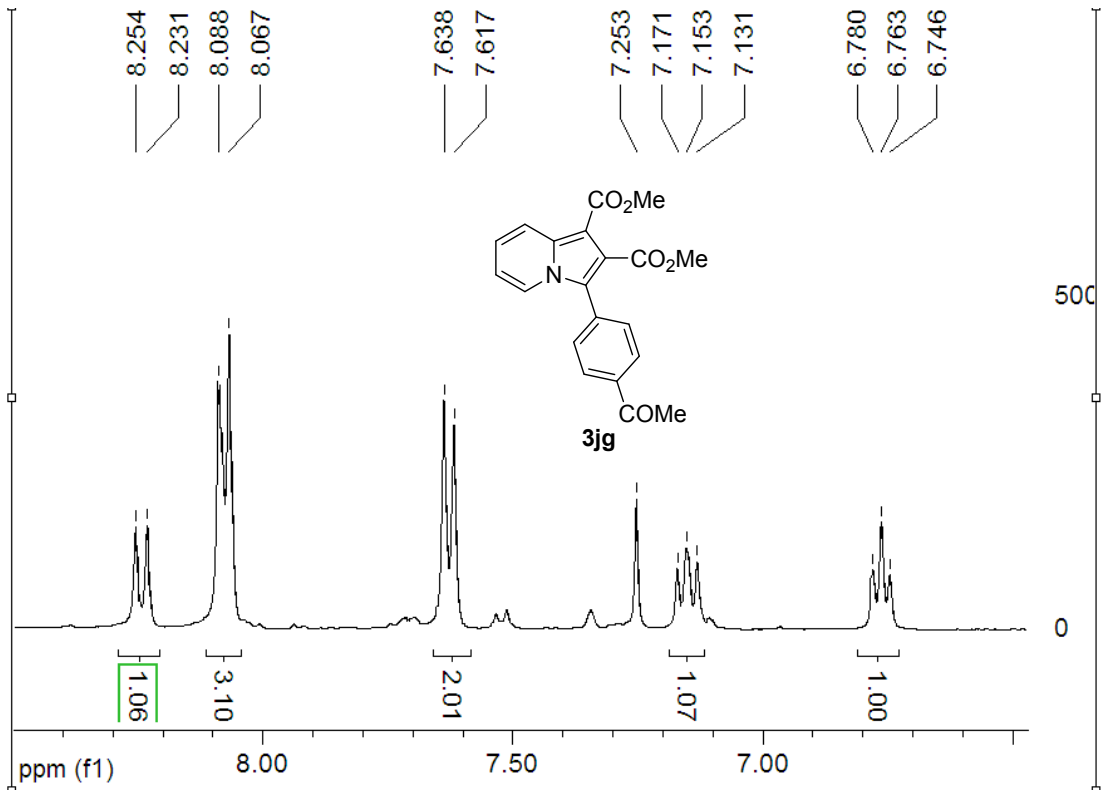
7.2528
7.1708
7.1530
7.1313
6.7800
6.7630
6.7461
3.8806
3.8120
2.6457
CO2Me
CO2Me
N
COMe
3jg
1500
1000
500
0
1.01
2.35
1.86
1.04
0.90
2.00
3.00
3.02
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm (f1)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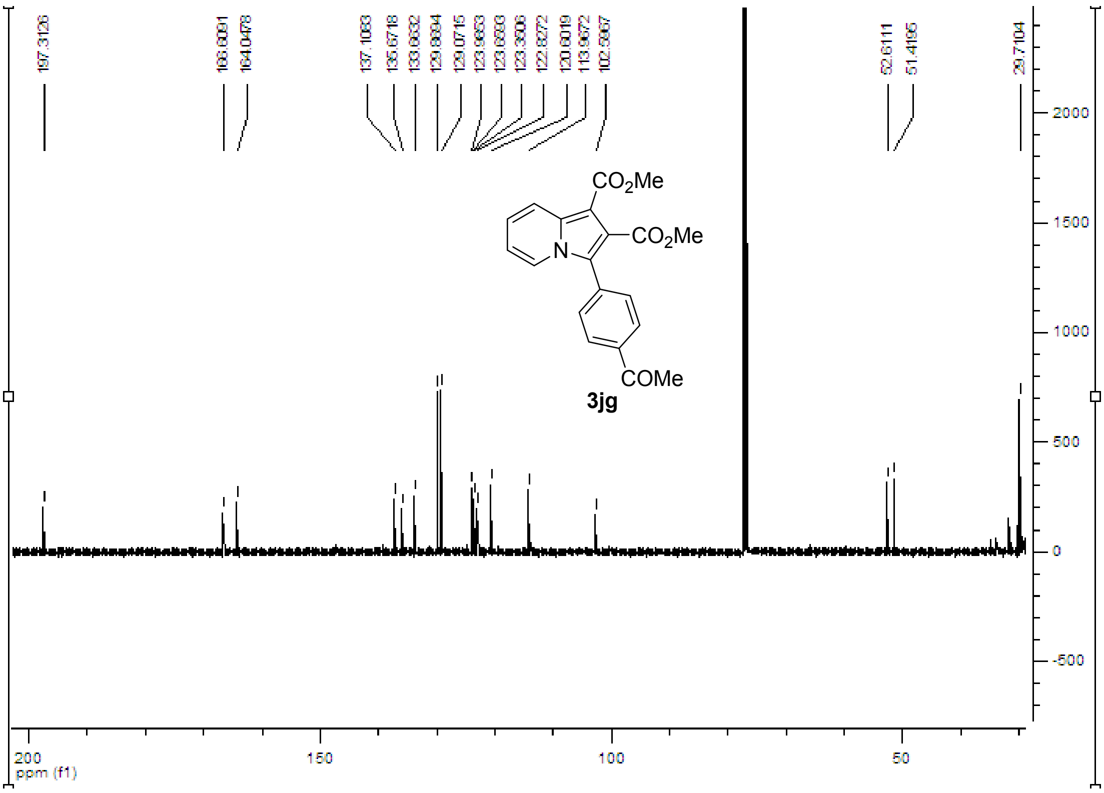
8.231
8.088
8.067
7.638
7.617
7.253
7.171
7.153
7.131
6.780
6.763
6.746
CO2Me
CO2Me
N
COMe
3jg
500
0
1.06
3.10
2.01
1.07
1.00
ppm (f1)
8.00
7.50
7.00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164.0478
137.1083
135.6718
133.6632
129.8894
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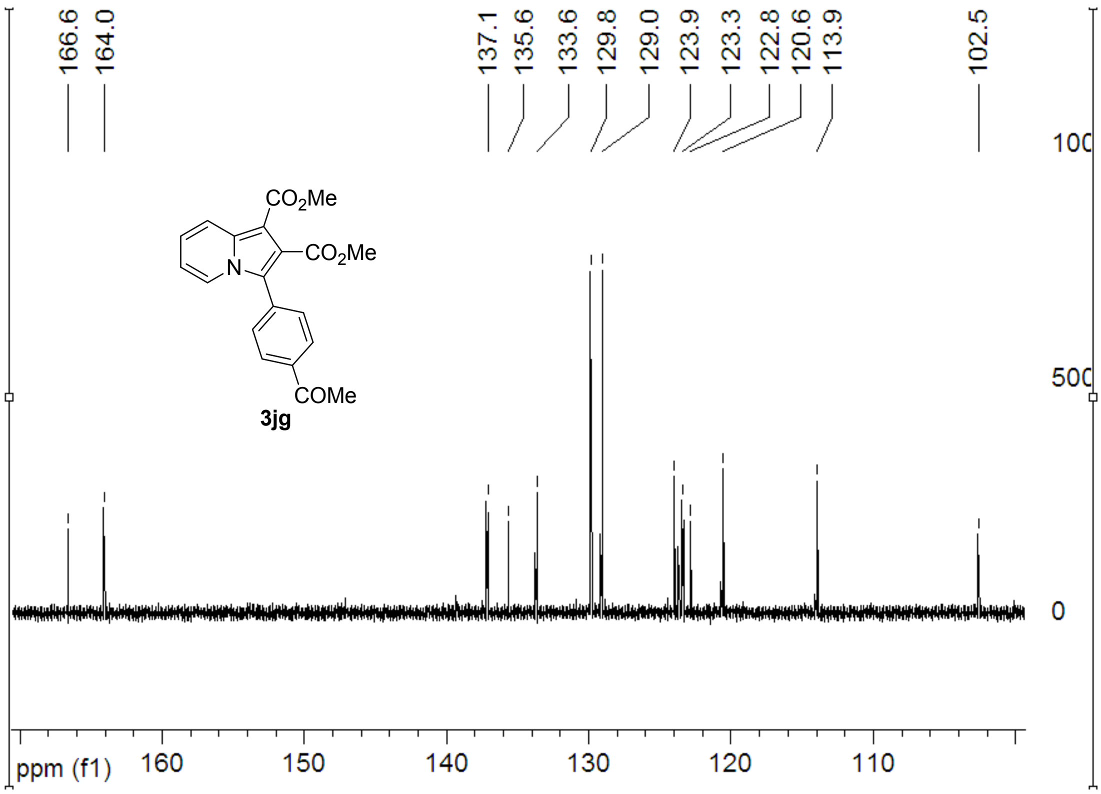
123.3506
122.8272
120.6019
113.9672
102.5967
52.6111
51.4195
29.7104
2000
1500
1000
500
0
-500
CO2Me
CO2Me
N
COMe
3jg
200
150
100
50
ppm (f1)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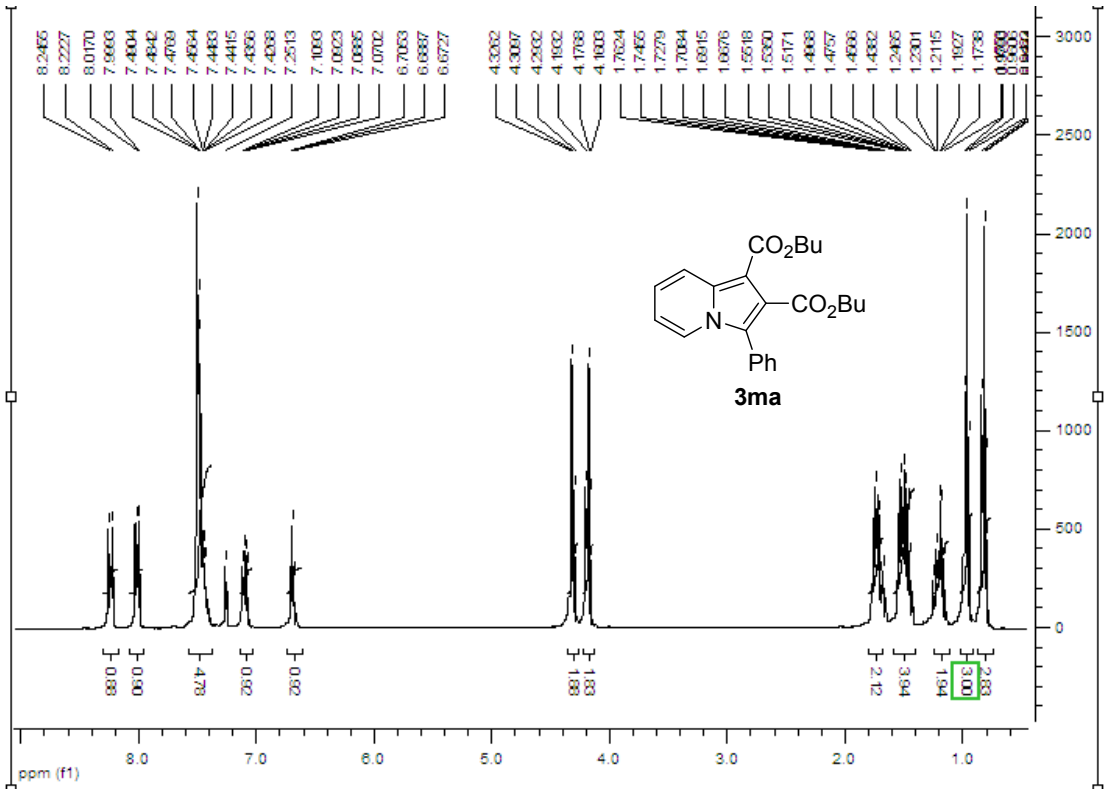
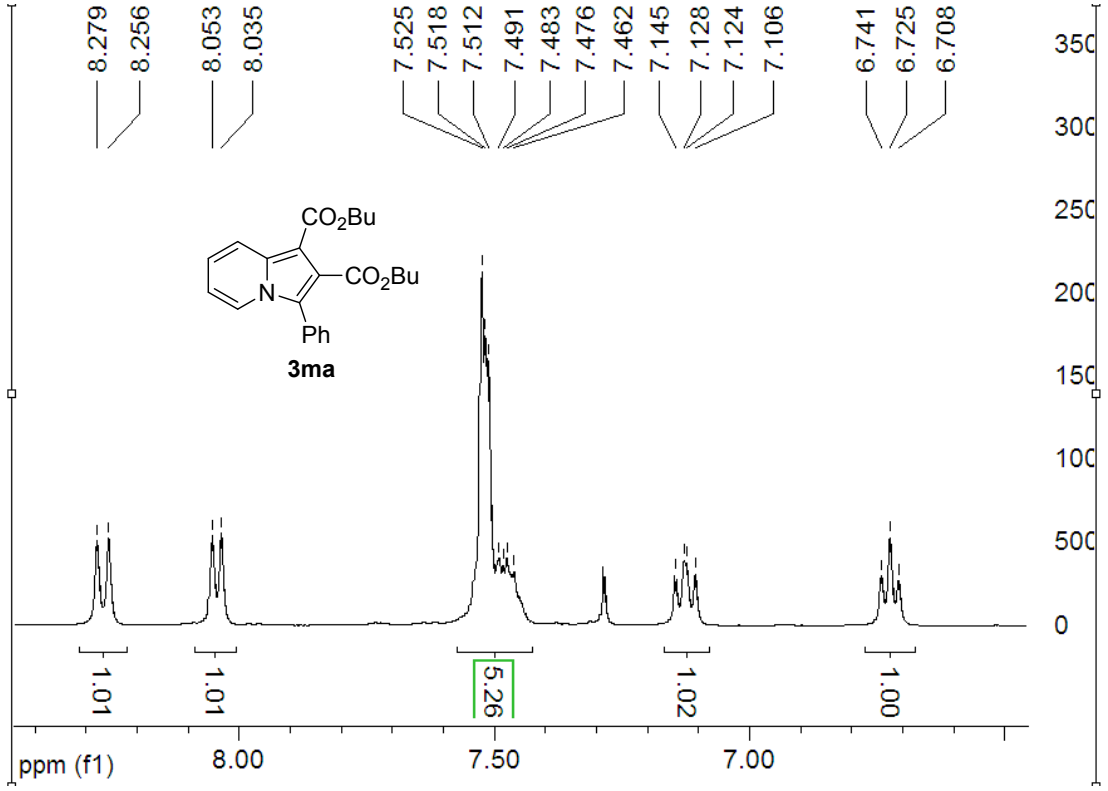
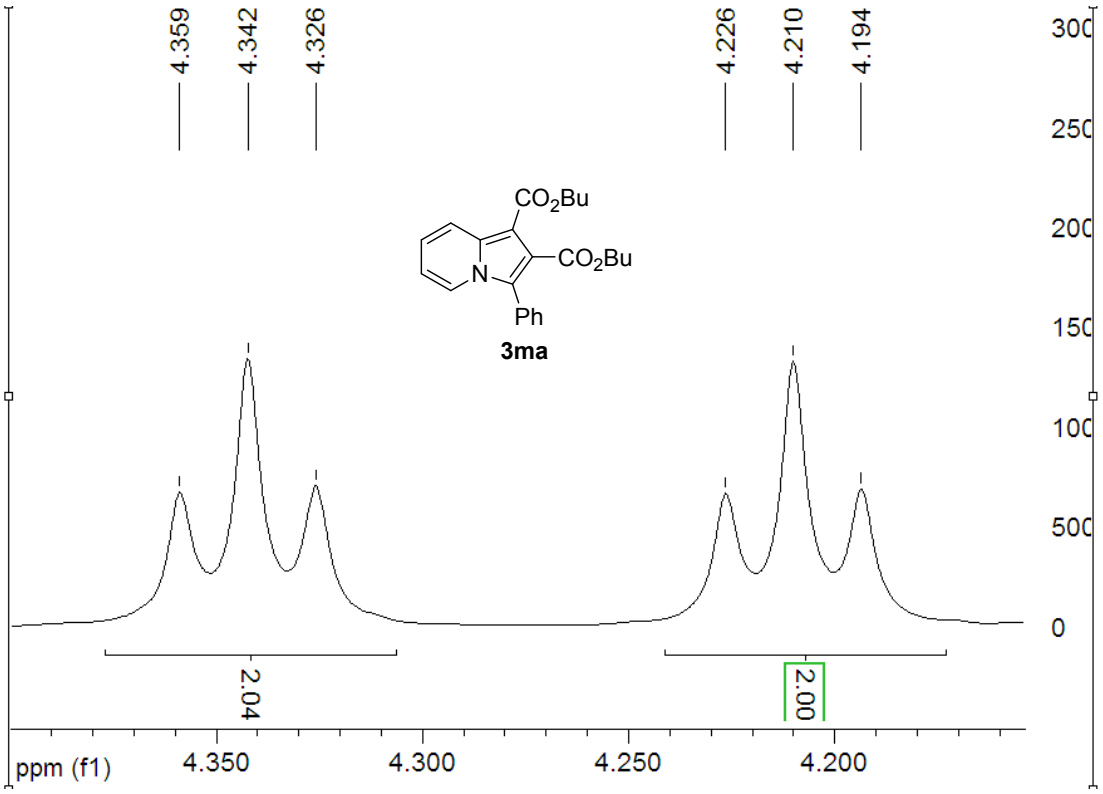
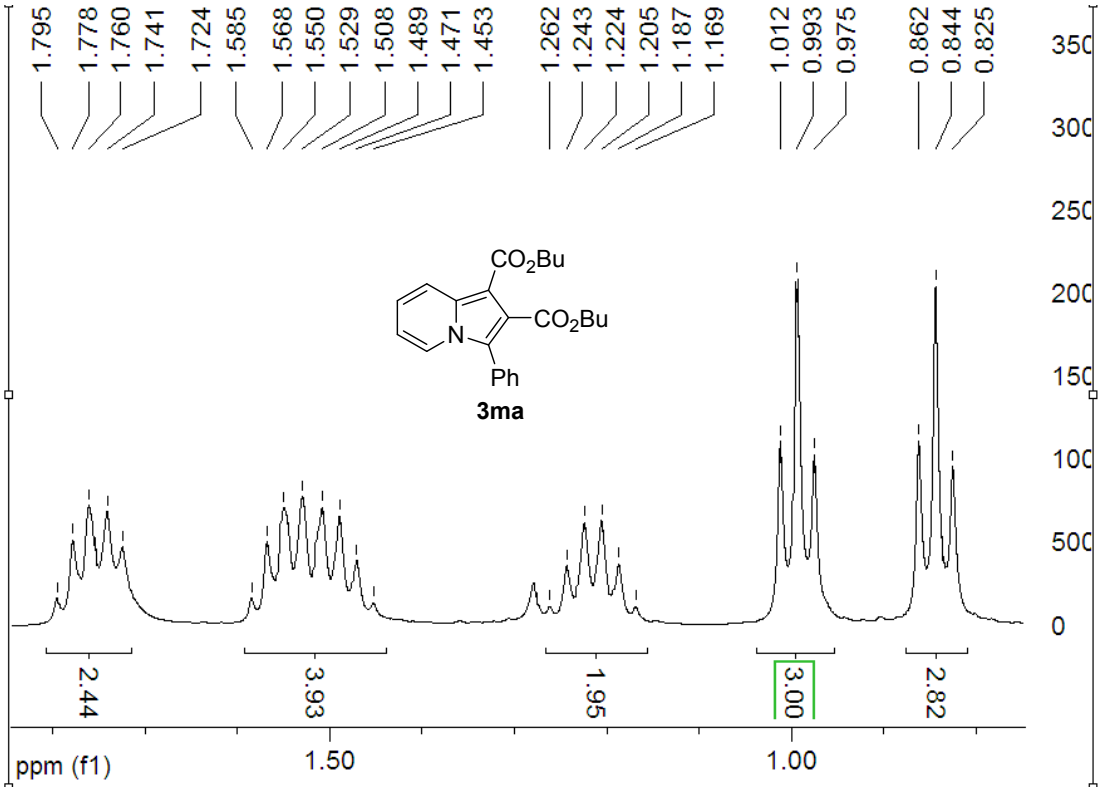
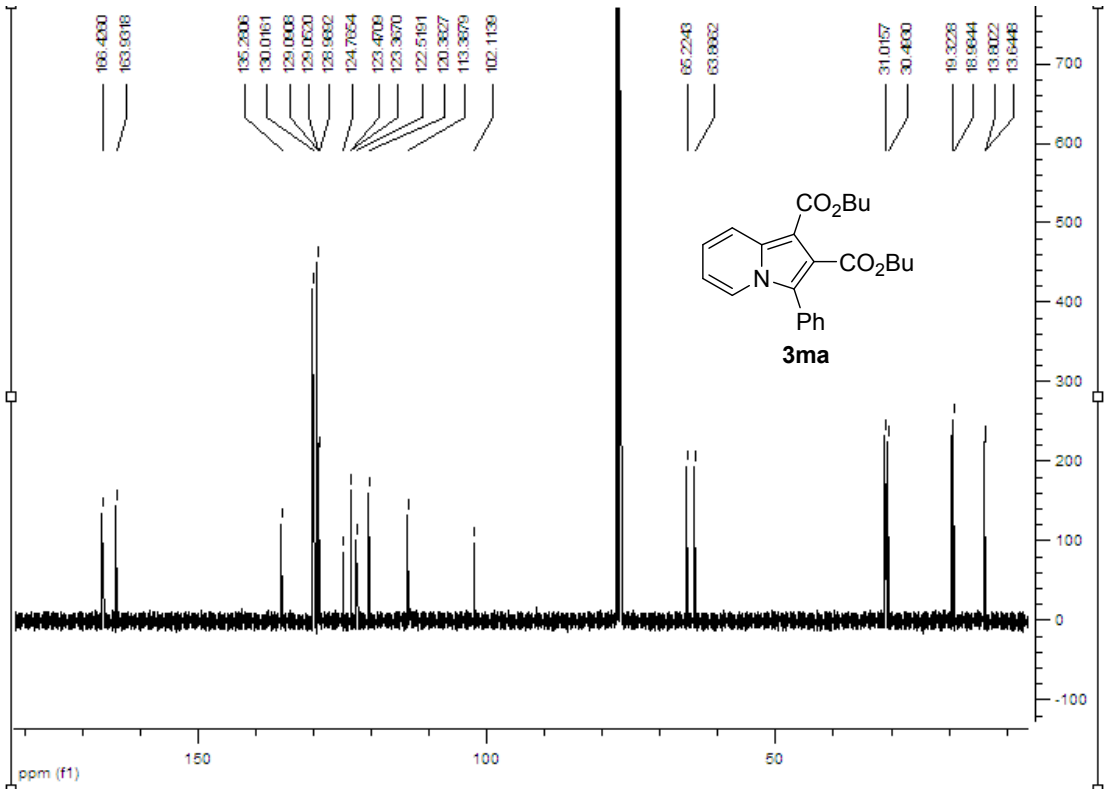
164.0
137.1
135.6
133.6
129.8
129.0
123.9
123.3
122.8
120.6
113.9
102.5
500
0
CO2Me
CO2Me
N
COMe
3jg
ppm (f1)
160
150
140
130
120
110

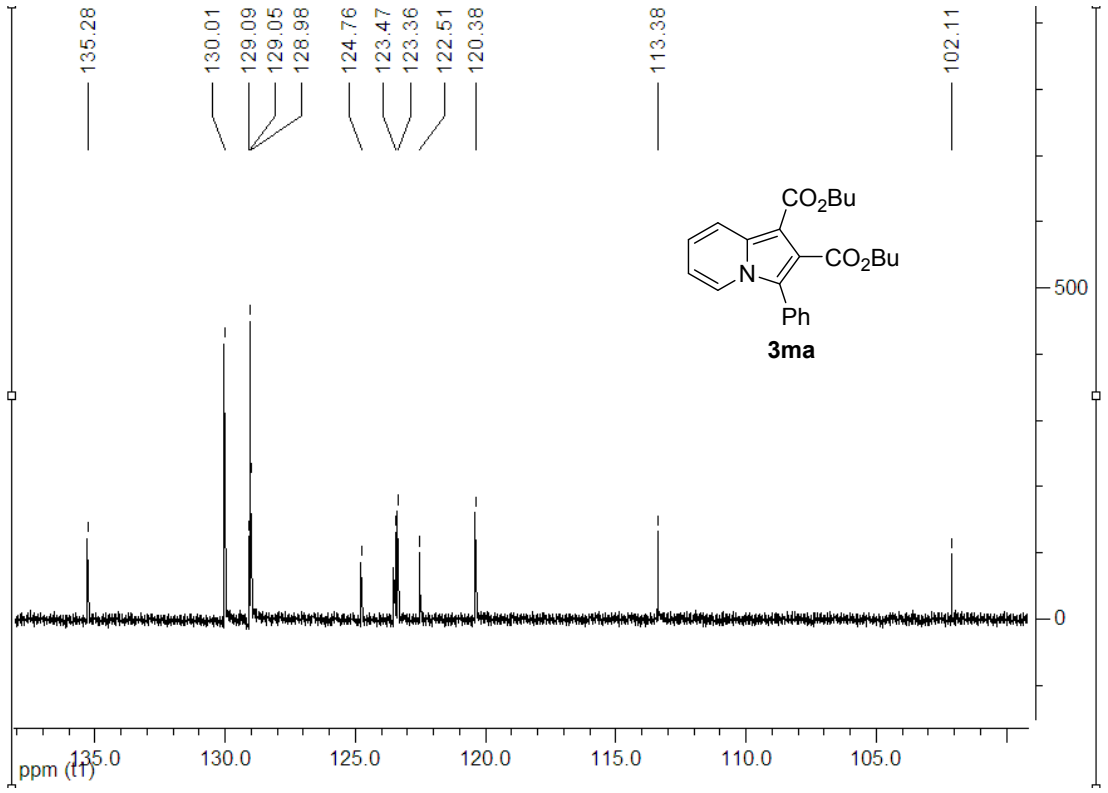

CO2Bu
CO2Bu
N
Ph
3ma
ppm (f1)


CO2Bu
CO2Bu
N
Ph
3ma
ppm (f1)


4.359
4.342
4.326
4.226
4.210
4.194
CO2Bu
CO2Bu
N
Ph
3ma
2.04
2.00
ppm (f1)
4.350
4.300
4.250
4.200


1.795
1.778
1.760
1.741
1.724
1.585
1.568
1.550
1.529
1.508
1.489
1.471
1.453
1.262
1.243
1.224
1.205
1.187
1.169
1.012
0.993
0.975
0.862
0.844
0.825
CO2Bu
CO2Bu
N
Ph
3ma
2.44
3.93
1.95
3.00
2.82
ppm (f1)
1.50
1.00


166.4300
163.9018
135.2906
130.0161
129.0008
129.0530
128.9882
124.7654
123.4709
123.3670
122.5191
120.3827
113.3879
102.1139
65.2243
63.8862
31.0157
30.4800
19.3228
18.9844
13.8022
13.6448
CO2Bu
CO2Bu
N
Ph
3ma
700
600
500
400
300
200
100
0
-100
150
100
50
ppm (f1)


135.28
130.01
129.09
129.05
128.98
124.76
123.47
123.36
122.51
120.38
113.38
102.11
CO2Bu
CO2Bu
N
Ph
3ma
500
0
135.0
130.0
125.0
120.0
115.0
110.0
105.0
ppm (f1)