Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Cobalt-Catalyzed Cross-Dehydrogenative Coupling of Imidazo[1,2-a]pyridines with Isochroman Using Molecular Oxygen as Oxidant

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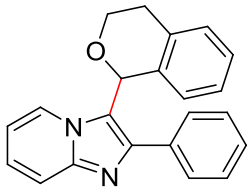
1. General information

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All the reactions were performed in Rotaflo®(England) resealable screw-cap tube (approx. 10 mL volume) in the presence of Teflon coated magnetic stirrer bar (4 mm × 10 mm). Thin layer chromatography was performed on precoated silica gel 60 F_{254} plates. Silica gel (200-300 mesh) was used for column chromatography. ^{1}H NMR spectra were recorded on a 400 MHz spectrometer. Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with TMS (δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were recorded on a 100 MHz spectrometer and the spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on an ESI-QToF mass spectrometer which the ionization method is electrospray ionization (ESI) and the mass analyzer is a quadrupole time-of-flight mass analyzer.

2. General procedures for cobalt-Catalyzed cross-dehydrogenative coupling of imidazo[1,2-a]pyridines with isochroman

$CoCl_2$•$6H_2O$ (0.03 mmol, 7.1 mg), phenylimidazo[1,2-a]pyridine **1a** (0.3 mmol, 58.2 mg) and isochroman (3 mmol, 0.38 mL) were added to a Schlenk tube at room temperature under oxygen atmosphere. The tube was then placed into a preheated oil bath (140 ℃) and stirred for 15 hours. After completion of reaction, the reaction tube was allowed to cool to room temperature and quenched with water and diluted with ethyl acetate. The organic layer was separated and the aqueous layer was washed with ethyl acetate. The filtrate was concentrated under reduced pressure. The crude products were purified by column chromatography on silica gel (200-300 mesh) to afford the desired product (85% yield).

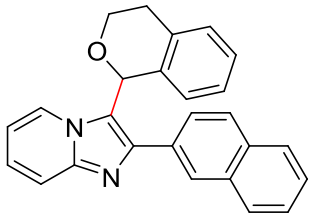
3. Characterization data (^{1}H NMR, ^{13}C NMR and HRMS) of the products



3a

3-(Isochroman-1-yl)-2-phenylimidazo[1,2-a]pyridine

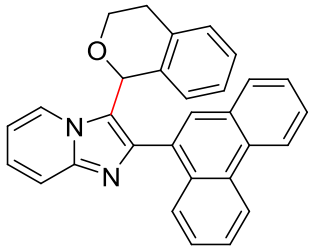
EA/PE = 1:1, R_f = 0.5, white solid, 85% yield, m.p. = 179-180 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 7.3 Hz, 2H), 7.75 (d, *J* = 6.6 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.52-7.41 (m, 3H), 7.28-7.21 (m, 2H), 7.15 (t, *J* = 7.5 Hz, 1H), 7.04 (t, *J* = 7.1 Hz, 1H), 6.73 (d, *J* = 7.4 Hz, 1H), 6.57 (t, *J* = 6.4 Hz, 1H), 6.44 (s, 1H), 4.44-4.40 (m, 1H), 4.07 (t, *J* = 10.1 Hz, 1H), 3.45-3.36 (m, 1H), 2.86 (d, *J* = 16.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.57, 145.63, 134.51, 134.35, 134.13, 129.24, 128.94, 128.63, 128.10, 127.52, 126.98, 125.85, 125.03, 124.99, 118.68, 117.49, 111.83, 71.79, 66.06, 28.68. IR ν_{max} 1635, 1389, 1280, 1082, 740, 699 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{19}N_2O$ $[M+H]^+$ 327.1492, found 327.1485.



3b

3-(Isochroman-1-yl)-2-(naphthalen-2-yl)imidazo[1,2-a]pyridine

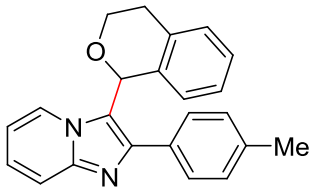
EA/PE = 1:1, R_f = 0.5, yellow solid, 74% yield, m.p. = 187-188 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (s, 1H), 8.05-7.90 (m, 4H), 7.76 (dd, *J* = 24.4, 6.8 Hz, 2H), 7.55-7.50 (m, 2H), 7.28-7.17 (m, 3H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 6.60 (t, *J* = 6.6 Hz, 1H), 6.55 (s, 1H), 4.47-4.43 (m, 1H), 4.12-4.06 (m, 1H), 3.47-3.38 (m, 1H), 2.87 (d, *J* = 15.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.44, 145.76, 134.46, 134.15, 133.49, 133.11, 131.73, 129.32, 128.42, 128.37, 127.97, 127.78, 127.60, 127.06, 126.89, 126.31, 126.30, 125.91, 125.25, 119.07, 117.50, 112.02, 71.88, 66.11, 28.63. IR ν_{max} 1633, 1387, 1281, 1084, 743, 695 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{26}H_{21}N_2O$ $[M+H]^+$ 377.1648, found 377.1639.



3c

3-(Isochroman-1-yl)-2-(phenanthren-9-yl)imidazo[1,2-a]pyridine

EA/PE = 1:1, R_f = 0.5, yellow solid, 85% yield, m.p. = 147-148 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81-8.75 (m, 2H), 8.35 (d, *J* = 7.6 Hz, 1H), 8.04 (s, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.86 (d, *J* = 6.9 Hz, 1H), 7.72-7.62 (m, 5H), 7.27-7.14 (m, 3H), 7.00 (t, *J* = 7.9 Hz, 1H), 6.75-66 (m, 2H), 6.66 (s, 1H), 4.41-4.37 (m, 1H), 3.92-3.86 (m, 1H), 3.41-3.32 (m, 1H), 2.78 (d, *J* = 16.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.69, 145.63, 134.35, 134.05, 131.65, 131.32, 130.66, 130.62, 130.28, 129.50, 129.13, 129.00, 127.36, 127.05, 126.94, 126.86, 126.75, 126.69, 125.78, 125.20, 125.03, 122.74, 122.62, 121.08, 117.63, 112.09, 71.65, 65.90, 28.65. IR v_{max} 1636, 1385, 1281 1080, 739, 695 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{30}H_{23}N_2O$ $[M+H]^+$ 427.1805, found 427.1790.

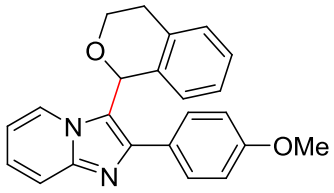


3d

3-(Isochroman-1-yl)-2-p-tolylimidazo[1,2-a]pyridine

EA/PE = 1:1, R_f = 0.5, white solid, 80% yield, m.p. = 155-158 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77-7.64 (m, 4H), 7.33-7.21 (m, 4H), 7.17-7.13 (m, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.59-6.55 (m, 1H), 6.43 (s, 1H), 4.44-4.40 (m, 1H), 4.10-4.04 (m, 1H), 3.45-3.37 (m, 1H), 2.78 (d, *J* = 16.8 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.54, 145.55, 137.96, 134.54, 134.13, 131.34, 129.38, 129.23, 128.79, 127.51, 126.98, 125.81, 125.07, 124.97, 118.41, 117.38, 111.80, 71.82, 66.09, 28.68, 21.35. IR v_{max} 1637, 1388, 1281, 1080, 738, 692 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O$ $[M]^+$ 341.1648,

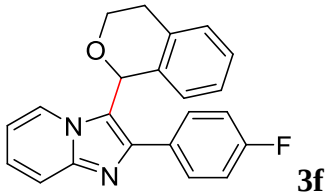
found 341.1640.



3e

3-(Isochroman-1-yl)-2-(4-methoxyphenyl)imidazo[1,2-a]pyridine)

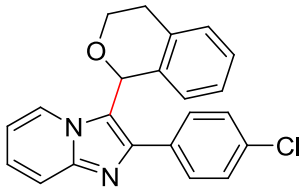
EA/PE = 1:1, R_f = 0.4, white solid, 74% yield, m.p. = 152-153 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80-7.63(m, 4H), 7.28-7.21 (m, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.05-7.03 (m, 3H), 6.73 (d, *J* = 7.9 Hz, 1H), 6.56 (t, *J* = 6.7 Hz, 1H), 6.41 (s, 1H), 4.44-4.40 (m, 1H), 4.11-4.04 (m, 1H), 3.88 (s, 3H), 3.45-3.36 (m, 1H), 2.87 (d, *J* = 15.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.68, 146.38, 145.52, 134.53, 134.14, 130.11, 129.24, 127.51, 126.98, 126.79, 125.76, 125.05, 124.93, 118.09, 117.29, 114.11, 111.76, 71.85, 66.08, 55.35, 28.68. IR ν_{max} 1608, 1388, 1282, 1083, 738 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O$ $[M]^+$ 357.1598, found 357.1588.



3f

2-(4-Fluorophenyl)-3-(isochroman-1-yl)imidazo[1,2-a]pyridine

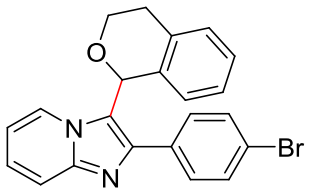
EA/PE = 1:1, R_f = 0.55, white solid, 70% yield, m.p. = 184-185 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84-7.80 (m, 2H), 7.73 (d, *J* = 6.8Hz, 1H), 7.64 (d, *J* = 9.3 Hz, 1H), 7.28-7.15 (m, 5H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 7.7 Hz, 1H), 6.61-6.57 (m, 1H), 6.37 (s, 1H), 4.45-4.41 (m, 1H), 4.11-4.04 (m, 1H), 3.45-3.36 (m, 1H), 2.87 (dd, *J* = 15.6, 2.4Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.84, 161.88, 145.57, 134.26, 134.12, 130.64, 130.58, 130.41, 130.39, 129.32, 127.62, 127.02, 125.82, 125.23, 124.92, 118.57, 117.41, 115.72, 115.55, 112.00, 71.70, 66.07, 28.63. IR ν_{max} 1634, 1489, 1387, 1281, 1087, 830 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}N_2OF$ $[M]^+$ 345.1398, found 345.1389.



3g

2-(4-chlorophenyl)-3-(isochroman-1-yl)imidazo[1,2-a]pyridine

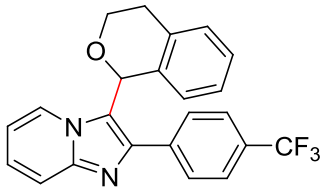
EA/PE = 1:1, R_f = 0.55, white solid, 81% yield, m.p. = 206-207 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81-7.72 (m, 3H), 7.64 (d, *J* = 9.1 Hz, 1H), 7.48-7.44 (m, 2H), 7.27-7.14 (m, 3H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.68 (d, *J* = 7.4 Hz, 1H), 6.60-6.56 (m, 1H), 6.37 (s, 1H), 4.43-4.39 (m, 1H), 4.09-4.03 (m, 1H), 3.44-3.35 (m, 1H), 2.86 (dd, *J* = 15.5, 2.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.64, 145.30,134.18, 134.16, 134.10, 132.82, 130.16, 129.35, 128.86, 127.65, 127.04, 125.86, 125.32, 124.89, 118.84, 117.47, 112.07, 71.67, 66.08, 28.62. IR ν_{max} 1635, 1488, 1389, 1282, 1087, 829 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}N_2OCl$ $[M]^+$ 361.1102, found 361.1094.



3h

2-(4-Bromophenyl)-3-(isochroman-1-yl)imidazo[1,2-a]pyridine

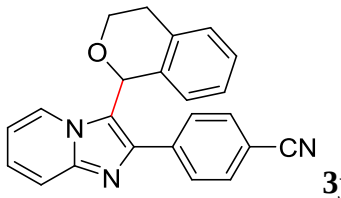
EA/PE = 1:1, R_f = 0.6, white solid, 77% yield, m.p. = 166-167 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74-7.61 (m, 6H), 7.27-7.16 (m, 3H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 7.60 Hz, 1H), 6.60 (t, *J* = 6.5 Hz, 1H), 6.37 (s, 1H), 4.45-4.41 (m, 1H), 4.11-4.04 (m, 1H), 3.45-3.36 (m, 1H), 2.88 (d, *J* = 15.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.68, 145.35, 134.19, 134.10, 133.27, 131.80, 130.45, 129.33, 127.65, 127.05, 125.86, 125.31, 124.91, 122.43, 118.83, 117.50, 112.06, 71.67, 66.09, 28.63. IR ν_{max} 1636, 1490, 1385, 1280, 1084, 830 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}N_2OBr$ $[M]^+$ 405.0597, found 405.0590.



3i

3-(Isochroman-1-yl)-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine

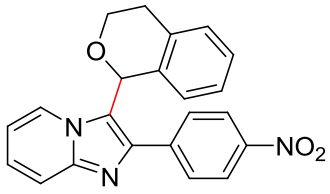
EA/PE = 1:1, R_f = 0.65, white solid, 63% yield, m.p. = 185-186 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 7.8 Hz, 3H), 7.67 (d, *J* = 9.1 Hz, 1H), 7.29-7.18 (m, 3H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 7.7 Hz, 1H), 6.61 (t, *J* = 6.8 Hz, 1H), 6.40 (s, 1H), 4.46-4.42 (m, 1H), 4.12-4.05 (m, 1H), 3.46-3.37 (m, 1H), 2.88 (d, *J* = 16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.79, 144.98, 137.95, 134.09, 134.05, 130.16, 129.84, 129.37, 129.15, 127.71, 127.07, 125.93, 125.62, 125.58, 125.54, 125.51, 124.87, 122.91, 119.42, 117.64, 112.24, 71.62, 66.09, 28.60. IR ν_{max} 1636, 1479, 1385, 1280, 1088 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{18}N_2OF_3$ $[M]^+$ 395.1366, found 395.1357.



3j

4-(3-(Isochroman-1-yl)imidazo[1,2-a]pyridin-2-yl)benzonitrile

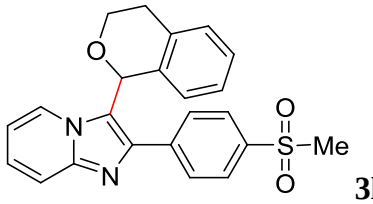
EA/PE = 1:1, R_f = 0.5, white solid, 77% yield, m.p. = 213-214 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.2 Hz, 2H), 7.78-7.75 (m, 3H), 7.66 (d, *J* = 9.1 Hz, 1H), 7.30-7.20 (m, 3H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.67-6.62 (m, 2H), 6.38 (s, 1H), 4.46-4.42 (m, 1H), 4.13-4.06 (m, 1H), 3.46-3.37 (m, 1H), 2.90 (d, *J* = 16.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.84, 144.31, 139.01, 134.09, 133.82, 132.40, 129.43, 129.39, 127.80, 127.09, 125.95, 125.77, 124.78, 119.81, 118.95, 117.67, 112.44, 111.52, 71.49, 66.09, 28.55. IR ν_{max} 1608, 1494, 1282, 1083, 738 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{18}N_3O$ $[M]^+$ 352.1444, found 352.1433.



3k

3-(Isochroman-1-yl)-2-(4-nitrophenyl)imidazo[1,2-a]pyridine

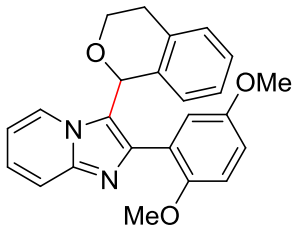
EA/PE = 1:1, R_f = 0.55, yellow solid, 52% yield, m.p. = 196-197 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, *J* = 8.7 Hz, 2H), 8.02 (d, *J* = 8.7 Hz, 2H), 7.77 (d, *J* = 7.0 Hz, 1H), 7.67 (d, *J* = 9.1 Hz, 1H), 7.30-7.21 (m, 3H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.68-6.63 (m, 2H), 6.40 (s, 1H), 4.47-4.43 (m, 1H), 4.14-4.07 (m, 1H), 3.46-3.38 (m, 1H), 2.91 (d, *J* = 16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.43, 145.91, 143.97, 140.94, 134.08, 133.77, 129.51, 129.45, 127.83, 127.13, 125.95, 125.87, 124.79, 123.90, 120.12, 117.75, 112.52, 71.52, 66.12, 28.56. IR ν_{max} 1637, 1515, 1347, 1281, 1082, 737 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}N_3O_3$ $[M]^+$ 372.1343, found 372.1329.



3l

3-(Isochroman-1-yl)-2-(4-(methylsulfonyl)phenyl)imidazo[1,2-a]pyridine

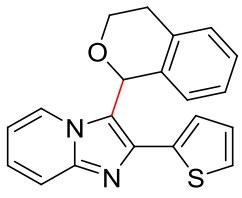
EA/PE = 3:1, R_f = 0.4, yellow solid, 74% yield, m.p. = 205-206 ℃.^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (s, 4H), 7.75 (d, *J* = 6.7 Hz, 1H), 7.64 (d, *J* = 8.9 Hz, 1H), 7.28-7.17(m, 3H), 7.01 (t, *J* = 7.1 Hz, 1H), 6.65-6.60 (m, 2H), 6.38 (s, 1H), 4.44-4.40 (m, 1H), 4.10-4.04 (m, 1H), 3.43-3.35 (m, 1H), 3.08 (s, 3H), 2.88 (d, *J* = 16.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.85, 144.27, 139.96, 139.70, 134.09, 133.82, 129.66, 129.42, 127.77, 127.68, 127.07, 125.94, 125.77, 124.78, 119.92, 117.68, 112.45, 71.51, 66.08, 44.62, 28.55. IR ν_{max} 1637, 1312, 1150, 741 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O_3S$ $[M]^+$ 405.1267, found 405.1254.



3m

2-(2,5-Dimethoxyphenyl)-3-(isochroman-1-yl)imidazo[1,2-a]pyridine

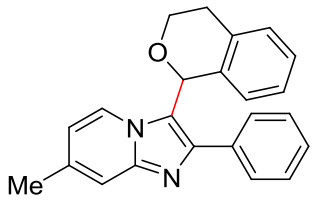
EA/PE = 1:1, R_f = 0.3, white solid, 72% yield, m.p. = 167-168 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72-7.63 (m, 2H), 7.30-7.28 (m, 1H), 7.24-7.19 (m, 2H), 7.14-7.11 (m, 1H), 7.03 (t, *J* = 7.7 Hz, 1H), 6.97-6.91 (m, 3H), 6.56 (t, *J* = 6.2 Hz, 1H), 6.17 (s, 1H), 4.39-4.35 (m, 1H), 4.03-3.96 (m, 1H), 3.84 (s, 3H), 3.73 (s, 3H), 3.41-3.33 (m, 1H), 2.83 (d, *J* = 16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.70, 151.18, 145.66, 143.01, 134.72, 134.09, 128.98, 127.28, 126.67, 125.70, 125.61, 124.56, 124.10, 120.40, 117.47, 117.31, 115.40, 112.25, 111.74, 71.96, 65.98, 55.89, 55.87, 28.70. IR ν_{max} 1603, 1378, 1280, 1084 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{24}H_{23}N_2O_3$ $[M]^+$ 387.1703, found 387.1693.



3n

3-(Isochroman-1-yl)-2-(thiophen-2-yl)imidazo[1,2-a]pyridine

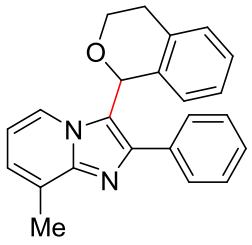
EA/PE = 1:1, R_f = 0.55, yellow solid, 75% yield, m.p. = 188-189 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78(d, *J* = 7.0 Hz, 1H), 7.63 (d, *J* = 9.1 Hz, 1H), 7.50-7.43 (m, 2H), 7.28-7.22 (m, 2H), 7.17-7.14 (m, 2H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.7 Hz, 1H), 6.63 (s, 1H), 6.58 (t, *J* = 6.6 Hz, 1H), 4.46-4.42 (m, 1H), 4.14-4.08 (m, 1H), 3.46-3.37 (m, 1H), 2.99 (d, *J* = 16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.60, 140.27, 136.89, 134.20, 134.05, 129.26, 127.68, 127.60, 127.04, 126.33, 125.85, 125.65, 125.32, 125.06, 118.37, 117.34, 112.01, 71.65, 66.16, 28.64. IR ν_{max} 1634, 1065, 695 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{20}H_{17}N_2OS$ $[M]^+$ 333.1056, found 333.1047.



3o

3-(Isochroman-1-yl)-7-methyl-2-phenylimidazo[1,2-a]pyridine

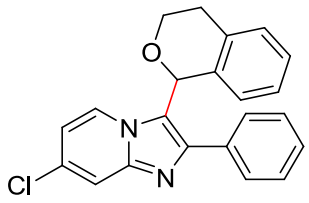
EA/PE = 1:1, R_f = 0.65, white solid, 76% yield, m.p. = 157-158 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.52-7.48 (m, 2H), 7.42-7.39 (m, 2H), 7.27-7.20 (m, 2H), 7.05 (t, *J* = 7.4 Hz, 1H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.63-6.44 (m, 2H), 4.44-4.40 (m, 1H), 4.10-4.03 (m, 1H), 3.44-3.35 (m, 1H), 2.86 (d, *J* = 16.4 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.15, 146.01, 136.12, 134.66, 134.32, 134.13, 129.21, 128.89, 128.61, 128.03, 127.48, 126.95, 125.10, 124.99, 118.08, 115.80, 114.59, 71.78, 66.05, 28.69, 21.32. IR v_{max} 1630, 1378, 1282, 1082, 740 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O$ $[M]^+$ 341.1648, found 341.1640.



3p

3-(Isochroman-1-yl)-8-methyl-2-phenylimidazo[1,2-a]pyridine

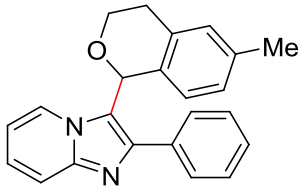
EA/PE = 1:1, R_f = 0.65, yellow solid, 72% yield, m.p. = 177-178 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.1 Hz, 2H), 7.62 (d, *J* = 6.9 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.27-7.21 (m, 2H), 7.06-6.95 (m, 2H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.50 (t, *J* = 6.9 Hz, 1H), 6.39 (s, 1H), 4.44-4.40 (m, 1H), 4.10-4.04 (m, 1H), 3.45-3.36 (m, 1H), 2.87 (d, *J* = 16.6 Hz, 1H), 2.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.17, 146.03, 134.73, 134.59, 134.13, 129.17, 129.13, 128.61, 127.97, 127.42, 127.35, 126.92, 125.14, 123.74, 123.62, 118.98, 111.86, 71.87, 66.06, 28.70, 17.23. IR v_{max} 1634, 1382, 1280, 1085, 739 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O$ $[M]^+$ 341.1648, found 341.1641.



3q

7-Chloro-3-(isochroman-1-yl)-2-phenylimidazo[1,2-a]pyridine

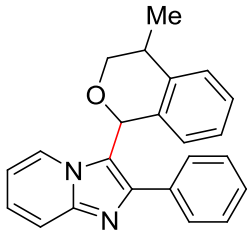
EA/PE = 3:1, R_f = 0.6, yellow solid, 80% yield, m.p. = 177-178 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85-7.82 (m, 2H), 7.67-7.65 (m, 2H), 7.53-7.49 (m, 2H), 7.46-7.42 (m, 1H), 7.27-7.22 (m, 2H), 7.06 (t, *J* = 7.9 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 6.57 (dd, *J* =7.3, 2.2 Hz, 1H), 6.41 (s, 1H), 4.45-4.40 (m, 1H), 4.10-4.04 (m, 1H), 3.45-3.35 (m, 1H), 2.88 (dd, *J* = 16.8, 2.9 Hz,1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.30, 145.39, 134.15, 134.06, 133.83, 131.63, 129.37, 128.85, 128.73, 128.37, 127.72, 127.09, 126.14, 124.95, 119.03, 116.31, 113.48, 71.61, 66.09, 28.60. IR ν_{max} 1638, 1375, 1280, 1084 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}N_2OCl$ $[M]^+$ 361.1102, found 361.1094.



5a

3-(6-Methylisochroman-1-yl)-2-phenylimidazo[1,2-a]pyridine

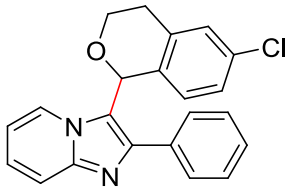
EA/PE = 1:1, R_f = 0.5, yellow oil, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.9 (d, *J* = 6.9 Hz, 2H), 7.78 (d, *J* = 6.9 Hz, 1H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 2H), 7.45-7.41 (m, 1H), 7.18-7.14 (m, 2H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.61-6.58 (m, 2H), 6.42 (s, 1H), 4.42-4.38 (m, 1H), 4.07 (td, *J* = 11.9, 3.2 Hz, 1H), 3.39-3.31 (m, 1H), 2.82 (d, *J* = 16.5 Hz, 1H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.28, 145.59, 136.69, 134.22, 134.19, 131.01, 129.13, 128.93, 128.66, 128.43, 128.13, 125.93, 125.34, 125.13, 118.80, 117.42, 111.95, 71.67, 66.17, 28.35, 21.08. IR ν_{max} 1636, 1387, 1283, 1087, 735, 699 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O$ $[M+H]^+$ 341.1654, found 341.1649.



5b

3-(4-Methylisochroman-1-yl)-2-phenylimidazo[1,2-a]pyridine

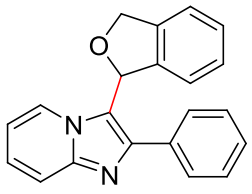
EA/PE = 1:1, R_f = 0.5, yellow oil, 71% yield (dr = 2:1). major isomer: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84-7.81 (m, 2H), 7.71-7.69 (m, 1H), 7.66-7.62 (m, 1H), 7.50-7.47 (m, 2H), 7.43-7.38 (m, 2H), 7.27-7.24 (m, 1H), 7.16-7.12 (m, 1H), 7.04-7.00 (m, 1H), 6.72-6.68 (m, 1H), 6.57-6.53 (m, 1H), 6.44 (s, 1H), 4.32-4.28 (m, 1H), 3.66 (t, *J* = 11.8 Hz, 1H), 3.46-3.41 (m, 1H), 1.33 (d, *J* = 6.8 Hz, 3H). minor isomer: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84-7.81(m, 2H), 7.77 (d, *J* = 6.9 Hz, 1H), 7.66-7.63 (m, 1H), 7.49-7.46 (m, 2H), 7.43-7.38 (m, 1H), 7.29 (d, *J* = 7.1 Hz, 1H), 7.27-7.24 (m, 1H), 7.16-7.11 (m, 1H), 7.04-7.00 (m, 1H), 6.72-6.68 (m, 1H), 6.57-6.53 (m, 1H), 6.34 (s, 1H), 4.180 (dd, *J* = 11.5, 3.5 Hz, 1H), 4.113 (d, *J* = 11.3 Hz, 1H), 2.99-2.97 (m, 1H), 1.62 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) (mixture): 147.04, 146.46, 145.69, 145.59, 139.66, 139.37, 134.29, 133.99, 133.91, 129.40, 128.98, 128.93, 128.64, 128.12, 127.86, 127.76, 127.00, 126.91, 126.80, 125.84, 125.04, 124.84, 124.63, 118.88, 118.15, 117.58, 117.47, 111.85, 111.80, 72.64, 72.44, 72.28, 71.78, 32.57, 31.58, 22.46, 15.93. IR ν_{max} 1653, 1647, 1392, 1378, 1291, 1287, 1091, 1088, 735, 729 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{23}H_{21}N_2O$ $[M+H]^+$ 341.1654, found 341.1658.



5c

3-(6-Chloroisochroman-1-yl)-2-phenylimidazo[1,2-a]pyridine

EA/PE = 1:1, R_f = 0.5, yellow oil, 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82-7.80 (m, 2H), 7.72 (dd, *J* = 16.5, 6.9 Hz, 2H), 7.51-7.48 (m, 2H), 7.43-7.40 (m, 1H), 7.20-7.16 (m, 3H), 6.70 (s, 1H), 6.61 (td, *J* = 6.8, 1.1 Hz, 1H), 6.34 (s, 1H), 4.42-4.38 (m, 1H), 4.01 (td, *J* = 11.8, 3.4 Hz, 1H), 3.36-3.28 (m, 1H), 2.80 (d, *J* = 16.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.73, 145.73, 136.35, 134.05, 132.67, 132.63, 130.63, 128.92, 128.72, 128.26, 127.85, 125.59, 125.30, 124.96, 117.87, 117.66, 112.18, 71.48, 65.88, 28.12. IR ν_{max} 1658, 1388, 1279, 1096, 741 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}ClN_2O$ $[M+H]^+$ 361.1108, found 361.1110.

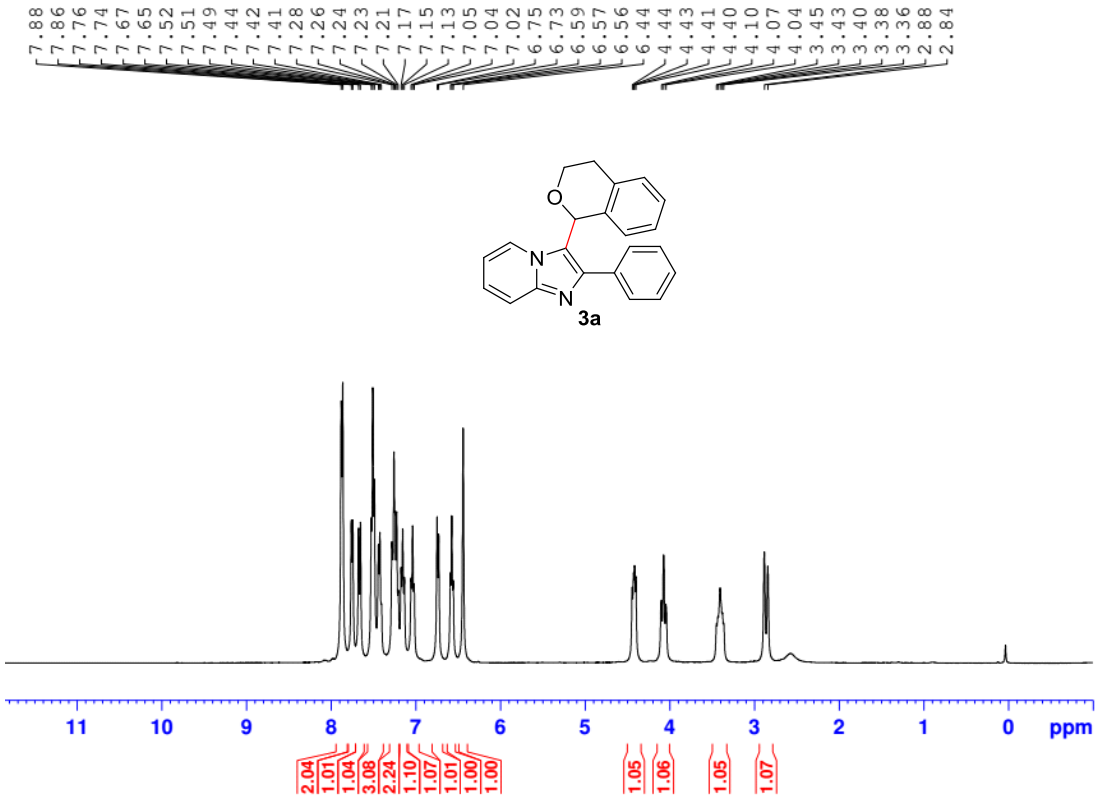


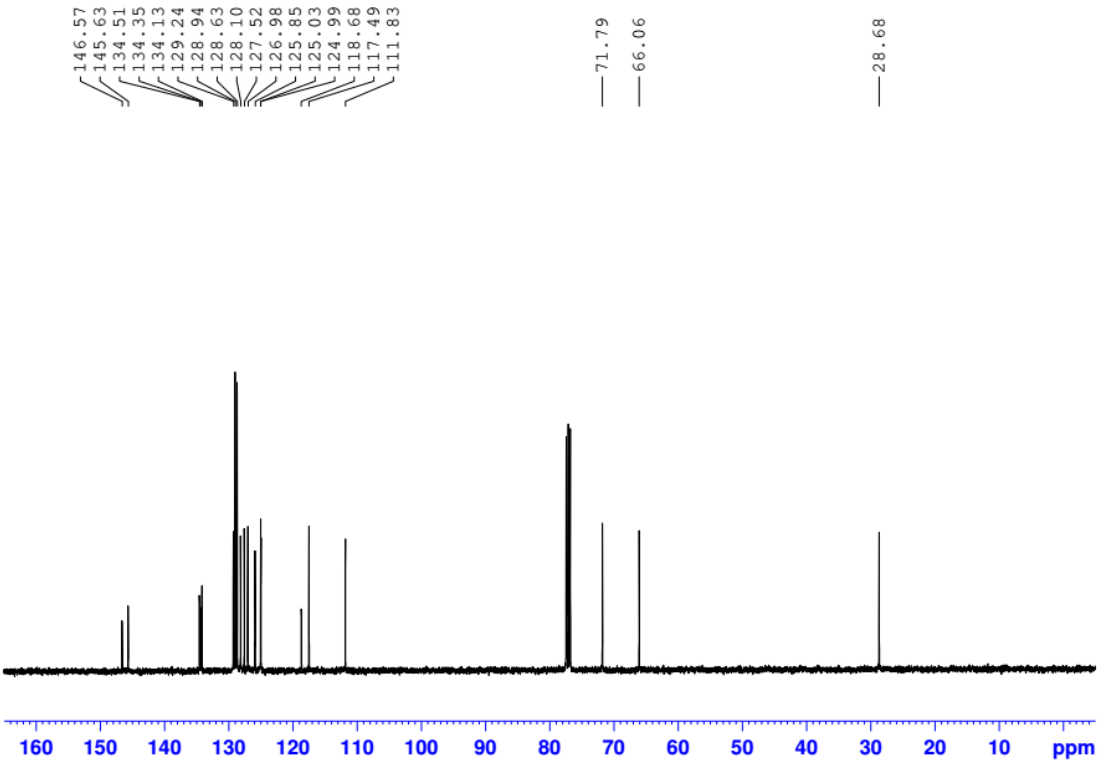
5d

3-(1,3-Dihydroisobenzofuran-1-yl)-2-phenylimidazo[1,2-a]pyridine

EA/PE = 1:1, R_f = 0.5, white solid, 70% yield, m.p. = 165-166 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86-7.84 (m, 2H), 7.66 (d, *J* = 9.0 Hz, 1H), 7.52-7.36 (m, 6H), 7.27-7.24 (m, 1H), 7.18-7.14 (m, 1H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.86 (s, 1H), 6.57-6.53 (m, 1H), 5.40 (dd, *J* = 12.5, 2.0 Hz, 1H), 5.27 (dd, *J* = 12.3, 2.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.04, 145.90, 139.65, 137.92, 134.07, 129.20, 128.61, 128.51, 128.21, 125.28, 125.17, 121.83, 121.62, 117.65, 117.40, 112.04, 77.76, 72.62. IR ν_{max} 1635, 1376, 1014, 746 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{21}H_{17}N_2O$ $[M]^+$ 313.1335, found 313.1327.

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

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128.63
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126.98
125.85
125.03
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117.49
111.83
71.79
66.06
28.68
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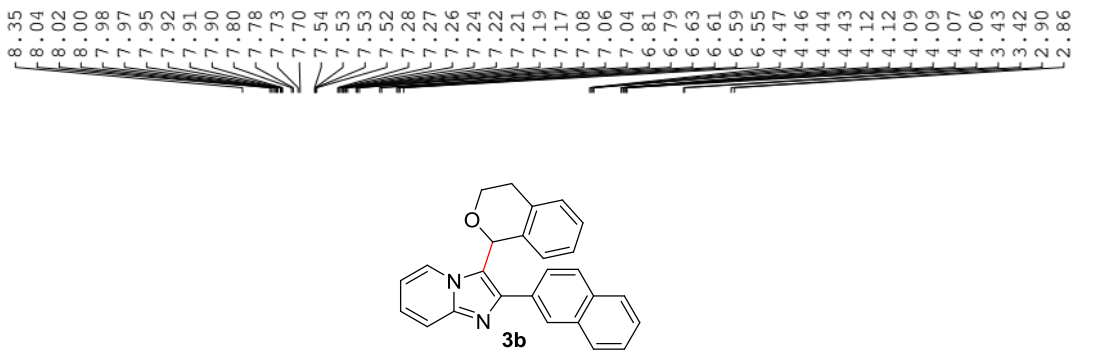
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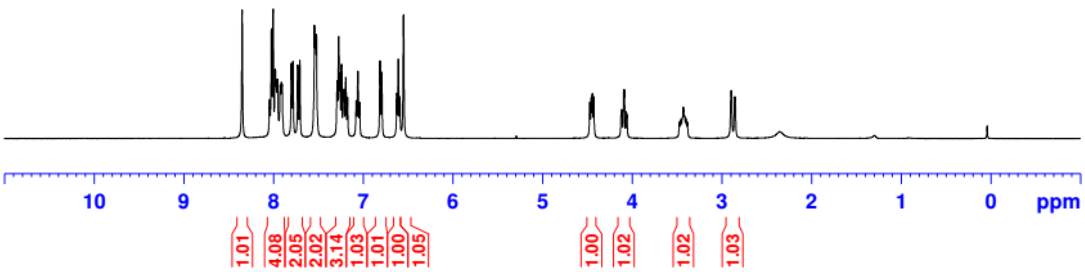
2.86

O
N
N

3b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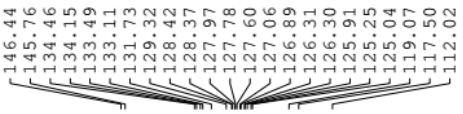
1.02
1.02
1.03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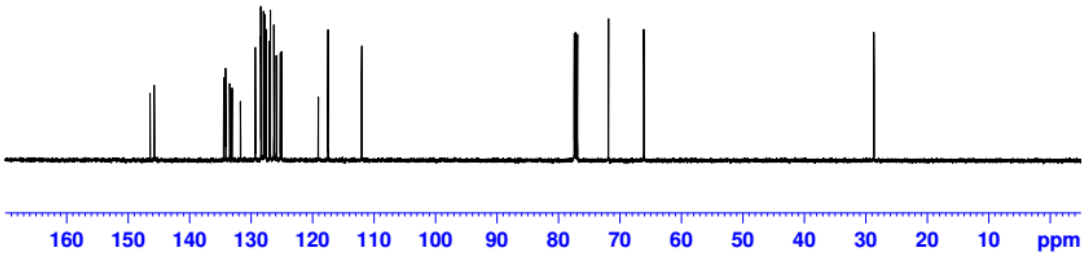
112.02


71.88
66.11
28.68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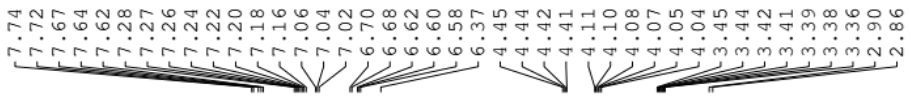
10
ppm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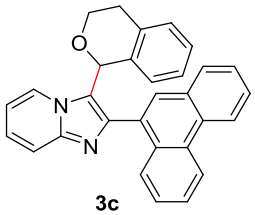
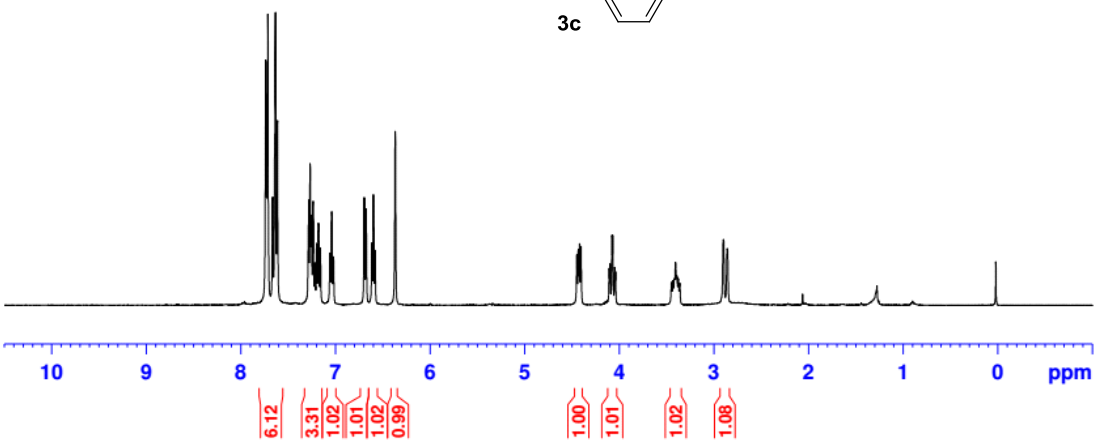

O
N
N

3c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1.00
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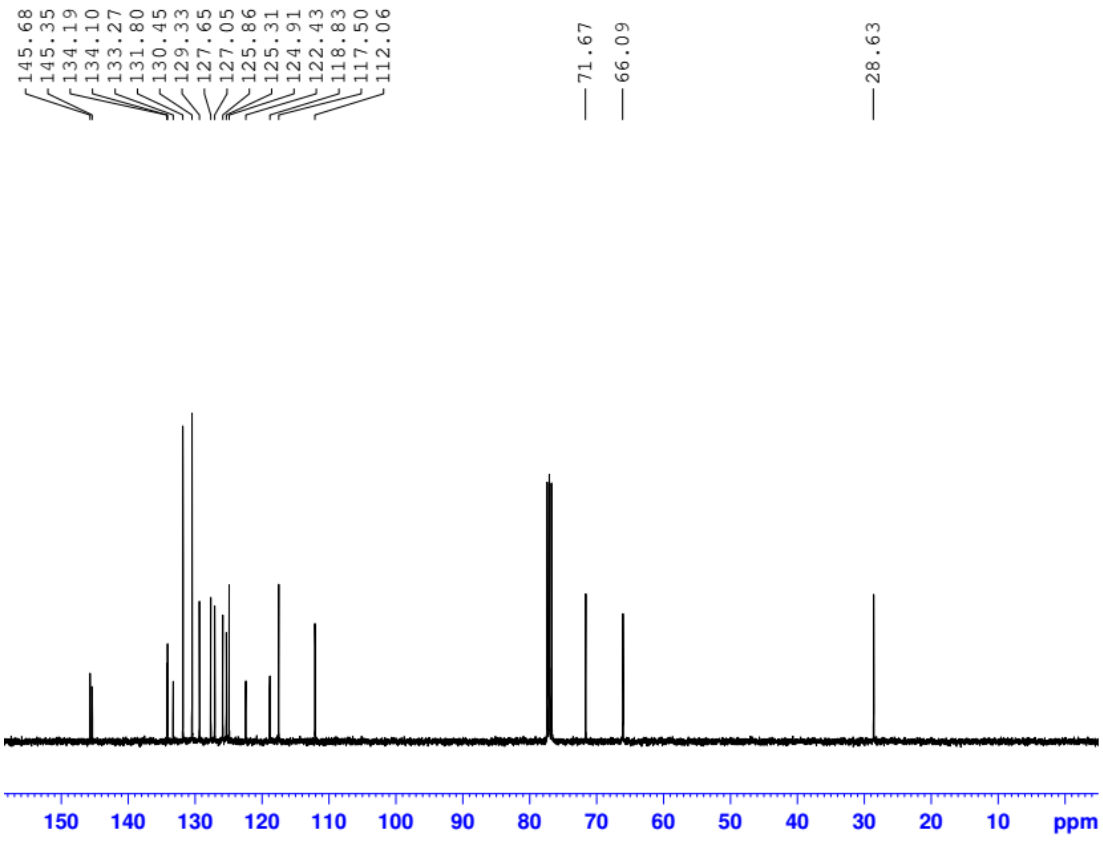
1.02
1.08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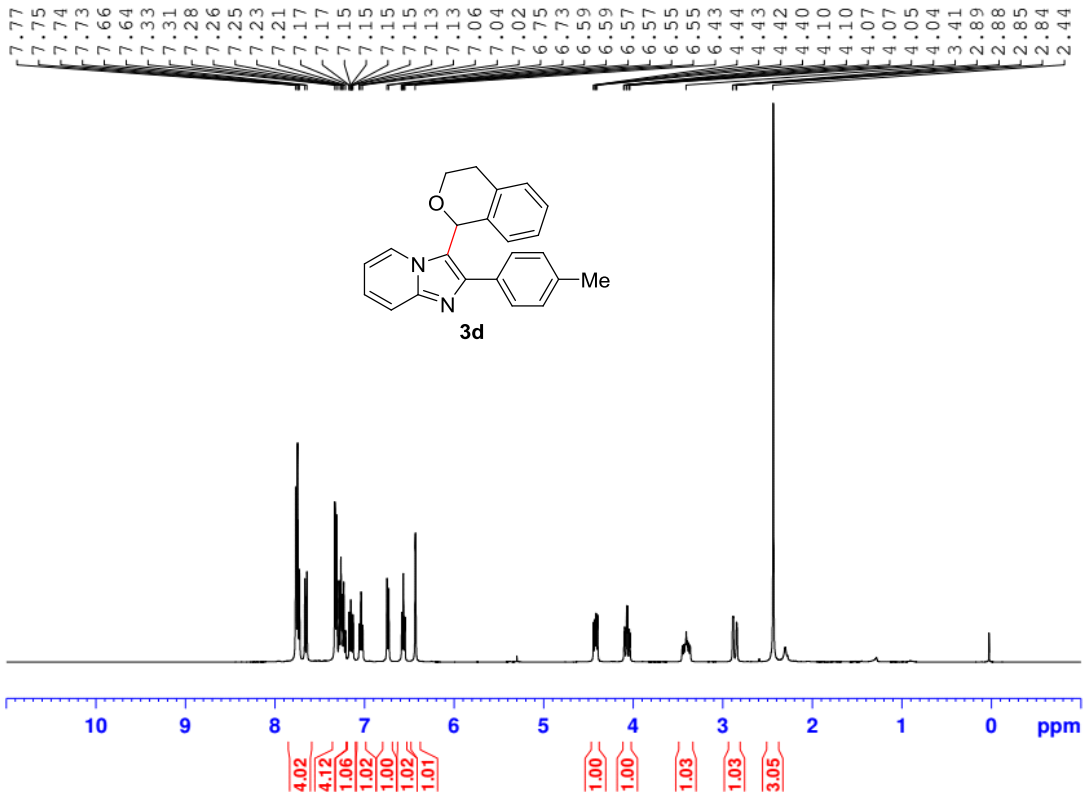
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2.85
2.84
2.44
O
N
N
Me
3d
10 9 8 7 6 5 4 3 2 1 0 ppm
4.02
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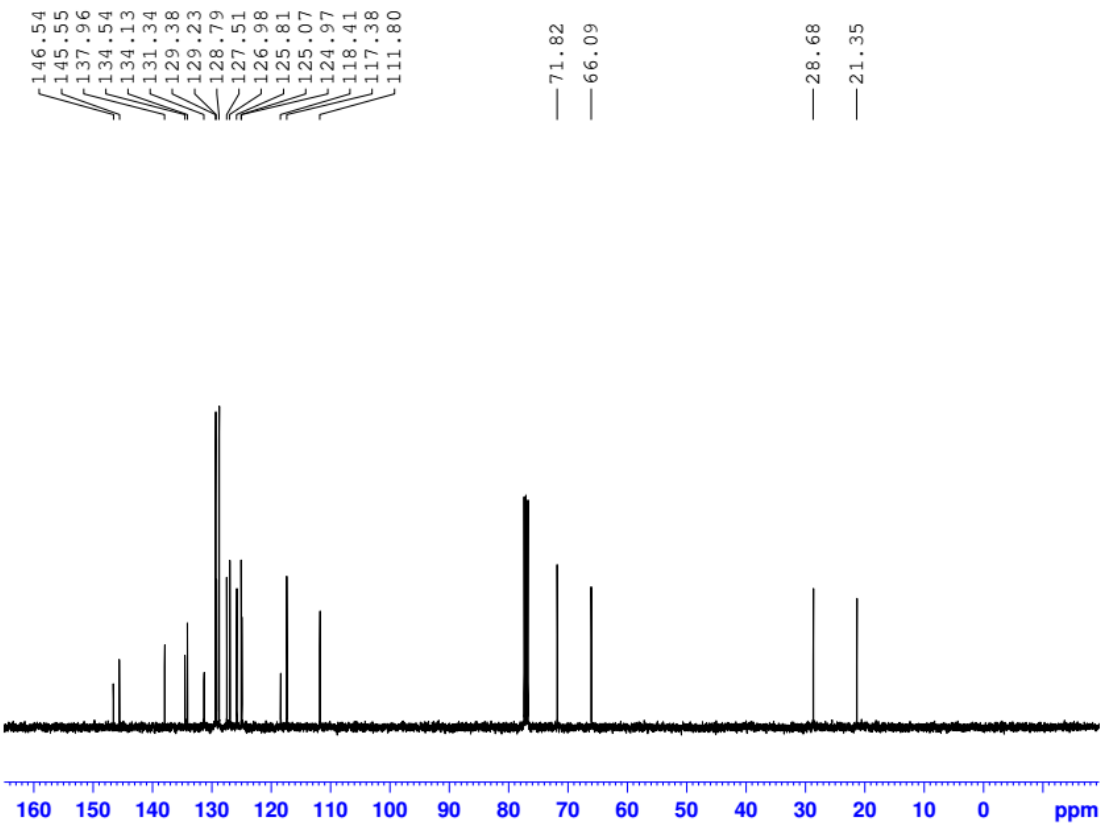
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125.07
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111.80
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66.09
28.68
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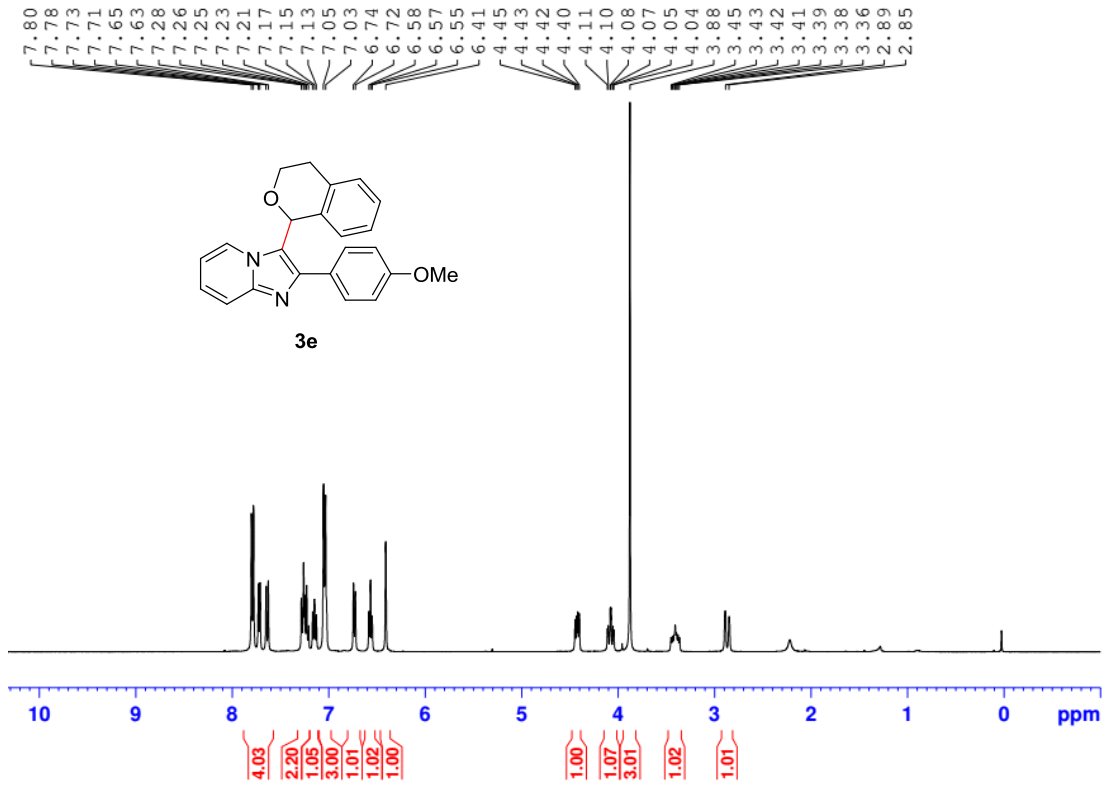
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7.13
7.05
7.03
6.74
6.72
6.58
6.57
6.55
6.41
4.45
4.43
4.42
4.40
4.11
4.10
4.08
4.07
4.05
4.04
3.88
3.45
3.43
3.42
3.41
3.39
3.38
3.36
2.89
2.85
O
N
N
OMe
3e
10 9 8 7 6 5 4 3 2 1 0 ppm
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3.00
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1.02
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1.00
1.07
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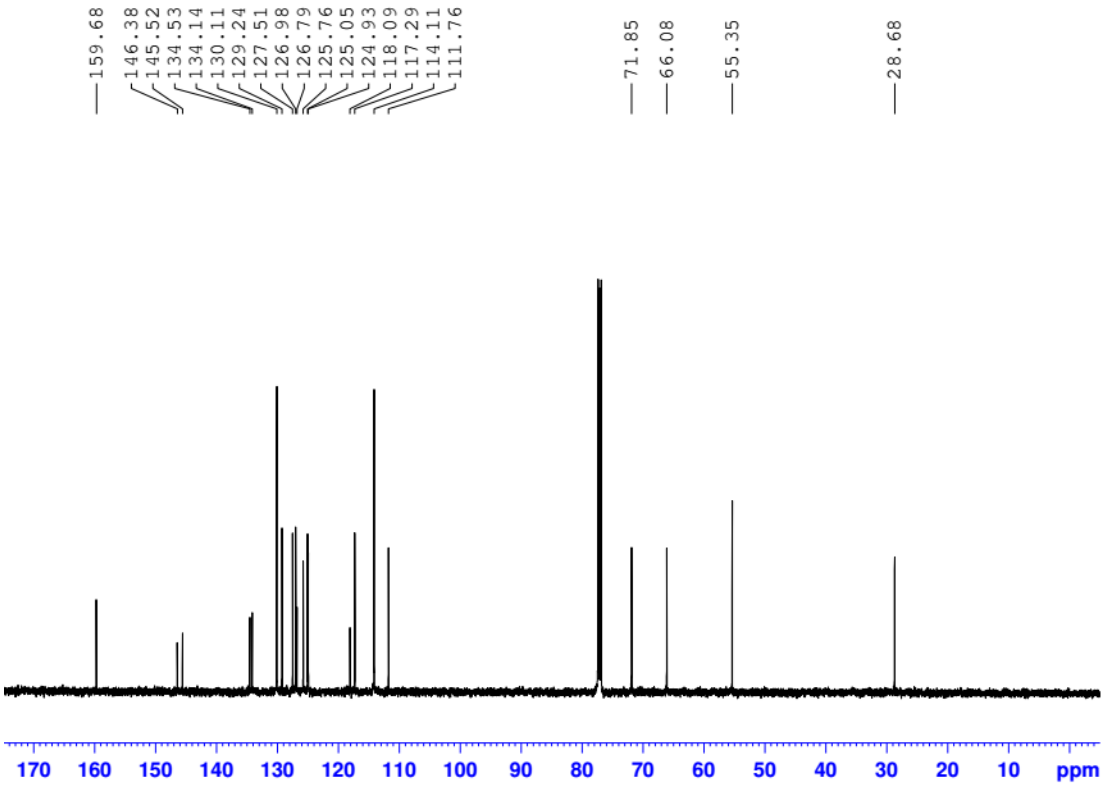
1.02
1.01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125.05
124.93
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111.76
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66.08
55.35
28.68
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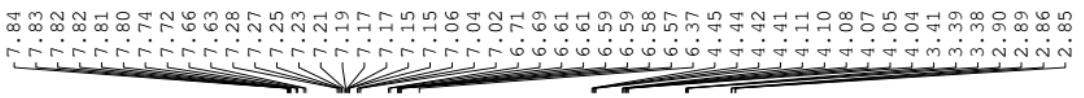
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7.23
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7.19
7.17
7.17
7.15
7.15
7.06
7.04
7.02
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6.69
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6.61
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6.59
6.58
6.57
6.37
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4.42
4.41
4.11
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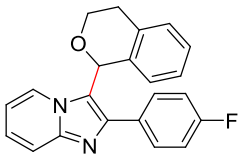
2.85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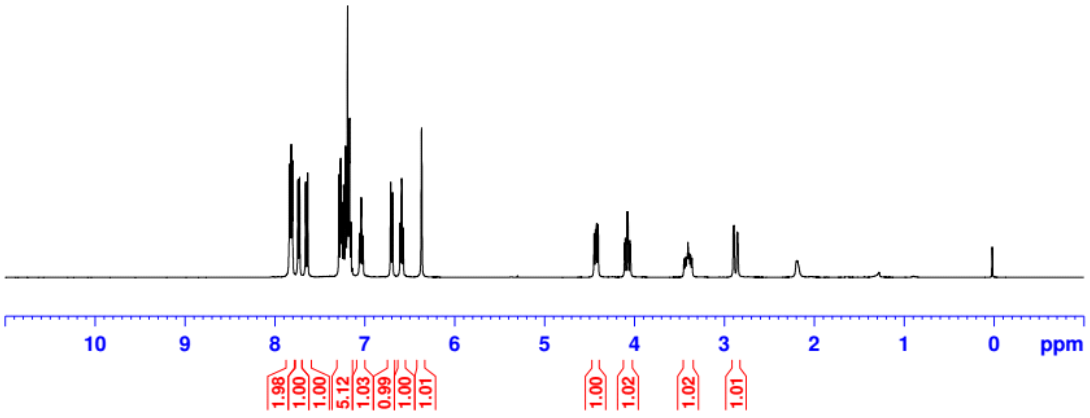
F

3f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1.01
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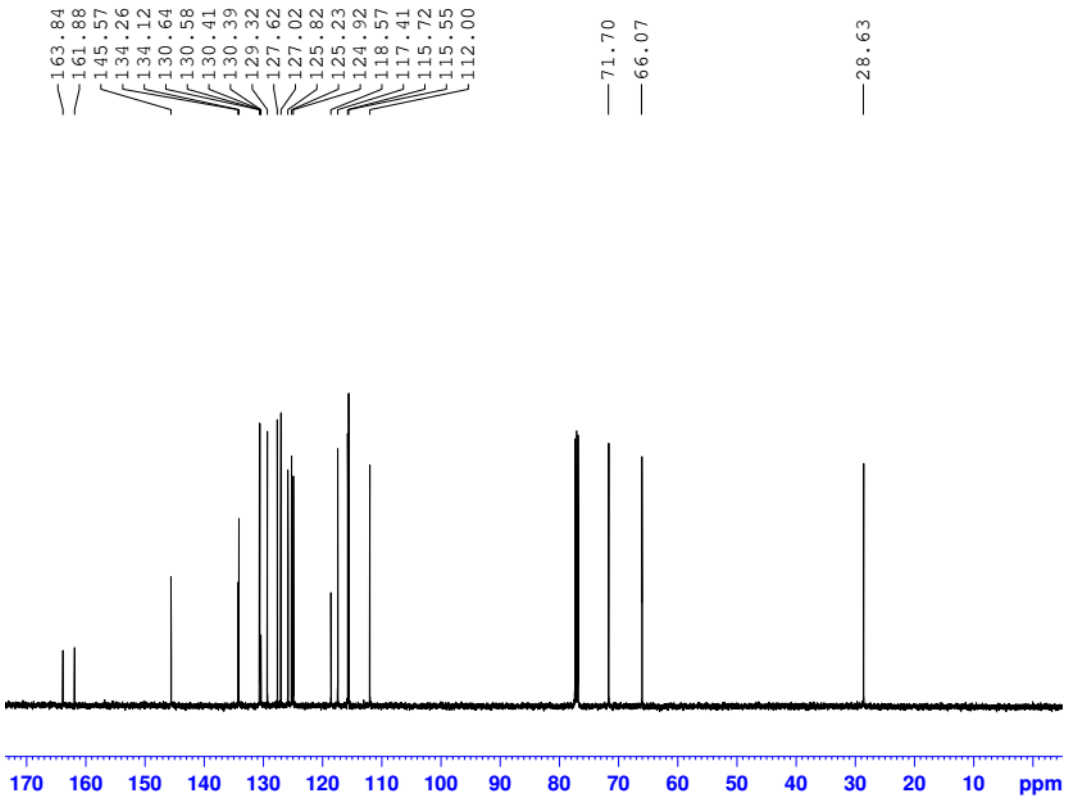
1.02
1.02
1.01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130.58
130.41
130.39
129.32
127.62
127.02
125.82
125.23
124.92
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115.55
112.00
71.70
66.07
28.63
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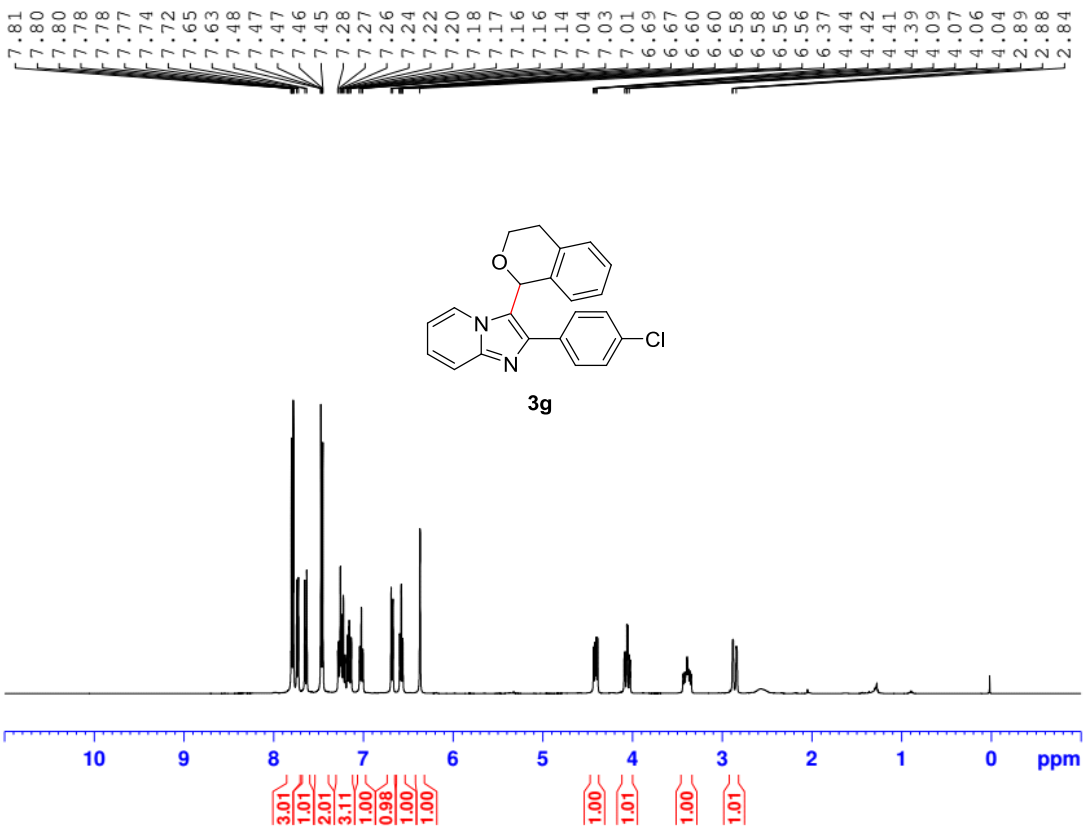
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7.77
7.74
7.72
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7.63
7.48
7.47
7.47
7.46
7.45
7.28
7.27
7.26
7.24
7.22
7.20
7.18
7.17
7.16
7.16
7.14
7.04
7.03
7.01
6.69
6.67
6.60
6.60
6.58
6.58
6.56
6.56
6.37
4.44
4.42
4.41
4.39
4.09
4.07
4.06
4.04
2.89
2.88
2.84
O
N
N
Cl
10 9 8 7 6 5 4 3 2 1 0 ppm
3.01
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3.11
1.00
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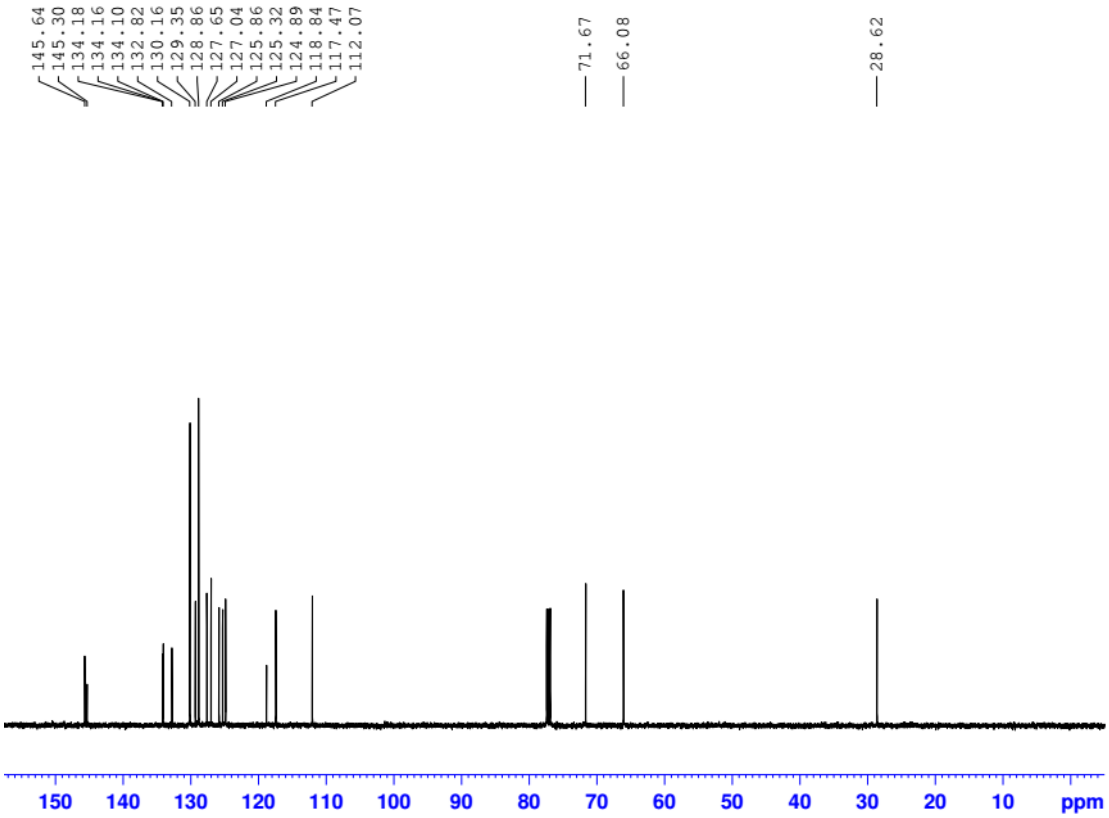
1.00
1.00
1.01
1.00
1.01

3g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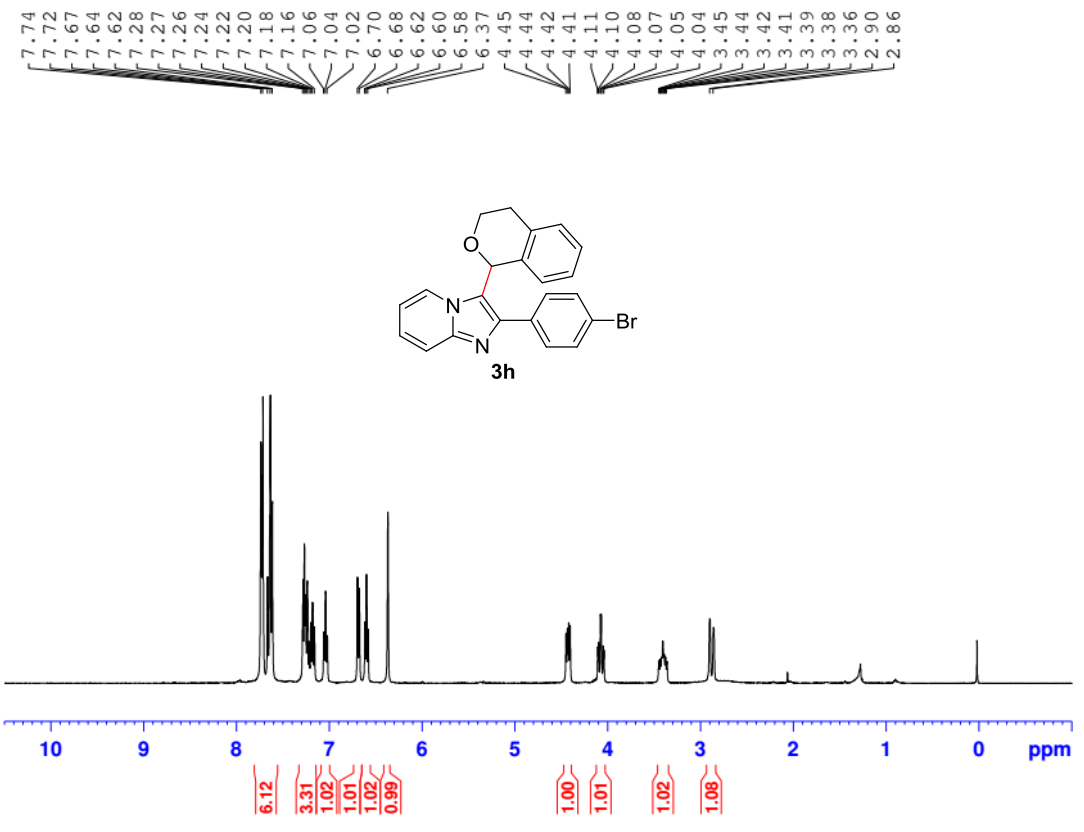
132.82
130.16
129.35
128.86
127.65
127.04
125.86
125.32
124.89
118.84
117.47
112.07
71.67
66.08
28.62
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.62
7.28
7.27
7.26
7.24
7.22
7.20
7.18
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7.06
7.04
7.02
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6.60
6.58
6.37
4.45
4.44
4.42
4.41
4.11
4.10
4.08
4.07
4.05
4.04
3.45
3.44
3.42
3.41
3.39
3.38
3.36
2.90
2.86
O
N
N
Br
3h
10
9
8
7
6
5
4
3
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3.31
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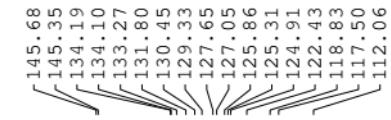
1.01
1.02
0.99
1.00
1.01
1.02
1.08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125.31
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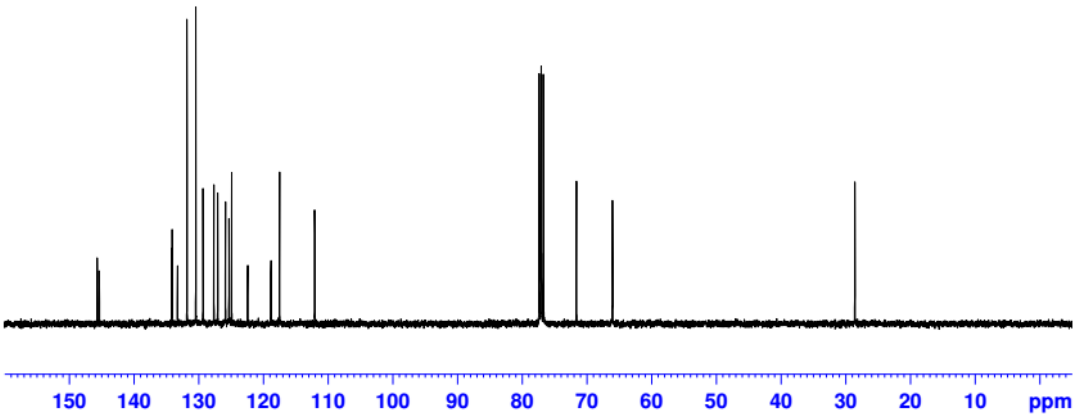
122.43
118.83
117.50
112.06


71.67
66.09
28.63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120
110
100
90
80
70
60
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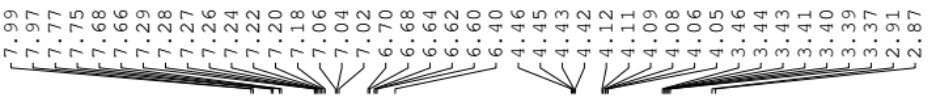
30
20
10
ppm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7.29
7.28
7.27
7.26
7.24
7.22
7.20
7.18
7.06
7.04
7.02
6.70
6.68
6.64
6.62
6.60
6.40
4.46
4.45
4.43
4.42
4.12
4.11
4.09
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3.46
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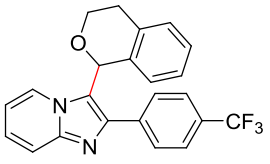
3.43
3.41
3.40
3.39
3.37
2.91
2.87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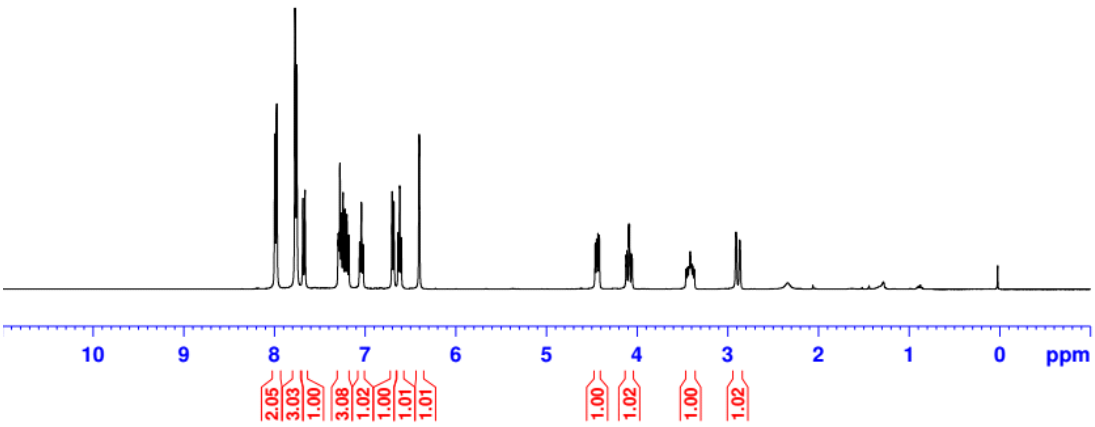
CF3

3i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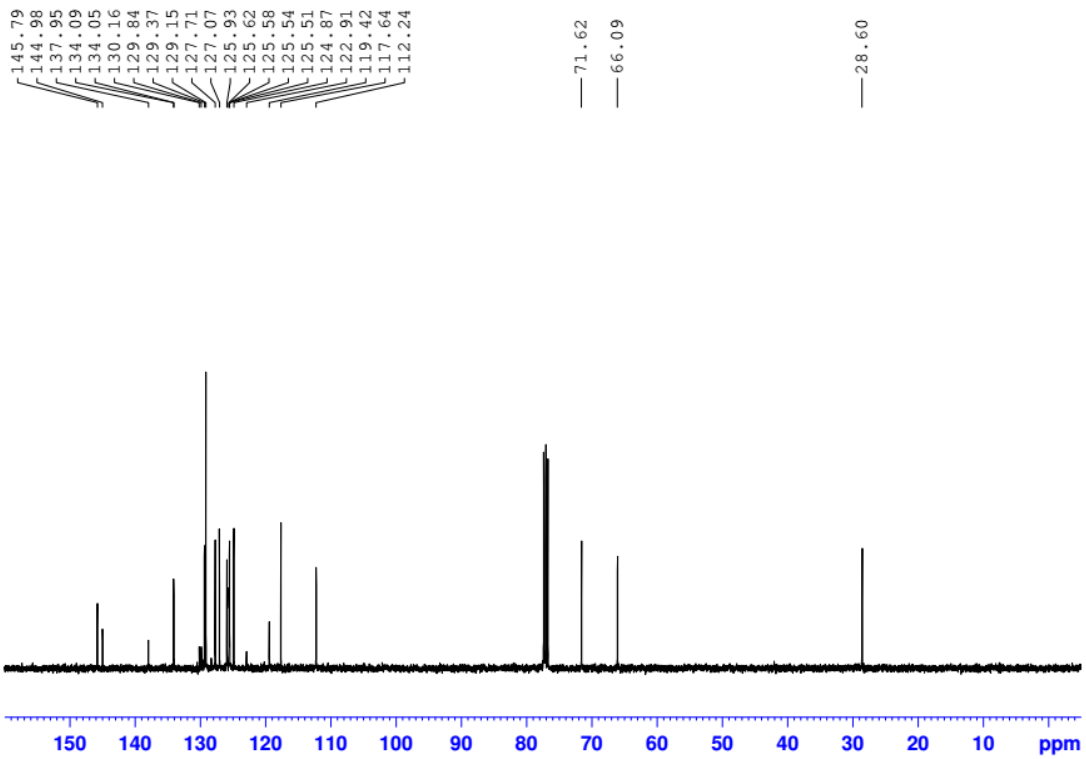
9
8
7
6
5
4
3
2
1
0
ppm
2.05
3.03
1.00
3.08
1.02
1.00
1.01
1.01
1.00
1.02
1.00
1.02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129.15
127.71
127.07
125.93
125.62
125.58
125.54
125.51
124.87
122.91
119.42
117.64
112.24
71.62
66.09
28.60
150
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120
110
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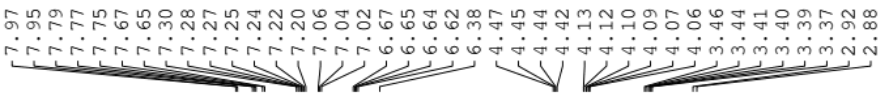
30
20
10
ppm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7.24
7.22
7.20
7.06
7.04
7.02
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6.65
6.64
6.62
6.38
4.47
4.45
4.44
4.42
4.13
4.12
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4.06
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3.44
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3.37
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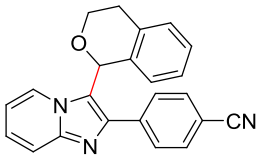
2.88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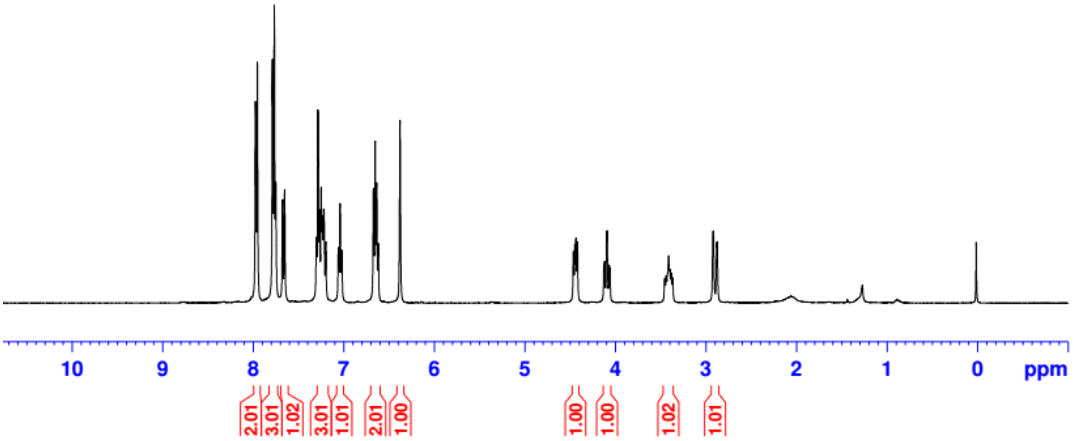
N
CN

3j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8
7
6
5
4
3
2
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ppm
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3.01
1.02
3.01
1.01
2.01
1.00
1.00
1.00
1.02
1.01


145.84
144.31
139.01
134.09
133.82
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129.39
127.80
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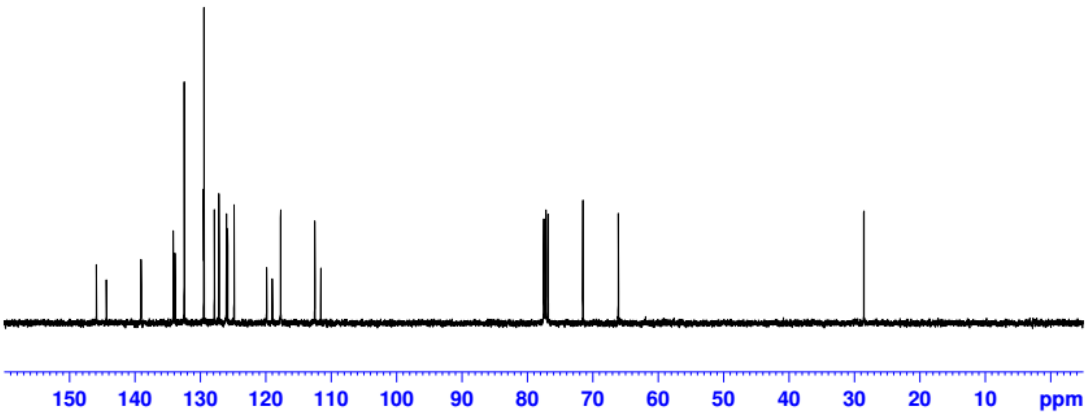
28.55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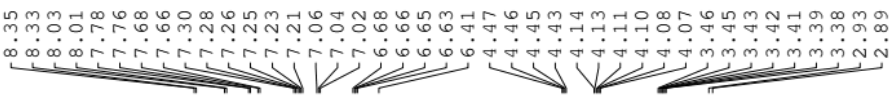
110
100
90
80
70
60
50
40
30
20
10
ppm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7.28
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7.25
7.23
7.21
7.06
7.04
7.02
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6.66
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6.63
6.41
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4.45
4.43
4.14
4.13
4.11
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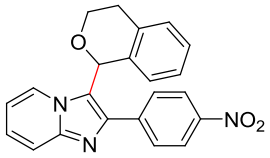
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NO2

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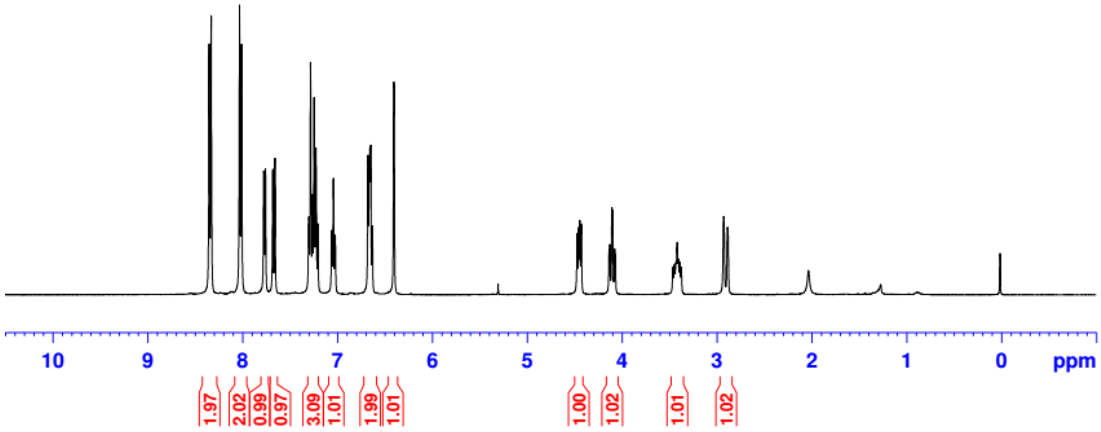
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
2.02
0.99
0.97
3.09
1.01
1.99
1.01
1.00
1.02
1.01
1.02


147.43
145.91
143.97
140.94
134.08
133.77
129.51
129.45
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117.75
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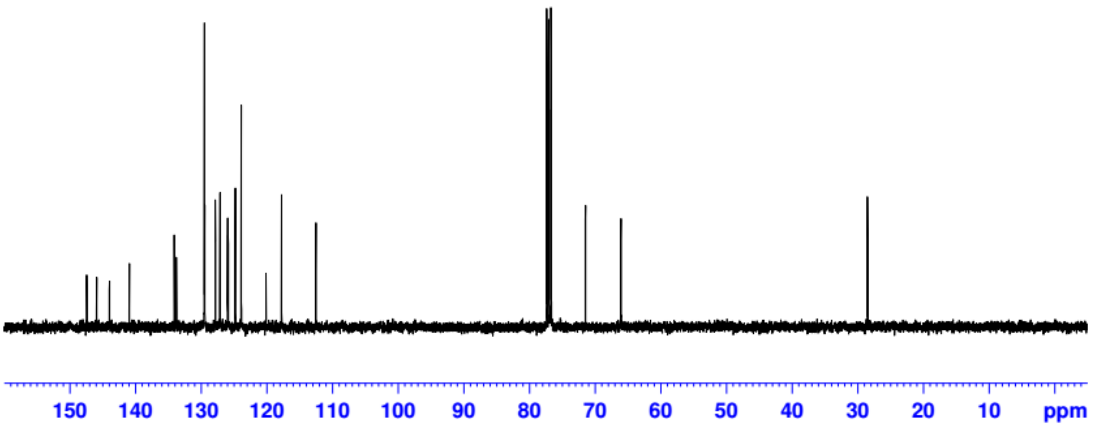
71.52
66.12
28.56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110
100
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70
60
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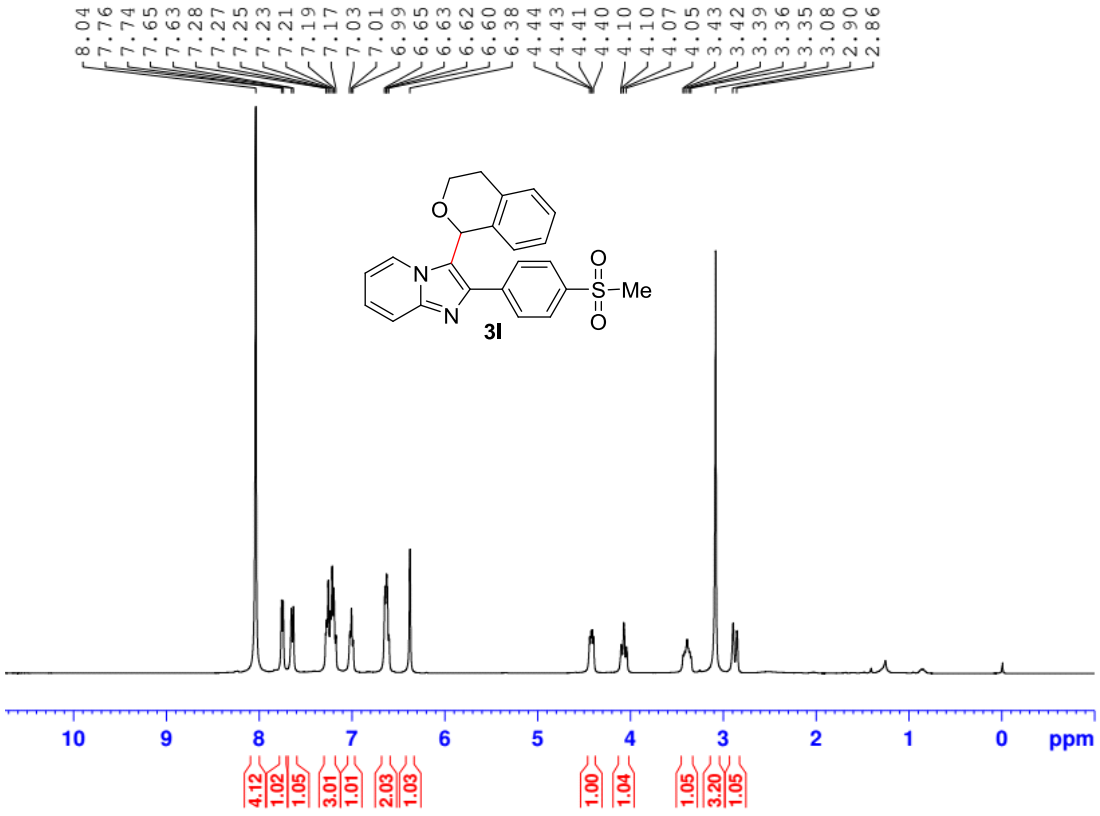
30
20
10
ppm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7.25
7.23
7.21
7.19
7.17
7.03
7.01
6.99
6.65
6.63
6.62
6.60
6.38
4.44
4.43
4.41
4.40
4.10
4.10
4.07
4.05
3.43
3.42
3.39
3.36
3.35
3.08
2.90
2.86
O
N
N
O
S
O
Me
3l
10
9
8
7
6
5
4
3
2
1
0
ppm
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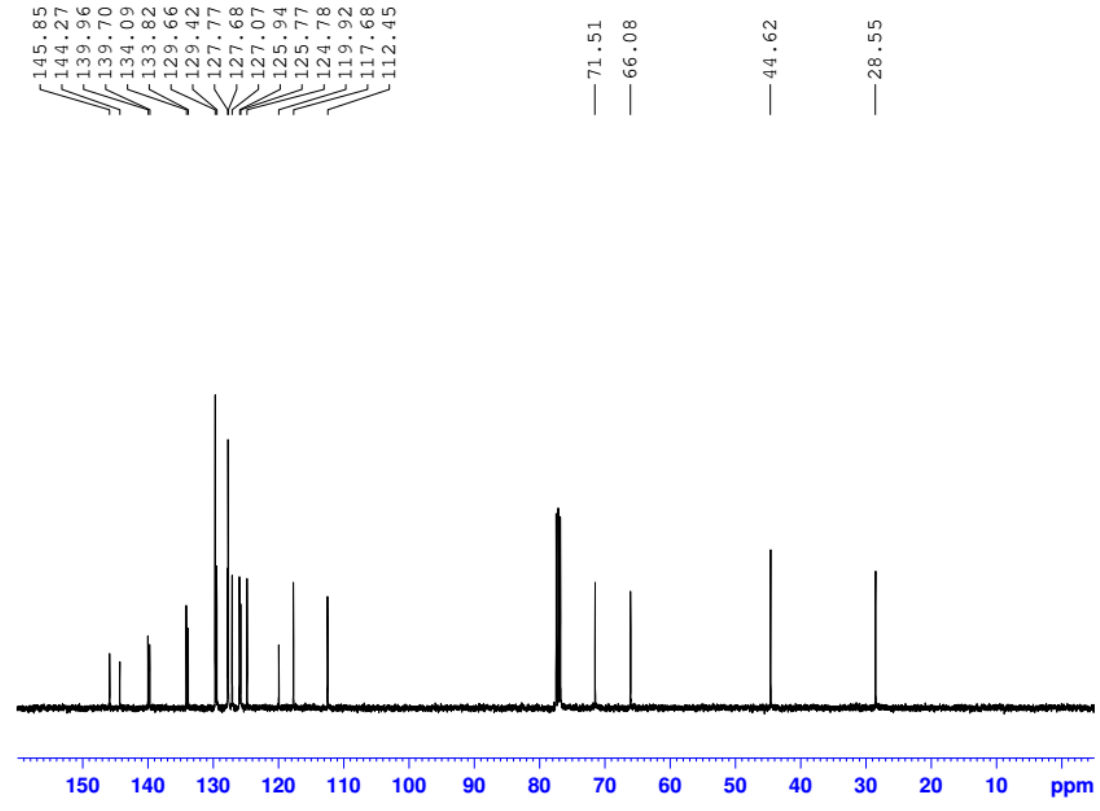
1.05
3.01
1.01
2.03
1.03
1.00
1.04
1.05
3.20
1.05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129.42
127.77
127.68
127.07
125.94
125.77
124.78
119.92
117.68
112.45
71.51
66.08
44.62
28.55
150
140
130
120
110
100
90
80
70
60
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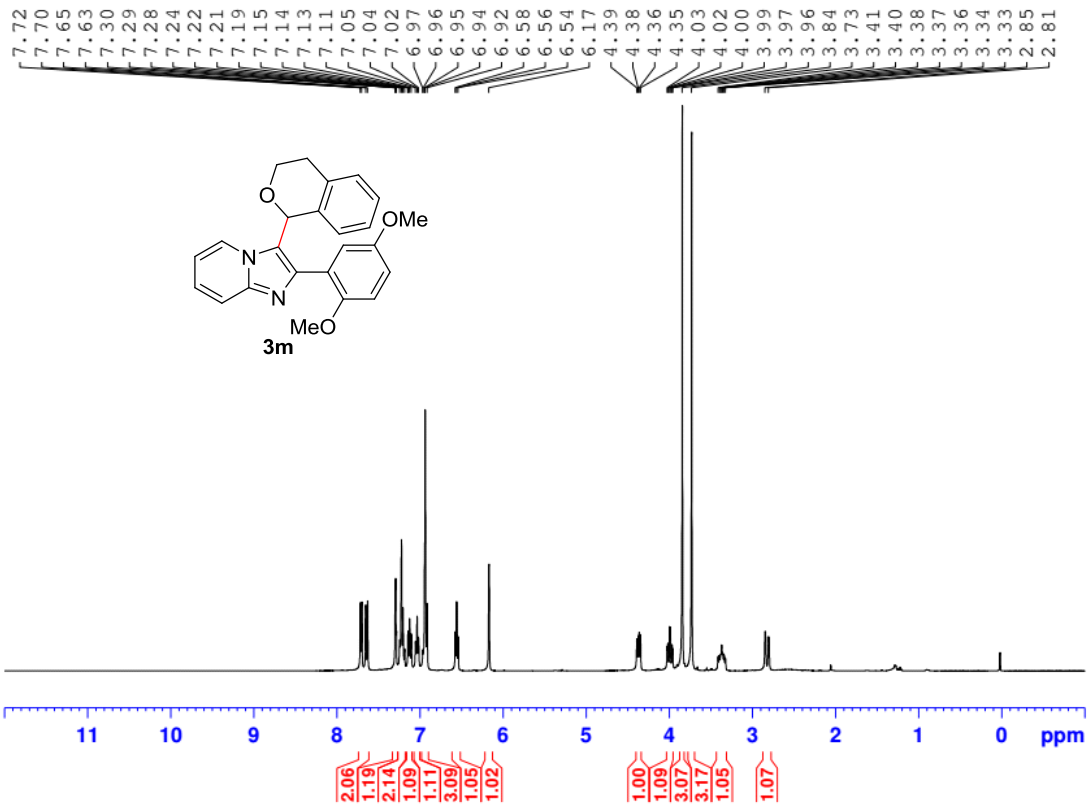
40
30
20
10
ppm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7.19
7.15
7.14
7.13
7.11
7.05
7.04
7.02
6.97
6.96
6.95
6.94
6.92
6.58
6.56
6.54
6.17
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4.36
4.35
4.03
4.02
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3.96
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3.73
3.41
3.40
3.38
3.37
3.36
3.34
3.33
2.85
2.81
O
OMe
N
N
MeO
3m
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
1.19
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3.09
1.05
1.02
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1.09
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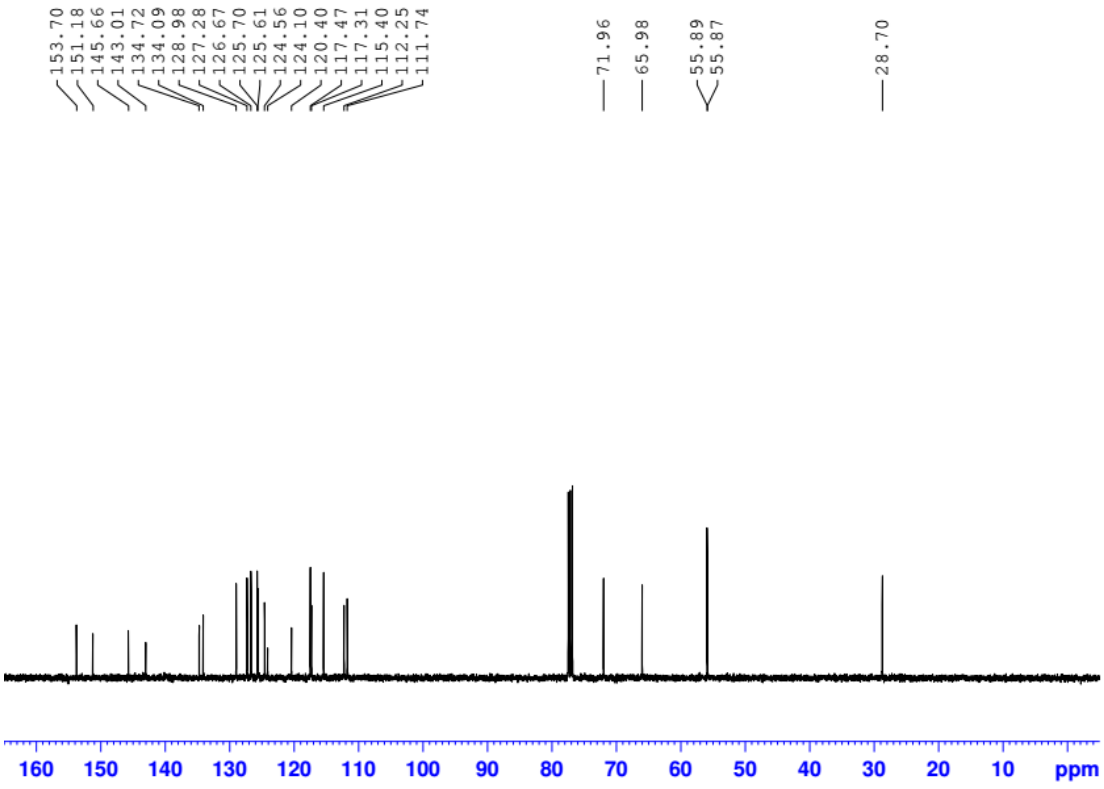
3.17
1.05
1.07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126.67
125.70
125.61
124.56
124.10
120.40
117.47
117.31
115.40
112.25
111.74
71.96
65.98
55.89
55.87
28.70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
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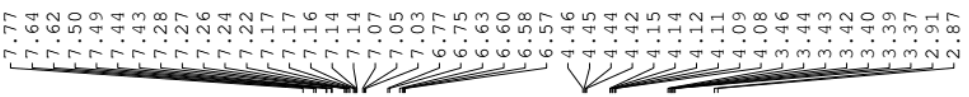
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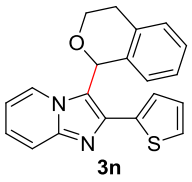
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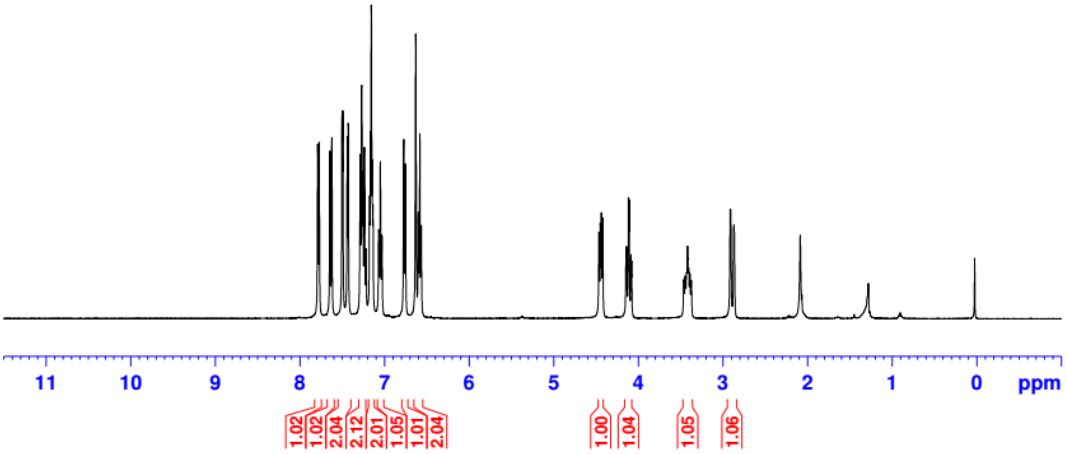
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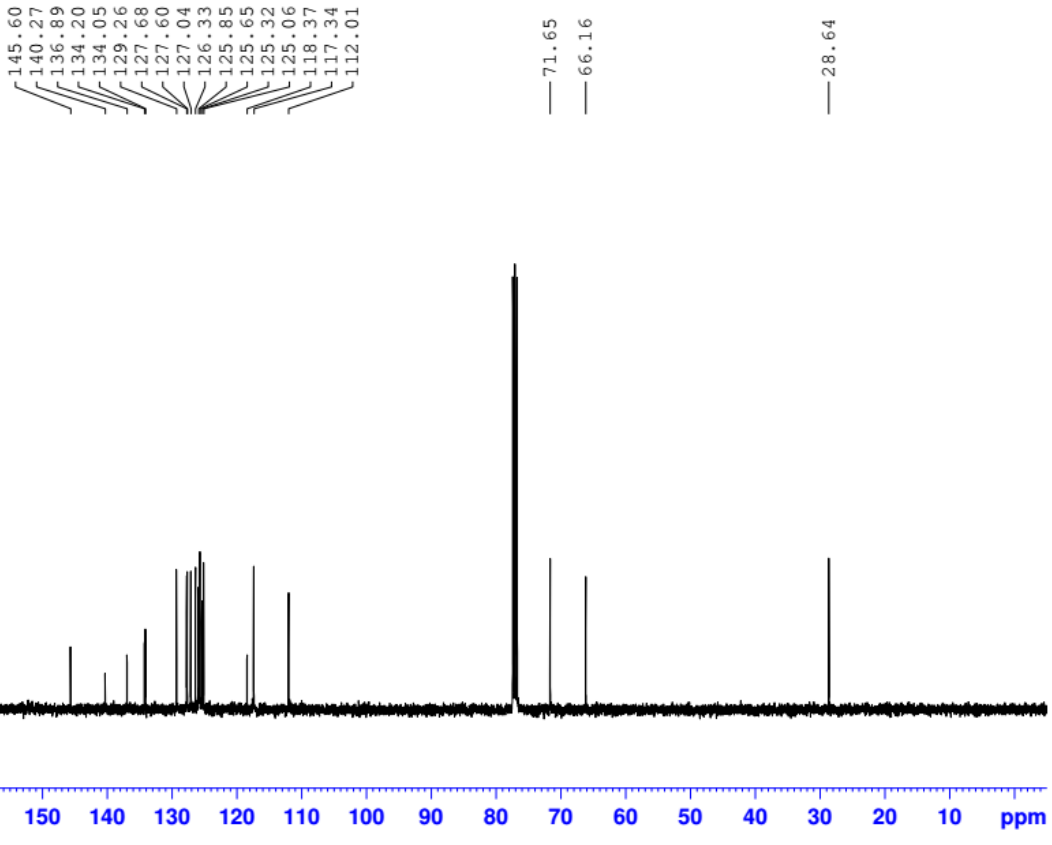
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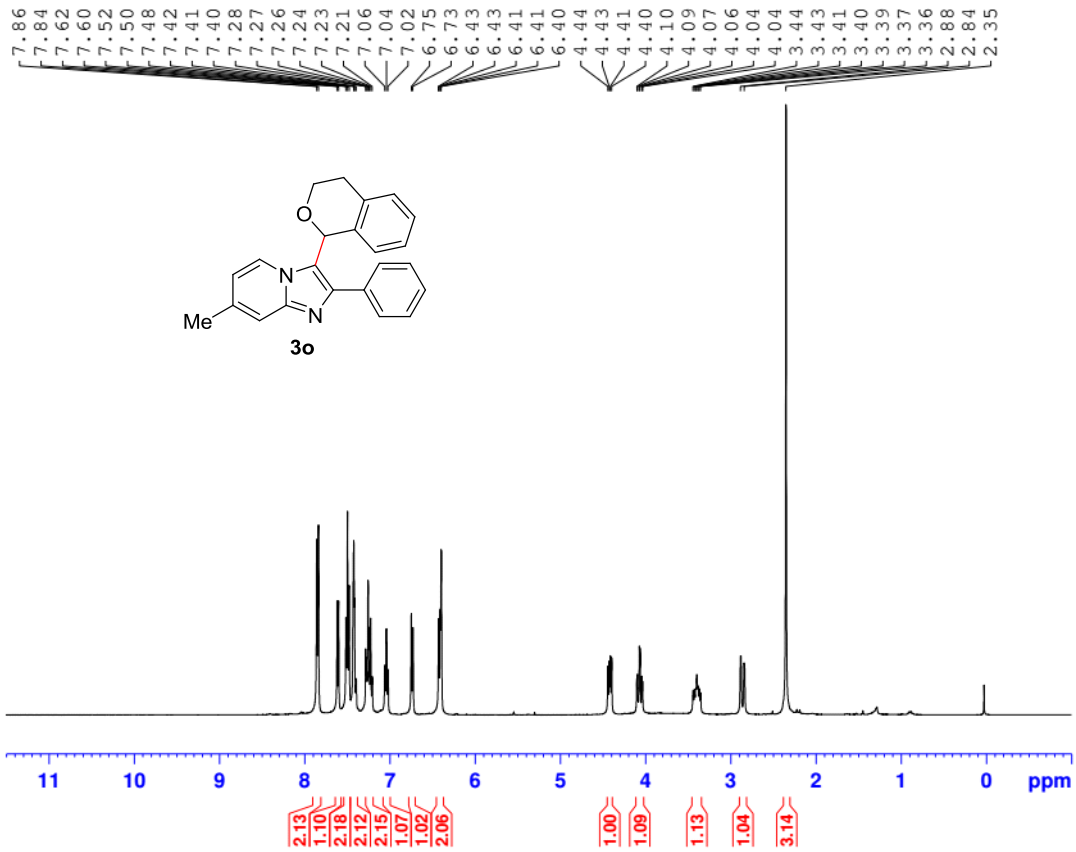
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6.41
6.40
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4.43
4.41
4.40
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N
Me
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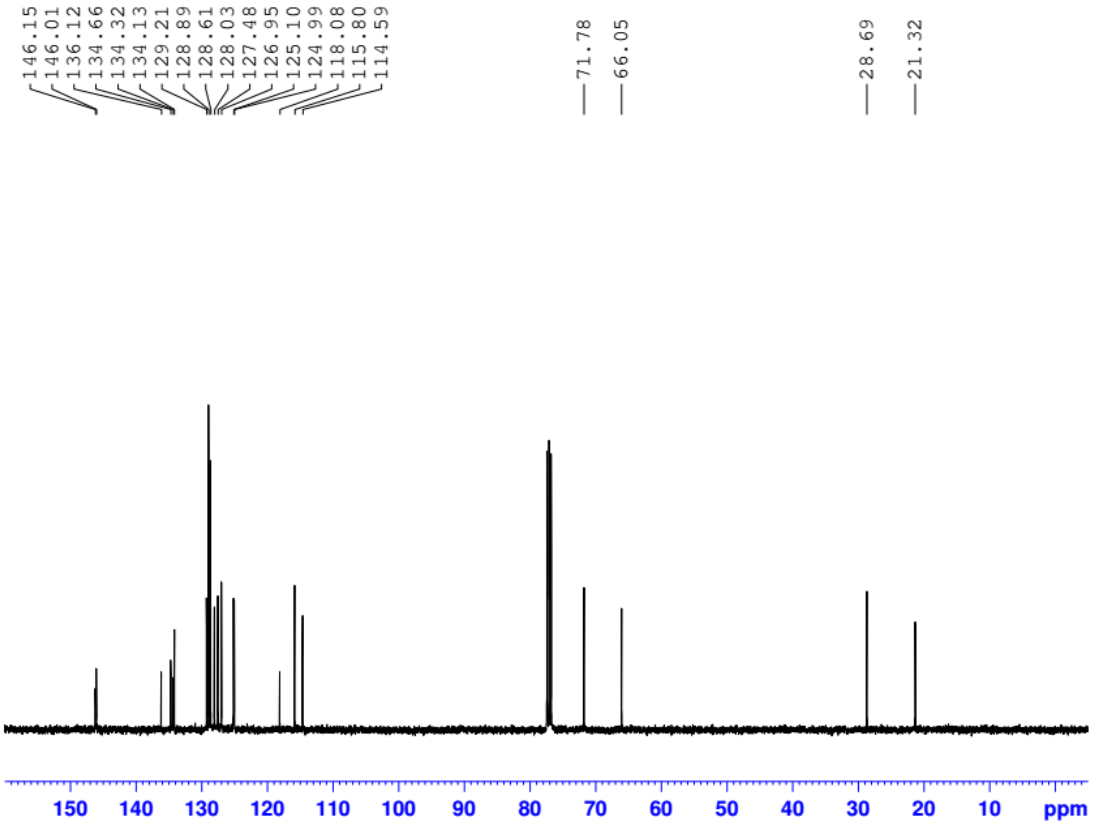
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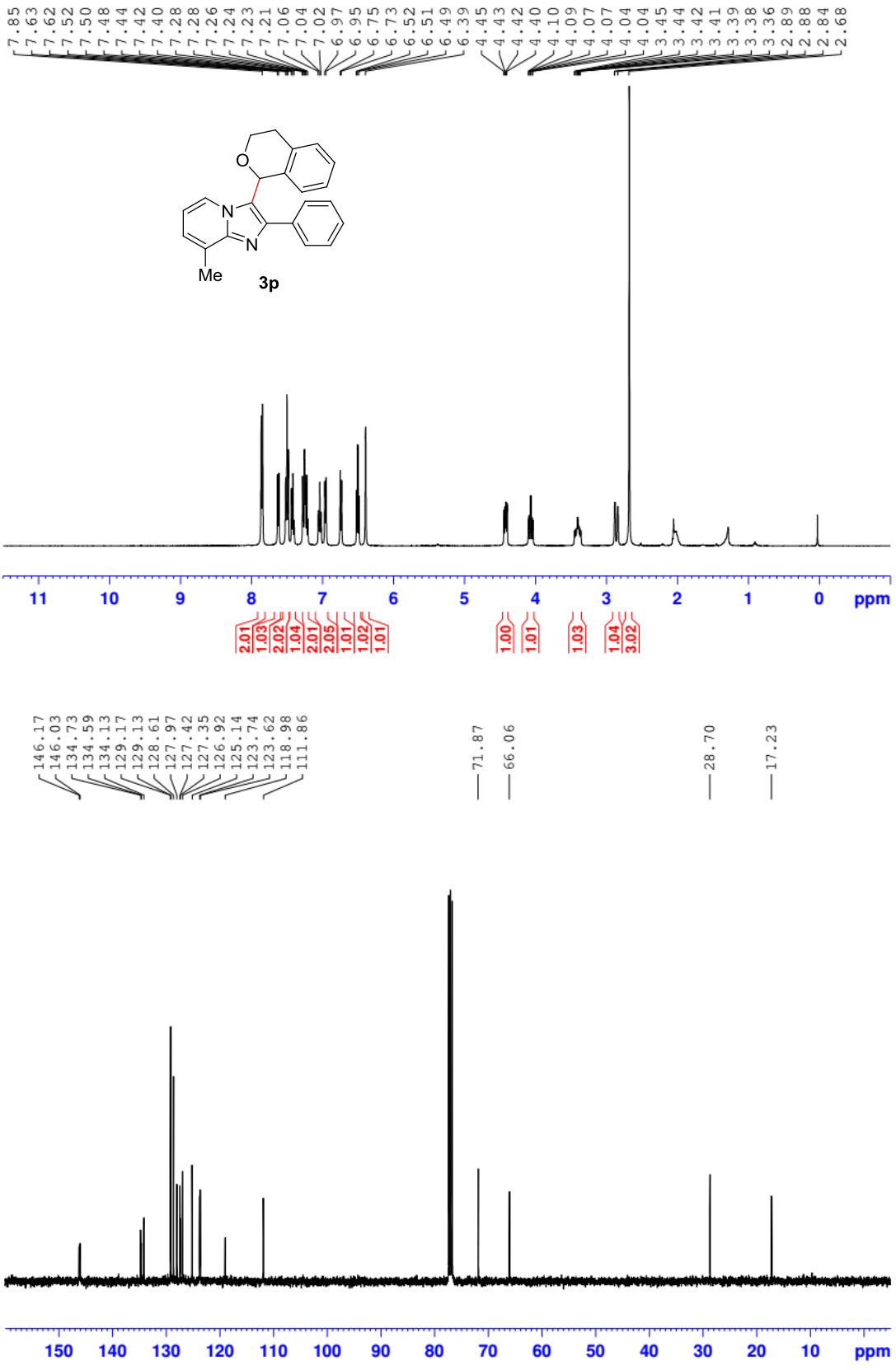
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N
Me
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4
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1.03
1.04
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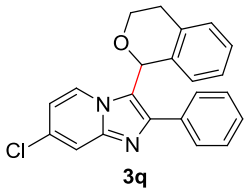
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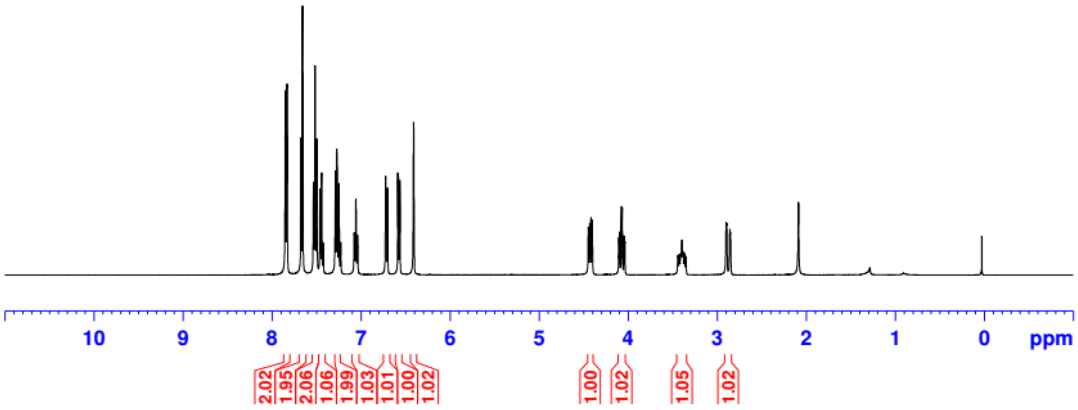
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1.01
1.00
1.02
1.00
1.02
1.05
1.02


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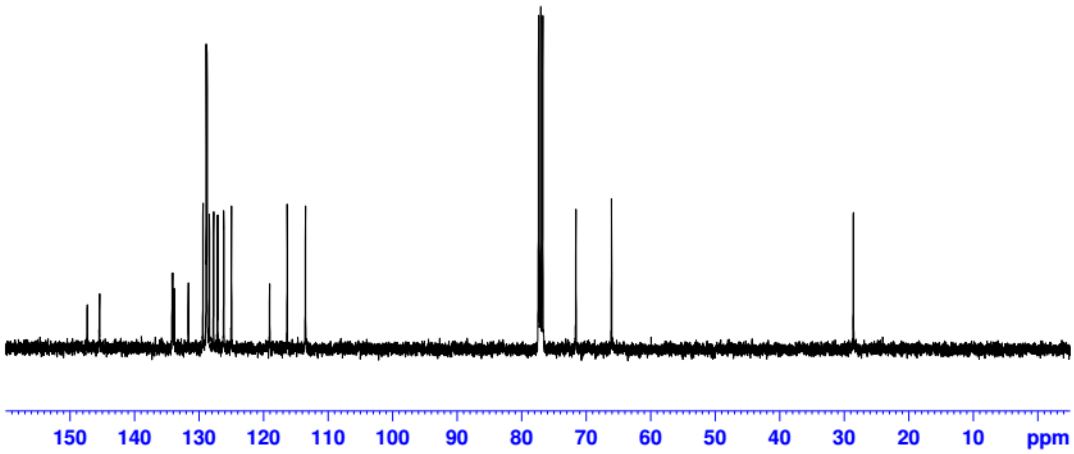
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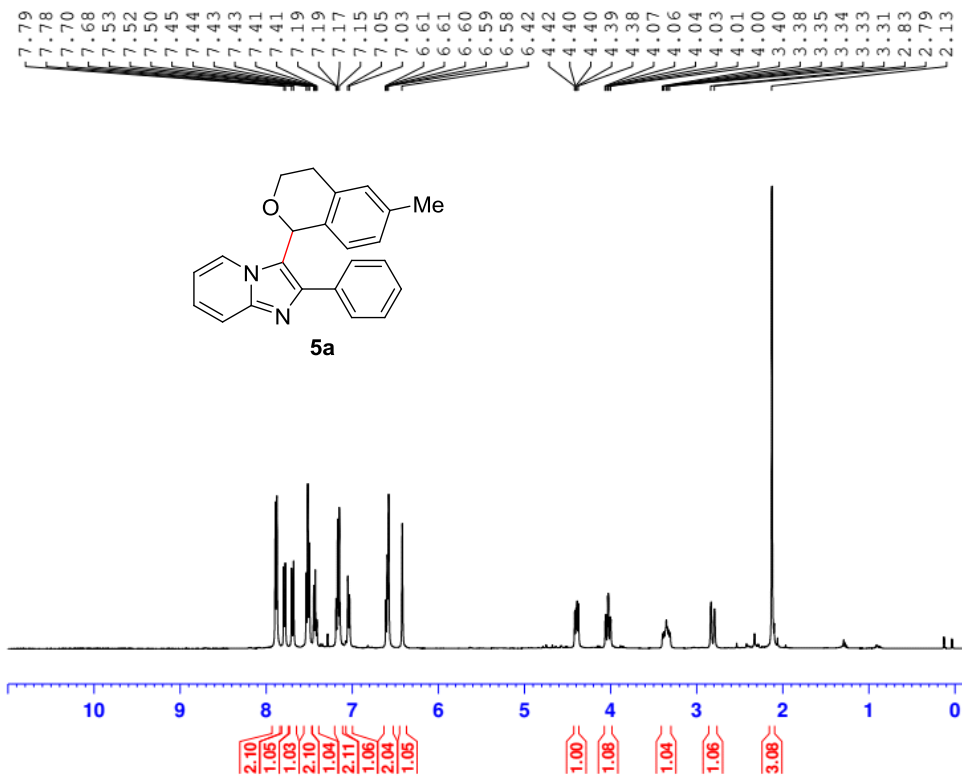
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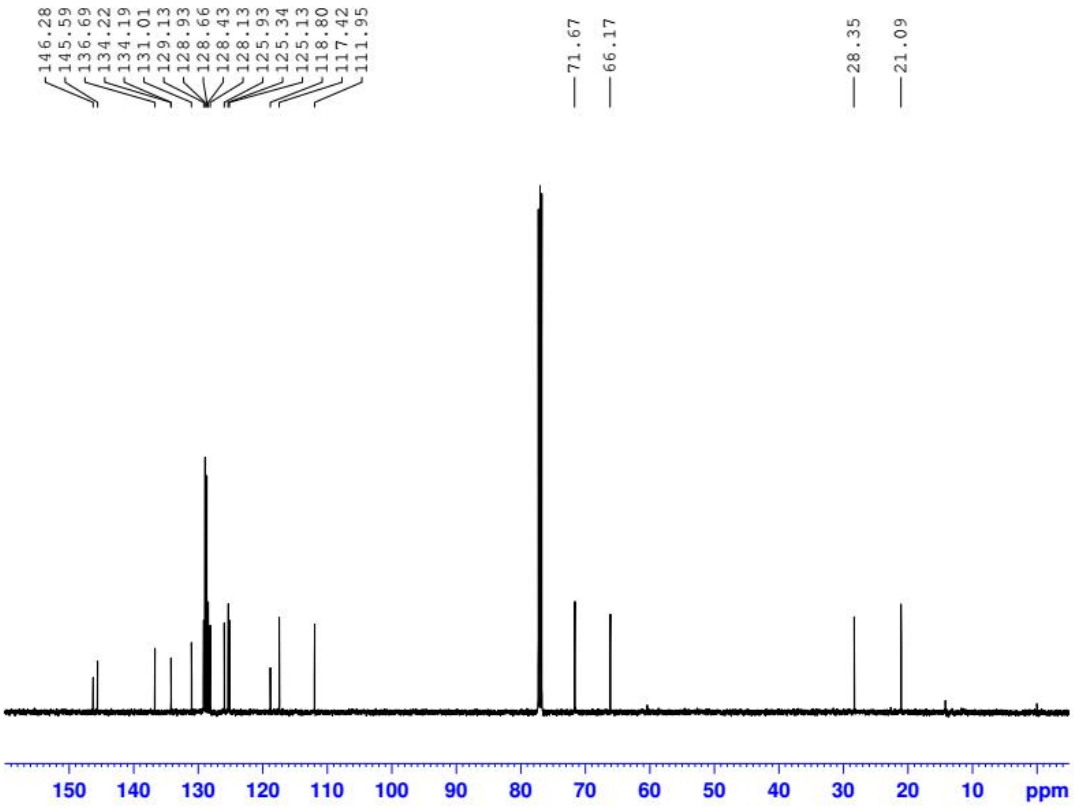
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ppm


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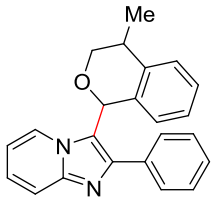
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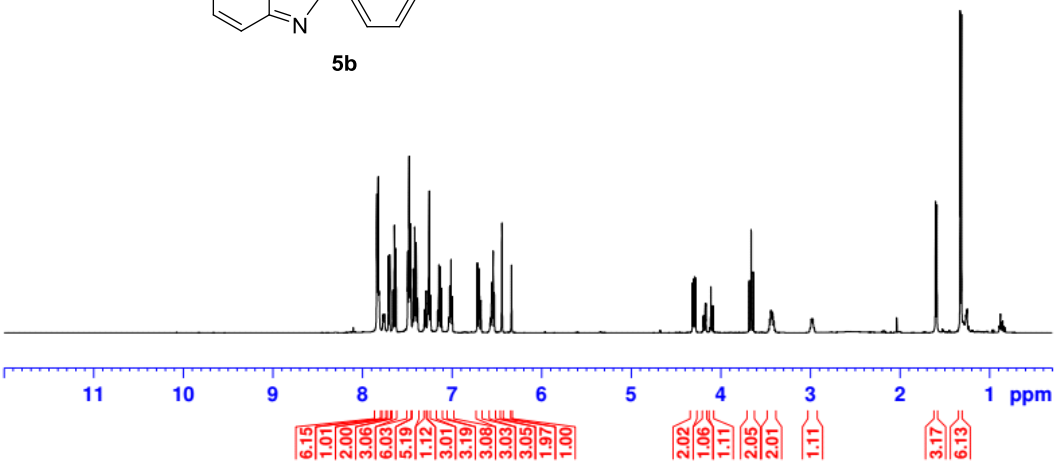
5b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ppm
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2.00
3.06
6.03
5.19
1.12
3.01
3.19
3.08
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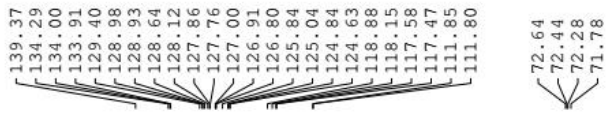
6.13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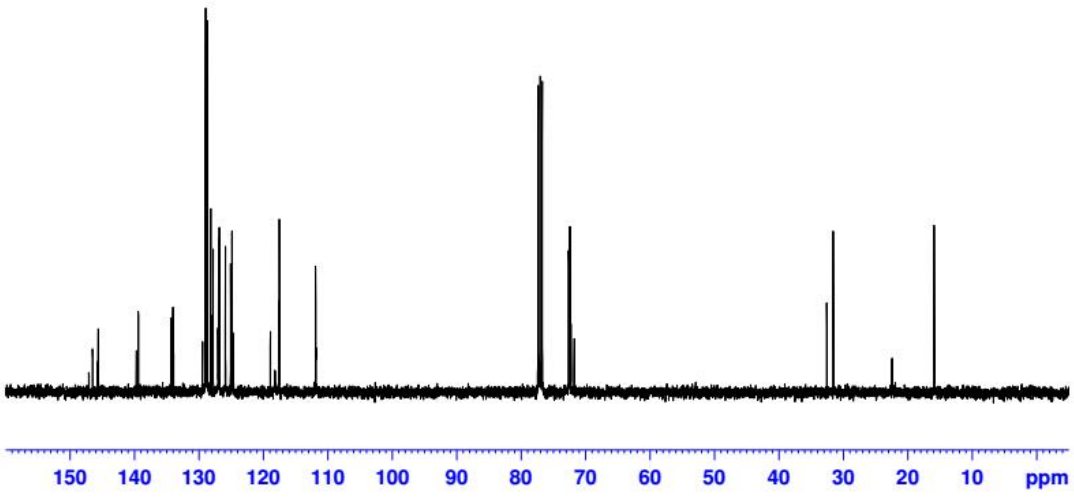
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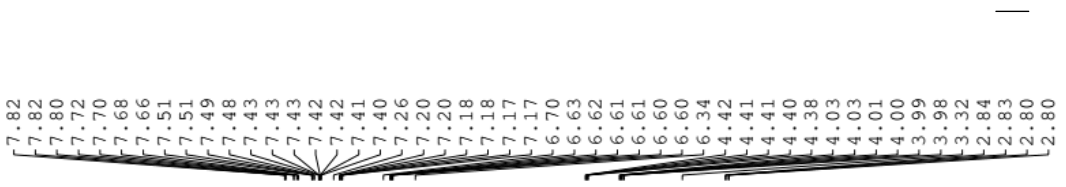
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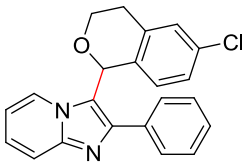
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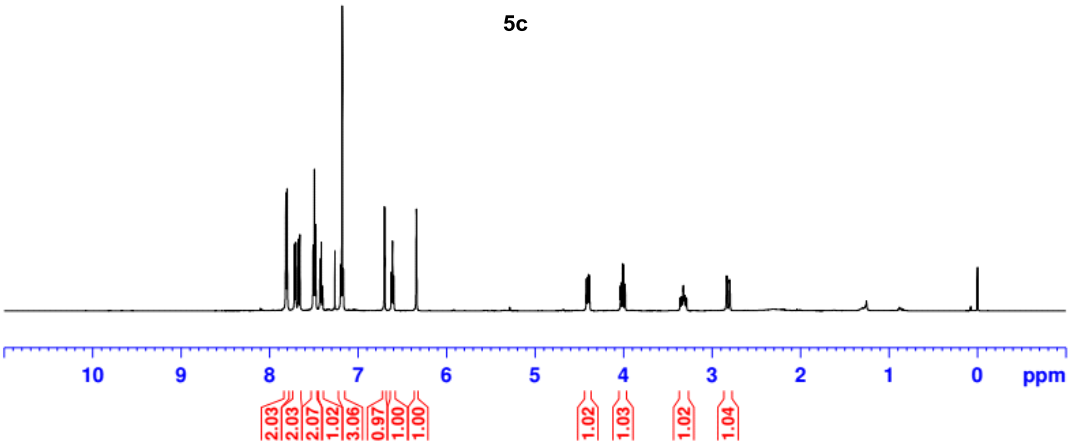
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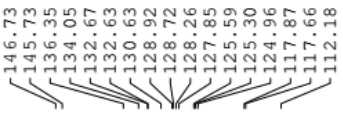
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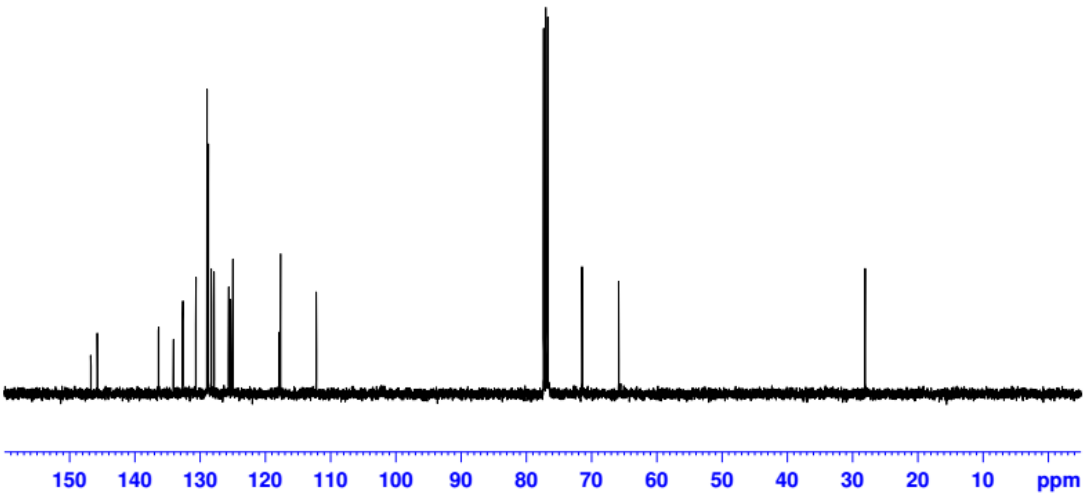
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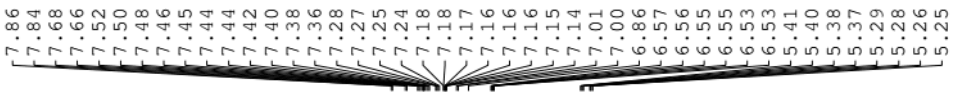
ppm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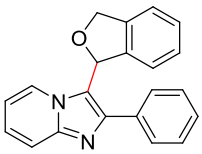
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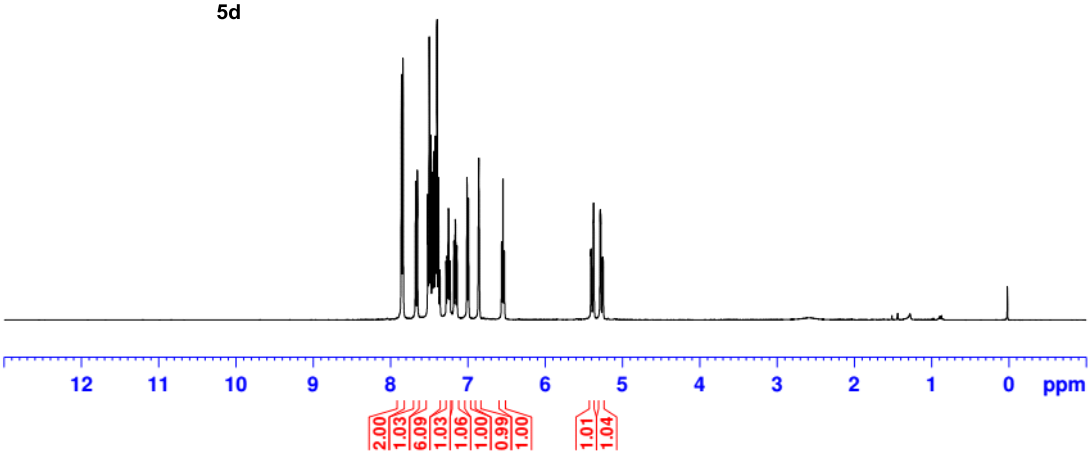
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1.03
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1.03
1.06
1.00
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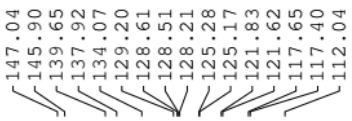
1.04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112.04


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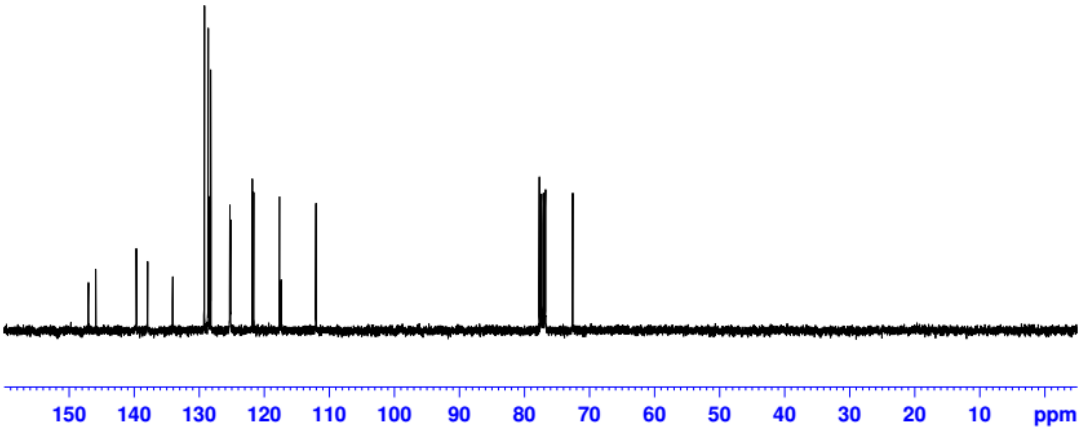
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ppm