Supporting Information

Carbonyl Group Directed Synthesis of 3-Boryl-3-Substituted Alkenyl Oxindoles and Tetrasubstituted β-Borylenones

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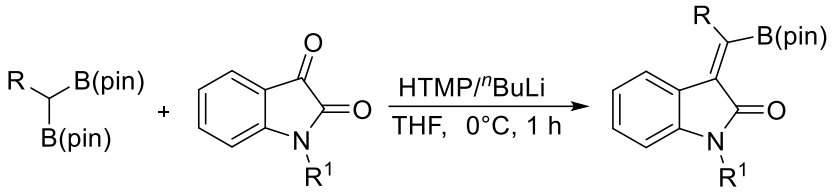
1. General information

General Methods: All the solvents were distilled prior to use. Dry solvents were prepared according to the standard procedures. All other reagents were used as received from either Aldrich or Lancaster chemical companies. Reactions requiring an inert atmosphere were carried out under an argon atmosphere. Infrared (IR) spectra were recorded on a JASCO 4100 FT-IR spectrometer. 1H NMR spectra were measured on Bruker AVANCE 400 MHz and 500 MHz spectrometers. Chemical shifts were reported in ppm relative to solvent signals. 13C NMR spectra were recorded on Bruker 100 MHz and 125 MHz spectrometers with complete proton decoupling. Chemical shifts were reported in ppm from the residual solvent as an internal standard. The high-resolution mass spectra (HRMS) were performed on Micromass QTOF micro mass spectrometer equipped with a Harvard apparatus syringe pump. X-ray crystallographic data were recorded using Bruker-AXS Kappa CCD-Diffractometer with graphite monochromator MoKα radiation (λ=0.7107 A). The structures were solved by direct methods (SHELXS-97) and refined by full-matrix least squares techniques against F2 (SHELXL-97). Hydrogen atoms were inserted from geometry consideration using the HFIX option of the program. For thin layer chromatography (TLC) analysis throughout this work, *E*-merck precoated TLC plates (silica gel 60 F254 grade, 0.25 mm) were used. Acme (India) silica gel (100-200 mesh) was used for column chromatography. Here all the geminal bis-pinacol-boronate esters have been synthesized by following ref [1] and all the keto-ester, keto-amide[2], and *N*-alkyl isatin were synthesized using literature reports.[3]

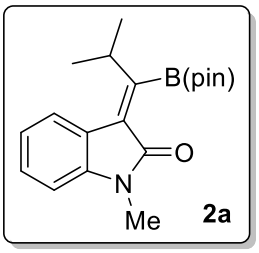
2. Experimental procedures:

2a. General procedure for the Boron-Wittig reaction with N-alkyl-oxindole:



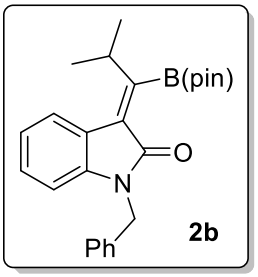
To a flame-dried reaction tube, 2,2,6,6-Tetramethylpiperidine (HTMP) (0.24 mmol, 1.2 equiv) in dry THF (1 mL) at -78 ^{o}C was added n-BuLi (l.2 equiv) drop-wise for 5 min under argon atmosphere. The reaction mixture was stirred for 30 min at the same temperature. The reaction was then cooled to 0 ^{o}C and stirred for another 30 min. Geminal-bis boronates (0.24 mmol, 1.2 equiv) dissolved in dry THF (1 ml) were added to the reaction mixture and stirred for 5 min. Then the reaction mixture was transferred to a solution of N-alkyl-oxindole (0.20 mmol) in THF at 0 ^{o}C and further stirred for 1h (for aromatic Geminal-bis boronates the reaction was stirred for 10 min). After completion of the reaction 2ml water was added and the product was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4 and concentrated in a vacuum to afford the crude product. This crude material was further purified by flash column chromatography using silica gel.

(*E*)-1-methyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2a):



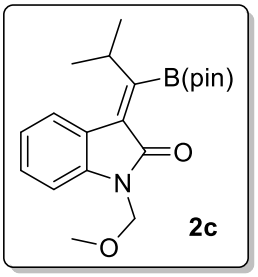
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid compound, yield (44 mg) 67%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.7 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.78 (d, *J* = 8.2 Hz, 1H), 3.51 (hept, *J* = 6.8 Hz, 1H), 1.44 (s, 12H), 1.27 (d, *J* = 6.9 Hz, 6H).; ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.07, 144.62, 130.72, 128.63, 124.12, 122.29, 122.09, 108.11, 84.25, 31.05, 26.16, 25.62, 21.52. HRMS (ESI): m/z calculated for $[C_{19}H_{26}BNO_3+ H]^+$ 328.2079, found: 328.2089. ^{11}B NMR (160 MHz, $CDCl_3$) δ 31.84.

(*E*)-1-benzyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2b):



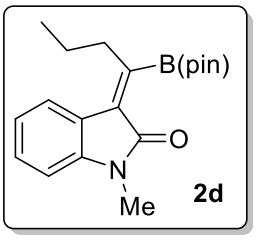
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (15% EtOAc/hexane), yellow gummy compound, yield (41 mg) 52%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.58 (d, *J* = 7.08 Hz, 1H), 7.31-7.21 (m, 5H), 7.11-7.07 (m, 1H), 6.99-6.94 (m, 1H), 6.63-6.61 (m, 1H), 4.91(s, 2H), 3.54 (h, *J* = 6.9, 5.8 Hz, 1H), 1.45 (s, 12H), 1.30-1.28 (m, 6H), ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.02, 143.71, 136.16, 130.64, 128.74, 128.58, 127.46, 127.32, 124.17, 122.36, 122.14, 109.33, 84.35, 43.73, 31.11, 25.62, 21.55. HRMS (ESI): m/z calculated for $[C_{25}H_{30}BNO_3 + H]^+$ 404.2392, found 404.2395.

(*E*)-1-(methoxymethyl)-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2c):



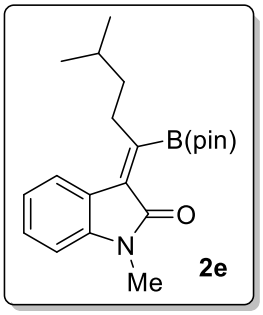
Synthesized using general procedure **2a**, purified by silica gel column chromatography (20% EtOAc/hexane), yellow gummy compound, yield (48 mg) 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.62-7.59 (m, 1H), 7.27-7.22 (m, 1H), 7.07-7.01 (m, 2H), 5.13 (s, 2H), 3.57-3.48 (m, 1H), 3.31 (s, 3H), 1.44 (s, 12H), 1.29-1.27 (m, 6H), ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.19, 142.83, 130.40, 128.75, 124.15, 122.60, 122.03, 109.60, 84.25, 71.34, 56.16, 31.00, 25.48, 21.37. HRMS (ESI): m/z calculated for $[C_{20}H_{28}BNO_4 + H]^+$ 358.2184, found 358.2163.

(*E*)-1-methyl-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butylidene)indolin-2-one (2d):



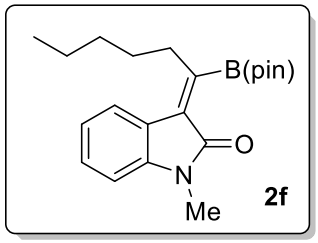
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (46 mg) 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.54 (d, *J* = 7.48 Hz, 1H), 7.26-7.22 (m, 1H), 7.01 (t, *J* = 7.44 Hz, 1H), 6.79 (d, *J* = 7.48 Hz, 1H), 3.19 (s, 3H), 2.73-2.68 (m, 2H), 1.75-1.65 (m, 2H) 1.41 (s, 12H), 1.06 (t, *J* = 6.4 Hz, 3H), ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.91, 144.59, 132.08, 128.71, 123.84, 122.52, 122.16, 108.18, 84.17, 34.33, 26.20, 25.14, 21.48, 14.77. HRMS (ESI): m/z calculated for $[C_{19}H_{26}BNO_3 + H]^+$ 328.2079, found: 328.2085.

(*E*)-1-methyl-3-(4-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentylidene)indolin-2-one (2e):



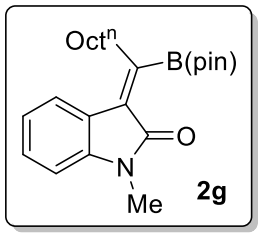
Synthesized using general procedure **2a**, purified by silica gel column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (50 mg) 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.54 (d, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.64, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.79 (d, *J* = 7.8 Hz, 1 H), 3.20 (s, 3H), 2.74-2.70 (m, 2H), 1.77-1.67 (m, 1H), 1.57-1.49 (m, 1H), 1.42(s, 12H), 0.97 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.88, 144.52, 131.68, 128.64, 123.65, 122.43, 122.15, 108.16, 84.14, 36.54, 30.07, 28.59, 26.17, 25.08, 22.51. HRMS (ESI): m/z calculated for $[C_{21}H_{30}BNO_3 + H]^+$ 356.2392, found: 356.2390.

(*E*)-1-methyl-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexylidene)indolin-2-one (2f):



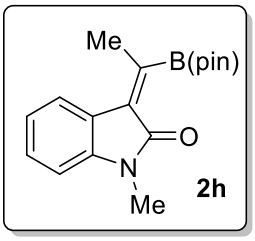
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (49 mg) 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.54 (d, *J* = 7.56 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.01(t, *J* = 7.52 Hz, 1H), 6.79 (d, *J* = 7.84 Hz, 1H), 3.20 (s, 3H), 2.72 (t, *J* = 8.08 Hz, 1H), 1.69-1.64 (m, 2H), 1.47-1.45 (m, 1H), 1.42 (s, 12H), 1.40-1.32 (m, 3H), 0.91 (t, *J* = 7.24 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.94, 144.65, 131.93, 128.68, 123.81, 122.61, 122.16, 108.16, 84.17, 32.37, 32.30, 27.68, 26.18, 25.16, 22.63, 14.08. HRMS (ESI): m/z calculated for $[C_{21}H_{30}BNO_3 + H]^+$ 356.2392, found: 356.2393.

(*E*)-1-methyl-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonylidene)indolin-2-one (2g):



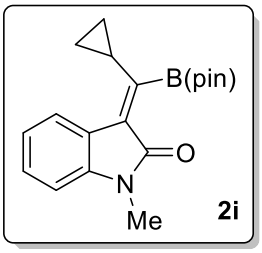
Synthesized using general procedure **2a**, purified by silica gel column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (56 mg) 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.54 (d, *J* = 7.56 Hz, 1H), 7.26-7.22 (m, 1H), 7.01 (t, *J* = 7.56 Hz, 1H), 6.79 (d, *J* = 7.76 Hz, 1H), 3.20 (s, 3H), 2.72 (t, *J* = 7.72 Hz, 2H), 1.69-1.63 (m, 2H), 1.42 (s, 12H), 1.34-1.22(m, 12H), 0.89-0.86 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.90, 144.54, 131.87, 128.66, 123.78, 122.50, 122.15, 108.16, 84.15, 32.31, 31.98, 30.19, 29.51, 29.30, 27.95, 26.18, 25.13, 22.80, 14.24. HRMS (ESI): m/z calculated for $[C_{24}H_{36}BNO_3 + H]^+$ 398.2861, found: 398.2877. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.99.

(*E*)-1-methyl-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)indolin-2-one (2h):



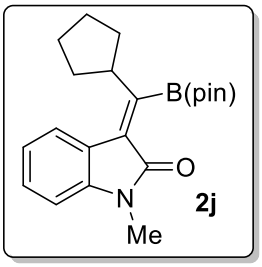
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (38 mg) 63%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.57 (d, *J* = 7.56 Hz, 1H), 7.27-7.26 (m, 1H), 7.03 (t, *J* = 7.56 Hz, 1H), 6.80 (d, *J* = 7.84, 1H), 3.21 (s, 3H), 2.32 (s, 3H), 1.42 (m, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.74, 144.63, 132.61, 128.76, 123.97, 122.95, 122.18, 108.15, 84.22, 26.18, 24.99, 17.85. HRMS (ESI): m/z calculated for $[C_{17}H_{22}BNO_3+ H]^+$ 300.1766, found: 300.1768.

(*E*)-3-(cyclopropyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methylene)-1-methylindolin-2-one (2i):



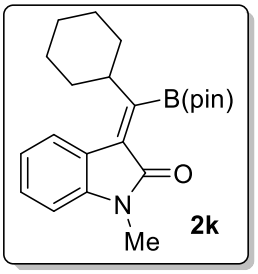
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (48 mg) 74%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.72 (d, *J* = 7.0 Hz, 1H), 7.27-7.22 (m, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.80 (d, *J* = 7.72 Hz, 1H), 3.21 (s, 1H), 2.42-2.39 (m, 1H), 1.41 (s, 12H), 1.12-1.04 (m, 4H), ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.76, 144.17, 131.76, 128.30, 123.38, 122.96, 121.98, 108.07, 84.40, 26.18, 25.49, 15.45, 8.91. HRMS (ESI): m/z calculated for $[C_{19}H_{24}BNO_3+ H]^+$ 326.1922, found: 326.1922. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.84.

(*E*)-3-(cyclopentyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methylene)-1-methylindolin-2-one (2j):



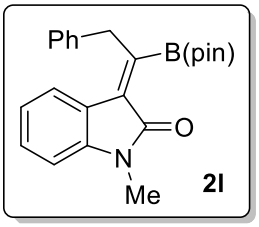
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (46 mg) 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.58 (d, *J* = 7.48 Hz, 1H), 7.24-7.20 (m, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.78 (d, *J* = 7.76 Hz, 1H), 3.59-3.51 (m, 1H), 3.19 (s, 3H), 2.06-1.98 (m, 2H), 1.74-1.64 (m, 6H) 1.43 (s, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.90, 144.46, 131.50, 128.51, 123.86, 122.58, 122.04, 108.07, 84.21, 42.89, 31.84, 26.13, 25.81, 25.61. HRMS (ESI): m/z calculated for $[C_{21}H_{28}BNO_3+ H]^+$ 354.2235, found: 354.2235. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.80.

(*E*)-3-(cyclohexyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methylene)-1-methylindolin-2-one (2k):



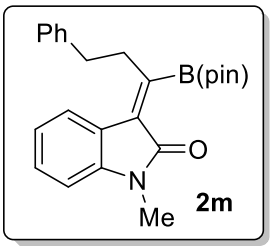
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (45 mg) 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.52 (d, *J* = 7.64 Hz, 1H), 7.20 (d, *J* = 7.96 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.78 (d, *J* = 7.84 Hz, 1H), 3.19 (s, 3H), 3.12-3.08 (m, 1H), 1.91-1.84 (m, 4H), 1.77 (d, *J* = 12.8Hz, 1H), 1.44 (s, 12H), 1.29-1.24 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.08, 144.57, 130.95, 128.60, 123.97, 122.33, 122.12, 108.12, 84.23, 41.73, 31.49, 26.52, 26.16, 26.13, 25.63. HRMS (ESI): m/z calculated for $[C_{22}H_{30}BNO_3+ H]^+$ 368.2392, found: 368.2390.

(E)-1-methyl-3-(2-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)indolin-2-one (2l):



Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (52 mg) 70%. ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.58 (d, *J* = 7.55 Hz, 1H), 7.32-7.27 (m, 4H), 7.24-7.19 (m, 2H), 6.98 (td, *J* = 7.65 Hz, *J* = 1.05 Hz, 1H), 6.81 (d, *J* = 7.85 Hz, 1H), 4.13 (s, 2H) 3.22 (s, 3H), 1.18 (s, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.72, 144.86, 137.66, 132.97, 129.70, 129.17, 128.59, 126.80, 124.02, 122.54, 122.26, 108.24, 84.14, 38.32, 26.22, 25.03. HRMS (ESI): m/z calculated for $[C_{23}H_{26}BNO_3+ H]^+$ 376.2079, found: 376.2077.

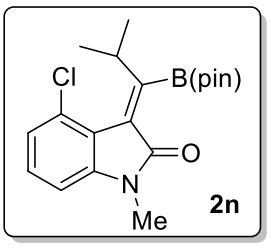
(E)-1-methyl-3-(3-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2 yl)propylidene)indolin-2-one (2m):



Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (57 mg) 73%. ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.51(d, *J* = 7.35 Hz, 1H), 7.33-7.26 (m, 4H), 7.23-7.18 (m, 2H), 6.98 (td, *J* = 7.65 Hz, *J* = 1.05 Hz, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 3.19 (s, 3H), 3.04-3.00 (m, 2H), 2.97-2.93 (m, 2H), 1.44 (s, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.81, 144.62, 141.49, 132.33, 128.88, 128.67, 128.45, 128.33, 126.30, 123.67, 122.20,

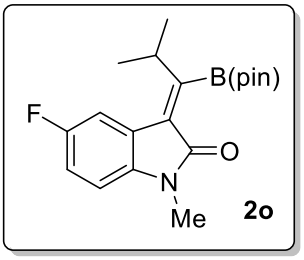
108.19, 84.24, 34.29, 33.93, 26.14, 25.12. HRMS (ESI): m/z calculated for $[C_{24}H_{28}BNO_3 + H]^+$ 390.2235, found: 390.2245. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.53.

(*E*)-4-chloro-1-methyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2n):



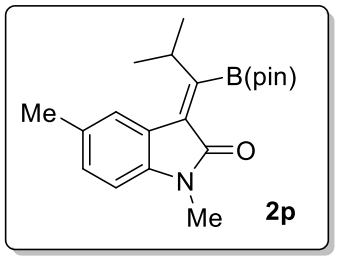
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid compound, yield (42 mg) 58%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.15 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.2 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 1H), 4.15 – 4.07 (m, 1H), 3.19 (s, 1H), 1.43 (s, 7H), 1.24 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.86, 146.82, 129.63, 128.93, 128.84, 124.94, 121.02, 106.69, 83.93, 33.16, 26.65, 25.84, 22.22. HRMS (ESI): m/z calculated for $[C_{19}H_{25}BClNO_3 + H]^+$ 362.1689, found: 362.1694.

(*E*)-5-fluoro-1-methyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2o):



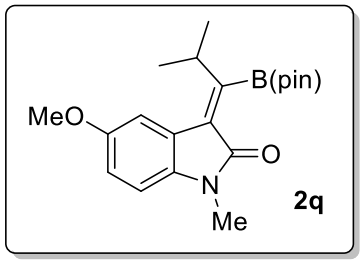
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid compound, yield (49 mg) 71%. ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.33-7.29 (m, 1H), 6.98-6.92 (m, 1H), 6.71-6.67 (m, 1H) 3.46-3.38 (m, 1H), 3.19-3.17 (m, 3H), 1.45-1.44 (m, 12H), 1.29-1.26 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.90, 160.12, 157.76, 140.62, 130.34, 123.05 (d, *J* = 34.48 Hz), 114.65 (d, *J* = 94.8Hz), 111.95 (d, *J* = 102.96), 108.33 (d, *J* = 33.38 Hz) 84.42, 31.13, 26.29, 25.60, 21.46. HRMS (ESI): m/z calculated for $[C_{19}H_{25}BFNO_3 + H]^+$ 346.1984, found: 346.1990.

(*E*)-1,5-dimethyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2p):



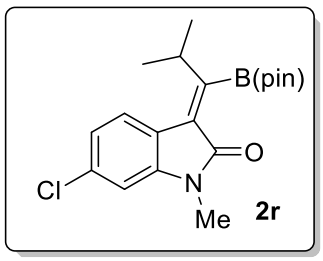
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid compound, yield (42 mg) 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.03 (d, *J* = 7.9 Hz, 1H), 6.66 (d, *J* = 7.8 Hz, 1H), 3.51 (hept, *J* = 7.0 Hz, 1H), 3.16 (s, 3H), 2.34 (s, 3H), 1.44 (s, 12H), 1.27 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.10, 142.39, 131.30, 130.86, 128.92, 124.94, 122.29, 107.79, 84.18, 30.97, 26.17, 25.60, 21.53, 21.44. HRMS (ESI): m/z calculated for $[C_{20}H_{28}BNO_3 + H]^+$ 342.2235, found: 342.2239. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.69.

(*E*)-5-methoxy-1-methyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2q):



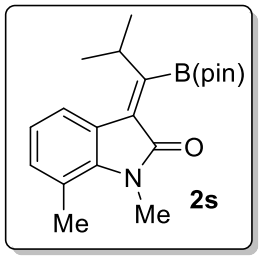
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid, yield (48 mg) 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.19 (s, 1H), 6.78-6.76 (m, 1H), 6.67 (d, *J* = 8.08 Hz, 1H), 3.79 (s, 3H), 3.45 ((h, *J* = 6.9 Hz, 1H), 3.16 (s, 3H), 1.4 (s, 12H) 1.26 (d, *J* = 6.88 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ ppm 168.94, 155.47, 138.59, 130.94, 123.19, 112.35, 112.21, 108.00, 84.25, 56.02, 31.00, 26.23, 25.61, 21.49. HRMS (ESI): m/z calculated for $[C_{20}H_{28}BNO_4 + H]^+$ 358.2184, found: 358.2194.

(*E*)-6-chloro-1-methyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2r):



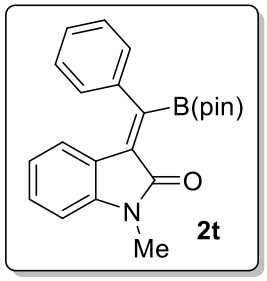
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid, yield (47 mg) 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.47 (d, *J* = 8.12 Hz, 1H) 6.97 (d, *J* = 6.7 Hz, 1H), 6.77 (s, 1H) 3.43 (p, *J* = 7.0 Hz, 1H), 3.17 (s, 3H), 1.43 (s, 12H), 1.25 (d, *J* = 8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.03, 145.65, 134.42, 129.75, 124.85, 121.94, 120.67, 108.85, 84.40, 31.20, 26.27, 25.59, 21.45. HRMS (ESI): m/z calculated for $[C_{19}H_{25}BClNO_3 + H]^+$ 362.1689, found: 362.1694. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.64.

(*E*)-1,7-dimethyl-3-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)indolin-2-one (2s):



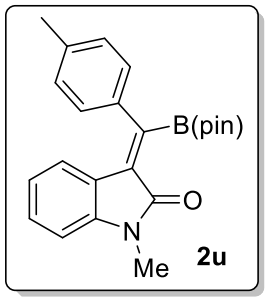
Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow solid, yield (46 mg) 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.44 (d, *J* = 7.52 Hz, 1H) 6.96 (d, *J* = 7.72 Hz, 1H), 6.90-6.86 (m, 1H) 3.52-3.45 (m, 4H), 2.54 (s, 3H), 1.43 (s, 12H), 1.26-1.24 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.95, 142.49, 132.49, 130.44, 122.89, 122.22, 121.98, 119.71, 84.14, 30.78, 29.81, 25.62, 21.47, 19.41. HRMS (ESI): m/z calculated for $[C_{20}H_{28}BNO_3 + H]^+$ 342.2235, found: 342.2243.

(*E*)-1-methyl-3-(phenyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methylene)indolin-2-one (2t):



Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (42 mg) 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.49-7.36 (m, 5H), 7.18 (t, *J* = 7.72 Hz, 1H) 6.98 (d, *J* = 7.76 Hz, 1H), 6.78-6.72 (m, 2H), 3.24 (s, 3H), 1.37 (s, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.24, 145.02, 138.12, 132.42, 129.58, 128.86, 128.40, 127.59, 123.32, 121.95, 121.55, 108.23, 84.42, 26.31, 24.94. HRMS (ESI): m/z calculated for $[C_{22}H_{24}BNO_3 + H]^+$ 362.1922, found: 362.1924. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.74.

(*E*)-1-methyl-3-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)(p-tolyl)methylene)indolin-2-one (2u):



Synthesized using general procedure **2a**, purified by silica gel flash column chromatography (25% EtOAc/hexane), yellow gummy compound, yield (44 mg) 59%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.39-7.36 (m, 2H), 7.24-7.16 (m, 3H) 7.12-7.08 (m, 1H), 6.77-6.73 (m, 2H), 3.24 (s, 3H), 2.41 (s, 3H), 1.37 (s, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.34, 144.94, 138.43, 135.00, 131.97, 129.53, 129.41, 127.69, 123.24, 121.87, 121.67, 108.18, 84.34, 26.29, 24.97, 21.55. HRMS (ESI): m/z calculated for $[C_{23}H_{26}BNO_3 + H]^+$ 376.2079, found: 376.2081. ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.91.

2b. Optimization of Boron-Wittig reaction between α-boryl cabanion and 1,2-diketones and α-keto-ester/amide:

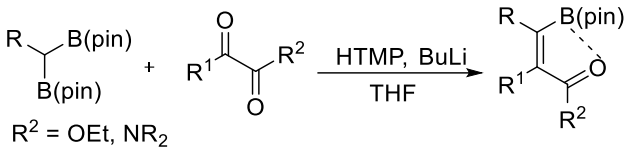
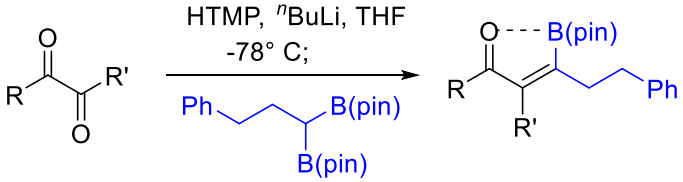


Table 1. Optimization of Reaction Condition[a]



Entry	R	R'	Reaction condition	Yield(%)[b]
1	Ph	Ph	A	nd[d]
2	Ph	Ph	C	nd[d]
3[c]	Ph	Ph	C	nd[d]
4	Ph	Ph	B	nd[d]
5	4-OMeC$_6$H$_4$	OEt	A	60
6	4-OMeC$_6$H$_4$	OEt	B	72
7[c]	4-OMeC$_6$H$_4$	OEt	B	55
8	4-OMeC$_6$H$_4$	OEt	C	45
9	Ph	NR_2	A	65
10	Ph	NR_2	B	69
11	Ph	NR_2	C	50

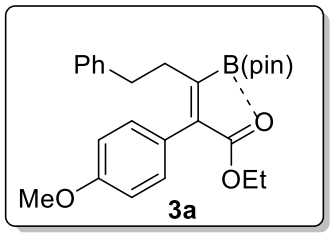
[a]Condition: The LTMP solution of geminal bis boronate was generated in situ using HTMP/^{n}BuLi at 0 °C, which was slowly added to the THF solution of 1,2-diketo compounds at -78 °C, HTMP (1.2 equiv.), ^{n}BuLi (1.2 equiv.); geminal-B(pin) (1.2 equiv.) at 0 °C then added Di-keto (1 equiv.) and stirred at below condition; [b] Isolated yield; [c] Di-keto (1 equiv.), HTMP (2 equiv.); ^{n}BuLi (2 equiv.); geminal-B(pin) (2 equiv.); **Condition A** : the lithiated geminal B(pin) was added to the keto at -78 °C then stirred at RT for 1 h; **Condition B**: the lithiated geminal B(pin) was added to the keto at -78 °C then stirred at 0 °C for 1h; C: added at -78 °C and stirred for 1h at -78 °C; [d]multiple inseparable spots.

2b.1. General procedure for the Boron-Wittig reaction with α-keto-ester/amide:

To a flame-dried reaction tube, 2,2,6,6-Tetramethylpiperidine (HTMP) (0.24 mmol, 1.2 equiv) in dry THF (1 mL) at -78 °C was added n-BuLi (l.2 equiv) drop-wise for 5 min under argon

atmosphere. The reaction mixture was stirred for 30 min at the same temperature. The reaction was then cooled to 0 °C and stirred for another 30 min. Geminal-bis boronates (0.24 mmol, 1.2 equiv) were dissolved in dry THF (1 ml) added to the reaction mixture and stirred for 5 min. Then the reaction mixture was transferred to a solution of α-keto ester (0.2 mmol) in THF at -78 °C and further stirred for 1h at 0 °C. In the case of keto-amide, the reaction is stirred for 2h at 0 °C. After completion of the reaction 1ml water was added and the product was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4 and concentrated in a vacuum to afford the crude product. This crude material was further purified by flash column chromatography. We are unable to detect the minor diastereoisomer from the crude reaction mixture.

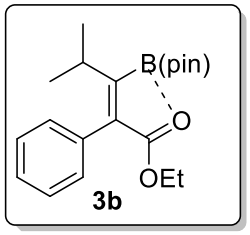
Ethyl (*E*)-2-(4-methoxyphenyl)-5-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-2-enoate (3a):



3a

Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), colorless oil, yield (63 mg) 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.20 (m, 2H), 7.14 (td, *J* = 5.3, 4.9, 2.5 Hz, 1H), 7.06 – 7.04 (m, 2H), 6.91-6.81 (m, 4H), 4.23 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 3H), 2.78 – 2.73 (m, 2H), 2.45 – 2.41 (m, 2H), 1.44 (s, 12H), 1.19 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.00, 158.90, 141.90, 137.99, 130.71, 128.51, 128.45, 127.49, 125.99, 113.52, 83.57, 62.28, 55.31, 34.65, 30.73, 25.27, 14.27. HRMS (ESI): m/z calculated for $[C_{26}H_{33}BO_5$+ H]$^+$ 437.2494 found: 437.2497. ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.33.

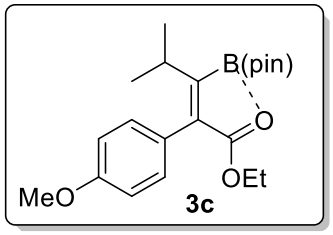
Ethyl (E)-4-methyl-2-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-2-enoate (3b):



3b

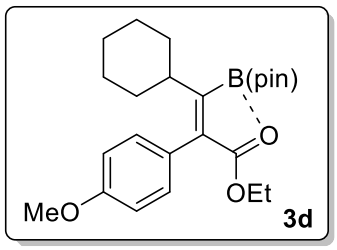
Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), colorless oil, yield (47 mg) 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.29(m, 3H), 7.13-7.09 (m, 2H), 2.56-2.49 (m 1H), 1.41 (s, 12H), 1.16-1.12(m,3H), 1.05-1.03(m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.96, 136.61, 136.29, 129.53, 127.97, 127.15, 83.72, 77.48, 76.85, 61.77, 31.82, 25.54, 21.71, 14.23. HRMS (ESI): m/z calculated for $[C_{20}H_{29}BO_4$+ H]$^+$ 345.2232 found: 345.2249.

Ethyl (*E*)-2-(4-methoxyphenyl)-4-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-2-enoate (3c):



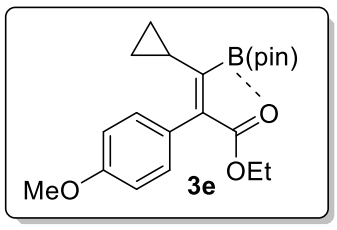
Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), colorless oil, yield (55 mg) 74%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (d, *J* = 8.5 Hz, 2H), 6.87 (d, *J* = 8.5 Hz, 2H), 4.19 – 4.12 (m, 2H), 3.81 (s, 3H), 2.57 (p, *J* = 7.0 Hz, 1H), 1.40 (s, 12H), 1.15 (t, *J* = 7.1 Hz, 3H), 1.03 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.31, 158.76, 136.27, 130.70, 128.54, 113.47, 83.66, 61.75, 55.26, 31.81, 25.57, 21.73, 14.27. HRMS (ESI): m/z calculated for $[C_{21}H_{231}BO_5 + H]^+$ 375.2337 found: 375.2367.

Ethyl (*E*)-3-cyclohexyl-2-(4-methoxyphenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate (3d):



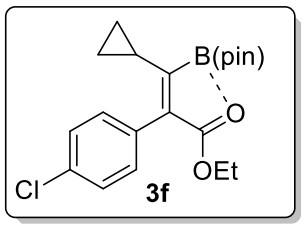
Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), colorless oil, yield (65 mg) 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (d, *J* = 7.5 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 2H), 4.16 (q, *J* = 7.3 Hz, 2H), 3.82 (s, 3H), 2.23 (tt, *J* = 12.1, 3.5 Hz, 1H), 1.67-1.64 (m, 2H), 1.57-1.54 (m, 3H), 1.41 (s, 12H), 1.27-1.21(m, 2H), 1.15 (t, *J* = 7.1 Hz, 3H), 1.06 – 1.01 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.50, 158.66, 136.50, 130.70, 128.49, 113.41, 83.61, 61.82, 55.27, 42.47, 31.51, 26.18, 26.09, 25.60, 14.30. HRMS (ESI): m/z calculated for $[C_{24}H_{35}BO_5 + H]^+$ 415.2650 found: 415.2676.

Ethyl (*E*)-3-cyclopropyl-2-(4-methoxyphenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate (3e):



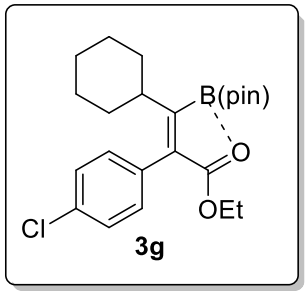
Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), colorless oilly compound, yield (53 mg) 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.64 Hz, 2H), 6.89 (d, *J* = 8.64 Hz, 2H), 4.22 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 1H), 1.66 – 1.59 (m, 1H), 1.36 (s, 12H), 1.19 (t, *J* = 7.08 Hz, 3H), 1.07 – 1.03 (m, 2H), 0.79 – 0.74 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.30, 158.79, 135.57, 131.47, 127.97, 113.50, 83.48, 62.22, 55.30, 25.70, 16.15, 14.31, 8.55. HRMS (ESI): m/z calculated for $[C_{21}H_{29}BO_5 + H]^+$ 373.2181. found: 373.2185.

Ethyl-(*E*)-2-(4-chlorophenyl)-3-cyclopropyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate (3f):



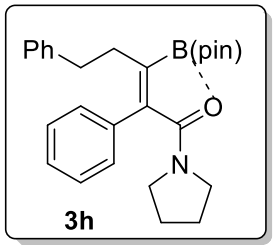
Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), white solid, yield (56 mg) 75%. ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.31 (d, *J* = 8.25 Hz, 2H), 7.17 (d, *J* = 8.15 Hz, 2H), 4.20 (q, *J* = 7.1 Hz, 2H) 1.53 (tt, *J* = 8.5Hz, 4.8 Hz, 1H), 1.36 (s, 12H), 1.18 (t, *J* = 7.1 Hz, 3H), 1.04 (dt, *J* = 6.7Hz, 3.4 Hz, 2H) 0.79-0.75 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.23, 134.96, 134.35, 133.17, 131.69, 128.30, 83.74, 62.17, 25.64, 16.15, 14.25, 8.68. HRMS (ESI): m/z calculated for $[C_{20}H_{26}BClO_4 + H]^+$ 377.1685 found: 377.1689. ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.42.

Ethyl (*E*)-2-(4-chlorophenyl)-3-cyclohexyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate (3g):



Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (5% EtOAc/hexane), white solid, yield (60 mg) 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dt, *J* = 6.6, 2.3 Hz, 2H), 7.04 (d, *J* = 8.5 Hz, 2H), 4.15 (q, *J* = 6.9 Hz, 1H), 2.19-2.11(m, 1H), 1.68-1.53(m, 7H), 1.42(s, 12H),1.14 (t, *J* = 7.1 Hz, 3H), 1.07-0.97 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.57, 135.79, 134.80, 133.10, 130.92, 128.28, 83.81, 61.85, 42.60, 31.44, 30.68, 25.98, 25.56, 14.23. HRMS (ESI): m/z calculated for $[C_{23}H_{32}BClO_4 + H]^+$ 419.2155 found: 419.2160. ^{11}B NMR (160 MHz, $CDCl_3$) δ 12.04.

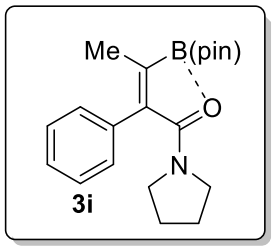
(*E*)-2,5-diphenyl-1-(pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-2-en-1-one (3h):



Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (35% EtOAc/hexane), white solid compound, yield (58 mg) 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.28-7.23 (m, 3H), 7.19-7.09 (m, 3H), 7.05-6.99 (m, 2H), 6.87-6.82 (m, 2H), 3.75-3.71 (m, 2H), 2.84-2.74 (m, 4H) 2.43-2.38 (m, 2H), 1.75-1.63 (m, 4H), 1.33 (s, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.77, 142.69, 135.45, 133.88, 129.75, 128.64,

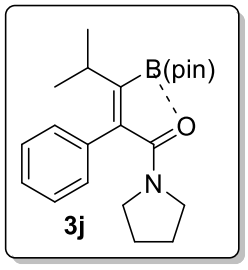
128.57, 128.26, 127.72, 125.60, 80.24, 49.59, 48.86, 34.40, 32.59, 26.37, 25.75, 23.42. HRMS (ESI): m/z calculated for $[C_{27}H_{34}BNO_3 + H]^+$ 432.2705, found: 432.2711. ^{11}B NMR (160 MHz, $CDCl_3$) δ 11.99.

(*E*)-2-phenyl-1-(pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)but-2-en-1-one (3i):



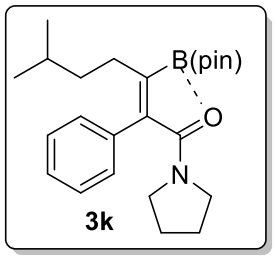
Synthesized using general procedure **2b.1**, purified by silica gel column chromatography (35% EtOAc/hexane), colorless liquid compound, yield (46 mg) 67%. ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.35-7.29 (m, 3H), 7.08-7.06 (m, 2H), 3.75 (t, *J* = 6.76Hz, 2H), 2.84 (t, *J* = 6.76Hz, 2H), 1.78 (s, 3H), 1.76-1.67 (m, 4H), 1.26 (s, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.97, 135.81, 133.13, 129.84, 128.69, 127.71, 80.07, 49.51, 49.06, 26.40, 25.56, 23.46, 15.91. HRMS (ESI): m/z calculated for $[C_{20}H_{28}BNO_3 + H]^+$ 342.2235, found: 342.2245. . ^{11}B NMR (160 MHz, $CDCl_3$) δ 12.45.

(*E*)-4-methyl-2-phenyl-1-(pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-2-en-1-one (3j):



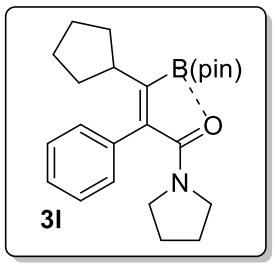
Synthesized using general procedure **2b.1**, purified by silica gel column chromatography (35% EtOAc/hexane), white solid compound, yield (51 mg) 69%. ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.35-7.32 (m, 3H), 7.12-7.08 (m, 2H), 3.72-3.68 (m, 2H), 2.78-2.74 (m, 2H), 2.55-2.49 (m, 1H), 1.74-1.67 (m, 4H), 1.31(s, 12H), 1.11-1.08 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.53, 136.52, 132.20, 130.04, 128.62, 127.73, 80.27, 49.54, 48.57, 31.28, 26.50, 26.35, 24.97, 23.38, 21.25. HRMS (ESI): m/z calculated for $[C_{22}H_{32}BNO_3 + H]^+$ 370.2548, found: 370.2533.

(*E*)-6-methyl-2-phenyl-1-(pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hept-2-en-1-one (3k):



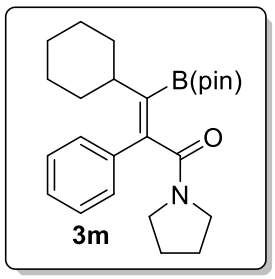
Synthesized using general procedure **2b.1**, purified by silica gel flash column chromatography (35% EtOAc/hexane), white solid compound, yield (62 mg) 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.35-7.29 (m, 3H), 7.09-7.07 (m, 2H), 3.73 (t, *J* = 7.16Hz, 2H), 2.81 (t, *J* = 6.8Hz, 2H), 2.11 (t, *J* = 8.52 Hz, 2H), 1.79-1.71(m, 4H), 1.43-1.34 (m, 3H), 1.27 (s, 12H), 0.73 (d, *J* = 6.2 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.01, 135.88, 132.99, 129.92, 128.60, 127.71, 80.08, 49.54, 48.91, 37.36, 28.74, 28.37, 26.45, 25.70, 23.46, 22.48. HRMS (ESI): m/z calculated for $[C_{24}H_{36}BNO_3+ H]^+$ 398.2861, found: 398.2870. ^{11}B NMR (160 MHz, $CDCl_3$) δ 12.16.

(*E*)-3-cyclopentyl-2-phenyl-1-(pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)prop-2-en-1-one (3l):



Synthesized using general procedure **2b.1**, purified by silica gel column chromatography (35% EtOAc/hexane), white solid compound, yield (56 mg) 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.34-7.29 (m, 3H), 7.10-7.08 (m, 2H), 3.68 (t, *J* =6.84 Hz, 2H), 2.75 (t, *J* = 6.88Hz, 2H), 2.49-2.43 (m, 1H), 2.09-2.04 (m, 2H), 1.76-1.66 (m, 6H), 1.55-1.38 (m, 4H), 1.27 (s, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.37, 136.63, 133.35, 130.17, 128.62, 127.69, 80.30, 49.46, 48.60, 43.61, 31.46, 26.53, 26.48, 26.18, 23.42. HRMS (ESI): m/z calculated for $[C_{24}H_{34}BNO_3+ H]^+$ 396.2705, found: 396.2713.

(*E*)-3-cyclohexyl-2-phenyl-1-(pyrrolidin-1-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)prop-2-en-1-one (3m):

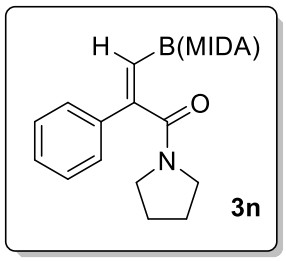


Synthesized using general procedure **2b.1**, purified by silica gel column chromatography (35% EtOAc/hexane), white solid compound, yield (57 mg) 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.33-7.30 (m, 3H), 7.09-7.08 (m, 2H), 3.69 (t, *J* =6.95 Hz, 2H), 2.73 (t, *J* = 6.9Hz, 2H), 2.23-2.16 (m, 1H), 1.75-1.61(m, 10H), 1.56-1.49 (m, 4H), 1.31 (s, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.81, 136.73, 132.40, 130.17, 128.61, 127.73, 80.29, 49.58, 48.56, 42.30, 30.52, 29.85, 26.48, 26.43, 26.23, 23.41. HRMS (ESI): m/z calculated for $[C_{25}H_{36}BNO_3+ H]^+$ 410.2861, found: 410.2871.

2b.2. Synthesis of tri-substituted MIDA-based organoboronates

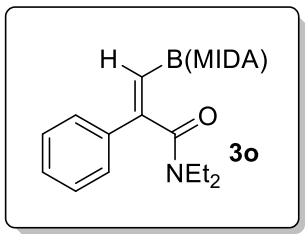
To a flame-dried reaction tube, 2,2,6,6-Tetramethylpiperidine (HTMP) (0.24 mmol, 1.2 equiv) in dry THF (1 mL) at -78 ^{o}C was added n-BuLi (l.2 equiv) drop-wise for 5 min under argon atmosphere. The reaction mixture was stirred for 30 min at the same temperature. The reaction was then cooled to 0 ^{o}C and stirred for another 30 min. Geminal-bis boronates (0.24 mmol, 1.2 equiv) were dissolved in dry THF (1 ml) added to the reaction mixture and stirred for 5 min. After that, a THF solution of keto-amide (0.2mmol) was added and stirred for 2h. Next, the reaction was worked up with EtOAc, and the crude was further dissolved in dry DMSO, MIDA(0.4 mmol, 2 equiv.) was added and degassed. $HC(OMe)_3$ (0.6 mmol, 3 equiv.) was added and stirred for 12 h at 100 ^{o}C.

(*Z*)-4-methyl-8-(3-oxo-2-phenyl-3-(pyrrolidin-1-yl)prop-1-en-1-yl)dihydro-4l4,8l4-[1,3,2]oxazaborolo[2,3-b][1,3,2]oxazaborole-2,6(3H,5H)-dione (3n):



Synthesized using general procedure **2b.2**, purified by silica gel column chromatography (25% EtOAc/hexane), yellow oil, yield (44 mg) 62%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.9 Hz, 2H), 7.37 – 7.29 (m, 3H), 6.01 (s, 1H), 4.15 – 4.07 (m, 1H), 3.81 (d, *J* = 16.5 Hz, 2H), 3.50 (t, *J* = 6.9 Hz, 2H), 3.15 (s, 2H), 3.03 (s, 1H), 1.90-1.78 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.25, 168.00, 152.90, 136.62, 128.98, 128.90, 125.90, 63.18, 48.10, 47.54, 45.49, 25.79, 24.49. HRMS (ESI): m/z calculated for $[C_{18}H_{21}BN_2O_5 + H]^+$ 357.1616, found: 357.1626.

(Z)-*N*,*N*-diethyl-3-(4-methyl-2,6-dioxotetrahydro-2H-4l4,8l4-[1,3,2]oxazaborolo[2,3-b][1,3,2]oxazaborol-8-yl)-2-phenylacrylamide (3o):

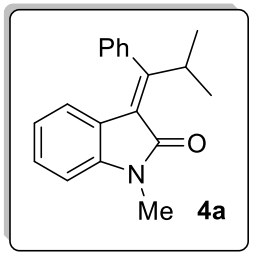


Synthesized using general procedure **2b.2**, purified by silica gel column chromatography (25% EtOAc/hexane), white solid, yield (47mg) 66%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.26 (m, 6H), 5.98 (s, 1H), 3.92-3.65 (m, 4H), 3.22-3.09 (m, 4H), 3.01 (s, 3H), 1.19 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.01, 152.48, 137.60, 128.99, 128.87, 125.74, 63.10, 47.96, 43.20, 39.07, 13.07, 12.71. HRMS (ESI): m/z calculated for $[C_{18}H_{23}BN_2O_5 + H]^+$ 359.1773, found: 359.1792. ^{11}B NMR (160 MHz, $CDCl_3$) δ 10.90.

2c. General procedure for the Zweifel Olefination Reaction

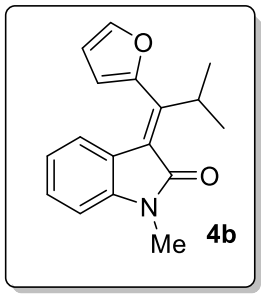
In a flame-dried reaction tube 4a (0.11mmol, 1 equiv.) was taken in dry THF (1ml) and cooled to -78 ^{o}C, Ar-Li (1.2 equiv.) was added dropwise and stirred for 30 mins. Then stirred for another 30 mins at rt and cooled to 0 ^{o}C. NaOMe (0.1ml) and I_2 (0.14 mmol, 1.3 equiv) in MeOH:THF (1:3) were added successively and stirred for 45 mins. After completion of the reaction sodium thiosulphate solution was added, and MeOH was evaporated in the rota and work-up with EtOAc. The organic layer was dried over Na_2SO_4 and concentrated in a vacuum. The crude product was purified by flash column chromatography.

(*E*)-1-methyl-3-(2-methyl-1-phenylpropylidene)indolin-2-one (4a):[4]



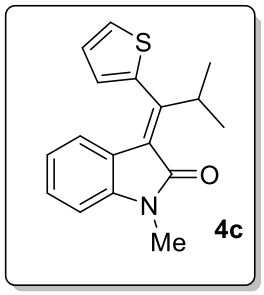
Synthesized using general procedure **2c**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (19 mg) 62%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 3H), 7.14 – 7.08 (m, 3H), 6.72 (d, *J* = 7.7 Hz, 1H), 6.57 (td, *J* = 7.8 Hz, 1.2 Hz, 1H), 5.59 (d, *J* = 7.7 Hz, 1H), 5.01 (hept, *J* = 6.9 Hz, 1H), 3.26 (s, 3H), 1.07 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.89, 164.48, 142.52, 138.29, 128.92, 128.11, 127.93, 127.49, 123.39, 123.23, 122.97, 121.57, 107.41, 28.62, 25.82, 20.89. HRMS (ESI): m/z calculated for $[C_{19}H_{19}NO+ H]^+$ 278.1539, found: 278.1534.

(*E*)-3-(1-(furan-2-yl)-2-methylpropylidene)-1-methylindolin-2-one (4b):



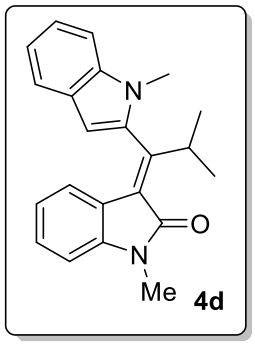
Synthesized using general procedure **2c**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (18 mg) 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.59-7.58 (m, 1H), 7.19-7.15(m, 1H), 6.79-6.73 (m, 2H), 6.57-6.55 (m, 1H), 6.42-6.40 (m, 1H), 5.96-5.93 (m, 1H), 4.95-4.90 (m, 1H), 3.24 (3H, s), 1.11-1.08 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.53, 151.39, 149.84, 142.75, 142.62, 128.85, 126.62, 123.13, 122.62, 121.97, 111.23, 110.06, 107.64, 28.30, 25.90, 20.66. HRMS (ESI): m/z calculated for $[C_{17}H_{17}NO_2+ H]^+$ 268.1332, found: 268.1332.

(*E*)-1-methyl-3-(2-methyl-1-(thiophen-2-yl)propylidene)indolin-2-one (4c):



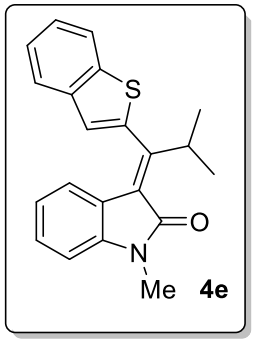
Synthesized using general procedure **2c**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (18 mg) 59%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.48 (d, *J* = 5 Hz, 1H), 7.18-7.13 (m, 2H), 6.85-6.84 (m, 1H), 6.73 (d, *J* = 7.76 Hz, 1H), 6.68 (t, *J* = 7.64Hz, 1H), 5.84 (d, *J* = 7.76 Hz, 1H), 4.97 (h, *J* = 6.7Hz. 1H), 3.24 (3H, s), 1.10 (d, *J* = 6.92, Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.26, 157.26, 142.62, 137.71, 128.70, 127.58, 126.31, 126.14, 126.02, 123.50, 122.83, 121.85, 107.54, 28.55, 25.87, 20.71. HRMS (ESI): m/z calculated for $[C_{17}H_{17}NOS+H]^+$ 284.1104, found: 284.1098.

(*E*)-1-methyl-3-(2-methyl-1-(1-methyl-1H-indol-2-yl)propylidene)indolin-2-one (4d):



Synthesized using general procedure **2c**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (26 mg) 72%. ^{1}H NMR (400 MHz,) δ 7.71 (d, *J* = 8.2 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.75 (d, *J* = 7.7 Hz, 1H), 6.58 (t, *J* = 7.4 Hz, 1H), 6.43 (m, 1H), 5.38 (d, *J* = 7.5 Hz, 1H), 5.07-5.00 (m, 1H), 3.49 (s, 1H), 3.29 (s, 1H), 1.32 (d, *J* = 5.8 Hz, 3H), 0.95 (d, *J* = 6.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.21, 153.35, 142.71, 137.27, 135.44, 128.97, 128.02, 127.18, 122.67, 122.59, 122.40, 121.94, 121.14, 120.18, 109.96, 107.58, 100.28, 30.27, 29.05, 25.90, 21.14, 19.99. HRMS (ESI): m/z calculated for $[C_{22}H_{22}N_2O+H]^+$ 331.1805, found: 331.1809.

(*E*)-3-(1-(benzo[b]thiophen-2-yl)-2-methylpropylidene)-1-methylindolin-2-one (4e):

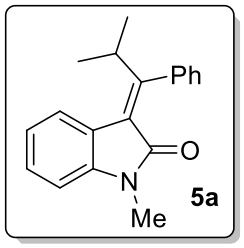


Synthesized using general procedure **2c**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (21 mg) 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.91 (d, *J* = 7.0 Hz, 1H), 7.84 (d, *J* = 8.9 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.14 (t, *J* = 7.7 Hz, 1H), 7.10 (s, 1H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.61 (t, *J* = 7.7 Hz, 1H), 6.12 (d, *J* = 7.8 Hz, 1H), 5.03 (hept, *J* = 6.8 Hz, 1H), 3.26 (s, 3H), 1.15 (d, *J* = 6.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.28, 156.54, 142.73, 140.40, 139.96, 138.40, 128.94, 125.85, 124.68, 124.10, 123.84, 122.71, 122.60, 122.50, 122.04, 107.64, 28.64, 25.95. HRMS (ESI): m/z calculated for $[C_{21}H_{19}NOS+H]^+$ 334.1260, found: 334.1267.

2d. General procedure for the Suzuki-Miyaura Cross-Coupling Reaction

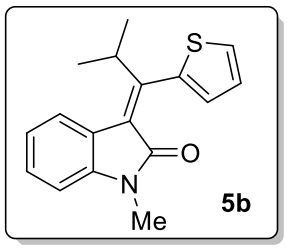
A mixture of 4 (0.083 mmol), aryl iodide (0.099 mmol), NaOH (3M, 0.249 mmol) and [Pd(P-^{t}Bu$_3$)$_2$] (5 mol%) in dioxane (2 ml) were degassed and heated at 90 ^{o}C for 16 h. After cooling the mixture, was filtered through celite and washed with EtOAc. The organic part was concentrated in vaccuo and further purified using flash column chromatography.

(*Z*)-1-methyl-3-(2-methyl-1-phenylpropylidene)indolin-2-one (5a):



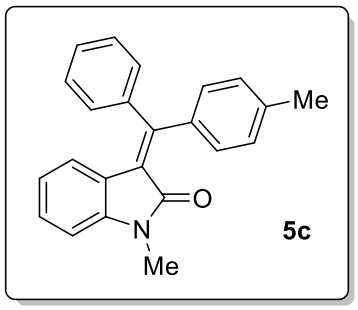
Synthesized using general procedure **2d**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellow solid compound, yield (16 mg) 71%. ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.72(d, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.15Hz, 2H), 7.39-7.36 (m, 1H), 7.31 (t, *J* = 7.7Hz, 1H), 7.11-7.07 (m, 3H), 6.82 (d, *J* = 7.95Hz, 1H), 3.78 (hept., *J* = 6.85Hz, 1H), 3.11 (s, 3H), 1.14 (d, *J* = 6.85Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.92, 162.59, 143.77, 138.56, 128.70, 128.03, 127.18, 127.15, 124.29, 123.17, 122.41, 121.89, 107.92, 32.08, 25.76, 20.43. HRMS (ESI): m/z calculated for $[C_{19}H_{19}NO+ H]^+$ 278.1539, found 278.1553.

(*Z*)-1-methyl-3-(2-methyl-1-(thiophen-2-yl)propylidene)indolin-2-one (5b):



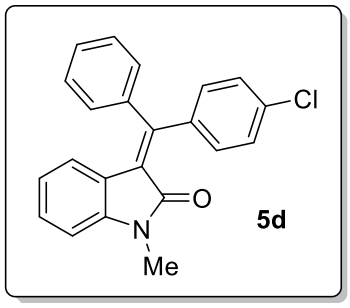
Synthesized using general procedure **2d**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (15 mg) 64%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.7 Hz, 1H), 7.42 (d, *J* = 6.0 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.13-7.11 (m, 1H), 7.07 (t, *J* = 8.15 Hz, 1H), 6.82 – 6.79 (m, 2H), 3.75 (hept, *J* = 6.9 Hz, 1H), 3.13 (s, 3H), 1.18 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.42, 155.02, 143.89, 137.82, 129.24, 126.95, 126.12, 125.73, 125.63, 124.53, 122.13, 121.98, 108.03, 32.19, 25.86, 20.24. HRMS (ESI): m/z calculated for $[C_{17}H_{17}NOS+ H]^+$ 284.1104, found: 284.1105.

(*Z*)-1-methyl-3-(phenyl(p-tolyl)methylene)indolin-2-one (5c):



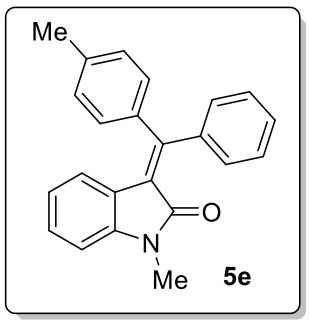
Synthesized using general procedure **2d**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (18 mg) 67%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.44-7.41 (m, 3H), 7.32-7.30 (m, 2H), 7.25-7.23 (m, 3H), 7.17-7.13 (m, 3H), 6.76 (d, *J* = 7.84, 1H), 6.67 (t, *J* = 7.64 Hz, 1H), 6.39 (d, *J* = 7.76 Hz, 1H), 3.21 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.00, 155.05, 143.24, 141.57, 139.54, 137.60, 137.08, 130.38, 129.60, 129.26, 128.98, 128.66, 128.63, 123.91, 123.59, 123.14, 121.42, 107.74, 25.97, 21.64. HRMS (ESI): m/z calculated for $[C_{23}H_{19}NO+ H]^+$ 326.1539, found: 326.1541.

(*Z*)-3-((4-chlorophenyl)(phenyl)methylene)-1-methylindolin-2-one (5d):[5]



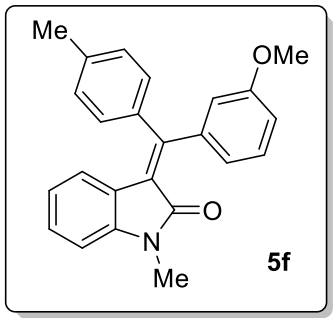
Synthesized using general procedure **2d**, purified by silica gel column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (20 mg) 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.42 (m, 3H), 7.34 – 7.23 (m, 6H), 7.18 (t, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 6.69 (t, *J* = 7.9 Hz, 1H), 6.42 (d, *J* = 8.0 Hz, 1H), 3.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.85, 153.02, 143.45, 140.97, 138.37, 135.33, 131.66, 129.53, 129.50, 129.16, 129.13, 128.23, 124.71, 123.33, 123.16, 121.63, 107.92, 26.00. HRMS (ESI): m/z calculated for $[C_{22}H_{16}ClNO+ H]^+$ 346.0993, found: 346.0998.

(*E*)-1-methyl-3-(phenyl(p-tolyl)methylene)indolin-2-one (5e):



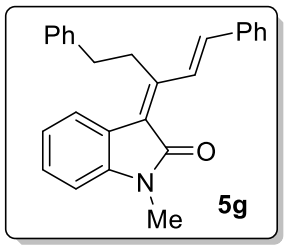
Synthesized using general procedure **2d**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (18 mg) 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.41-7.35 (m, 5H), 7.28-7.25 (m, 4H), 7.22-7.19 (m, 1H), 6.80 (d, *J* = 7.68 Hz, 1H), 6.75 (t, *J* = 7.44 Hz, 1H), 6.61 (d, *J* = 7.60 Hz, 1H), 3.24 (s, 3H), 2.46 (3H, s). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.04, 155.07, 143.32, 140.37, 139.54, 138.45, 130.21, 129.67, 129.65, 129.15, 128.69, 127.89, 123.95, 123.53, 123.14, 121.42, 107.76, 25.96, 21.61. HRMS (ESI): m/z calculated for $[C_{23}H_{19}NO+ H]^+$ 326.1539, found: 326.1544.

(*Z*)-3-((3-methoxyphenyl)(p-tolyl)methylene)-1-methylindolin-2-one (5f):



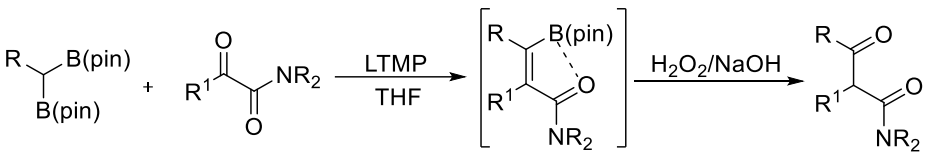
Synthesized using general procedure **2d**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish solid compound, yield (19 mg) 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.29-7.13 (m, 6H), 6.93-6.88 (m, 2H), 6.81-6.79 (m, 1H), 6.74 (d, *J* = 7.72 Hz, 1H), 6.69 (t, *J* = 7.64 Hz, 1H), 6.55 (d, *J* = 7.64 Hz, 1H), 3.75 (s, 3H), 3.19 (s, 3H), 2.41 (3H, s). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.91, 159.21, 154.68, 143.37, 141.83, 139.51, 138.25, 129.67, 129.51, 128.87, 128.76, 124.13, 123.46, 123.17, 122.60, 121.41, 115.74, 114.37, 107.75, 55.32, 25.98, 21.61. HRMS (ESI): m/z calculated for $[C_{24}H_{21}NO_2+ H]^+$ 356.1645, found: 356.1649.

(Z)-3-((E)-1,5-diphenylpent-1-en-3-ylidene)-1-methylindolin-2-one (5g):



Synthesized using general procedure **2d**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (22 mg) 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 9.35 (d, *J* = 16.44 Hz, 1H), 7.64-7.61 (m, 3H), 7.41-7.36 (m, 6H), 7.32-7.26 (m, 3H), 7.15 (d, *J* = 16.44Hz, 1H), 7.06 (t, *J* = 75.6Hz, 1 H), 6.86 (d, *J* = 7.68Hz, 1H), 3.32-3.29 (m, 5H), 3.02-2.98 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.33, 151.88, 143.06, 141.18, 137.33, 136.67, 129.05, 128.92, 128.46, 128.36, 128.01, 126.80, 126.65, 123.97, 123.23, 122.80, 122.12, 108.02, 34.57, 31.21, 25.89. HRMS (ESI): m/z calculated for $[C_{26}H_{23}NO+ H]^+$ 366.1852, found: 366.1856.

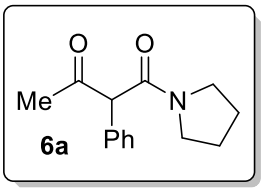
2e. General procedure for the synthesis of 1,3 di-carbonyl compound



To a flame-dried reaction tube 2,2,6,6-Tetramethylpiperidine (HTMP) (0.24 mmol, 1.2 equiv) in dry THF (1 mL) at -78 ºC was added n-BuLi (l.2 equiv) drop-wise for 5 min under argon atmosphere. The reaction mixture was stirred for 30 min at the same temperature. The reaction was then cooled to 0 ºC and stirred for another 30 min. Geminal-bis boronates (0.24 mmol, 1.2 equiv) were dissolved in dry THF (1 ml) added to the reaction mixture and stirred for 5 min. Then the reaction mixture was transferred to a solution of α-keto-amide / N-alkyl-oxindole (0.2 mmol) in THF at 0 ºC and further stirred for 2 h. After completion of the reaction 2ml water was added and the product was extracted with EtOAc (3 × 5 mL). The organic layer was dried

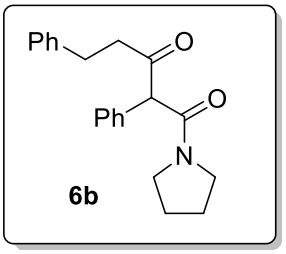
over Na_2SO_4 and concentrated in vacuum to afford the crude product. This crude material was further purified by flash column chromatography. Then the product was oxidized using H_2O_2/NaOH (1:1) in THF at 0 ^oC. After, 15 mins. the reaction was extracted with EtOAc and further purified using column chromatography.

2-phenyl-1-(pyrrolidin-1-yl)butane-1,3-dione (6a):



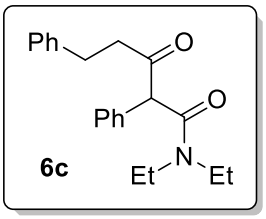
Synthesized using general procedure **2e**, purified by silica gel column chromatography (20% EtOAc/hexane), colorless oil, yield (30 mg) 65%. ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.39-7.32 (m, 5H), 4.67 (s, 1H), 3.59-3.54 (m,1H), 3.49-3.42 (m, 2H), 3.15-3.12 (m, 1H), 2.22 (s, 3H), 1.94-1.79 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.84, 167.15, 133.66, 129.15, 128.11, 65.75, 46.94, 46.24, 29.03, 26.15, 24.38. HRMS (ESI): m/z calculated for $[C_{14}H_{17}NO_2+ H]^+$ 232.1332, found: 232.1330.

2,5-diphenyl-1-(pyrrolidin-1-yl)pentane-1,3-dione (6b):



Synthesized using general procedure **2e**, purified by silica gel column chromatography (20% EtOAc/hexane), colorless oil, yield (43 mg) 67%. ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.37-7.30 (m, 3H), 7.28-7.22 (m, 4H), 7.17-7.11 (m, 3H), 4.63(s, 1H), 3.58-3.51 (m, 1H), 3.49-3.42 (m, 1H). 3.37-3.31 (m, 1H), 3.11-3.05 (m, 1H), 3.01-2.92 (m, 1H), 2.89-2.80 (m, 2H), 2.76 -2.69 (m 1H), 1.92-1.75 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.77, 167.17, 141.21, 133.33, 129.25, 129.09, 128.54, 128.50, 128.05, 126.09, 65.39, 46.88, 46.22, 43.13, 30.08, 26.11, 24.35. HRMS (ESI): m/z calculated for $[C_{21}H_{23}NO_2+ H]^+$ 322.1802, found: 322.1796.

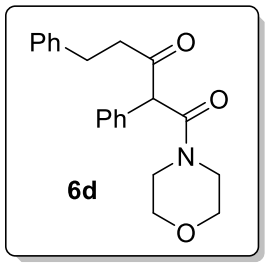
***N,N*-diethyl-3-oxo-2,5-diphenylpentanamide (6c):**



Synthesized using general procedure **2e**, purified by silica gel column chromatography (20% EtOAc/hexane), colorless oil, yield (47 mg) 72%. ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.37-7.30 (m, 3H), 7.26-7.22 (m, 4H), 7.18-7.11 (m, 3H), 4.67 (s, 1H), 3.54-3.45 (m, 1H), 3.31-3.23 (m, 1H). 3.20-3.13 (m, 1H), 3.10-3.01 (m, 1H), 2.99-2.80 (m, 3H), 2.73-2.65 (m, 1H) 1.12 (t, *J* = 6.8Hz, 3H), 1.00 (t, *J* = 6.96 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.86, 168.07, 141.27, 133.91, 129.13, 128.99, 128.53, 128.50, 128.05, 126.08, 63.68, 43.24, 42.43, 40.41,

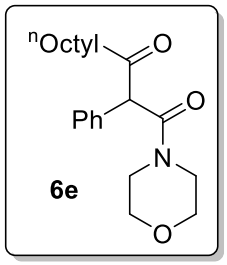
30.25, 14.24, 12.86. HRMS (ESI): m/z calculated for $[C_{21}H_{25}NO_2+ H]^+$ 324.1958, found: 324.1965.

1-morpholino-2,5-diphenylpentane-1,3-dione (6d):



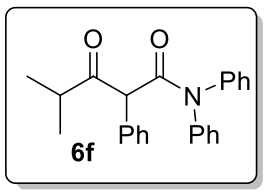
Synthesized using general procedure **2e**, purified by silica gel column chromatography (25% EtOAc/hexane), colorless oil, yield (46 mg) 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.38-7.32 (m, 3H), 7.26-7.16 (m, 5H), 7.15-7.11 (m, 2H), 4.68 (s, 1H), 3.76-3.66 (m, 2H), 3.60-3.44 (m, 3H). 3.25-3.11 (m, 3H), 2.97-2.84 (m, 3H), 2.73-2.66 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.52, 167.66, 141.09, 133.33, 129.36, 129.03, 128.56, 128.33, 126.20, 66.78, 66.29, 63.56, 46.52, 43.26, 42.40, 30.18. HRMS (ESI): m/z calculated for $[C_{21}H_{23}NO_3+ H]^+$ 338.1751, found: 338.1757.

1-morpholino-2-phenylundecane-1,3-dione (6e):



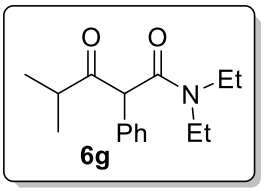
Synthesized using general procedure **2e**, purified by silica gel column chromatography (25% EtOAc/hexane), colorless oil, yield (46 mg) 66%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.40-7.32 (m, 3H), 7.26-7.23 (m, 2H), 4.76 (s, 1H), 3.80-3.67 (m, 2H), 3.61-3.52 (m, 3H), 3.37-3.31 (m, 1H), 3.25-3.20 (m, 2H), 2.63-2.54 (m, 1H), 2.40-2.31 (m, 1H), 1.55-1.48 (m, 2H), 1.24-1.20 (m, 10H), 0.87-0.82 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.47, 167.79, 133.66, 129.30, 129.02, 128.24, 66.80, 66.32, 63.34, 46.58, 42.41, 41.78, 31.93, 29.48, 29.23, 29.15, 23.89, 22.77, 14.23. HRMS (ESI): m/z calculated for $[C_{21}H_{31}NO_3+ H]^+$ 346.2377, found: 346.2388.

4-methyl-3-oxo-N,N,2-triphenylpentanamide (6f):



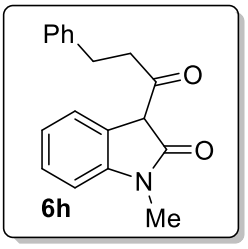
Synthesized using general procedure **2e**, purified by silica gel column chromatography (10% EtOAc/hexane), colorless oil, yield (46 mg) 64%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.41-7.29 (m, 10H), 7.24-7.17(m, 5H), 4.99 (s, 1H), 2.66-2.59 (m, 1H), 0.96 (d, J = 6.72 Hz, 3H), (0.80, J = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.35, 168.55, 142.88, 142.54, 133.62, 130.01, 129.94, 129.35, 129.19, 129.05, 128.70, 128.51, 127.99, 126.51, 62.52, 39.49, 18.75, 18.65. HRMS (ESI): m/z calculated for $[C_{24}H_{23}NO_2+ H]^+$ 358.1802, found: 358.1816.

***N,N*-diethyl-4-methyl-3-oxo-2-phenylpentanamide (6g):**



Synthesized using general procedure **2e**, purified by silica gel column chromatography (20% EtOAc/hexane), colorless oil, yield (34 mg) 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.38-7.31 (m, 3H), 7.28-7.26(m, 2H), 4.89(s, 1H), 3.52-3.44 (m, 1H), 3.34-3.22 (m, 2H), 3.17-3.08 (m, 1H), 2.97-2.85 (m, 1H), 1.14-1.11 (m, 6H), 1.04 (t, *J* = 7.08 Hz, 3H), 0.98-0.96 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.88, 168.09, 133.98, 129.26, 128.94, 127.90, 61.99, 42.43, 40.38, 39.66, 19.15, 19.04, 14.19, 12.82. HRMS (ESI): m/z calculated for $[C_{16}H_{23}NO_2+H]^+$ 262.1802, found: 262.1812.

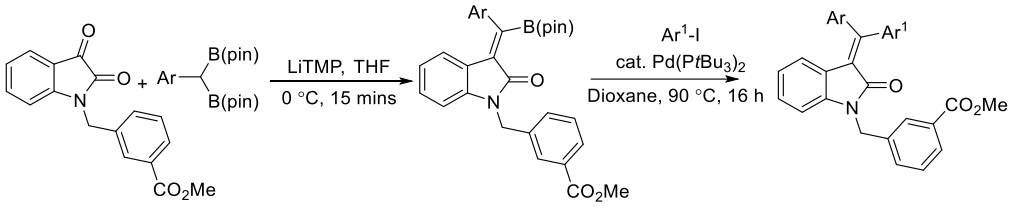
1-methyl-3-(3-phenylpropanoyl)indolin-2-one (6h):



Synthesized using general procedure **2e**, purified by silica gel column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (40 mg) 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.36-7.28 (m, 5H), 7.25-7.19 (m, 2H), 7.09 (t, *J* = 7.6Hz, 1 H), 6.95 (d, *J* = 7.68Hz, 1H), 4.78 (s, 0.5H), 3.55 (s, 3H), 3.12-3.03 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.49, 171.42, 140.53, 139.03, 128.79, 128.43, 126.58, 125.42, 122.32, 121.93, 119.84, 108.58, 101.55, 35.79, 31.96, 25.85. HRMS (ESI): m/z calculated for $[C_{18}H_{17}NO_2+H]^+$ 280.1332, found: 280.1317.

2f. General procedure for Bio-active compounds

Synthesis of AMPK activator

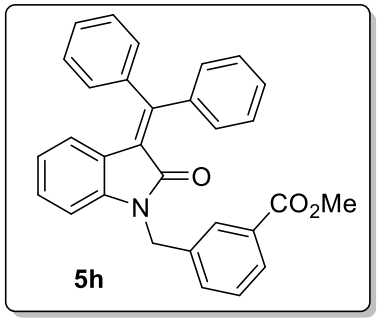


To a flame-dried reaction tube 2,2,6,6-Tetramethylpiperidine (HTMP) (0.24 mmol, 1.2 equiv) in dry THF (1 ml) at -78 ^{o}C was added n-BuLi (l.2 equiv) drop-wise for 5 min under argon atmosphere. The reaction mixture was stirred for 30 min at the same temperature. The reaction was then cooled to 0 ^{o}C and stirred for another 30 min. Geminal-bis boronates (0.24 mmol, 1.2 equiv) were dissolved in dry THF (1 ml) added to the reaction mixture, and stirred for 3 min. Then the reaction mixture was transferred to a solution of N-alkyl-oxindole (0.20 mmol) in THF at 0 ^{o}C and further stirred for 15 mins. After completion of the reaction 1ml water was added and the product was extracted with EtOAc (3 × 5 mL). The organic layer was dried over

Na_2SO_4 and concentrated in vacuum to afford the crude product. This crude material was further purified by flash column chromatography using silica gel.

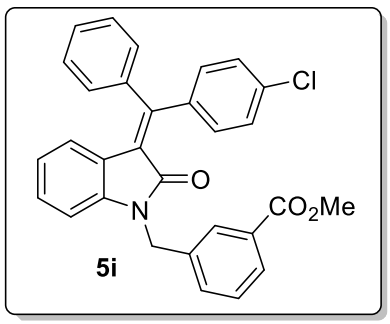
Next, the above product, aryl iodide (1.2 equiv.), NaOH (3M) and [Pd(P-^{t}Bu$_3$)$_2$] (5 mol%) in dioxane were degassed and heated at 90 ^{o}C for 16 h. After cooling the mixture, filtered through celite and washed with EtOAc. The organic part was concentrated in vaccuo and further purified using flash column chromatography.

methyl 3-((3-(diphenylmethylene)-2-oxoindolin-1-yl)methyl)benzoate (5h):



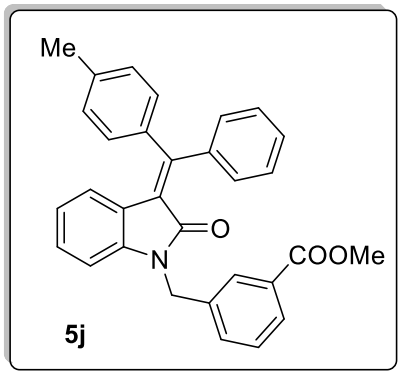
Synthesized using general procedure **2f**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound (64 mg), yield 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-8.01 (m, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.42 (m, 3H), 7.40-7.34 (m, 8H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.67 – 6.63 (m, 2H), 6.43 (d, *J* = 7.7 Hz, 1H), 4.97 (s, 2H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.02, 155.48, 142.27, 141.42, 139.98, 137.01, 132.12, 130.70, 130.33, 129.49, 129.42, 129.10, 129.05, 128.92, 128.86, 128.65, 128.00, 123.97, 123.57, 123.40, 121.74, 108.67, 77.48, 77.20, 77.16, 76.85, 52.32, 43.39. HRMS (ESI): m/z calculated for $[C_{30}H_{23}NO_3 + H]^+$ 446.1751, found: 446.1756.

methyl(*Z*)-3-((3-((4-chlorophenyl)(phenyl)methylene)-2-oxoindolin-1yl)methyl)benzoate (5i):



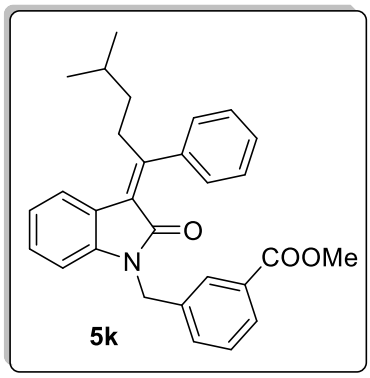
Synthesized using general procedure **2f**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (72 mg) 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 -7.92 (m, 2H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.31 (m, 9H), 7.26 (s,1H), 7.06 (t, *J* = 7.7 Hz, 1H), 6.66 (t, *J* = 7.7 Hz, 2H), 6.42 (d, *J* = 7.7 Hz, 1H), 4.96 (s, 2H), 3.91 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.96, 153.79, 142.33, 141.00, 138.28, 136.89, 135.56, 132.10, 131.84, 130.76, 129.66, 129.54, 129.22, 129.12, 129.09, 128.98, 128.66, 128.30, 124.35, 123.49, 123.37, 121.86, 108.75, 77.42, 76.91, 52.33, 43.44. HRMS (ESI): m/z calculated for $[C_{30}H_{22}ClNO_3 + H]^+$ 480.1361, found: 480.1372.

methyl (*E*)-3-((2-oxo-3-(phenyl(p-tolyl)methylene)indolin-1-yl)methyl)benzoate (5j):



Synthesized using general procedure **2f**, purified by silica gel flash column chromatography (10% EtOAc/hexane), yellowish gummy compound, yield (1.56 gm isolated) 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.93 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.44-7.28 (m, 6H), 7.24-7.21(m, 4H), 7.10-7.04 (m, 1H), 6.70 – 6.62 (m, 2H), 6.58 (d, *J* = 7.6 Hz, 1H), 4.96 (s, 2H), 3.91 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.12, 167.00, 155.86, 142.16, 140.29, 139.73, 138.47, 137.07, 132.13, 130.67, 130.44, 129.72, 129.37, 129.04, 128.90, 128.69, 128.65, 127.96, 123.75, 123.59, 123.27, 121.66, 108.62, 52.31, 43.36, 21.63. HRMS (ESI): m/z calculated for $[C_{31}H_{25}NO_3+H]^+$ 460.1907, found: 460.1914.

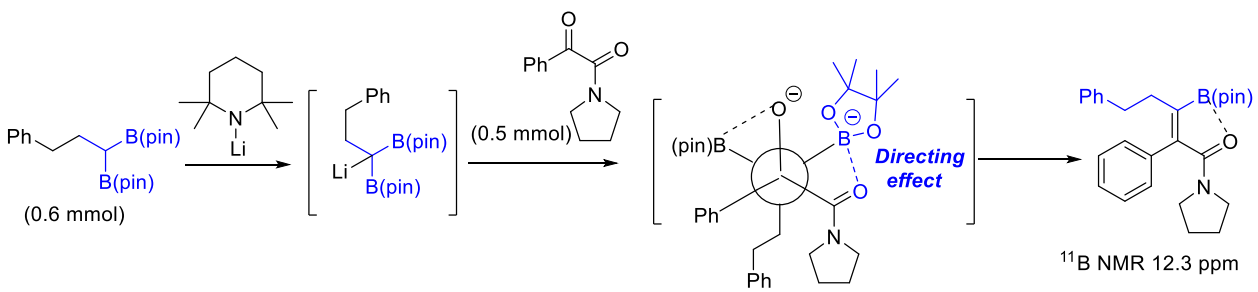
Methyl-(*Z*)-3-((3-(4-methyl-1-phenylpentylidene)-2-oxoindolin-1-yl)methyl)benzoate (5k):



Synthesized using general procedure **2f**, purified by silica gel flash column chromatography (25% EtOAc/hexane), gummy compound, yield (68 mg) 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.46-7.37 (m, 4H), 7.36- 7.29(m, 3H), 7.17 (t, *J* = 7.7 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.66(d, J = 7.84Hz, 1H), 4.90 (s, 2H), 3.89 (s, 3H), 2.99 – 2.94 (m, 2H), 1.73-1.67 (m,1H), 1.54-1.48 (m, 2H), 0.96 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.99, 166.64, 159.48, 142.39, 141.76, 137.08, 131.95, 130.69, 128.98, 128.83, 128.57, 128.53, 128.26, 128.15, 127.64, 123.65, 123.19, 122.86, 122.16, 108.88, 77.41, 76.91, 52.27, 43.22, 36.54, 35.a3, 28.92, 22.53. HRMS (ESI): m/z calculated for $[C_{19}H_{29}NO_3+H]^+$ 440.2220, found: 440.2227.

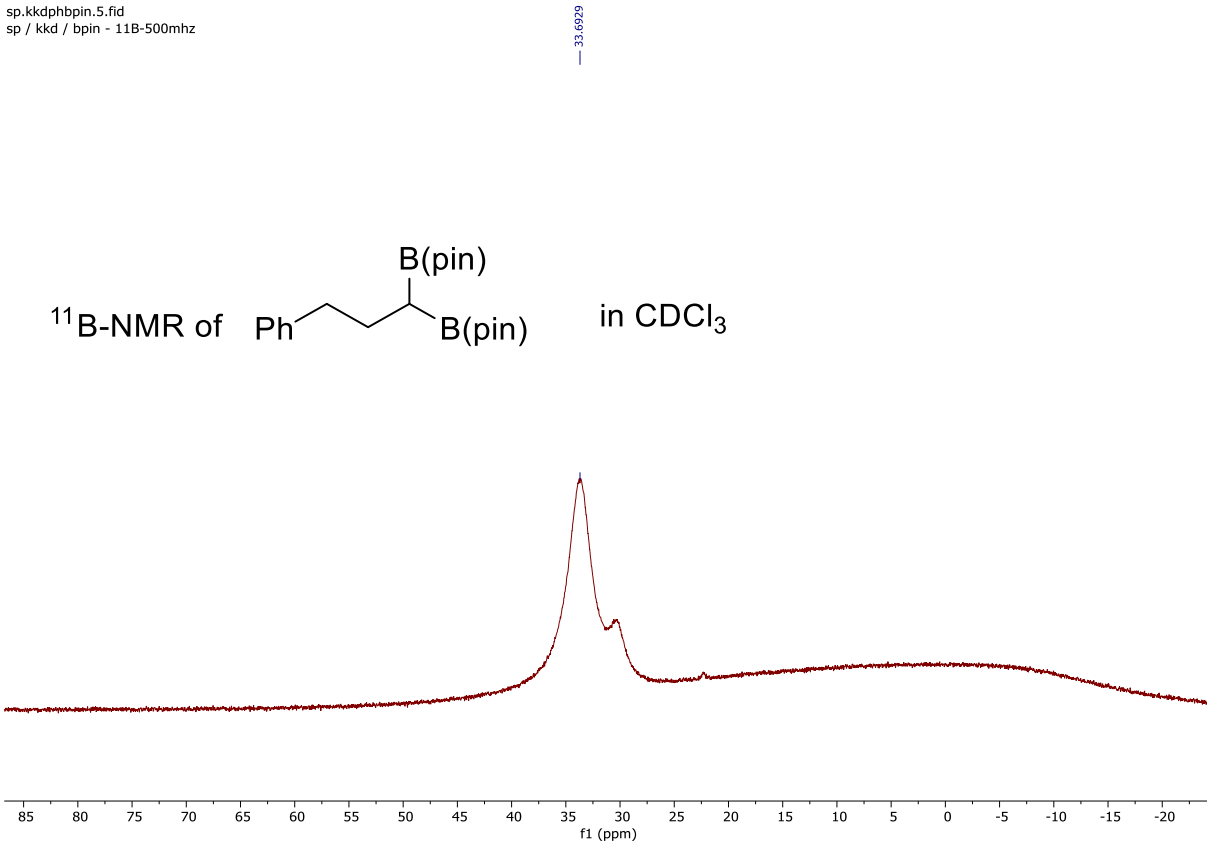
3. ^{11} B-NMR study of reaction with *α*-keto-amide:

^{11} B-NMR study with keto-amide



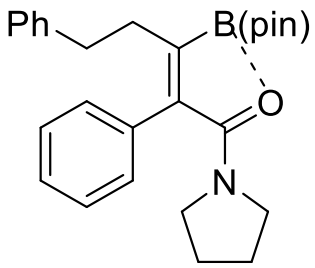
We have tried the *in situ* ^{11}B NMR studies to elucidate the reaction intermediates. We have taken 2,2,6,6-Tetramethylpiperidine (HTMP) (0.6 mmol, 1.2 equiv) in dry THF (2 mL) at -78 °C in

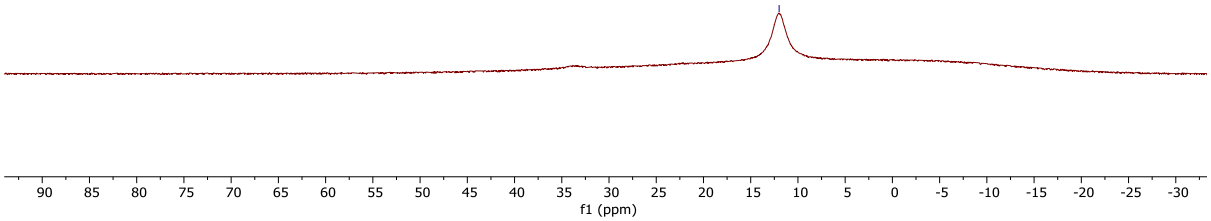
which n-BuLi (l.2 equiv) drop-wise for 5 min under argon atmosphere. The reaction mixture was stirred for 30 min at the same temperature. The reaction was then cooled to 0 °C and stirred for another 30 min. Geminal-bis boronates (0.6 mmol, 1.2 equiv) were dissolved in dry THF (2 ml) added to the reaction mixture, and stirred for 5 min. Then the reaction mixture was transferred to a solution of α-keto amide (0.5 mmol) in THF at -78 °C and further stirred for 30 mins at 0 °C. We have recorded the ^{11}B NMR in THF using $CDCl_3$ capillary inside the NMR tube for lock purposes. The ^{11}B NMR indicates the formation of the desired product at 12.3 ppm as well as a peak at 4.8 ppm indicating the formation of boronate species. We have also seen a peak ~ 34 ppm arise due to the presence of unreacted geminal bis boronates, which was taken in excess.



sp.dg672b.10.fid
sp / dg / 672 b - 11B -500mhz

11.9917

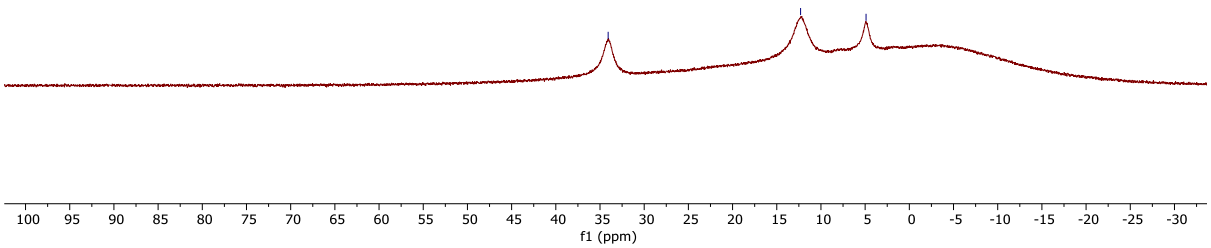
^{11}B-NMR of  in $CDCl_3$



sp.dg735b.5.fid
sp / dg / 735b - 11B -500mhz

34.0774
12.3033
4.8971

^{11}B-NMR of reaction mixture in THF after 30 mins, $CDCl_3$ capillary was inserted in the NMR tube for lock purpose



4. Crystallographic Data and Structure Refinements:

All the crystals grew as colorless prisms by slow evaporation from pet ether and ethyl acetate. First, the compound was taken in a small glass vial and dissolved in a minimum amount of ethyl acetate. Then dropwise pet ether was added until the solution became faint opaque. Next, the vial was closed with a plastic cap containing a small hole for slow solvent evaporation. After one week the growing crystal was found to be visible and submitted for further characterization. Good quality single crystals of each compounds were sorted out with the help of a polarizing microscope and immersed in paratone oil, which was then mounted on the tip of glass fiber and cemented using epoxy resin. The single-crystal XRD diffraction data were collected at 298 K on a Bruker AXS (D8 Quest System) X-ray diffractometer, equipped with a PHOTON 100 CMOS detector using graphite-monochromated Mo-Kα radiation (0.71073 Å). The linear absorption coefficients, scattering factors for the atoms, and the anomalous dispersion corrections were taken from International Tables for X-ray Crystallography. Bruker Apex III software was used for data collection, unit cell measurements, absorption corrections, scaling, and integration.5 The data were reduced and an empirical absorption correction was applied with the help of SAINTPLUS software and SADABS programs using XPREP, respectively.6 The structures were solved by the direct method using SHELXL-2014 in the WinGx programs. For all the cases, nonhydrogen atoms were refined anisotropically. All other hydrogen atoms were geometrically fixed using the riding atom model and assigned fixed isotropic displacement parameters. The “ACTA” command was used to generate the Crystallographic Information File (CIF). The structural details of all the compounds are presented in below. CCDC: 2266989, 2266990, 2266922, 2266991contain the crystallographic data of these compounds 3h, 2q, 4a, 5a respectively.

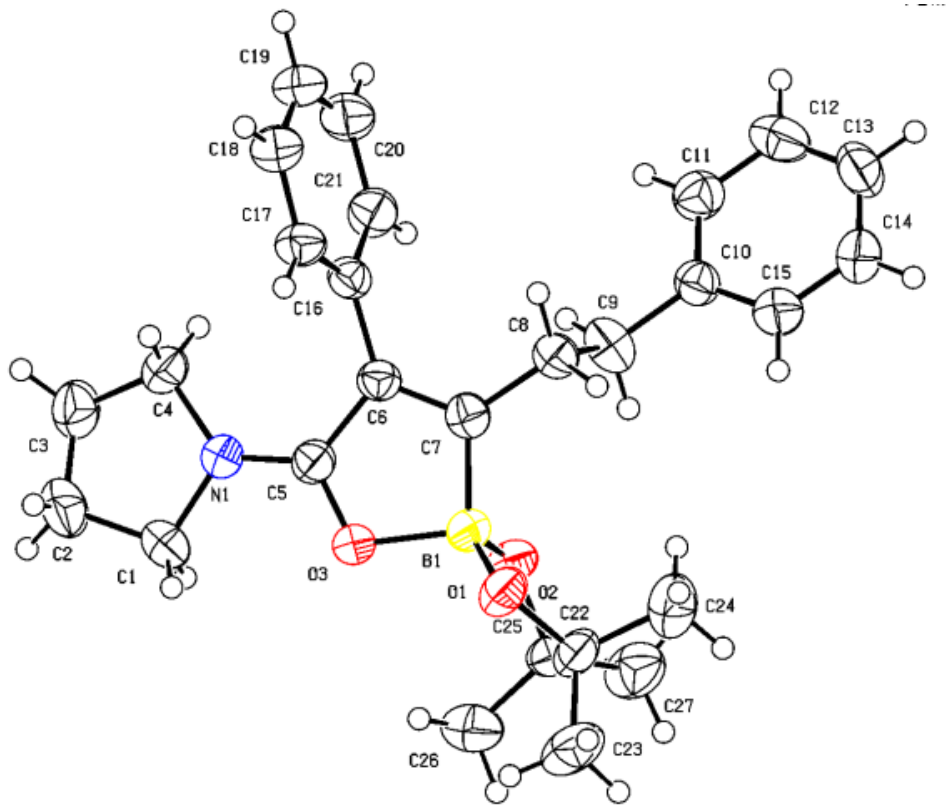


Figure 1. Perspective view of 3h with 50% thermal ellipsoid probability

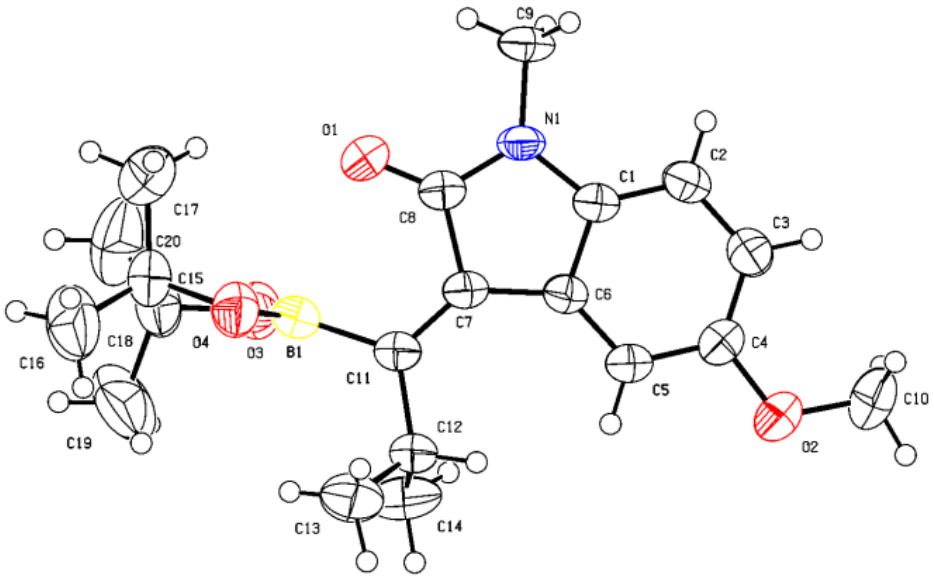


Figure 2. Perspective view of 2q with 50% thermal ellipsoid probability

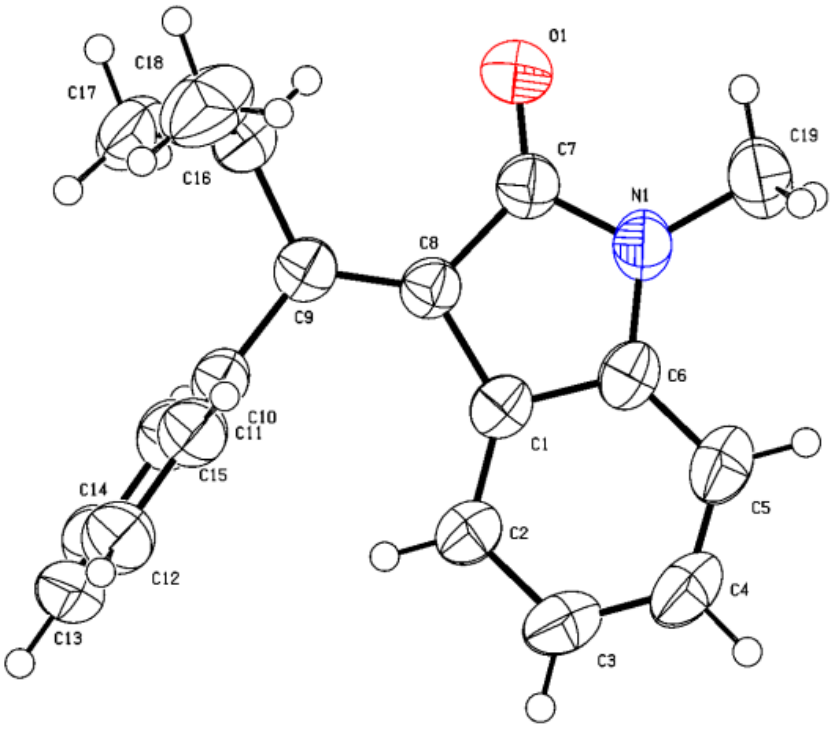


Figure 3. Perspective view of 4a with 50% thermal ellipsoid probability

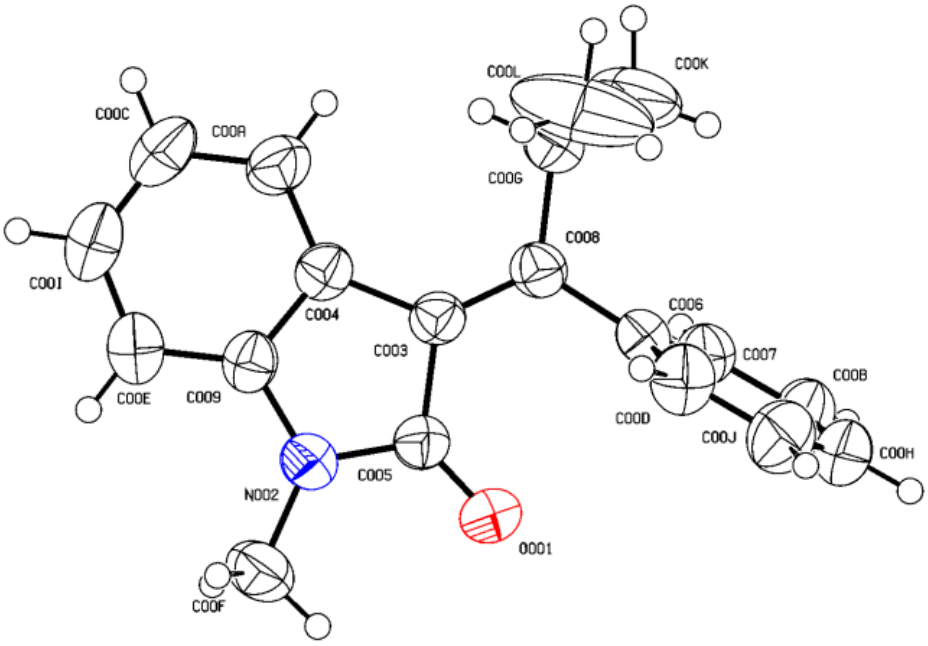


Figure 4. Perspective view of 5a with 50% thermal ellipsoid probability

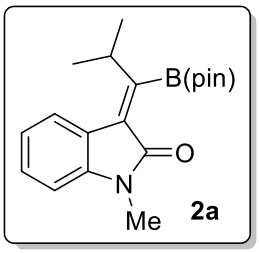
Table 1: Crystal data and structure refinements for the molecules **2h, 3q, 4a, 5a** respectively

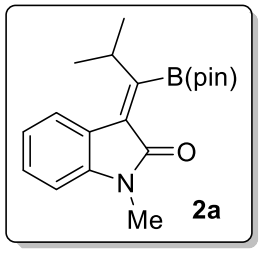
Entry	**3h**	**2q**	**4a**	**5a**
Empirical formula	$C_{27}H_{34}BNO_3$	$C_{20}H_{28}BNO_4$	$C_{19}H_{19}NO$	$C_{19}H_{19}NO$
Formula weight	431.36	357.24	277.35	277.35
Temperature (K)	296(2)	296(2)	296(2)	296(2)
Wave length [Å]	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	P -1	P b c a	P 2_1/n	P2_1/n
a [Å]	8.867(3)	8.6631(4)	11.7963(7)	9.004(12)
b [Å]	11.445(4)	13.5282(6)	8.2830(4)	9.504(11)
c [Å]	12.457(4)	35.3230(15)	15.9743(10)	18.11(2)
α [°]	102.292	90	90	90
β [°]	95.249	90	105.775(2)	94.20
γ [°]	98.197(11)°.	90	90	90
Volume [Å^3]	1212.8(6)	4139.7(3)	1502.04(15)	1546(3)
Z	2	8	4	4
Density (calculated) [mg/m^3]	1.181	1.146	1.226	1.192
Absorption coefficient [mm^{-1}]	0.075	0.078	0.075	0.073
F (000)	464	1536	592	592
Crystal size [mm^3]	0.200 x 0.180 x 0.150	0.350 x 0.250 x 0.150	0.250 x 0.150 x 0.100	0.12 x 0.090 x 0.080
Theta range for data collection	2.339 to 24.998°.	2.306 to 25.497°.	1.919 to 25.499°.	2.421 to 28.292
Limiting indices	-10<=h<=10, -13<=k<=13, -14<=l<=14	-10<=h<=10, -15<=k<=16, -42<=l<=42	-14<=h<=14, -10<=k<=10, -19<=l<=19	-11<=h<=12, -12<=k<=12, -24<=l<=24
Reflections collected / unique	17144/4267 [R(int) = 0.1311]	72526/ 3861 [R(int) = 0.0881]	26754/2795 [R(int) = 0.0806]	36315/3822 [R(int) = 0.0690]

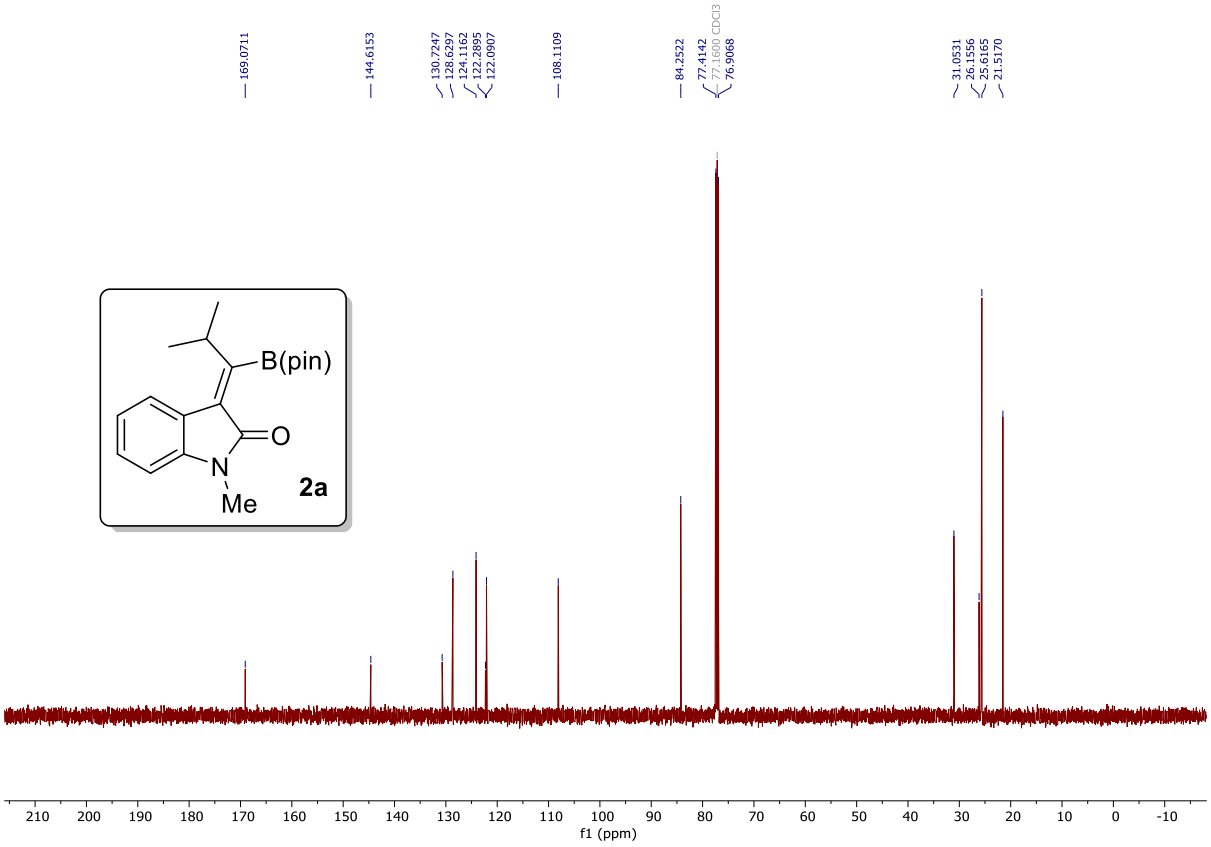
Goodness-of-fit on F^2	1.010	1.122	1.042	1.044
Final R indices [I>2sigma(I)]	R_1 = 0.0633, wR2 = 0.1336	R_1 = 0.0677, wR_2 = 0.1685	R_1 = 0.0605, wR_2 = 0.1654	R_1 =0.0555, wR_2 = 0.1360
R indices (all data)	R_1 = 0.1324, wR_2 = 0.1658	R_1 = 0.0885, wR_2 = 0.1817	R_1 = 0.0816, wR_2 = 0.1937	R_1 = 0.0990, wR_2 = 0.1587
CCDC	2266989	2266990	2266922	2266991

5. NMR spectra of compounds

^{1}H-NMR of crude reaction mixture



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31.0531
26.1556
25.6165
21.5170
B(pin)
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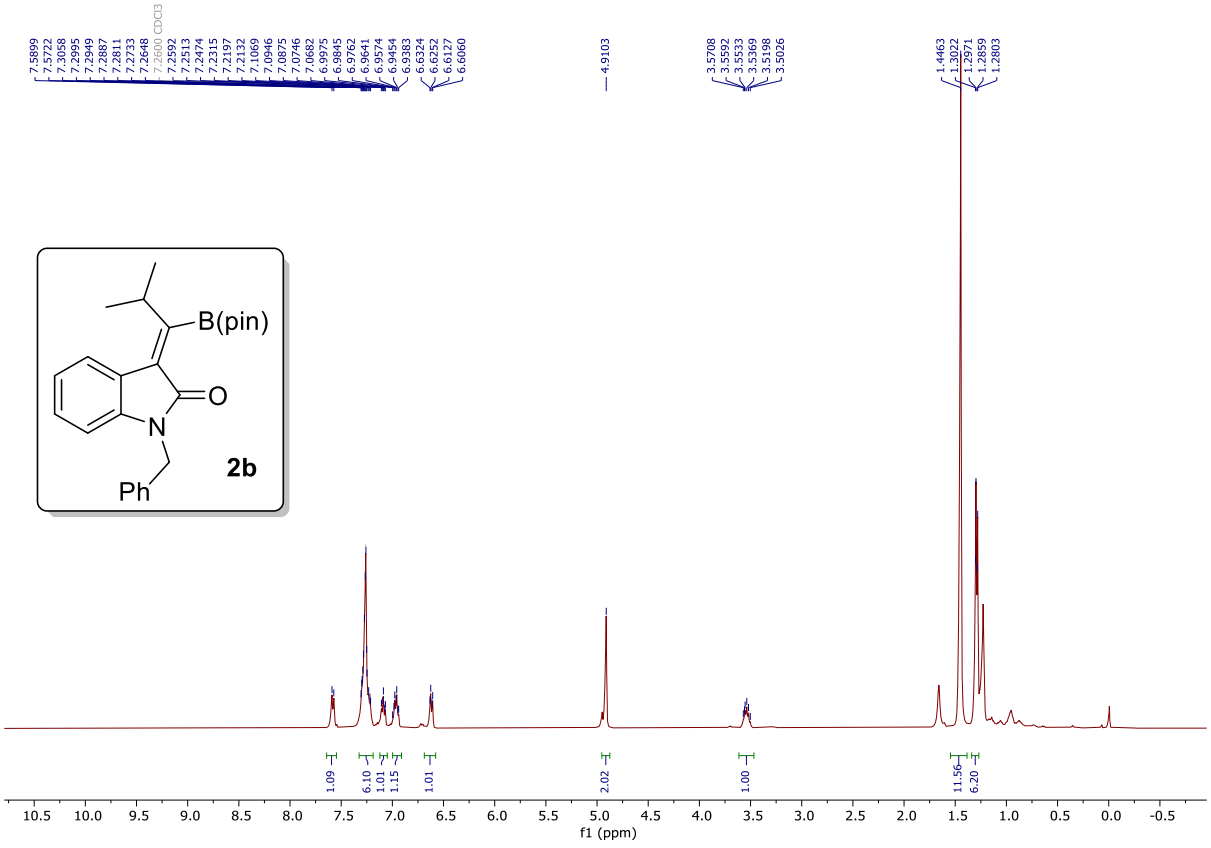
N
Me
2a
f1 (ppm)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3.5198
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1.2971
1.2859
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B(pin)
O
N
Ph
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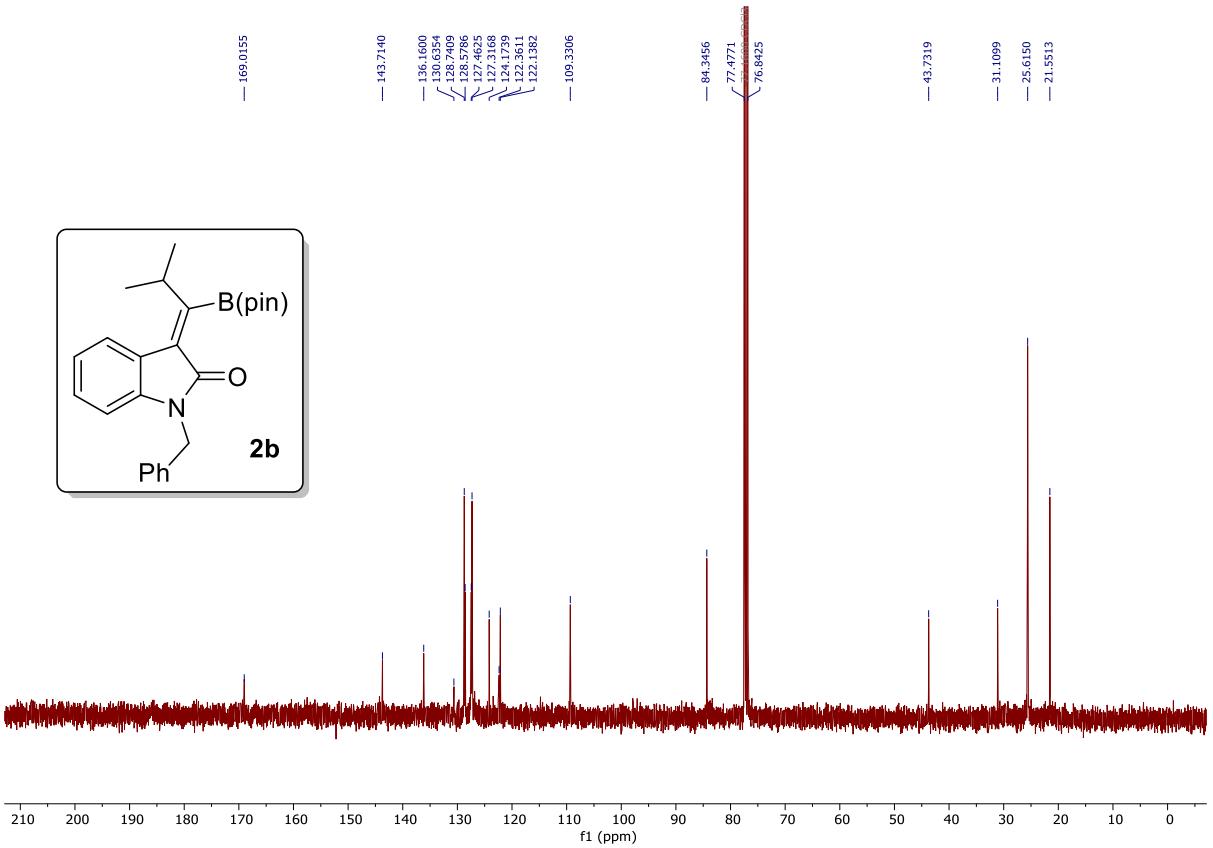
1.15
1.01
2.02
1.00
11.56
6.20
f1 (ppm)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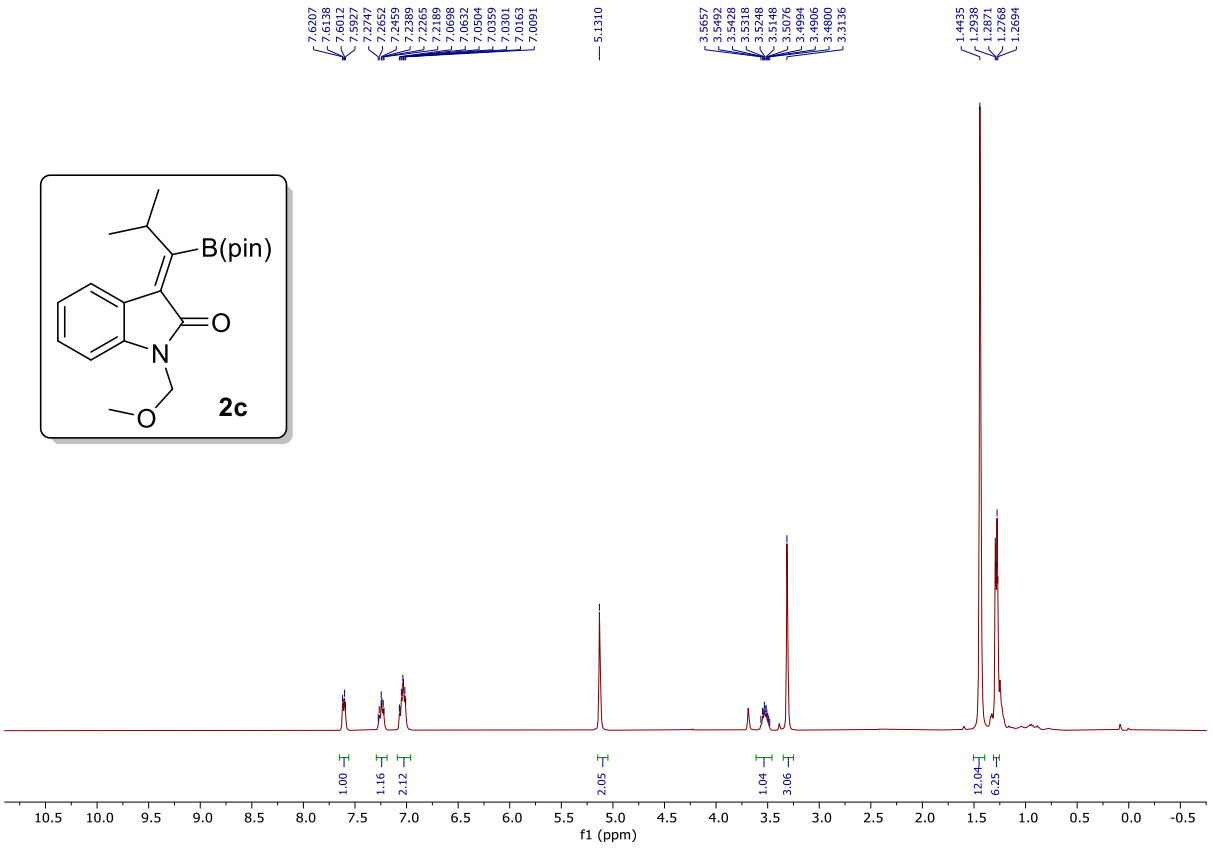
Ph
2b
f1 (ppm)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B(pin)
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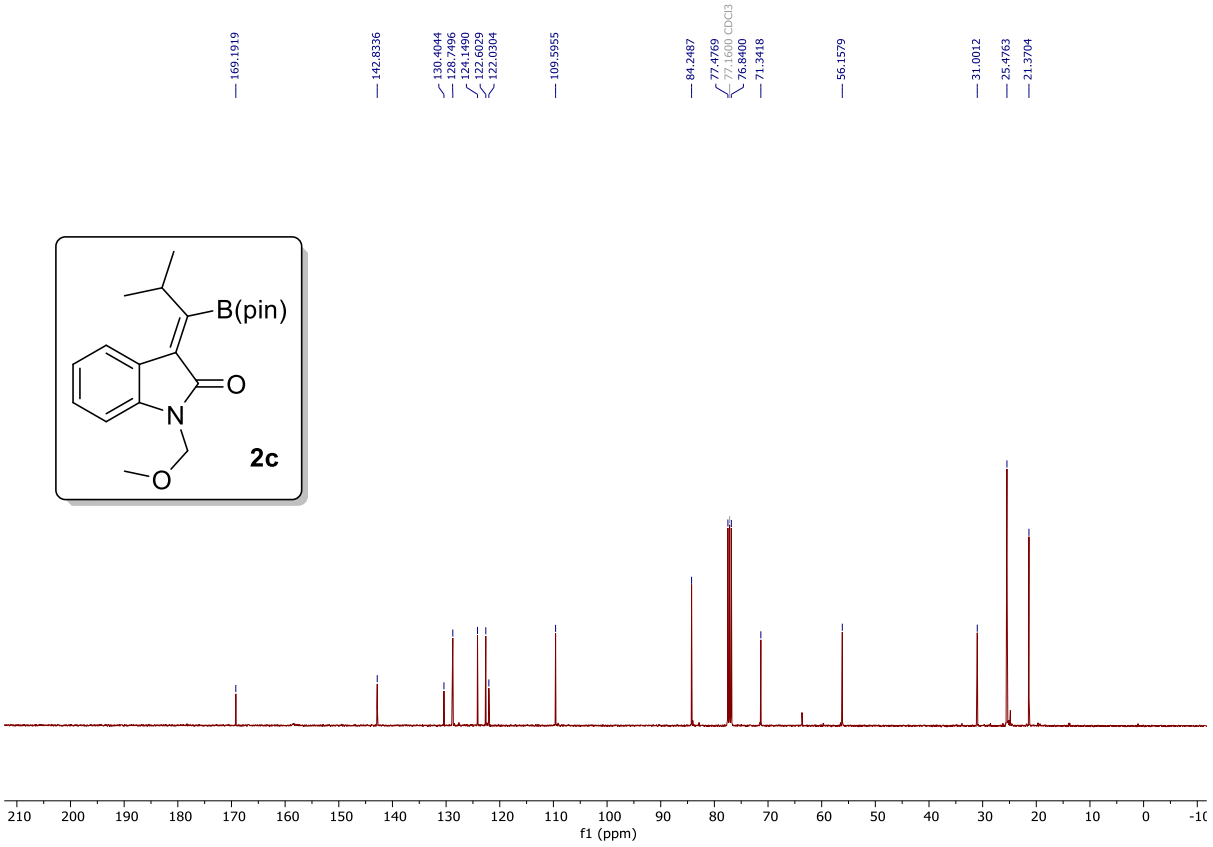
6.25
f1 (ppm)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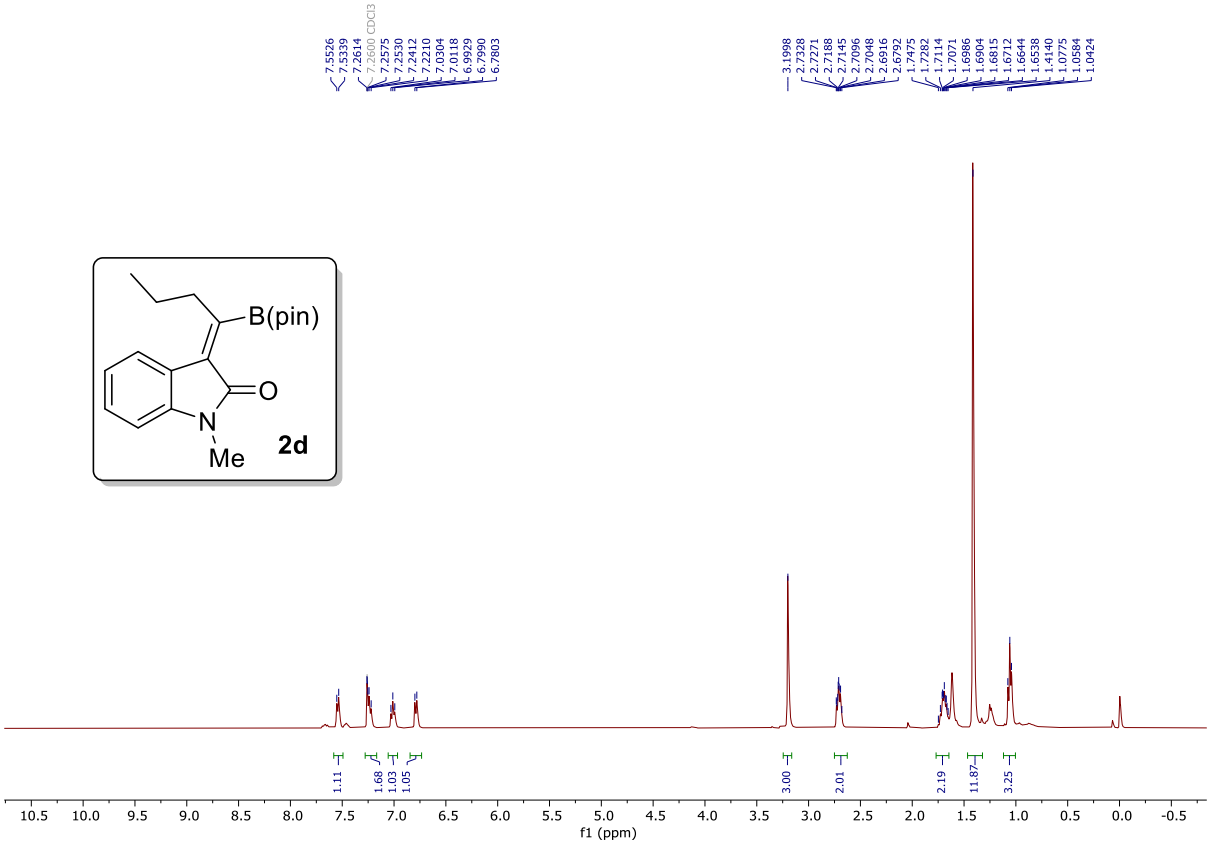
2c
f1 (ppm)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6.7803
3.1998
2.7328
2.7271
2.7188
2.7145
2.7096
2.7048
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2.6792
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1.6815
1.6712
1.6644
1.6538
1.4140
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1.0584
1.0424
B(pin)
O
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Me
2d
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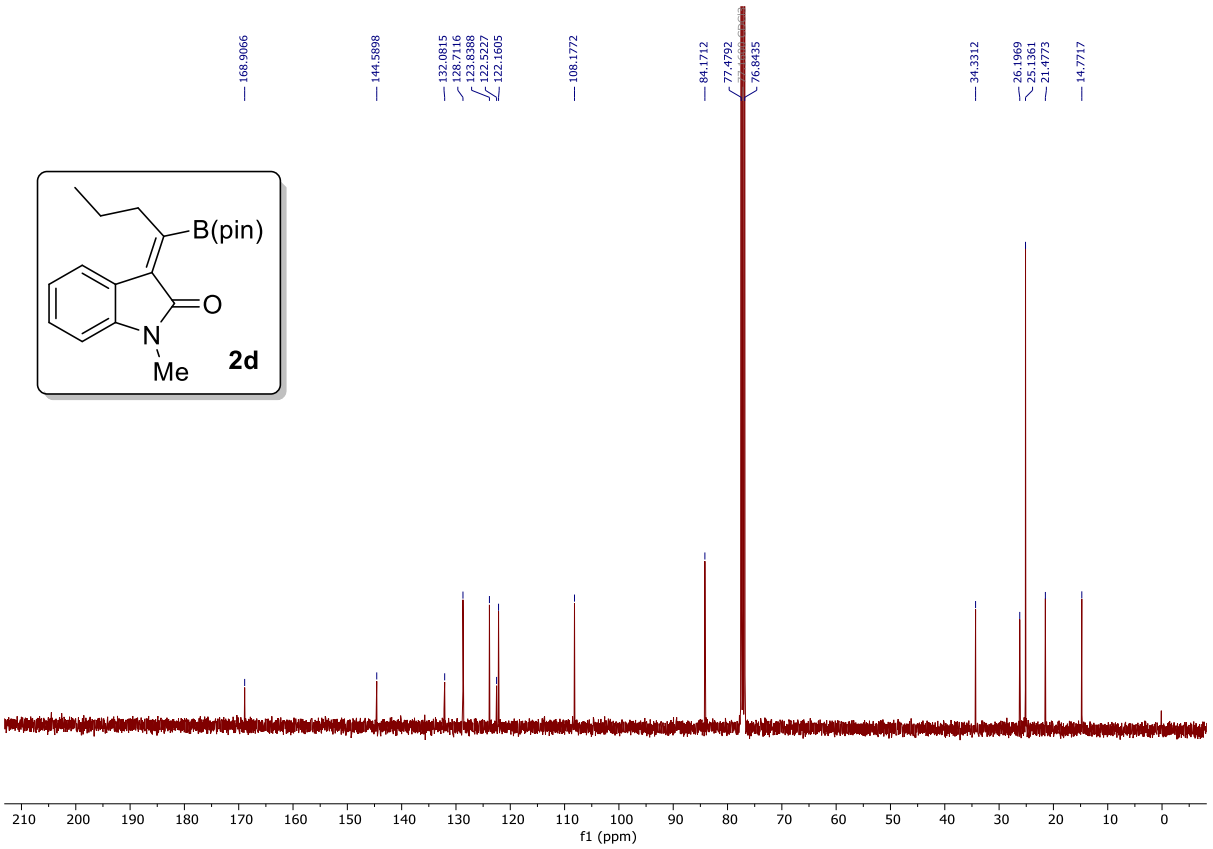
1.68
1.03
1.05
3.00
2.01
2.19
11.87
3.25
f1 (ppm)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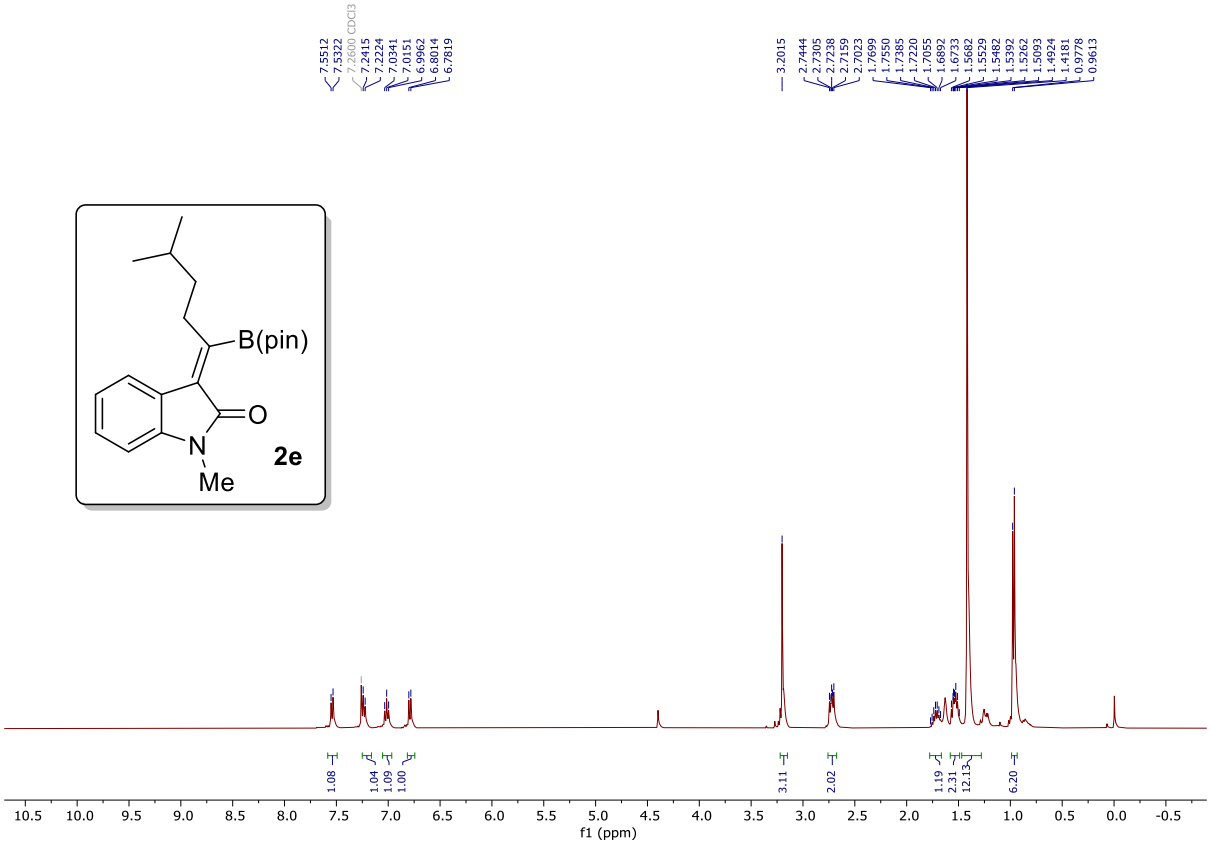
Me
2d
f1 (ppm)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2.7305
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0.9613
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1.04
1.09
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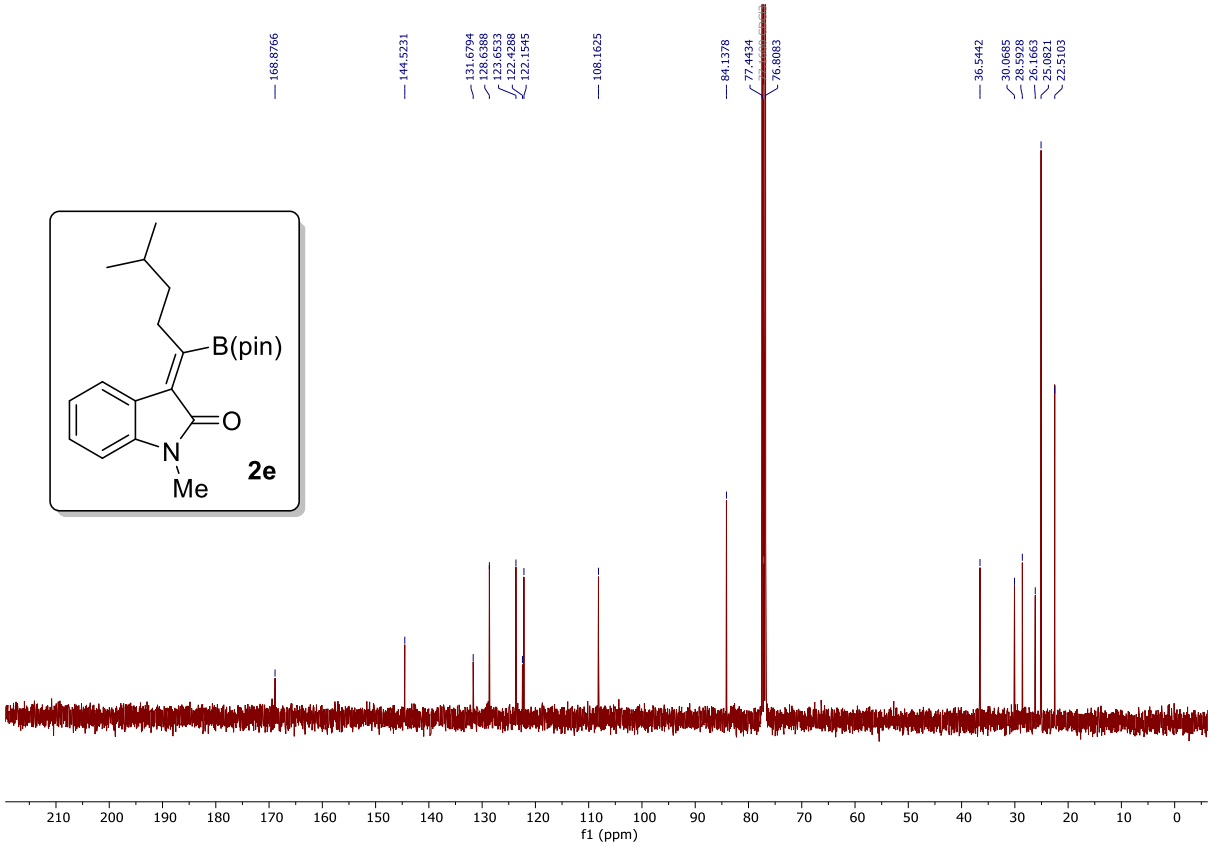
B(pin)
O
N
Me
2e
f1 (ppm)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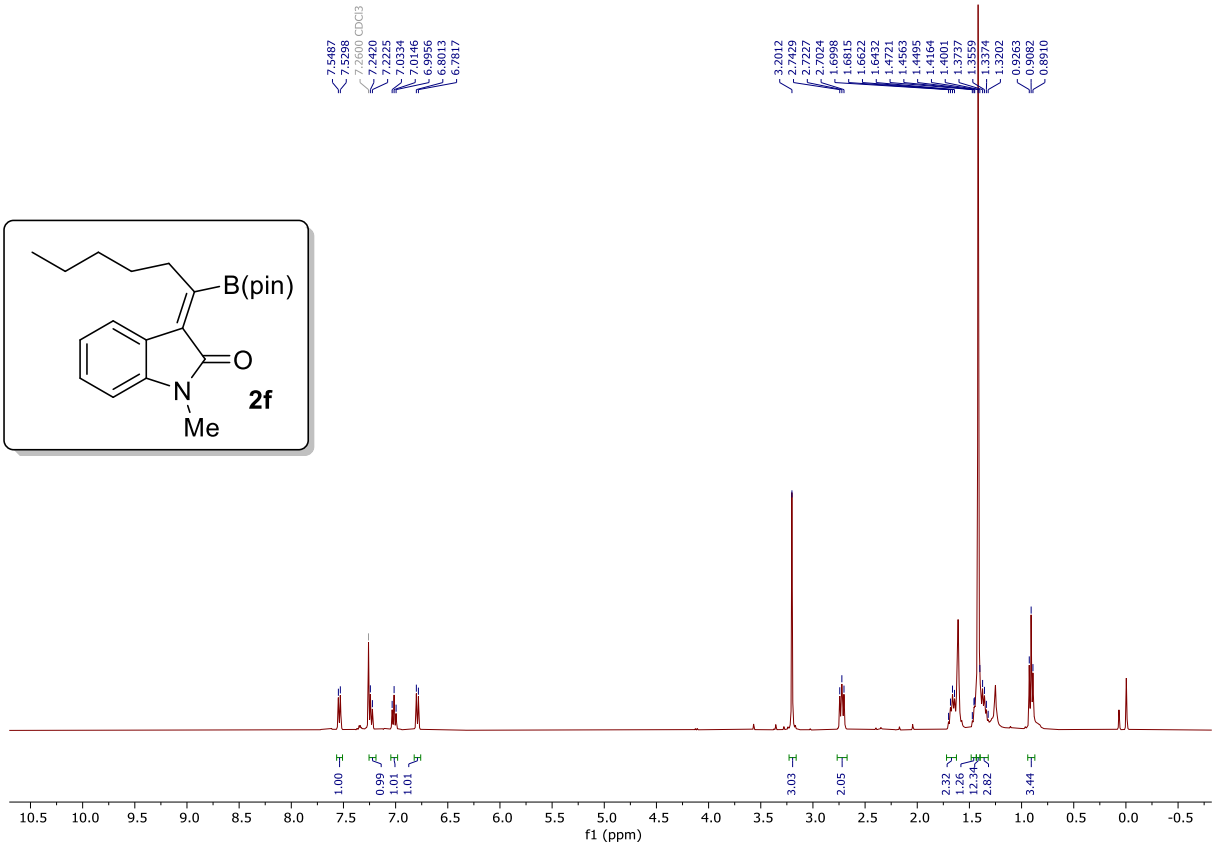
B(pin)
O
N
Me
2e
f1 (ppm)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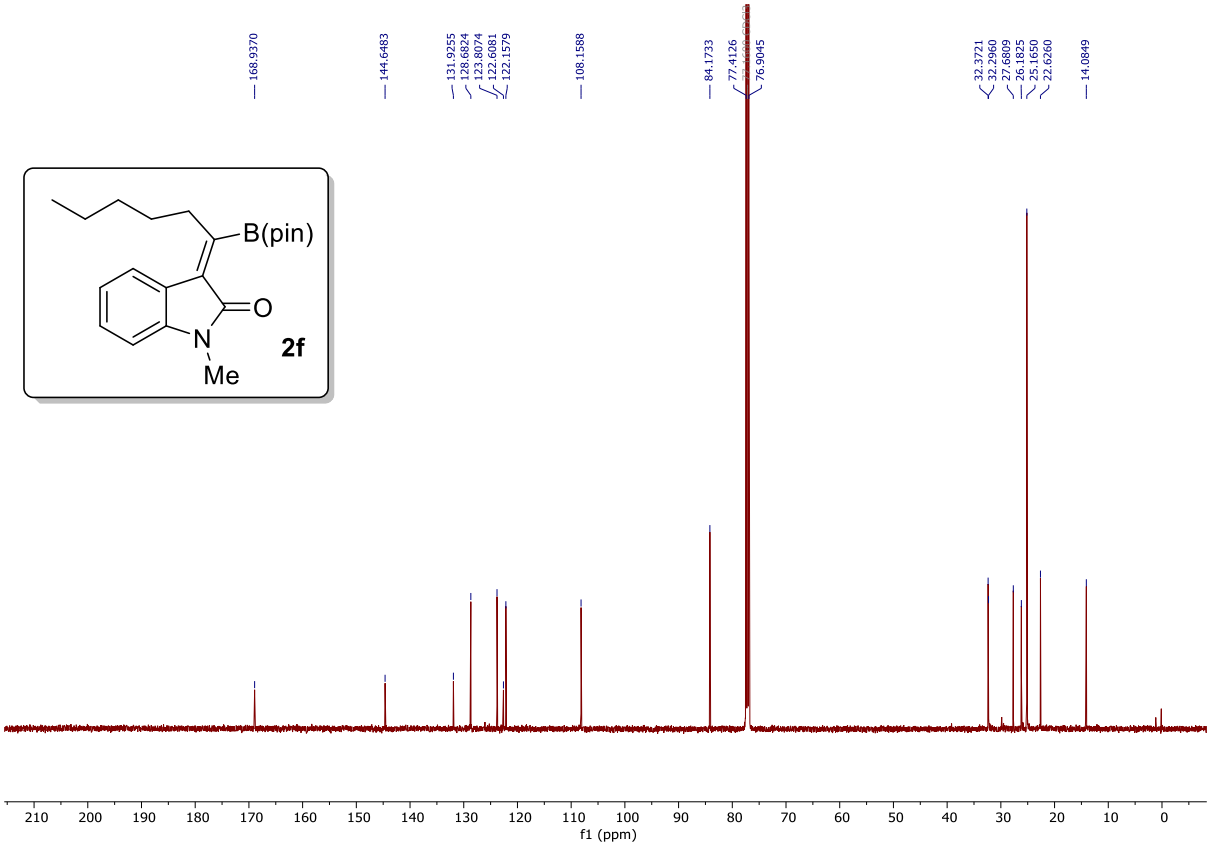
7.0334
7.0146
6.9956
6.8013
6.7817
3.2012
2.7429
2.7227
2.7024
1.6998
1.6815
1.6622
1.6432
1.4721
1.4563
1.4495
1.4164
1.4001
1.3737
1.3559
1.3374
1.3202
0.9263
0.9082
0.8910
B(pin)
O
N
Me
2f
1.00
0.99
1.01
1.01
3.03
2.05
2.32
1.26
12.34
2.82
3.44
f1 (ppm)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122.1579
108.1588
84.1733
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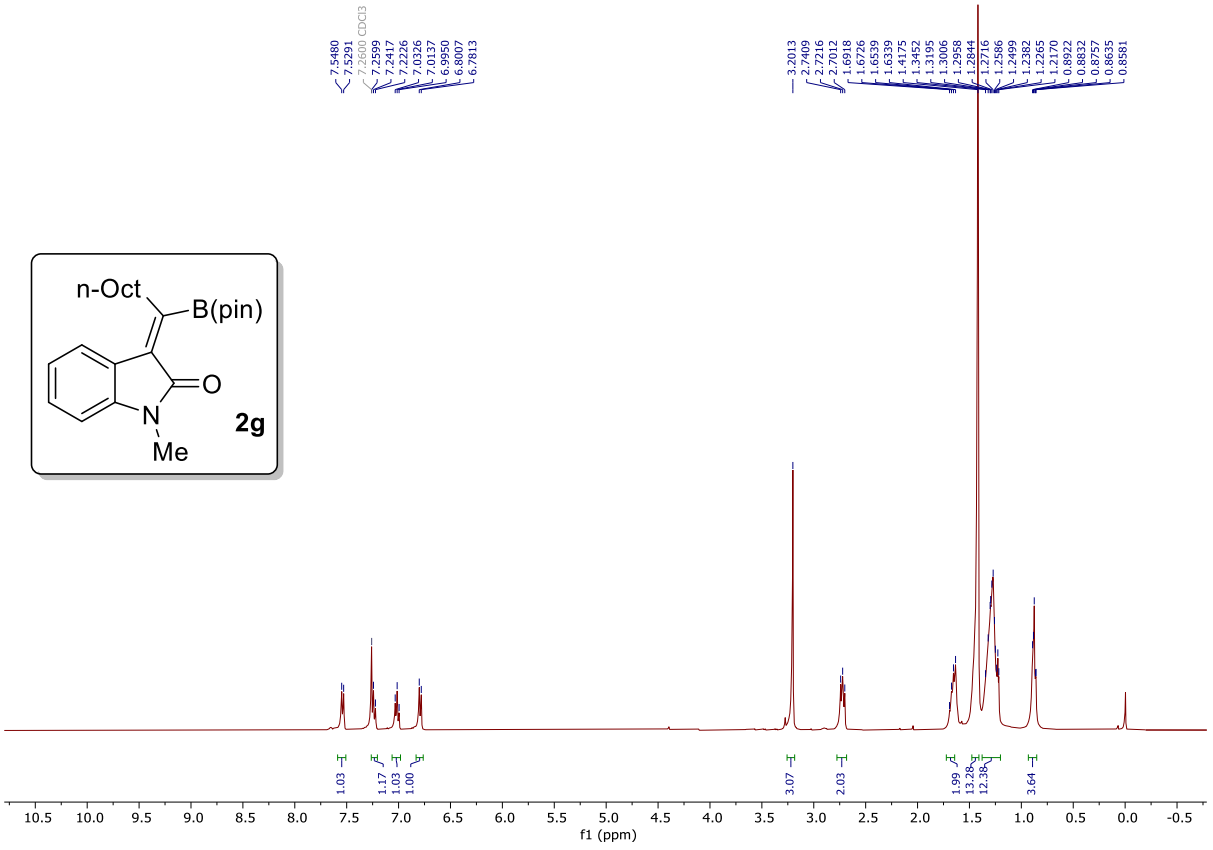
76.9045
32.3721
32.2960
27.6809
26.1825
25.1650
22.6260
14.0849
B(pin)
O
N
Me
2f
f1 (ppm)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7.2226
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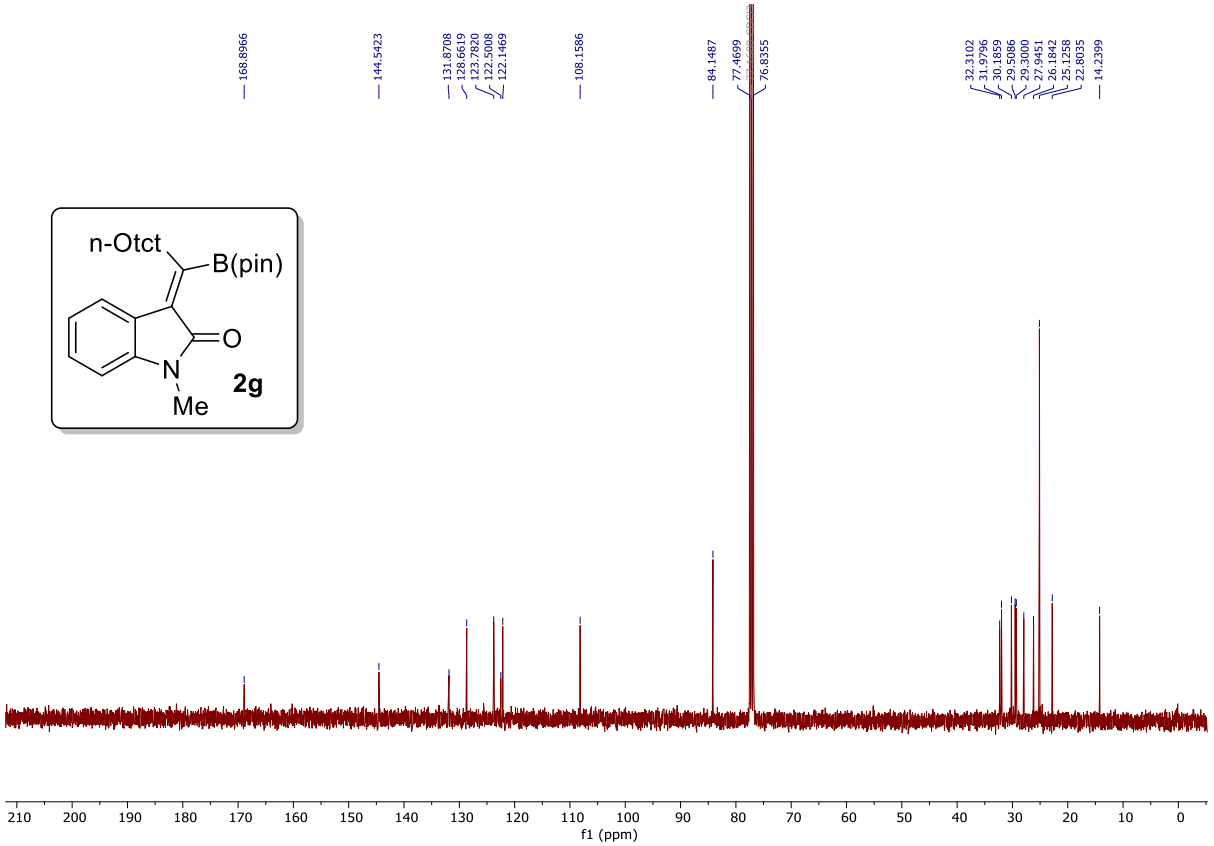
6.7813
3.2013
2.7409
2.7216
2.7012
1.6918
1.6726
1.6539
1.6339
1.4175
1.3452
1.3195
1.3006
1.2958
1.2844
1.2716
1.2586
1.2499
1.2382
1.2265
1.2170
0.8922
0.8832
0.8757
0.8635
0.8581
n-Oct
B(pin)
O
N
Me
2g
1.03
1.17
1.03
1.00
3.07
2.03
1.99
13.28
12.38
3.64
f1 (ppm)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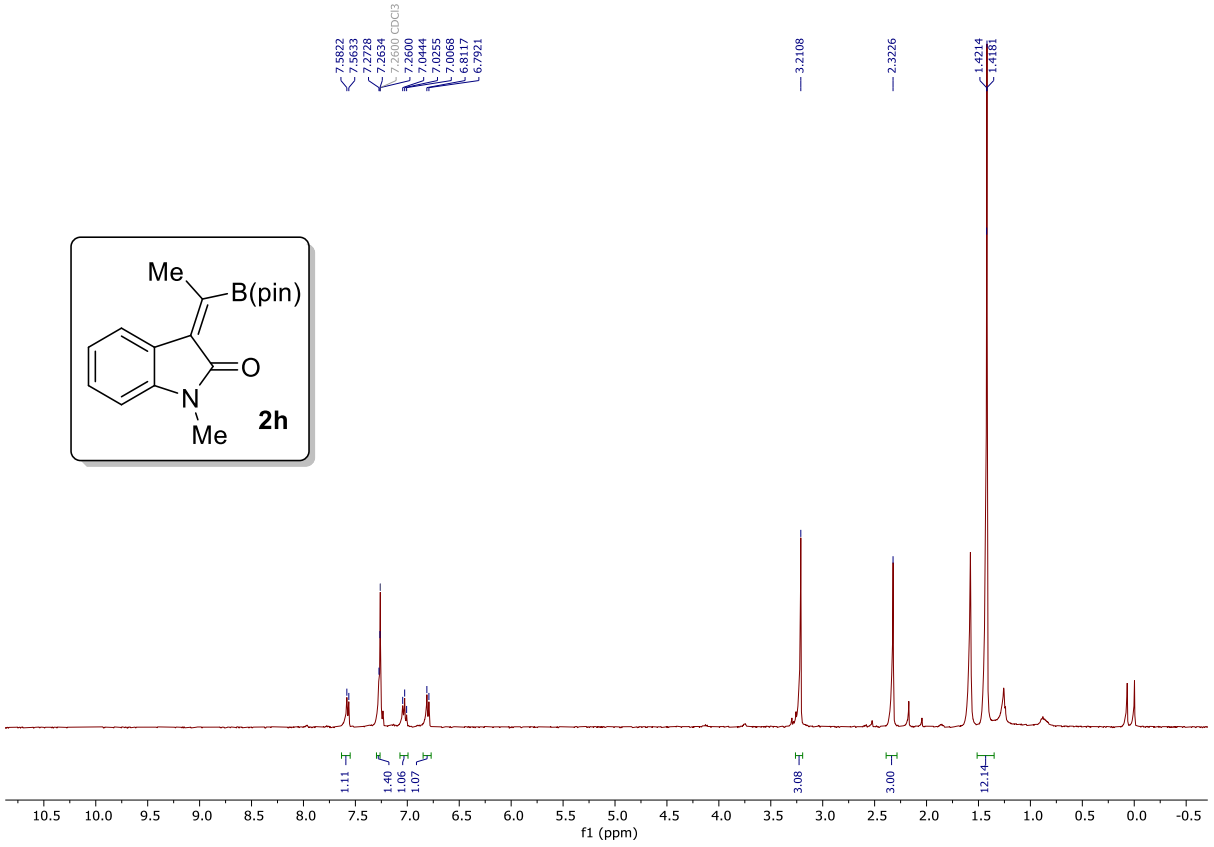
76.8355
32.3102
31.9796
30.1859
29.5086
29.3000
27.9451
26.1842
25.1258
22.8035
14.2399
n-Octct
B(pin)
O
N
Me
2g
f1 (ppm)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7.0255
7.0068
6.8117
6.7921
3.2108
2.3226
1.4214
1.4181
Me
B(pin)
O
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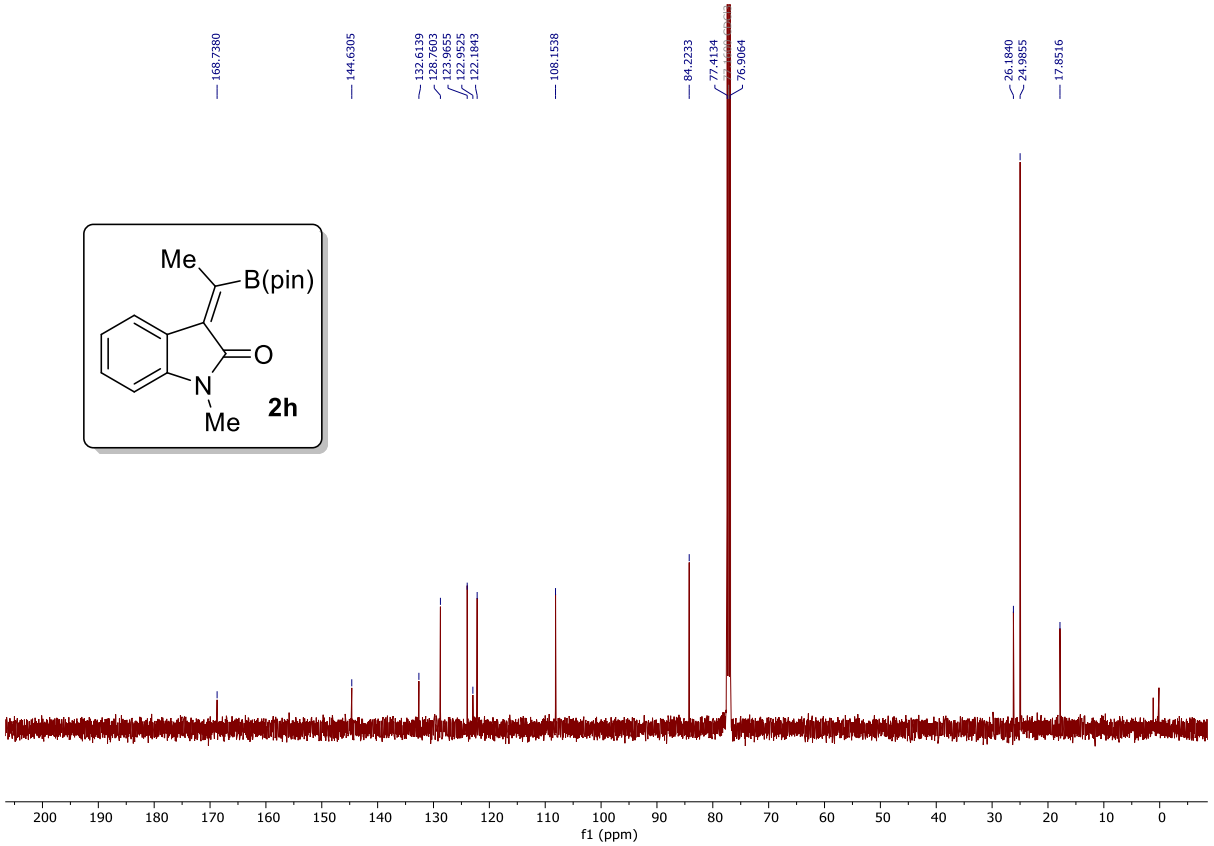
Me
2h
1.11
1.40
1.06
1.07
3.08
3.00
12.14
f1 (ppm)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122.1843
108.1538
84.2233
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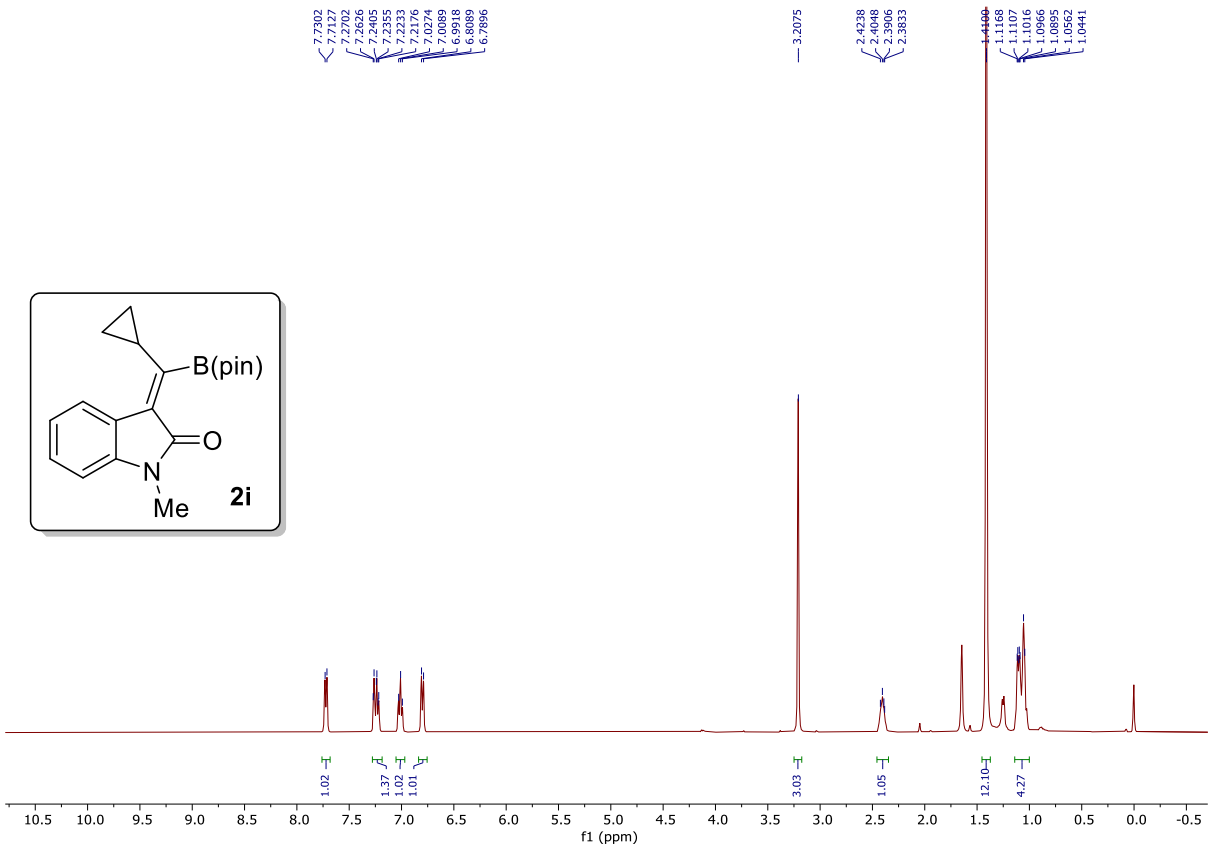
26.1840
24.9855
17.8516
Me
B(pin)
O
N
Me
2h
f1 (ppm)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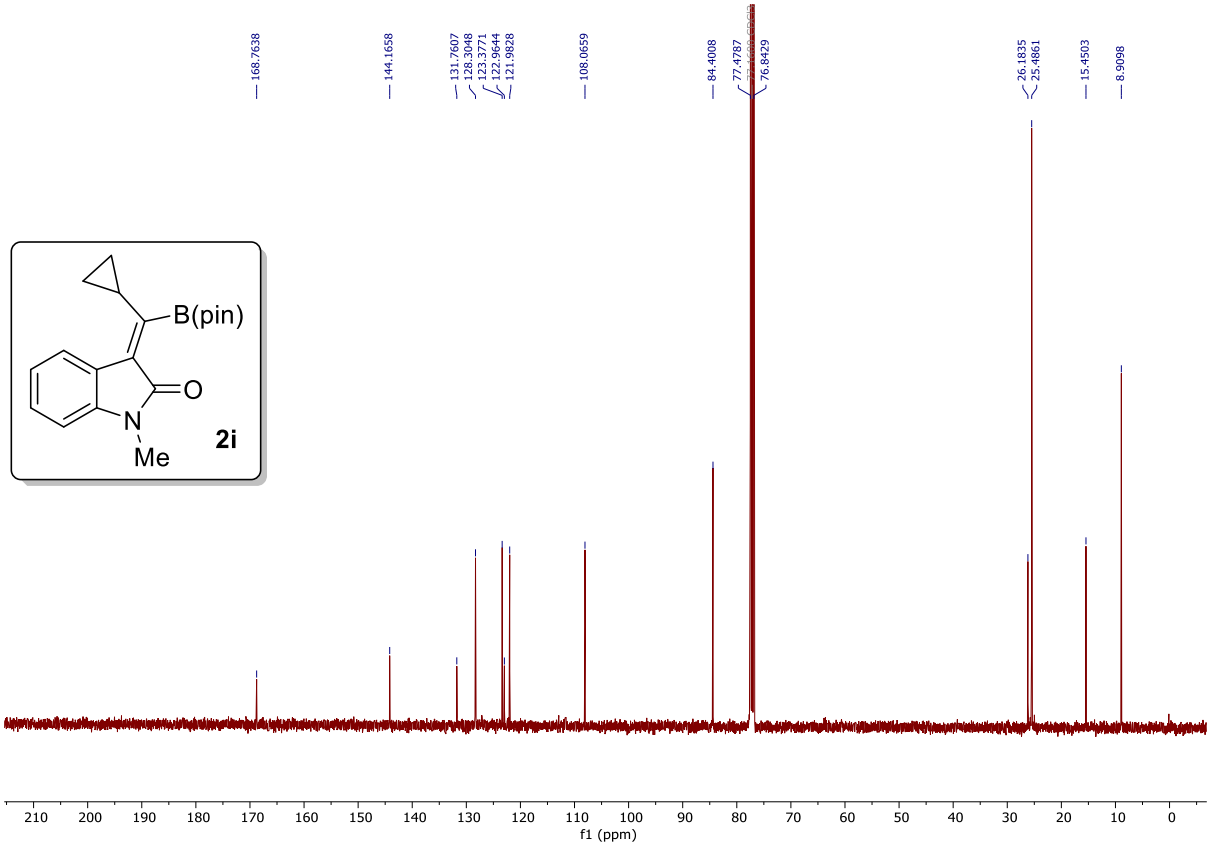
7.2702
7.2686
7.2465
7.2255
7.2233
7.2176
7.0274
7.0085
6.9918
6.8089
6.7896
3.2075
2.4238
2.4048
2.3906
2.3833
1.1168
1.1107
1.1016
1.0966
1.0895
1.0562
1.0441
1.02
1.37
1.02
1.01
3.03
1.05
12.10
4.27
B(pin)
O
N
Me
2i
f1 (ppm)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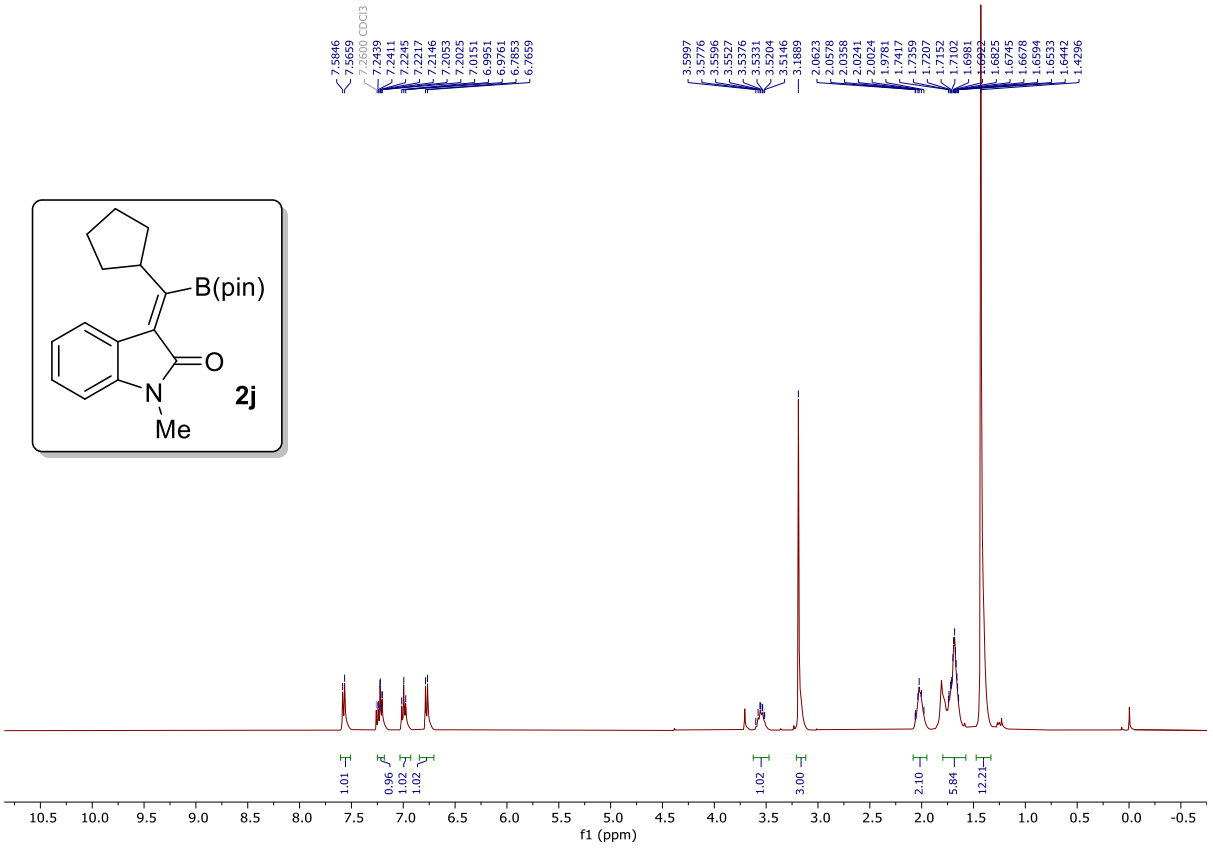
25.4861
15.4503
8.9098
B(pin)
O
N
Me
2i
f1 (ppm)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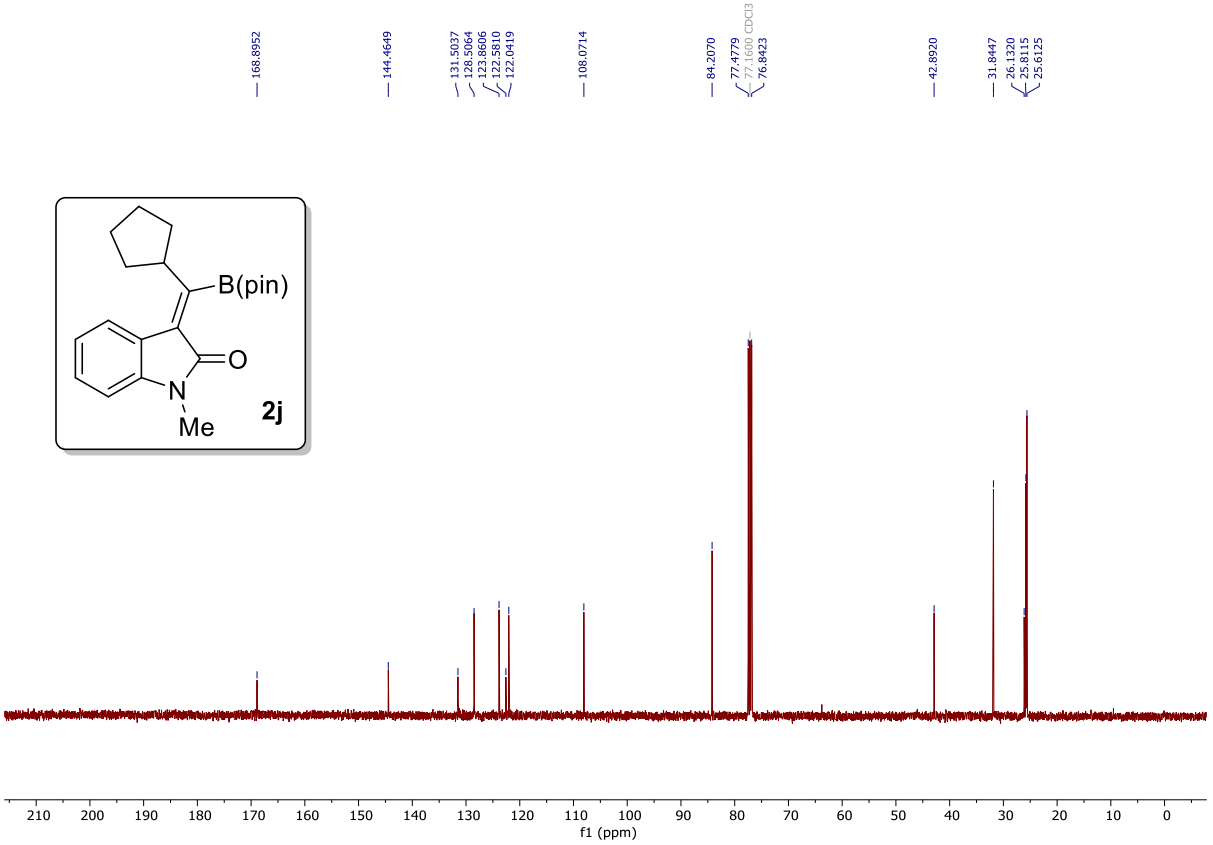
7.2600 CDCl3
7.2439
7.2411
7.2245
7.2217
7.2146
7.2053
7.2025
7.0151
6.9951
6.9761
6.7853
6.7659
3.5997
3.5776
3.5596
3.5527
3.5376
3.5331
3.5204
3.5146
3.1889
2.0623
2.0578
2.0358
2.0241
2.0024
1.9781
1.7417
1.7359
1.7207
1.7152
1.7102
1.6981
1.6822
1.6825
1.6745
1.6678
1.6594
1.6533
1.6442
1.4296
B(pin)
O
N
Me
2j
1.01
0.96
1.02
1.02
1.02
3.00
2.10
5.84
12.21
f1 (ppm)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122.0419
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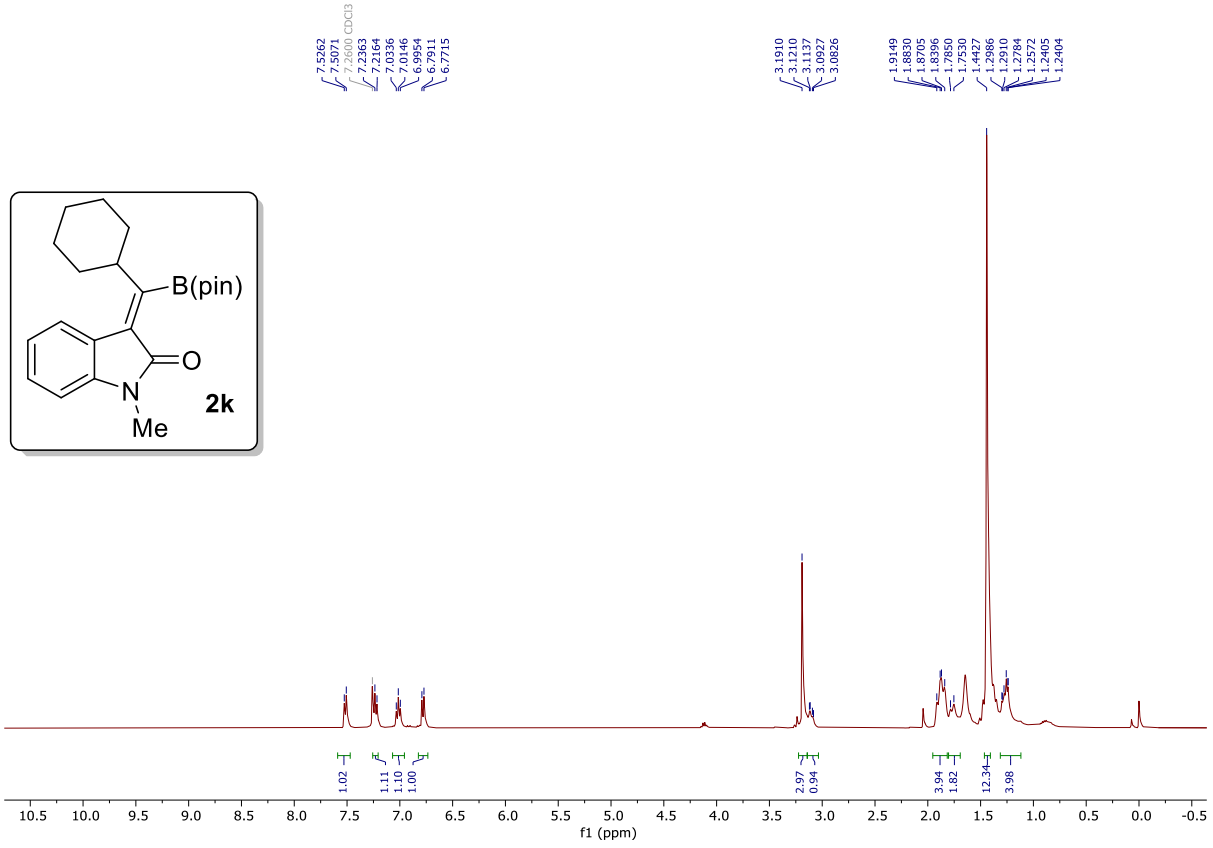
77.4779
77.1600 CDCl3
76.8423
42.8920
31.8447
26.1320
25.8115
25.6125
B(pin)
O
N
Me
2j
f1 (ppm)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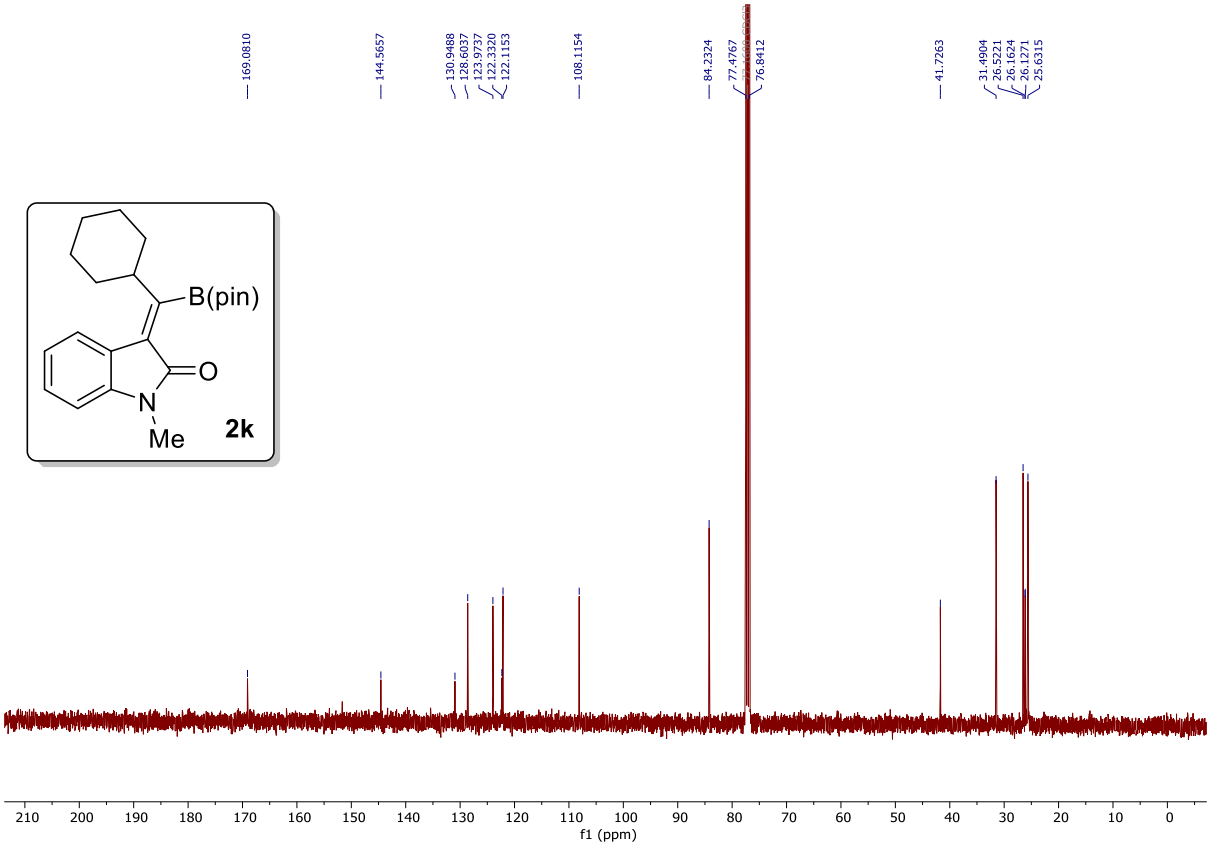
7.0336
7.0146
6.9954
6.7911
6.7715
3.1910
3.1210
3.1137
3.0927
3.0826
1.9149
1.8830
1.8705
1.8396
1.7850
1.7530
1.4427
1.2986
1.2910
1.2784
1.2572
1.2405
1.2404
B(pin)
O
N
Me
2k
1.02
1.11
1.10
1.00
2.97
0.94
3.94
1.82
12.34
3.98
f1 (ppm)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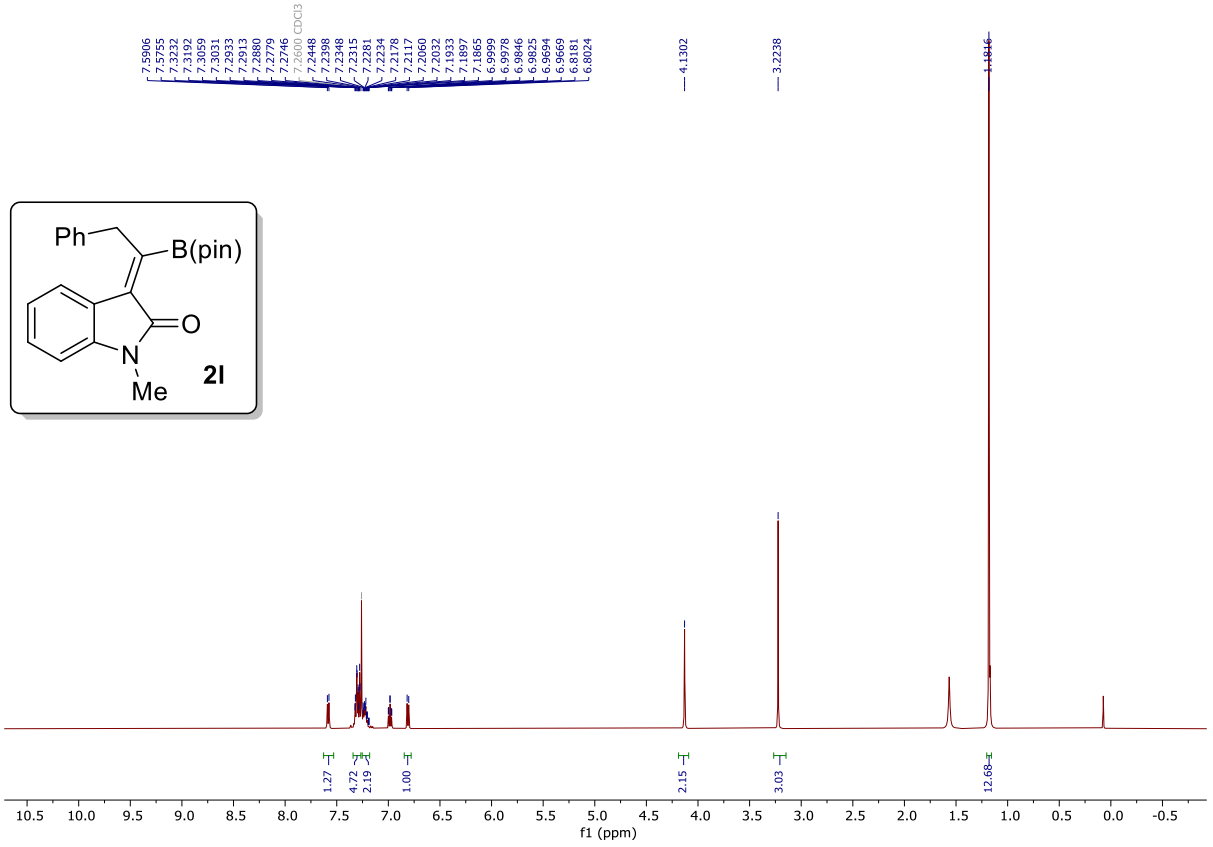
144.5657
130.9488
128.6037
123.9737
122.3320
122.1153
108.1154
84.2324
77.4767
76.8412
41.7263
31.4904
26.5221
26.1624
26.1271
25.6315
B(pin)
O
N
Me
2k
f1 (ppm)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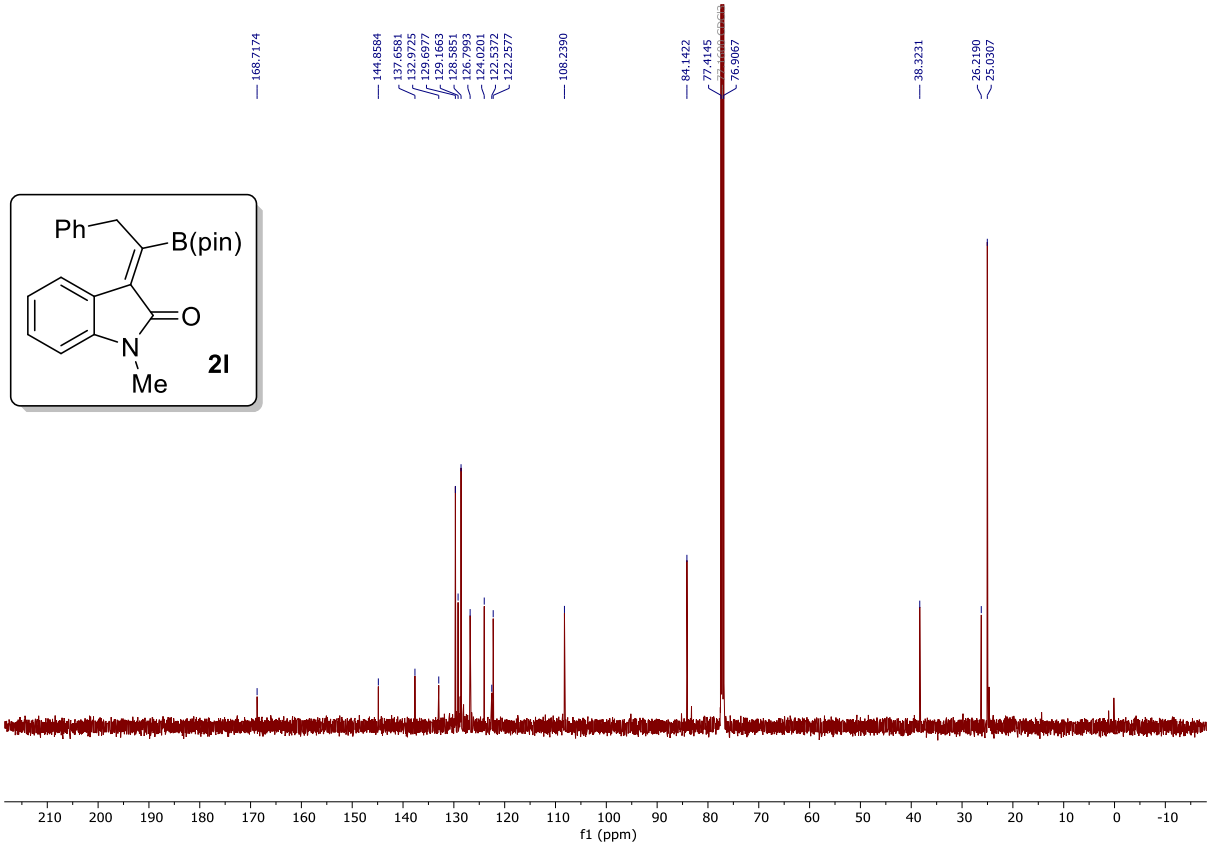
7.5755
7.3232
7.3192
7.3059
7.3031
7.2933
7.2913
7.2880
7.2779
7.2746
7.2600 CDCl3
7.2448
7.2398
7.2348
7.2315
7.2281
7.2234
7.2178
7.2117
7.2060
7.2032
7.1933
7.1897
7.1865
6.9999
6.9978
6.9846
6.9825
6.9694
6.9669
6.8181
6.8024
4.1302
3.2238
1.1816
Ph
B(pin)
O
N
Me
2l
1.27
4.72
2.19
1.00
2.15
3.03
12.68
f1 (ppm)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122.2577
108.2390
84.1422
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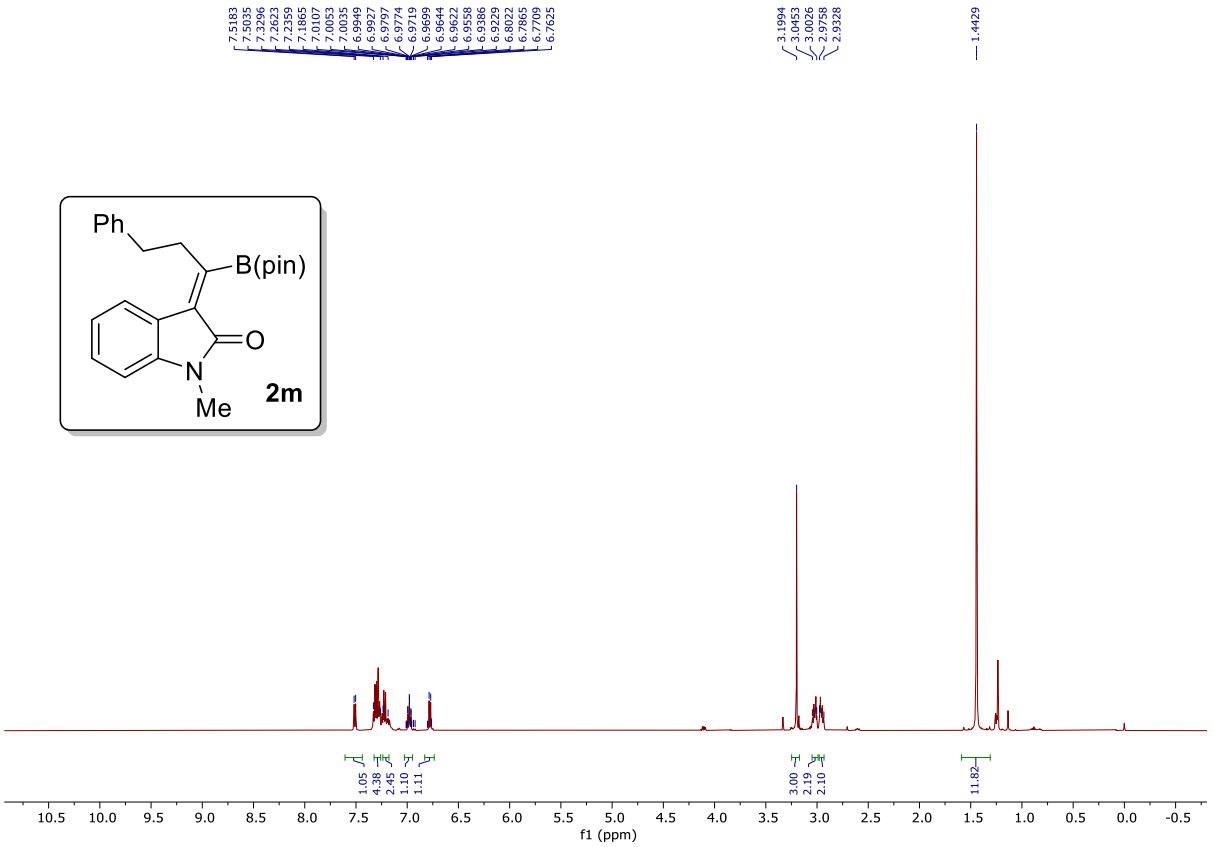
38.3231
26.2190
25.0307
Ph
B(pin)
O
N
Me
2l
f1 (ppm)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7.0053
7.0035
6.9948
6.9927
6.9797
6.9774
6.9719
6.9699
6.9644
6.9622
6.9558
6.9386
6.9229
6.8022
6.7865
6.7709
6.7625
3.1994
3.0453
3.0026
2.9758
2.9328
1.4429
Ph
B(pin)
O
N
Me
2m
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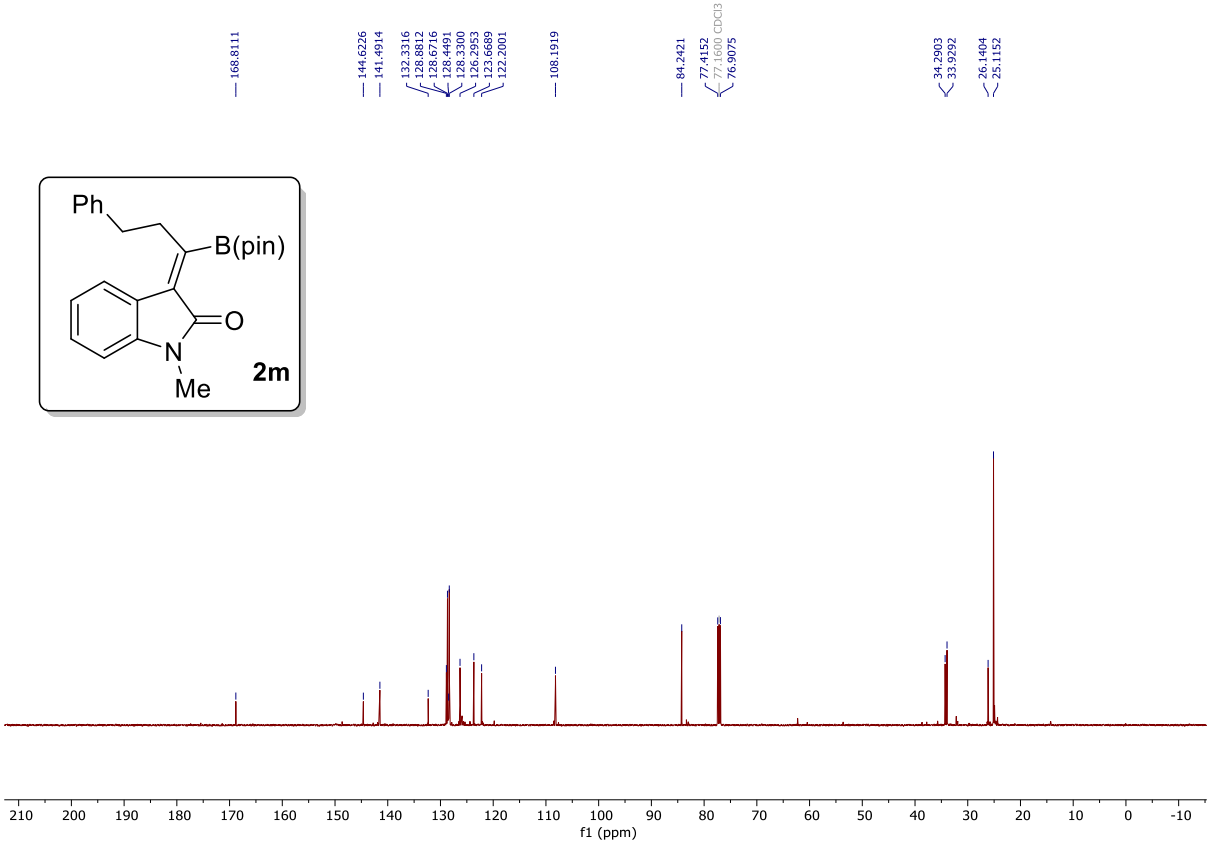
4.38
2.45
1.10
1.11
3.00
2.19
2.10
11.82
f1 (ppm)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126.2953
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122.2001
108.1919
84.2421
77.4152
77.1600 CDCl3
76.9075
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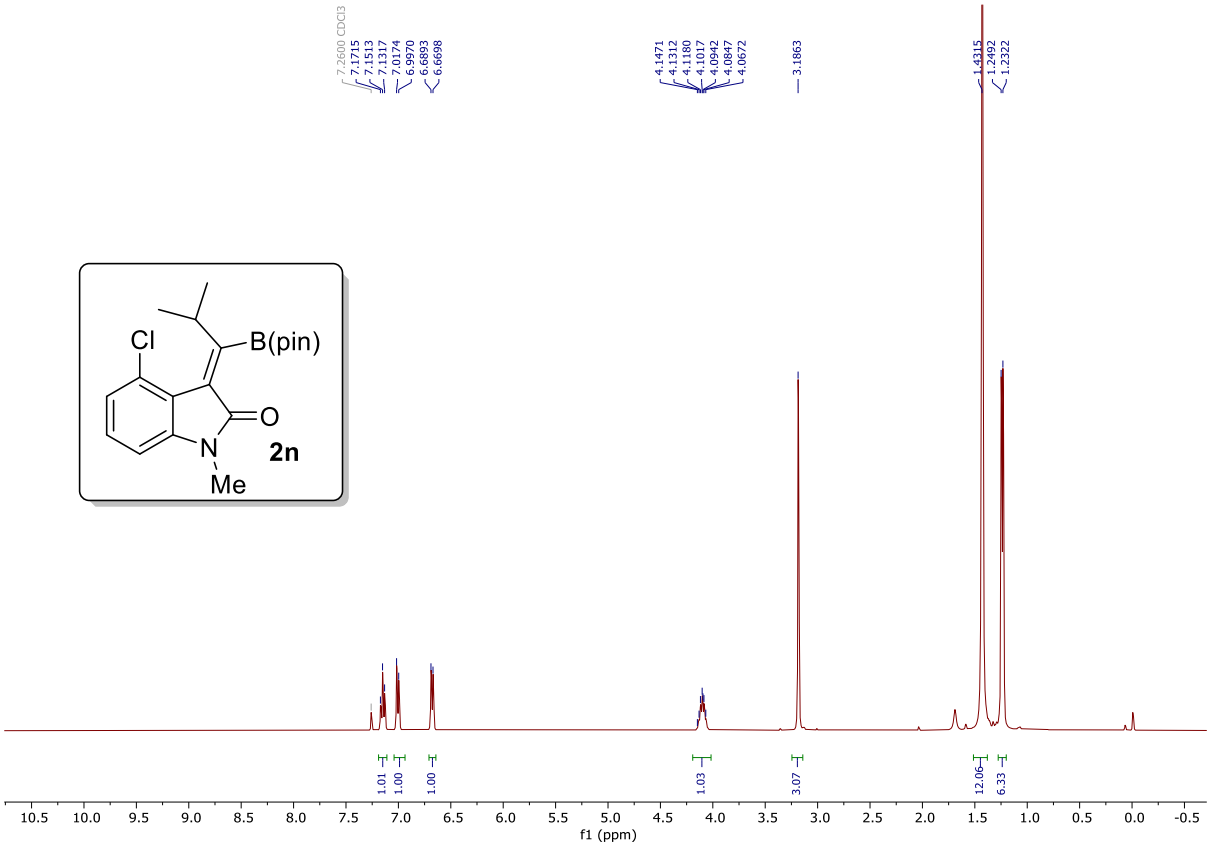
33.9292
26.1404
25.1152
Ph
B(pin)
O
N
Me
2m
f1 (ppm)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7.1317
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6.6893
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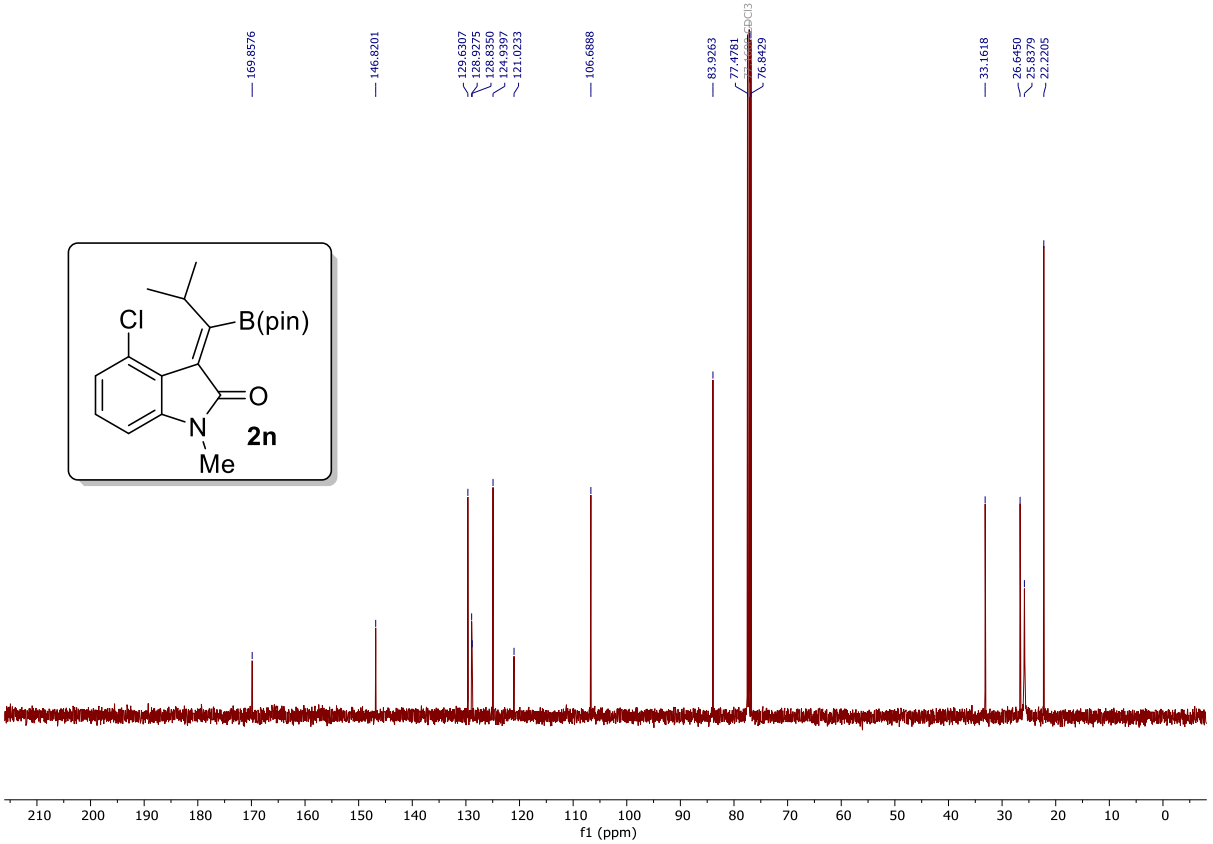
4.1471
4.1312
4.1180
4.1017
4.0942
4.0847
4.0672
3.1863
1.4315
1.2492
1.2322
Cl
B(pin)
O
N
Me
2n
1.01
1.00
1.00
1.03
3.07
12.06
6.33
f1 (ppm)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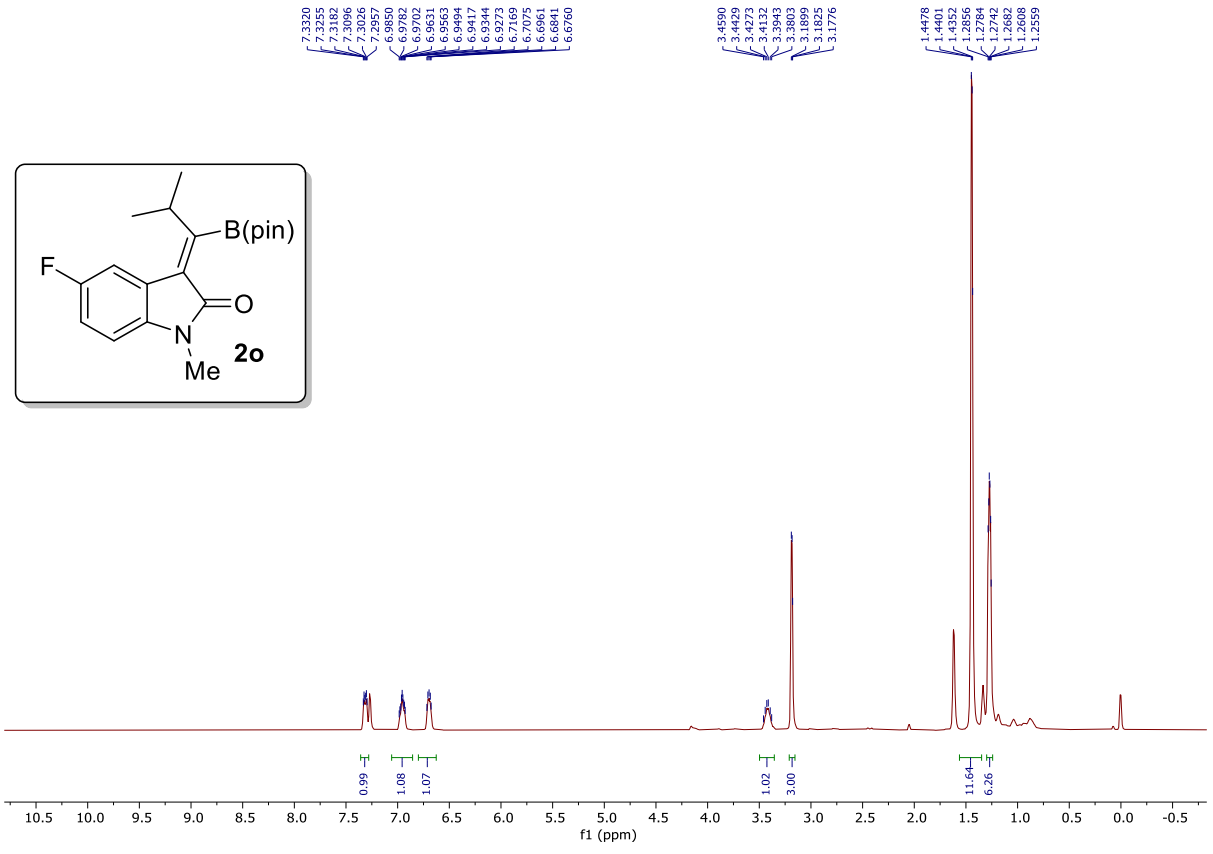
26.6450
25.8379
22.2205
Cl
B(pin)
O
N
Me
2n
f1 (ppm)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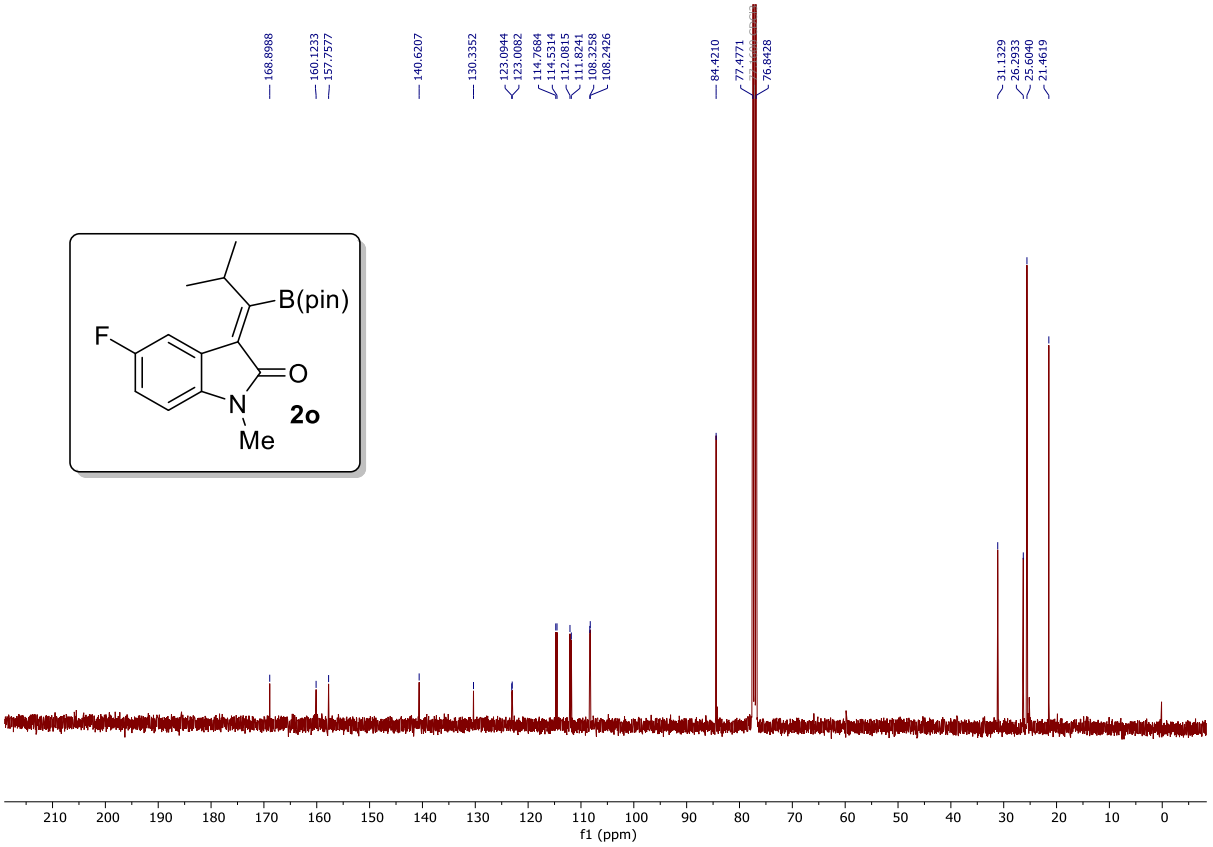
6.9417
6.9344
6.9273
6.7169
6.7075
6.6961
6.6841
6.6760
3.4590
3.4429
3.4273
3.4132
3.3943
3.3803
3.1899
3.1825
3.1776
1.4478
1.4401
1.4352
1.2856
1.2784
1.2742
1.2682
1.2608
1.2559
F
B(pin)
O
N
Me
2o
0.99
1.08
1.07
1.02
3.00
11.64
6.26
f1 (ppm)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112.0815
111.8241
108.3258
108.2426
84.4210
77.4771
76.8428
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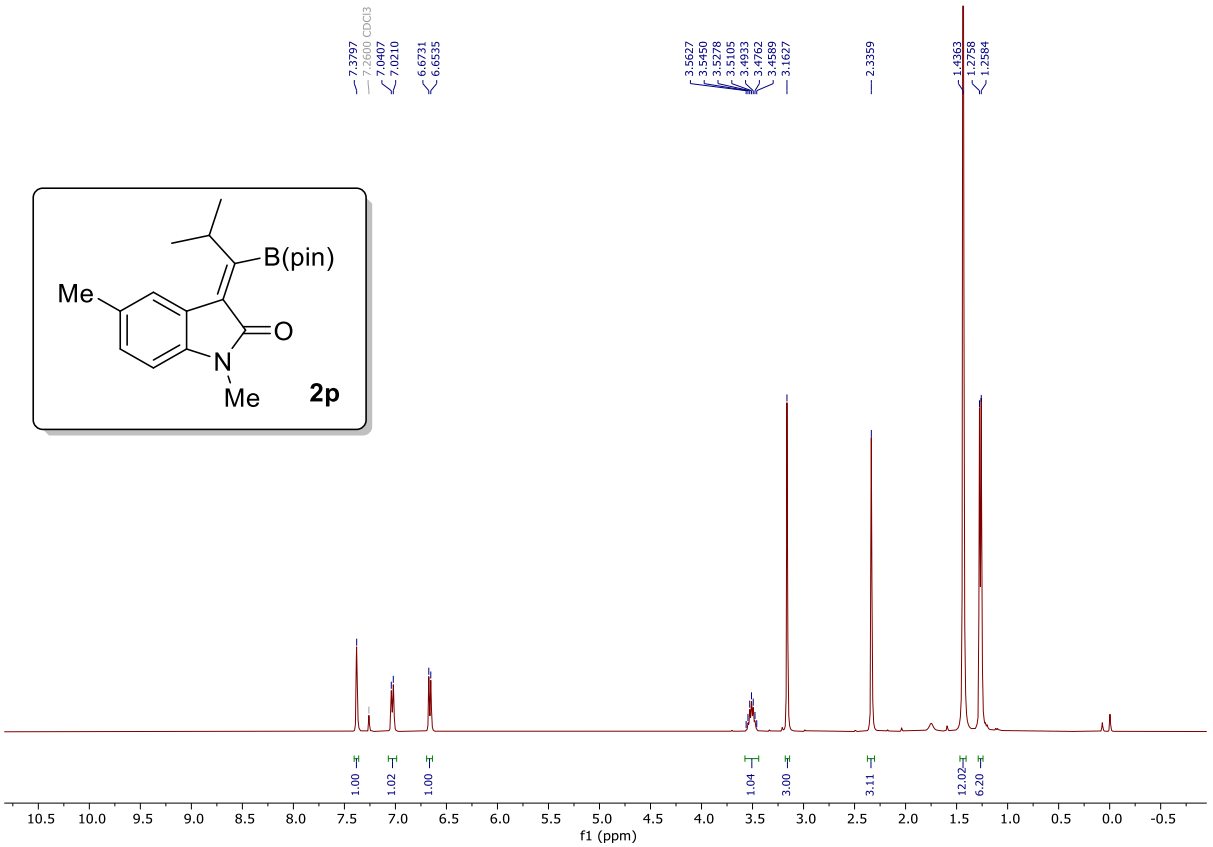
26.2933
25.6040
21.4619
B(pin)
F
O
N
Me
2o
f1 (ppm)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3.5105
3.4933
3.4762
3.4589
3.1627
2.3359
1.4363
1.2758
1.2584
B(pin)
Me
O
N
Me
2p
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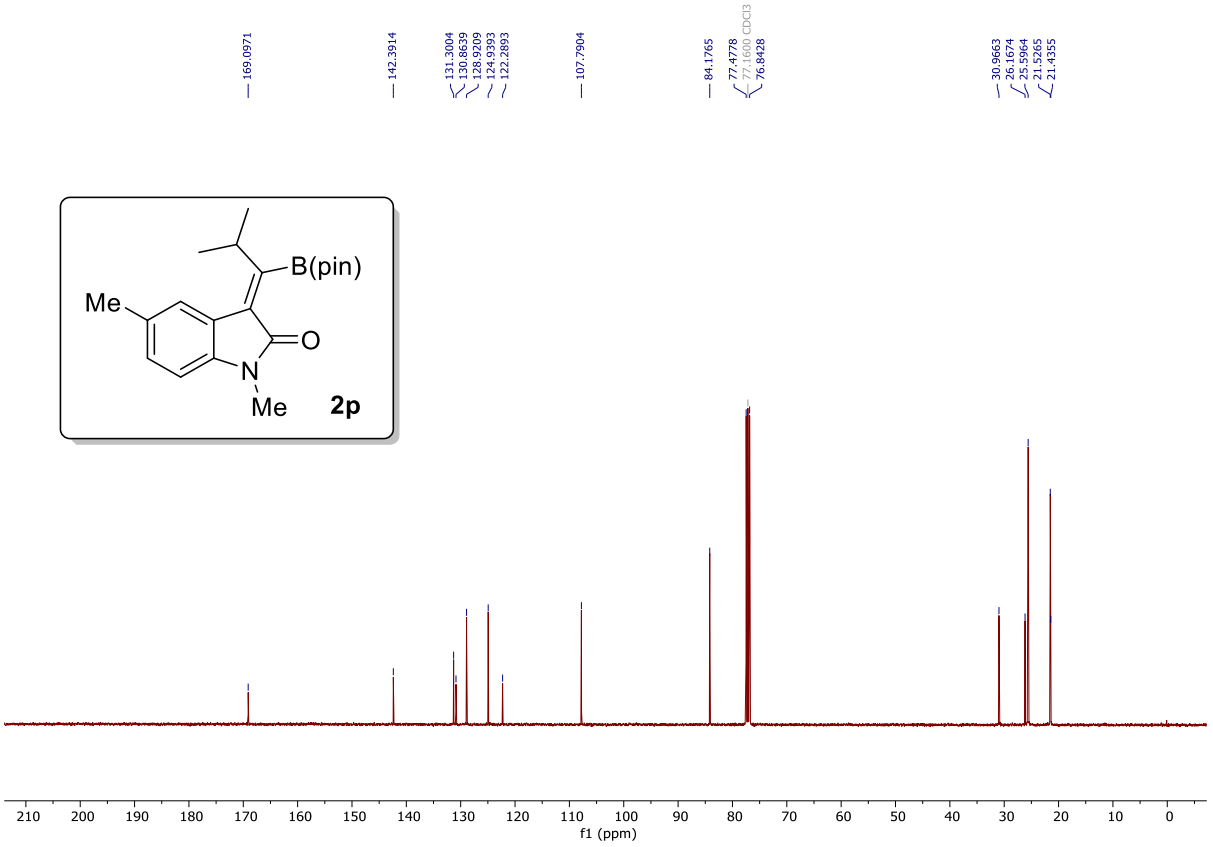
1.00
1.04
3.00
3.11
12.02
6.20
f1 (ppm)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122.2893
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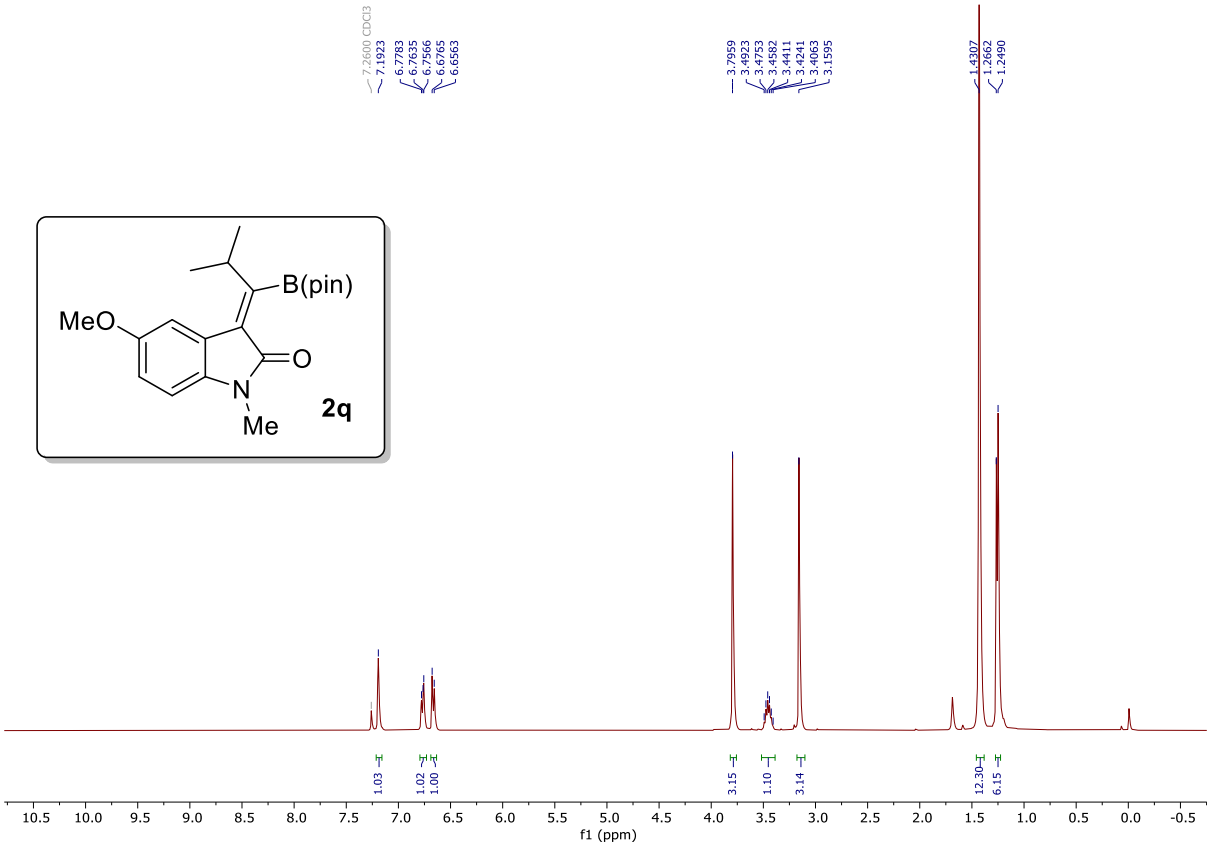
84.1765
77.4778
77.1600 CDCl3
76.8428
30.9663
26.1674
25.5964
21.5265
21.4355
B(pin)
Me
O
N
Me
2p
f1 (ppm)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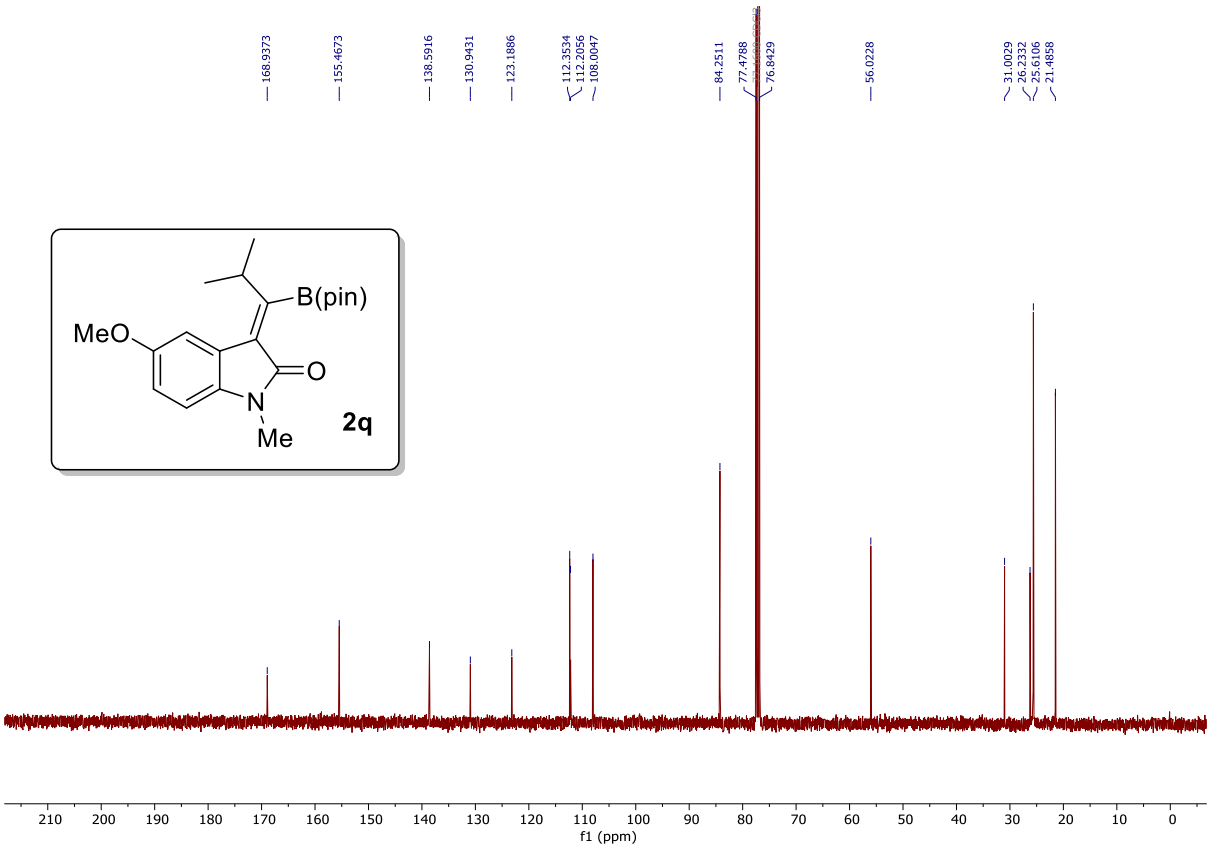
6.7566
6.6765
6.6563
3.7959
3.4923
3.4753
3.4582
3.4411
3.4241
3.4063
3.1595
1.4307
1.2662
1.2490
1.03
1.02
1.00
3.15
1.10
3.14
12.30
6.15
B(pin)
MeO
O
N
Me
2q
f1 (ppm)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77.4788
76.8429
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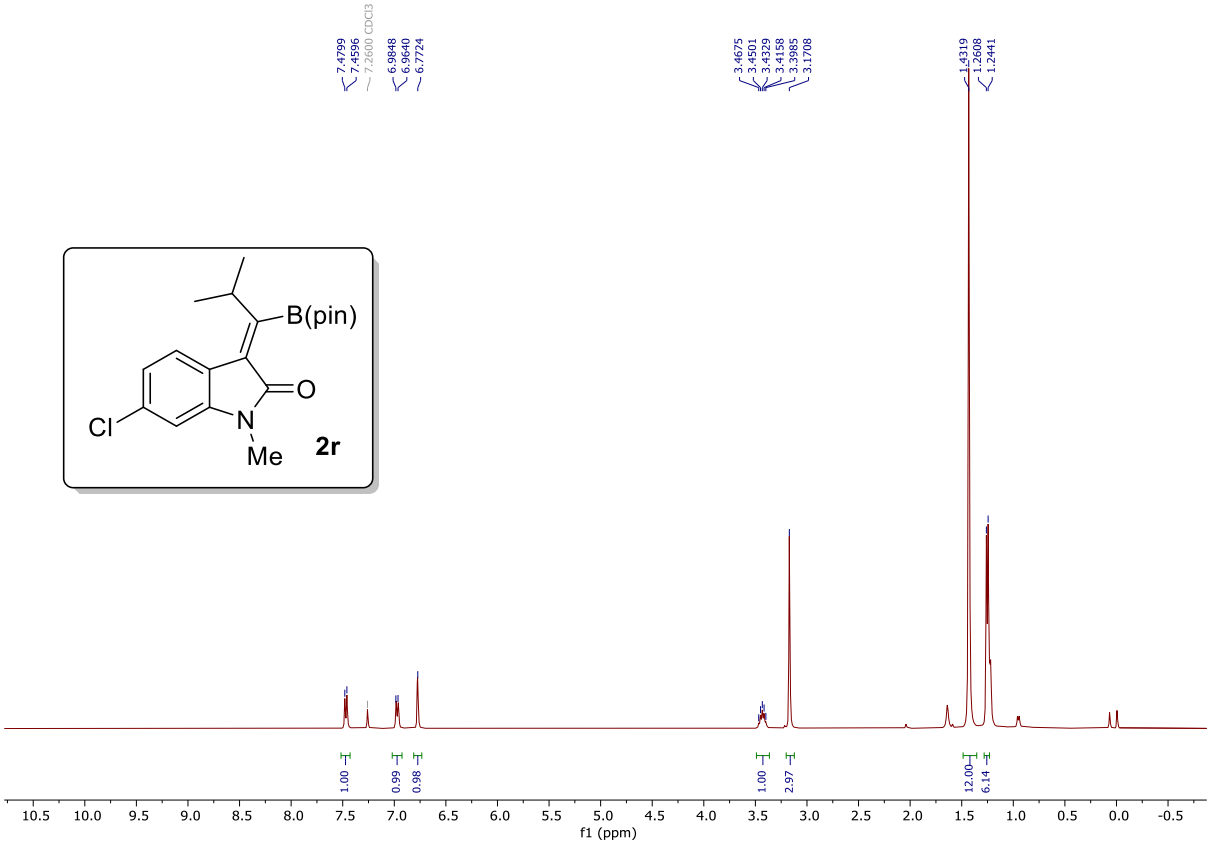
26.2332
25.6106
21.4858
B(pin)
MeO
O
N
Me
2q
f1 (ppm)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7.2600 CDCl3
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6.9640
6.7724
3.4675
3.4501
3.4329
3.4158
3.3985
3.1708
1.4319
1.2608
1.2441
B(pin)
Cl
O
N
Me
2r
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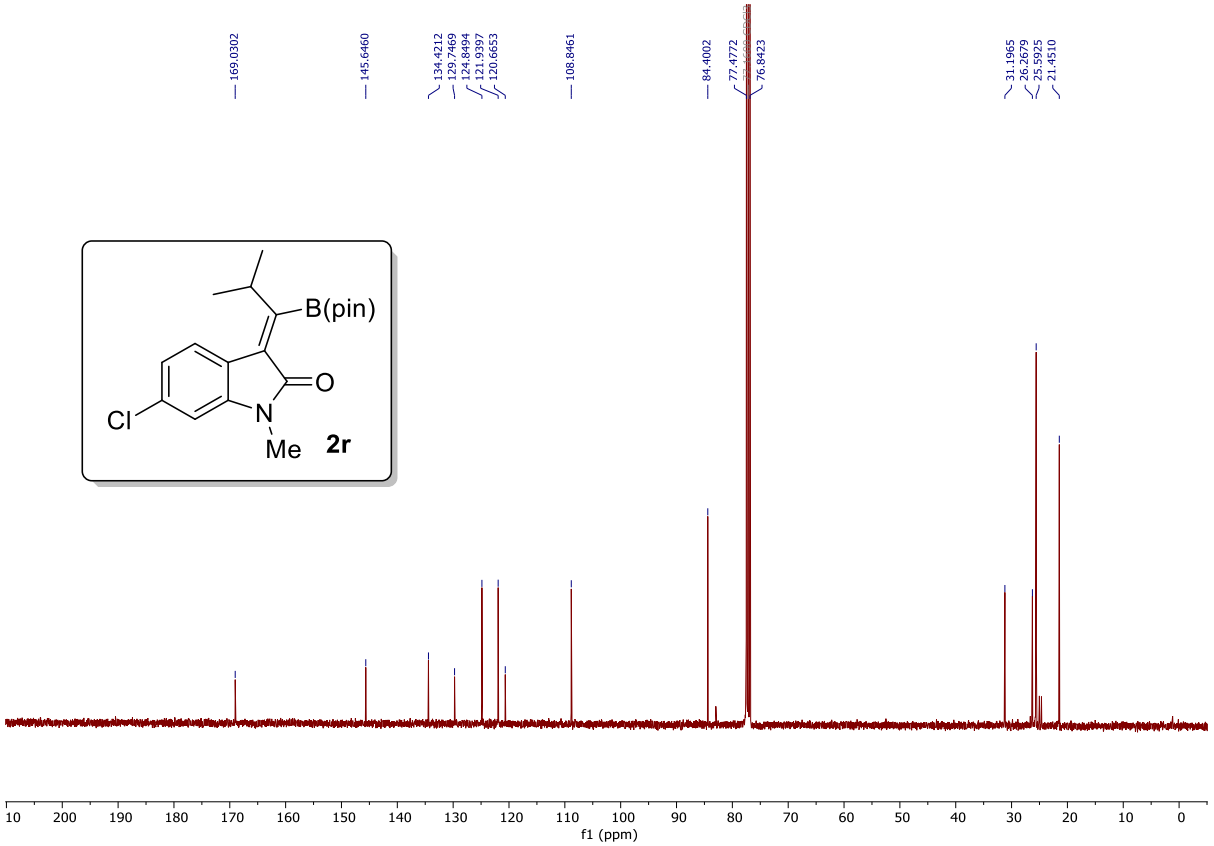
0.98
1.00
2.97
12.00
6.14
f1 (ppm)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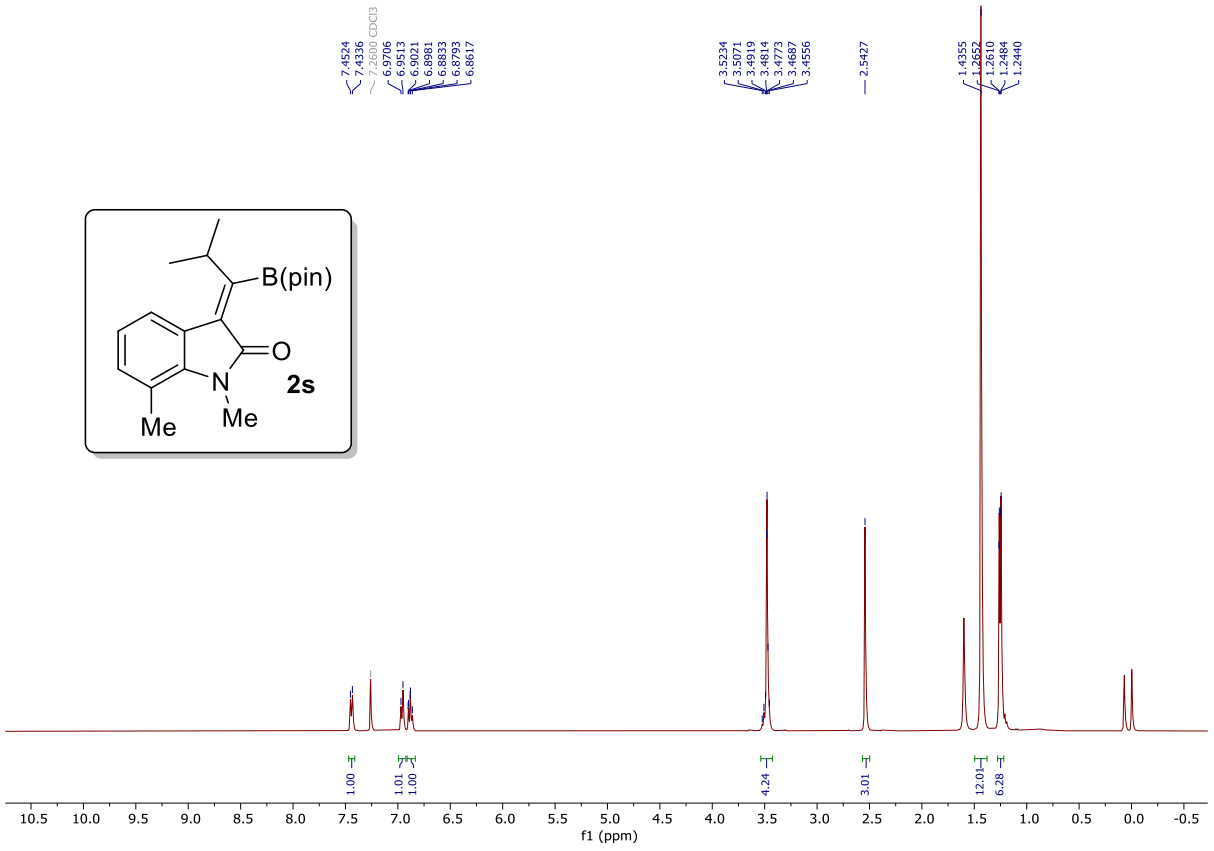
134.4212
129.7469
124.8494
121.9397
120.6653
108.8461
84.4002
77.4772
76.8423
31.1965
26.2679
25.5925
21.4510
B(pin)
O
N
Cl
Me
2r
f1 (ppm)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6.8883
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6.8617
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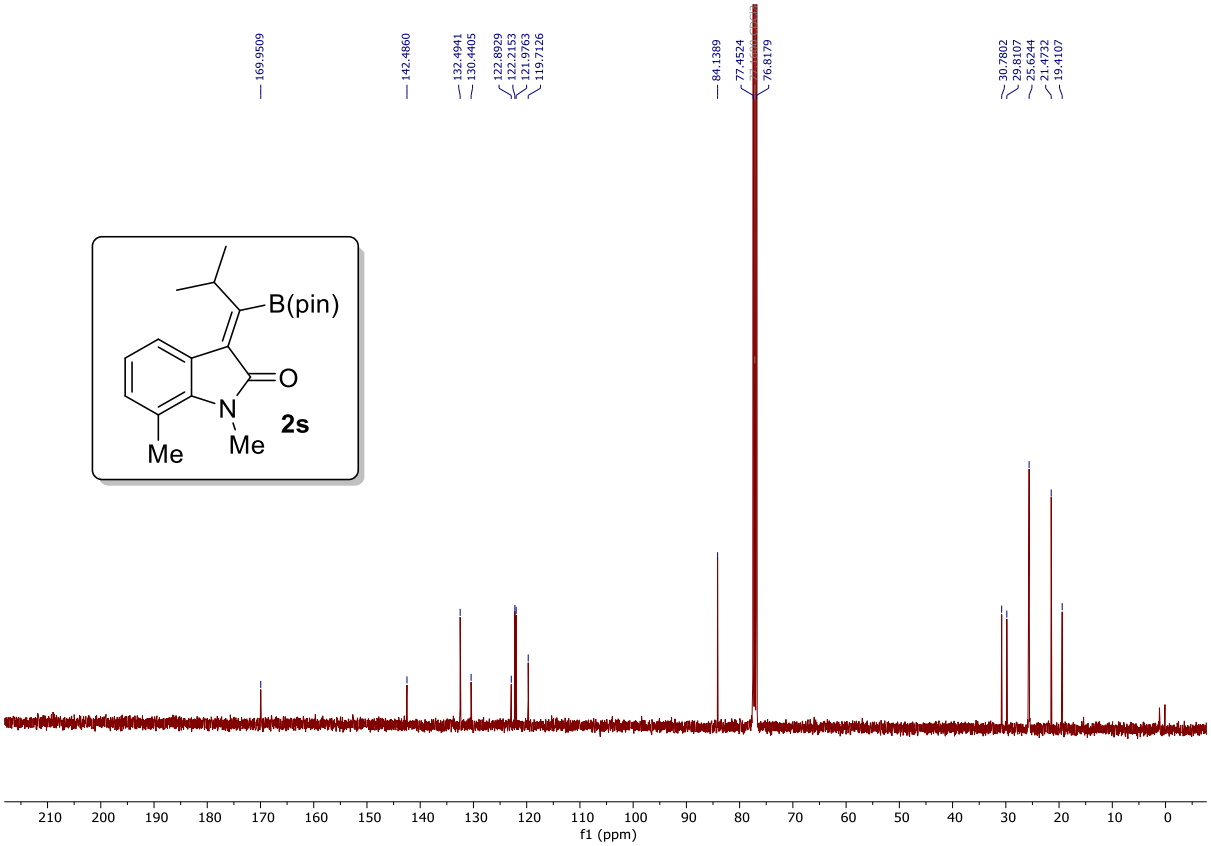
3.5071
3.4919
3.4814
3.4773
3.4687
3.4556
2.5427
1.4355
1.2652
1.2610
1.2484
1.2440
1.00
1.01
1.00
4.24
3.01
12.01
6.28
B(pin)
O
N
Me
Me
2s
f1 (ppm)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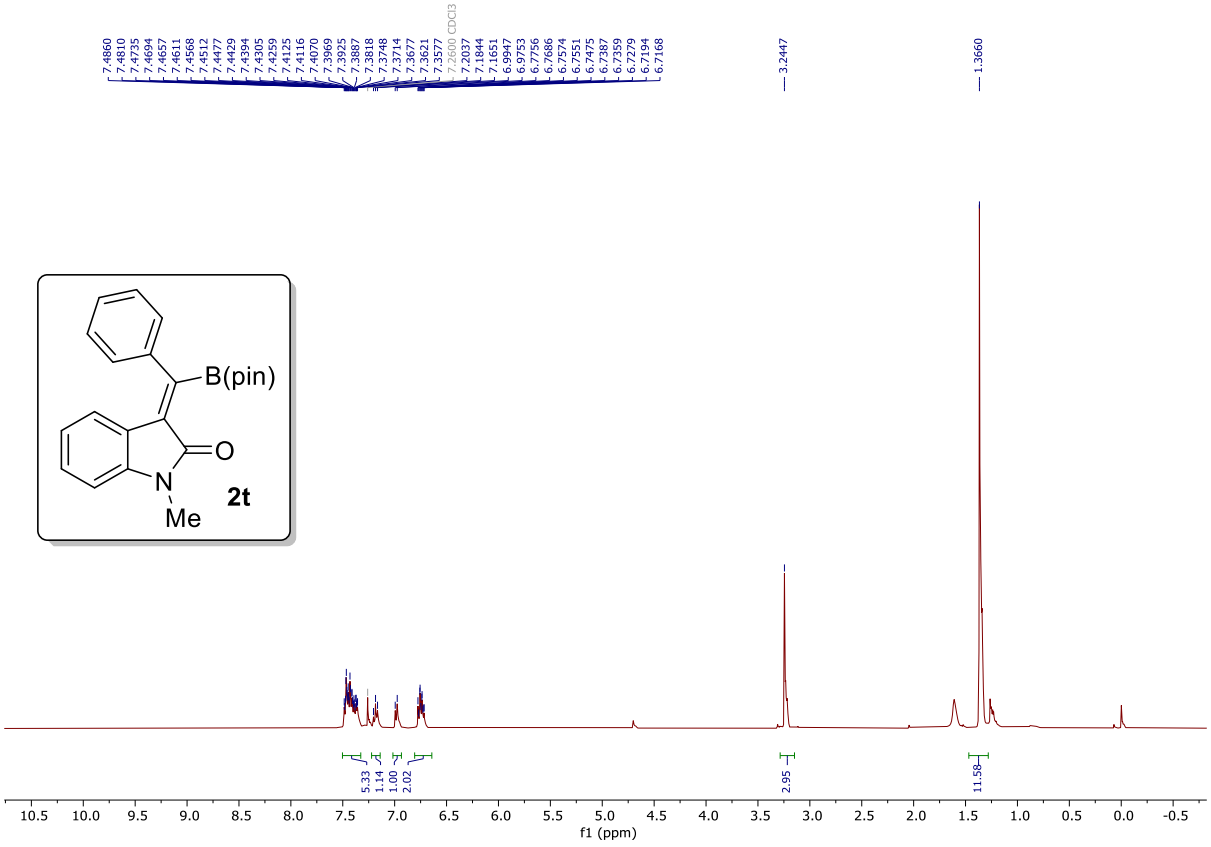
132.4941
130.4405
122.8929
122.2153
121.9763
119.7126
84.1389
77.4524
76.8179
30.7802
29.8107
25.6244
21.4732
19.4107
B(pin)
O
N
Me
Me
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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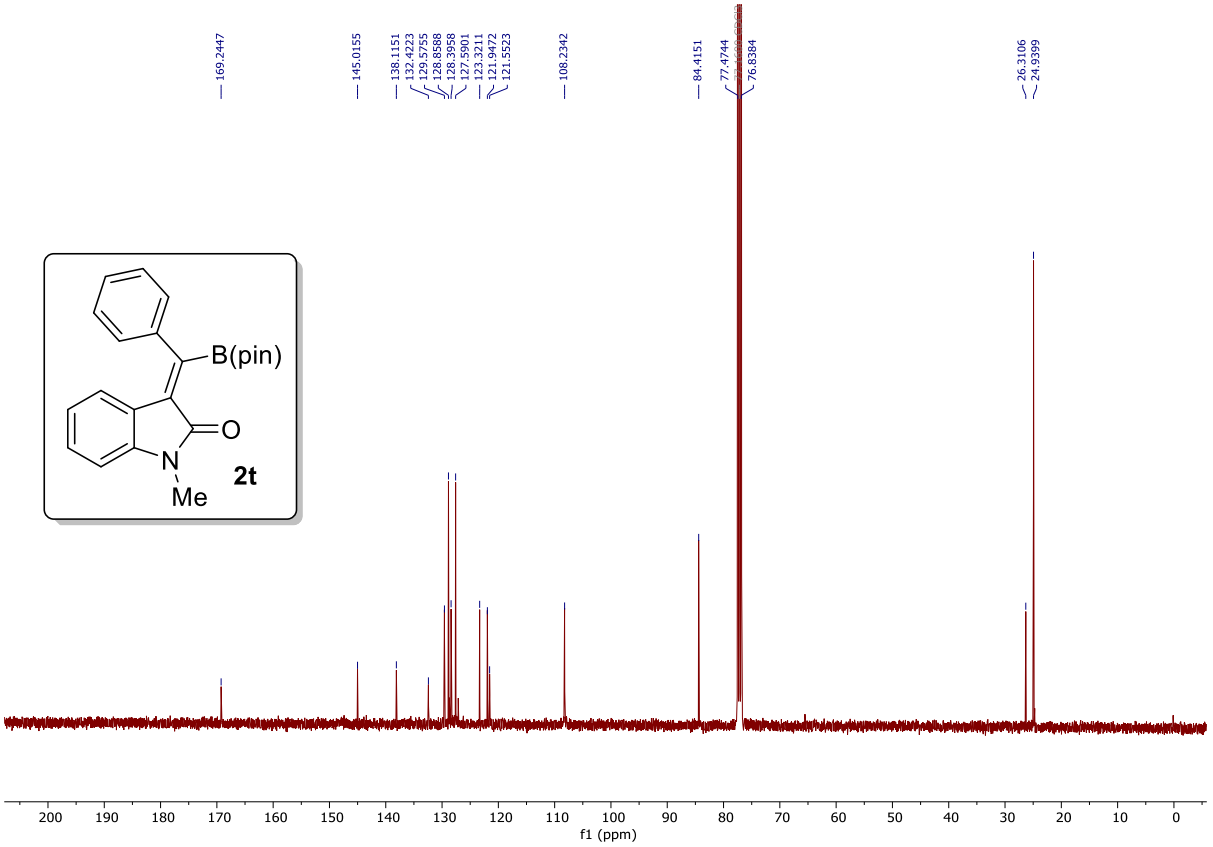
7.4477
7.4429
7.4394
7.4305
7.4259
7.4125
7.4116
7.4070
7.3969
7.3925
7.3887
7.3818
7.3748
7.3714
7.3677
7.3621
7.3577
7.2600 CDCl3
7.2037
7.1844
7.1651
6.9947
6.9753
6.7756
6.7686
6.7574
6.7551
6.7475
6.7387
6.7359
6.7279
6.7194
6.7168
3.2447
1.3660
B(pin)
O
N
Me
2t
5.33
1.14
1.00
2.02
2.95
11.58
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.5523
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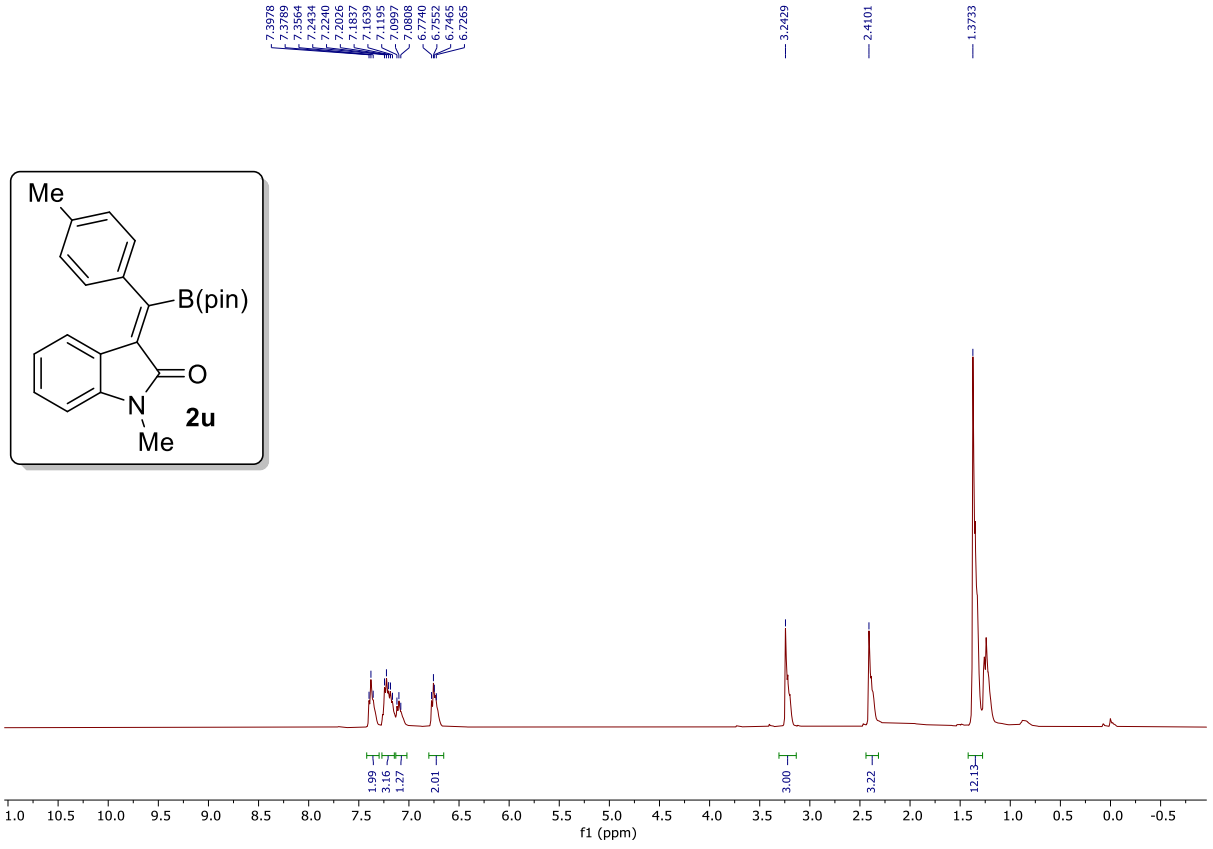
84.4151
77.4744
76.8384
26.3106
24.9399
B(pin)
O
N
Me
2t
f1 (ppm)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7.3564
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7.2240
7.2026
7.1837
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7.1195
7.0997
7.0808
6.7740
6.7552
6.7465
6.7265
3.2429
2.4101
1.3733
Me
B(pin)
O
N
Me
2u
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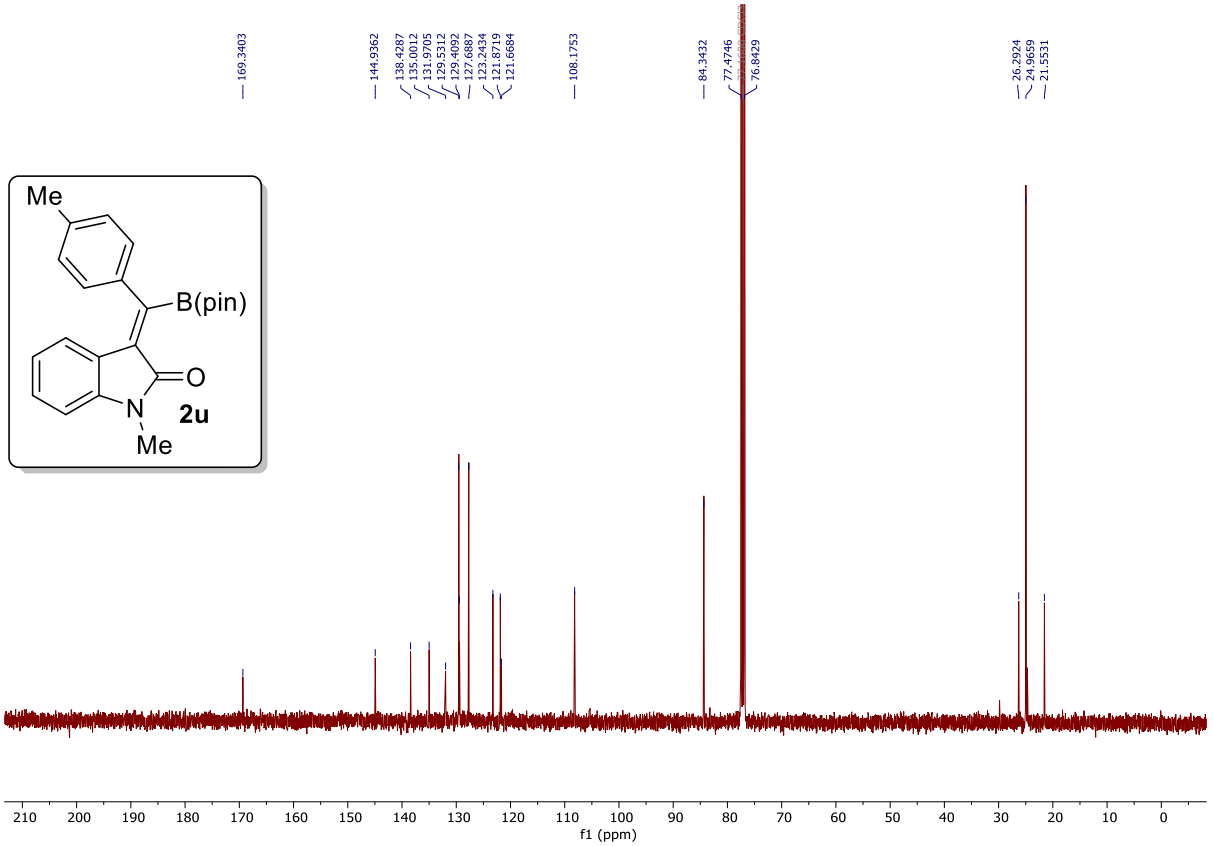
3.16
1.27
2.01
3.00
3.22
12.13
f1 (ppm)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B(pin)
O
N
Me
2u
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131.9705
129.5312
129.4092
127.6887
123.2434
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121.6684
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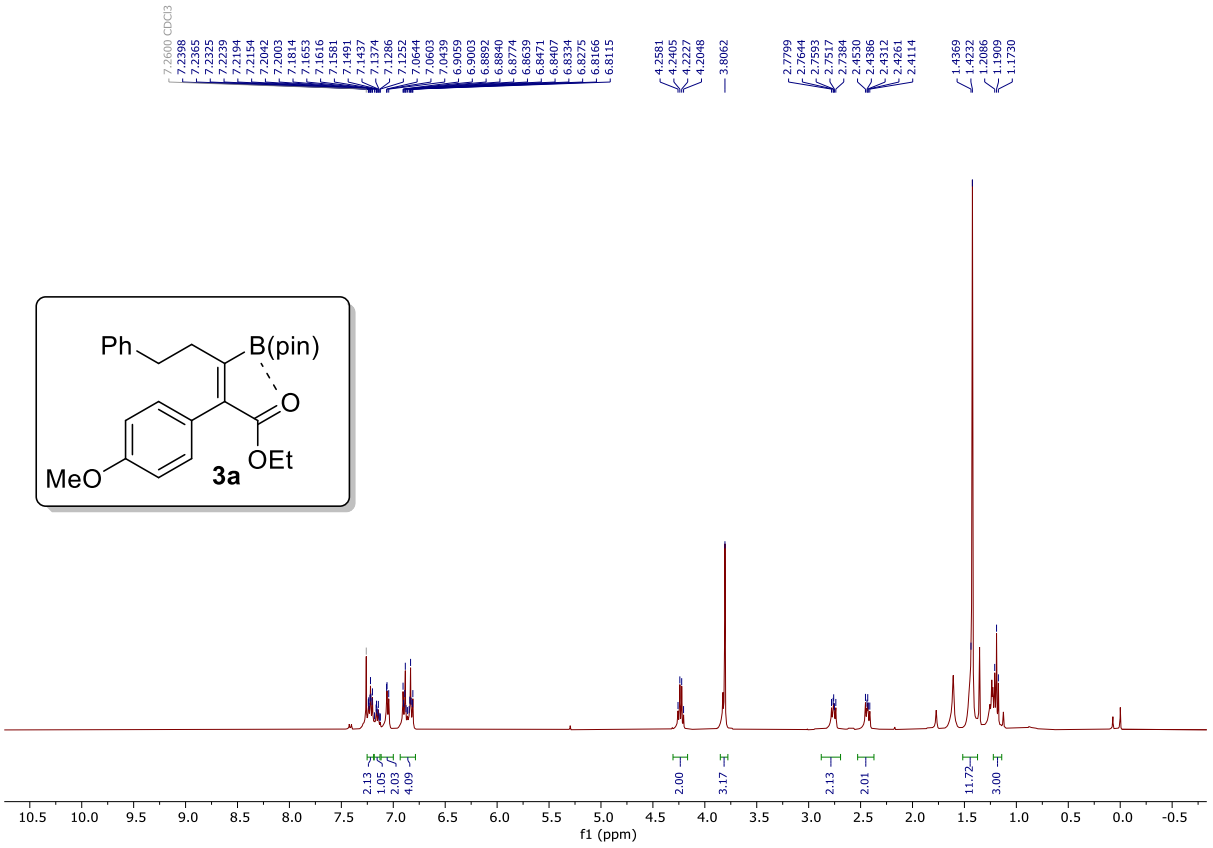
77.4746
76.8429
26.2924
24.9659
21.5531
f1 (ppm)


Ph
B(pin)
O
MeO
OEt
3a
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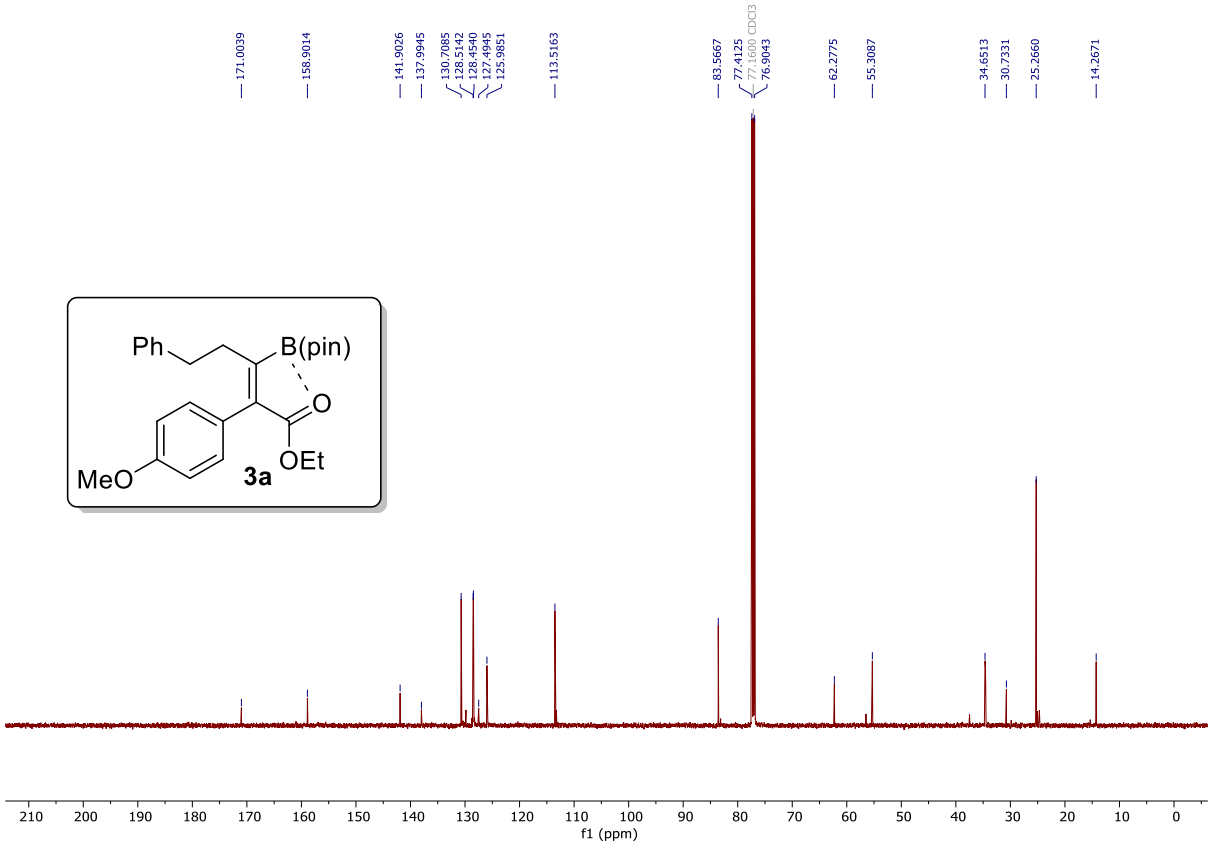
4.2581
4.2405
4.2227
4.2048
3.8062
2.7799
2.7644
2.7593
2.7517
2.7384
2.4530
2.4386
2.4312
2.4261
2.4114
1.4369
1.4232
1.2086
1.1909
1.1730
2.13
1.05
2.03
4.09
2.00
3.17
2.13
2.01
11.72
3.00
f1 (ppm)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113.5163
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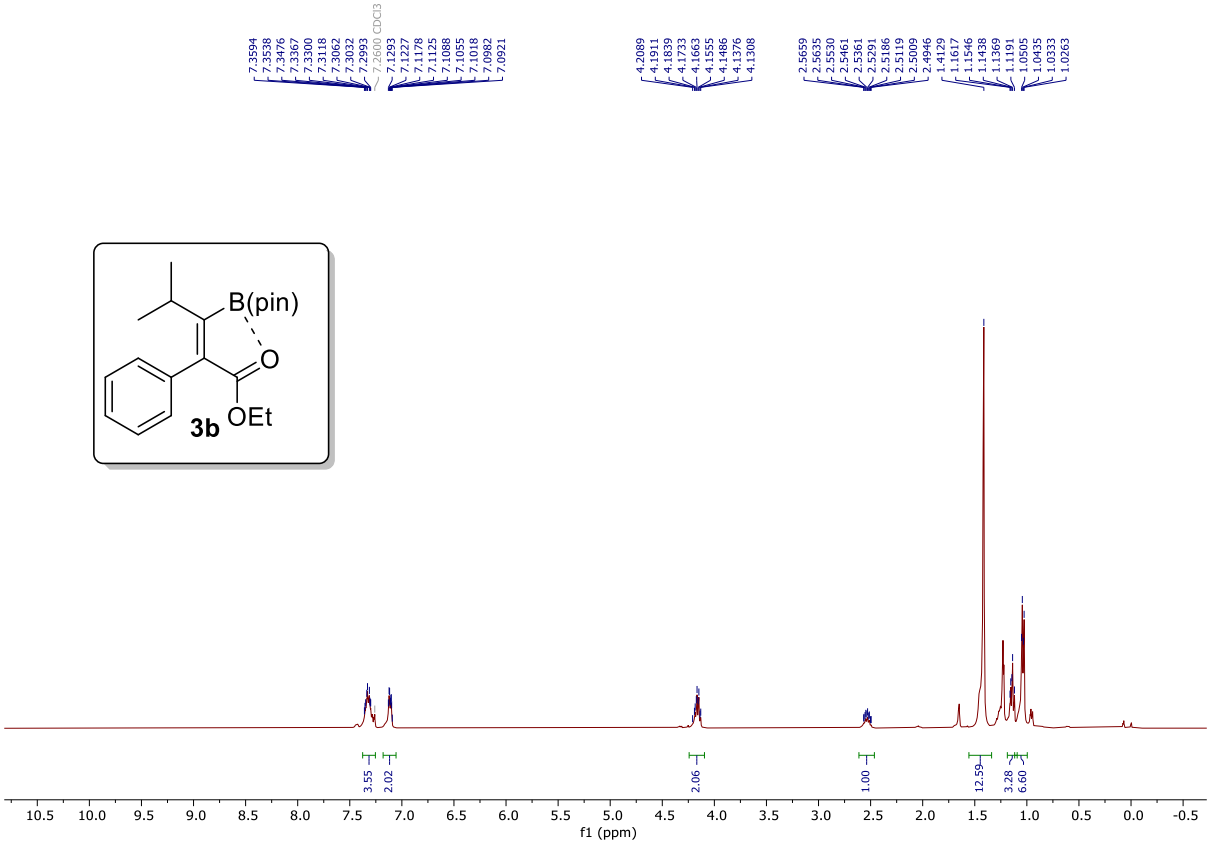
77.1660 CDCl3
76.9043
62.2775
55.3087
34.6513
30.7331
25.2660
14.2671
Ph
B(pin)
O
OEt
MeO
3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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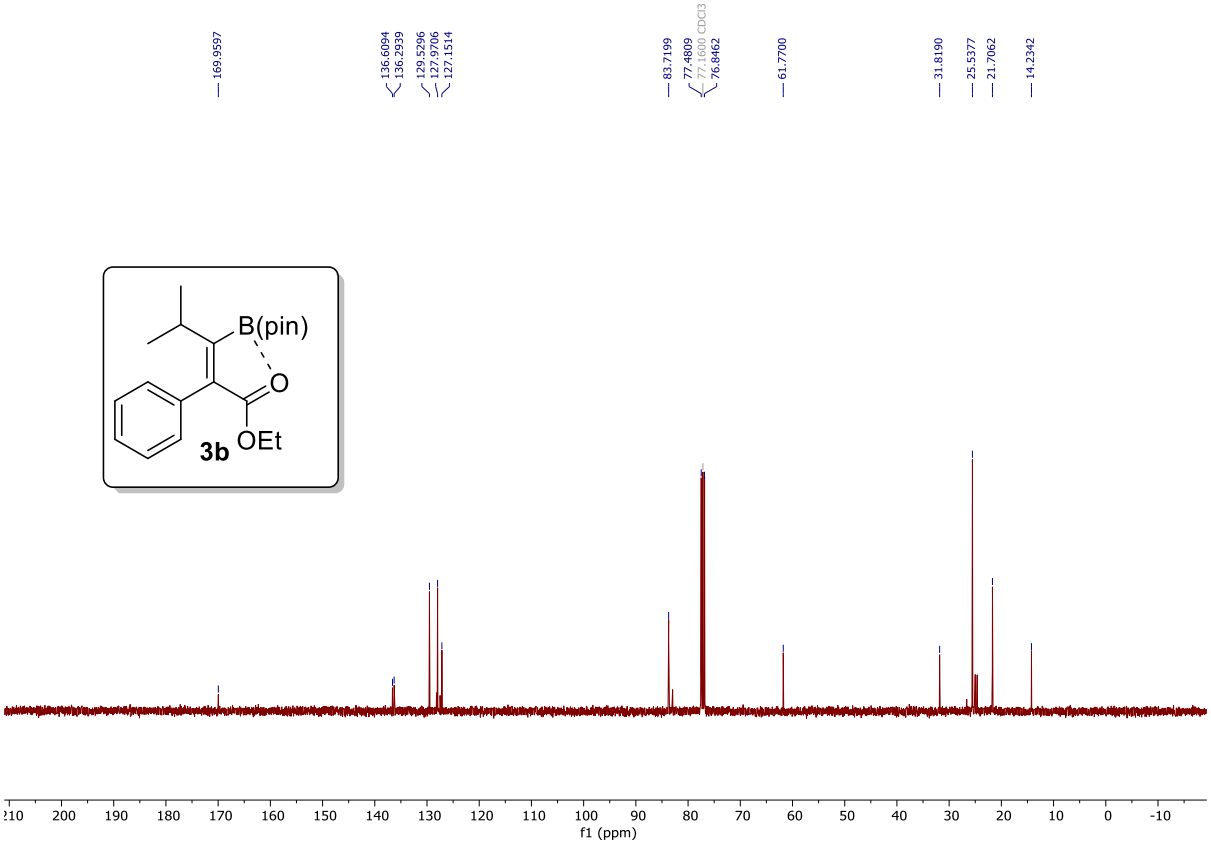
7.3476
7.3367
7.3300
7.3118
7.3062
7.3032
7.2993
7.2600 CDCl3
7.1293
7.1227
7.1178
7.1125
7.1088
7.1055
7.1018
7.0982
7.0921
4.2089
4.1911
4.1839
4.1733
4.1663
4.1555
4.1486
4.1376
4.1308
2.5659
2.5635
2.5530
2.5461
2.5361
2.5291
2.5186
2.5119
2.5009
2.4946
1.4129
1.1617
1.1546
1.1438
1.1369
1.1191
1.0505
1.0435
1.0333
1.0263
B(pin)
O
OEt
3b
3.55
2.02
2.06
1.00
12.59
3.28
6.60
f1 (ppm)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127.1514
83.7199
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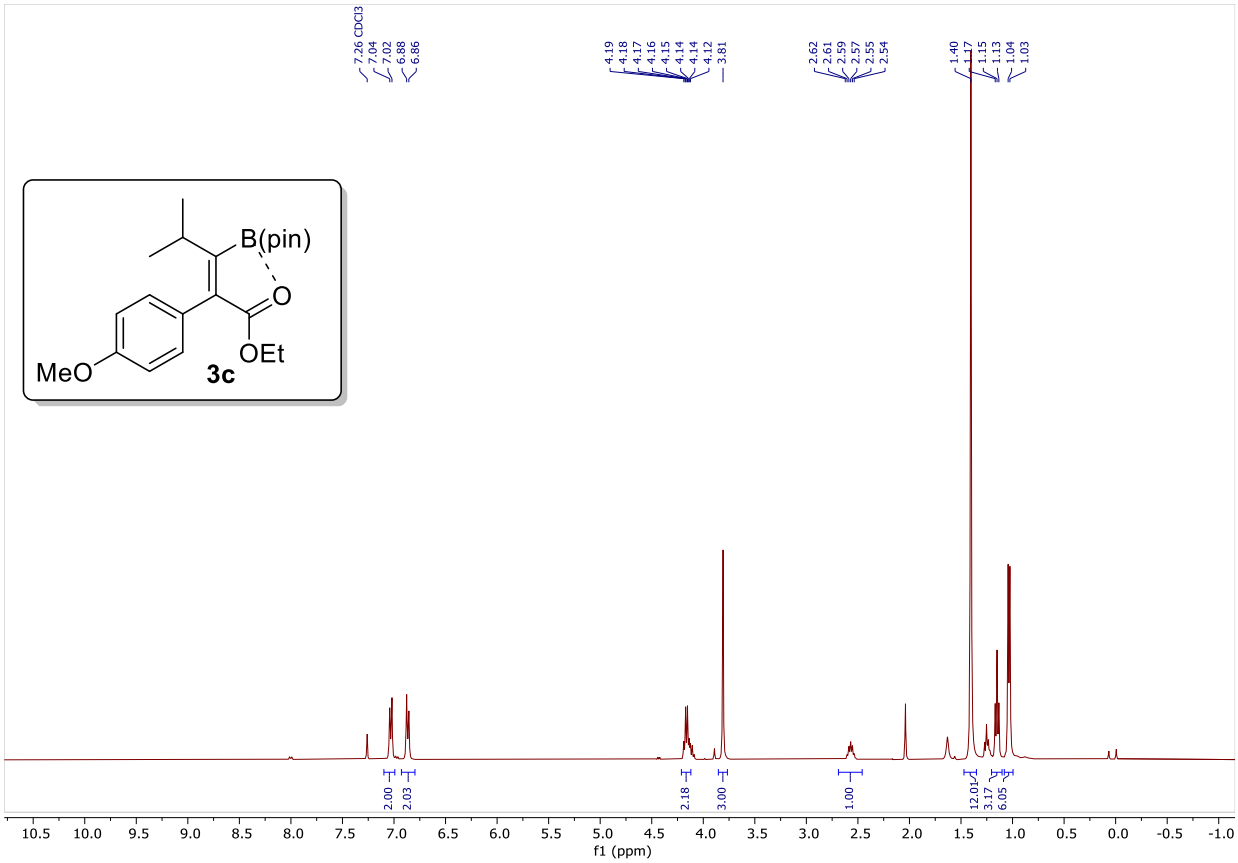
77.1600 CDCl3
76.8462
61.7700
31.8190
25.5377
21.7062
14.2342
B(pin)
O
OEt
3b
f1 (ppm)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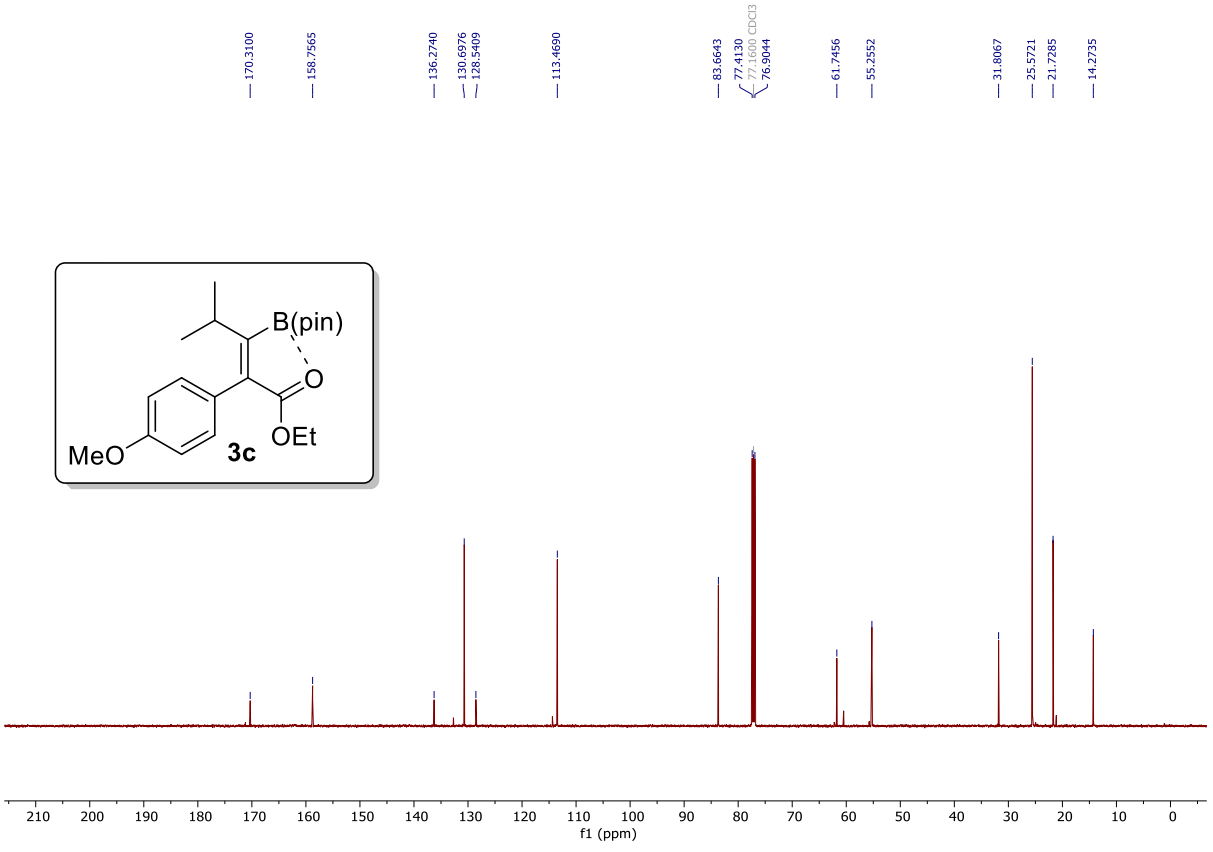
7.02
6.88
6.86
4.19
4.18
4.17
4.16
4.15
4.14
4.14
4.12
3.81
2.62
2.61
2.59
2.57
2.55
2.54
1.40
1.17
1.15
1.13
1.04
1.03
B(pin)
O
OEt
MeO
3c
2.00
2.03
2.18
3.00
1.00
12.01
3.17
6.05
f1 (ppm)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128.5409
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83.6643
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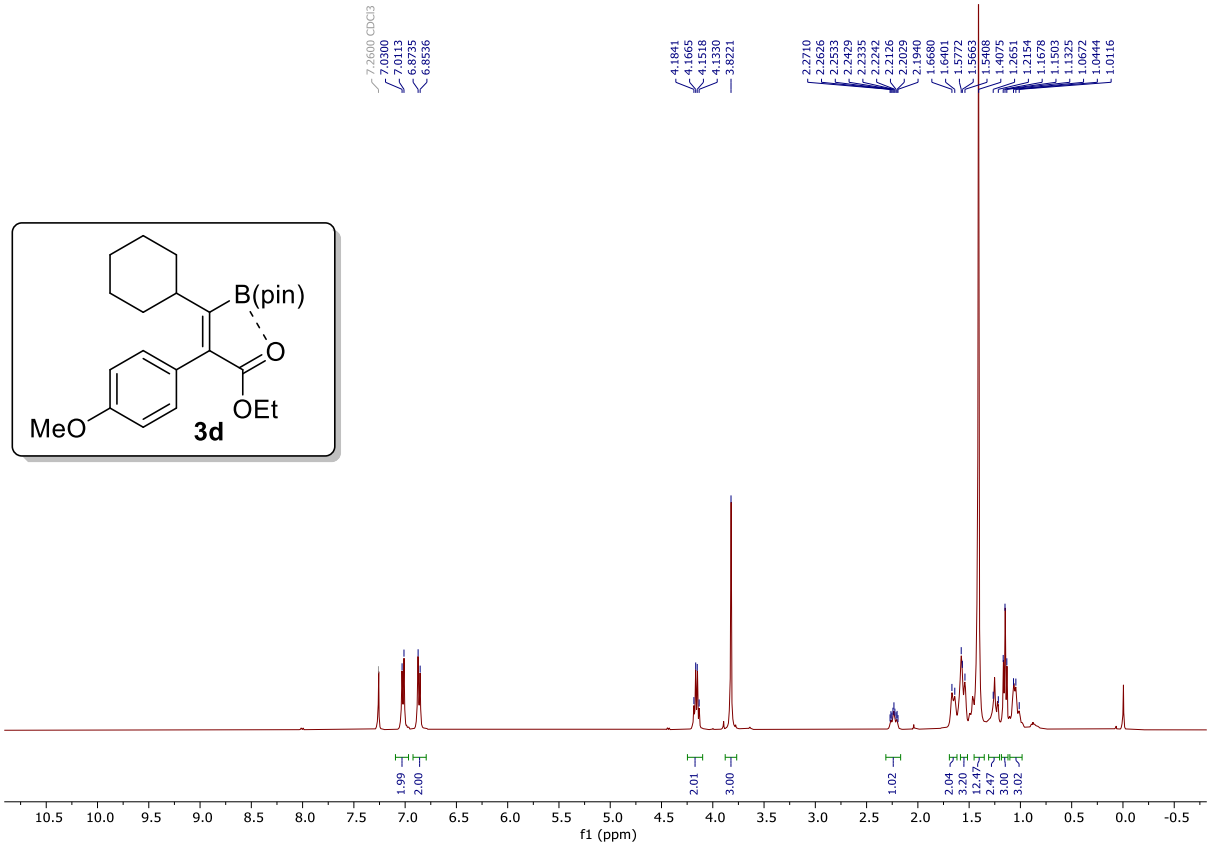
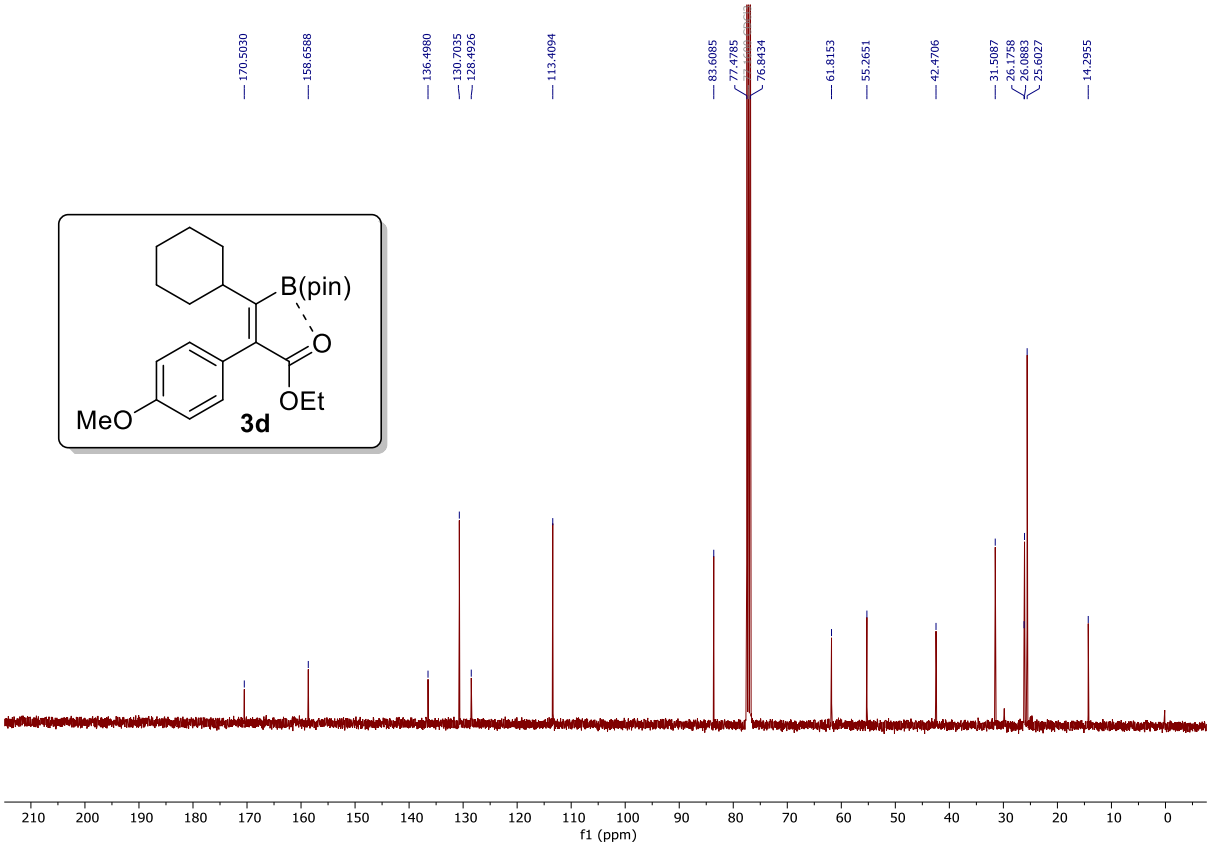
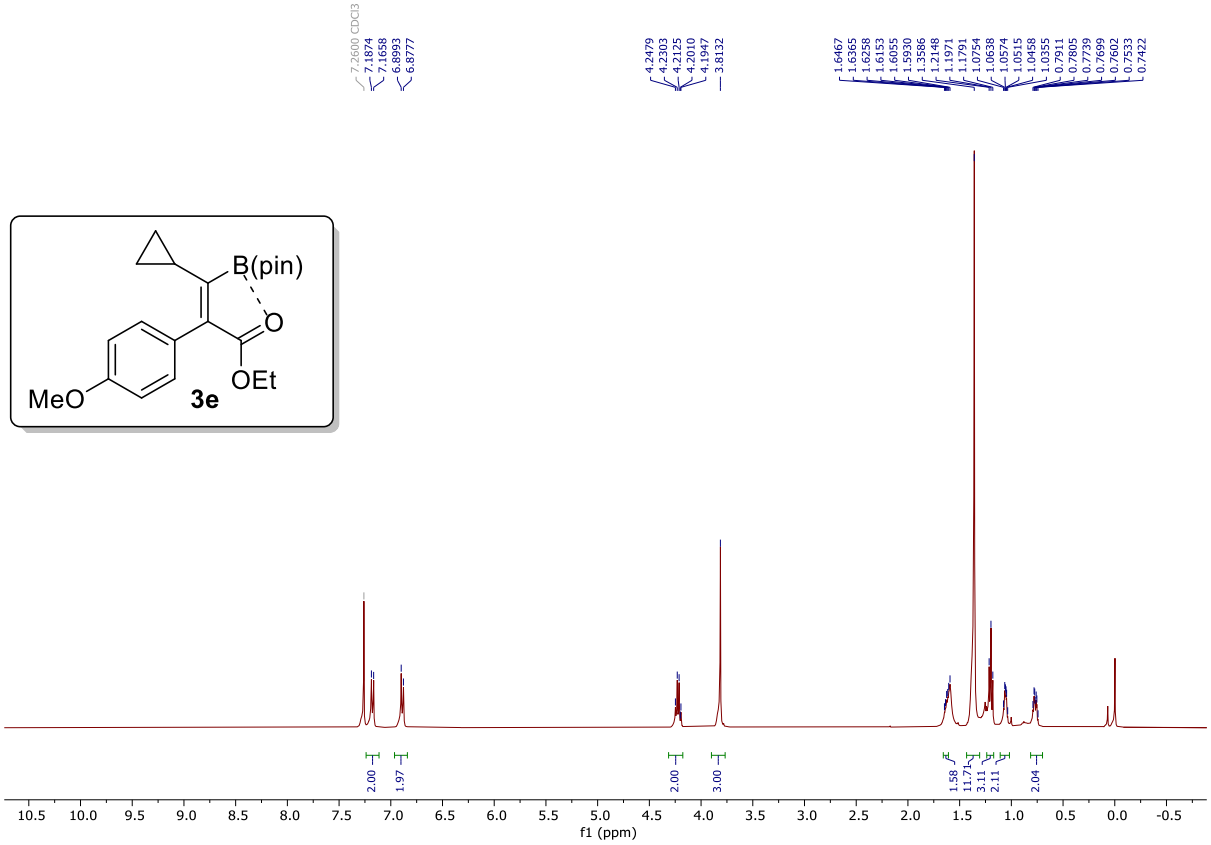
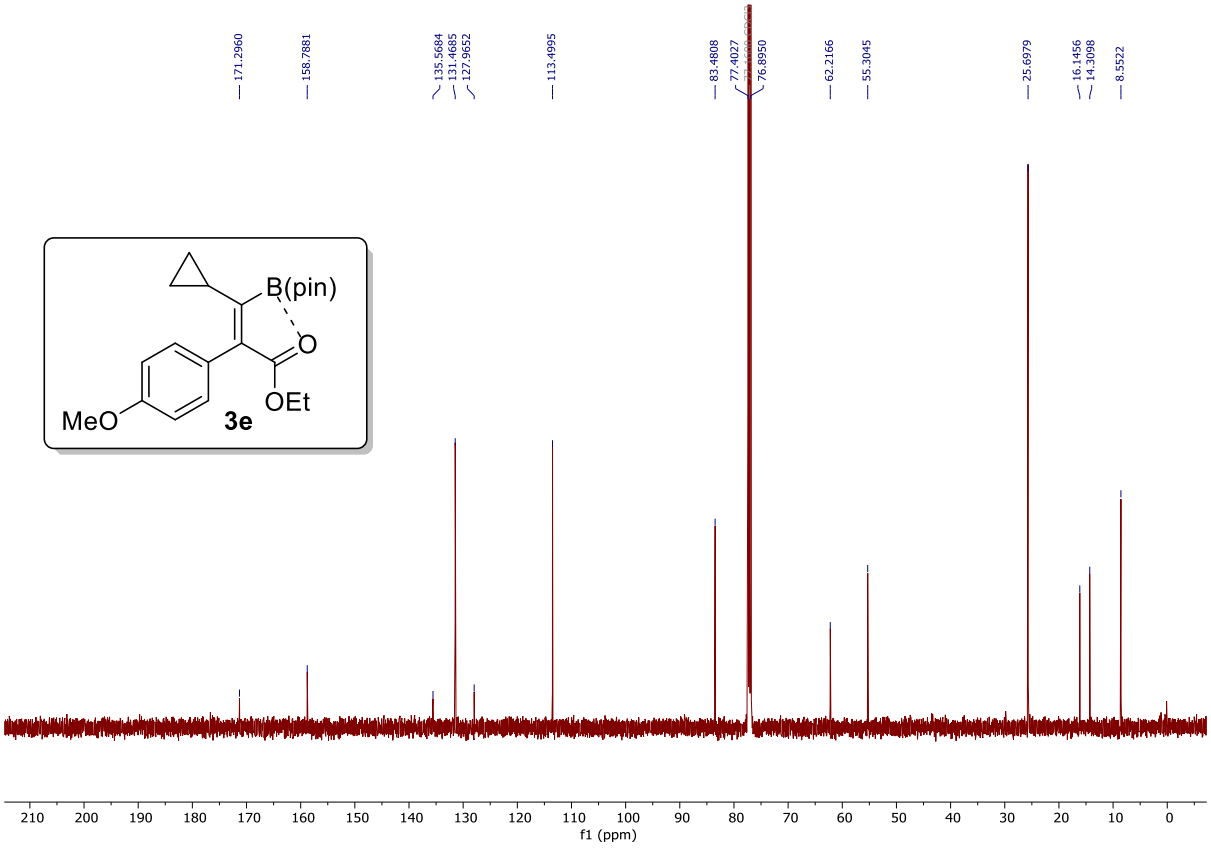
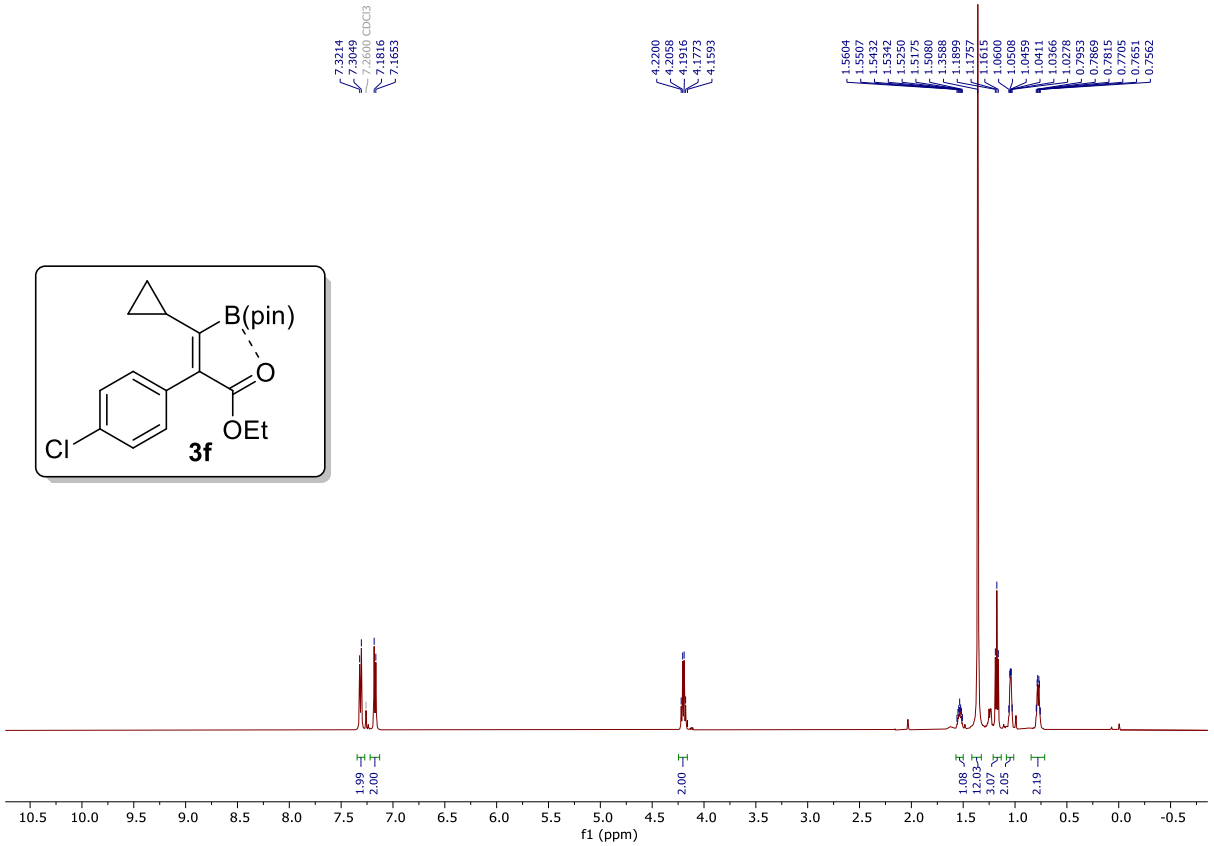
77.1600 CDCl3
76.9044
61.7456
55.2552
31.8067
25.5721
21.7285
14.2735
B(pin)
O
OEt
MeO
3c
f1 (ppm)


B(pin)
O
OEt
MeO
3d
f1 (ppm)


B(pin)
O
OEt
MeO
3d
f1 (ppm)


B(pin)
O
OEt
MeO
3e
f1 (ppm)


B(pin)
O
OEt
MeO
3e
f1 (ppm)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4.2200
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4.1773
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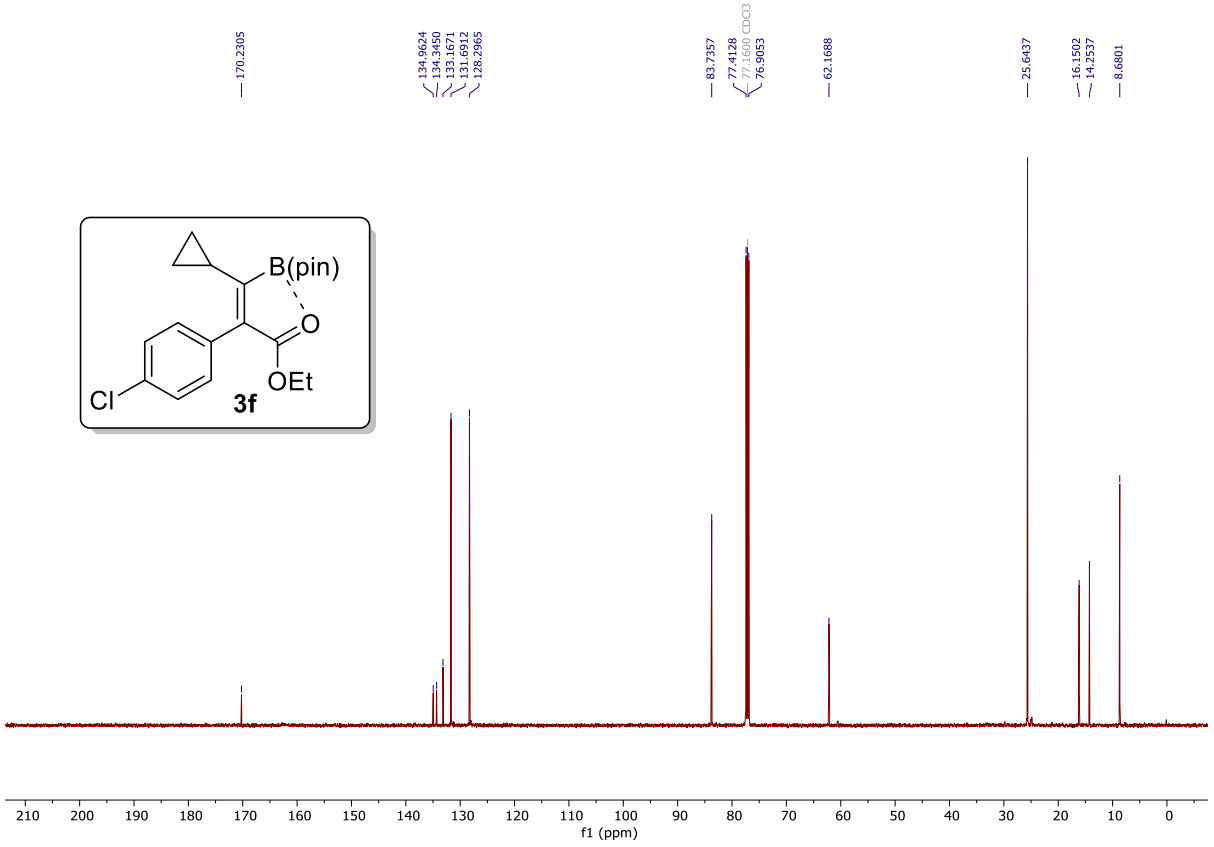
1.5604
1.5507
1.5432
1.5342
1.5250
1.5175
1.5080
1.3588
1.1899
1.1757
1.1615
1.0600
1.0508
1.0459
1.0411
1.0366
1.0278
0.7953
0.7869
0.7815
0.7705
0.7651
0.7562
B(pin)
O
OEt
Cl
3f
1.99
2.00
2.00
1.08
12.03
3.07
2.05
2.19
f1 (ppm)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133.1671
131.6912
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83.7357
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77.1600 CDCl3
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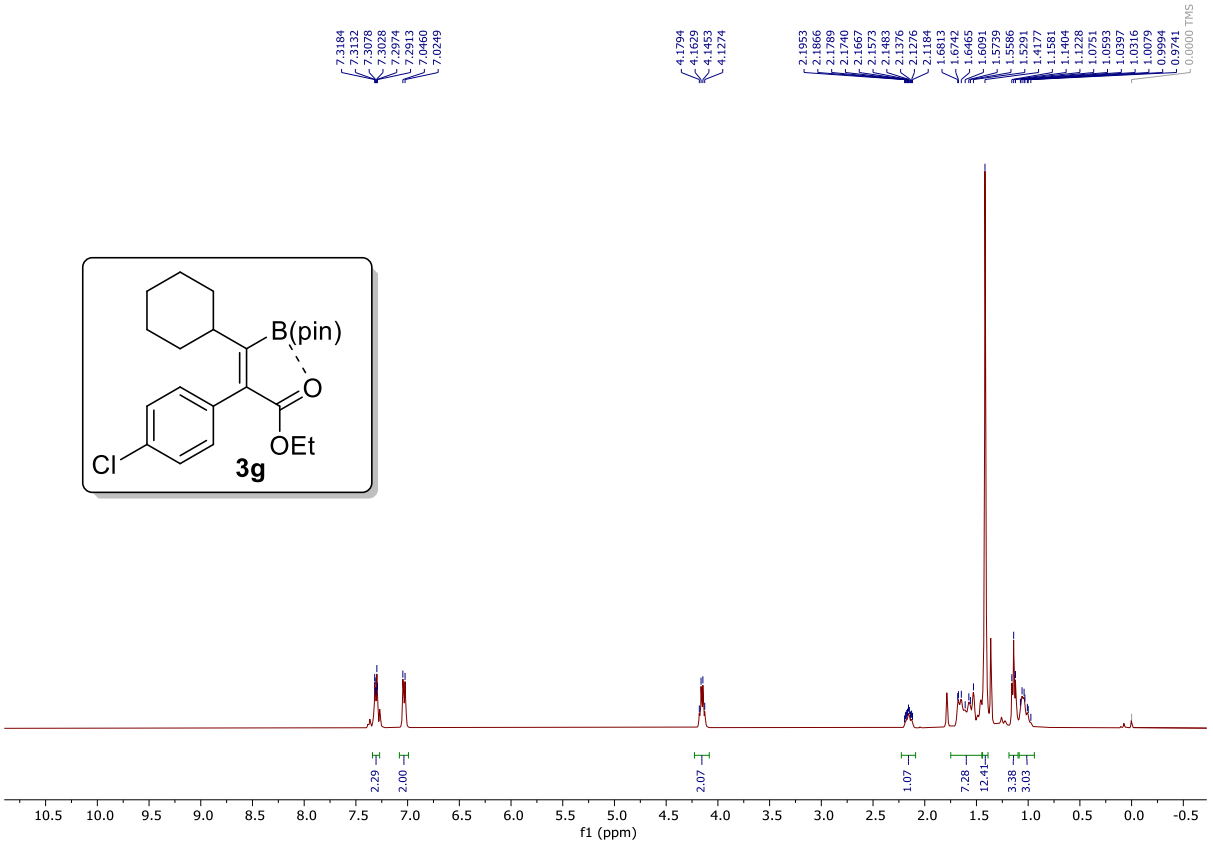
16.1502
14.2537
8.6801
B(pin)
O
OEt
Cl
3f
f1 (ppm)



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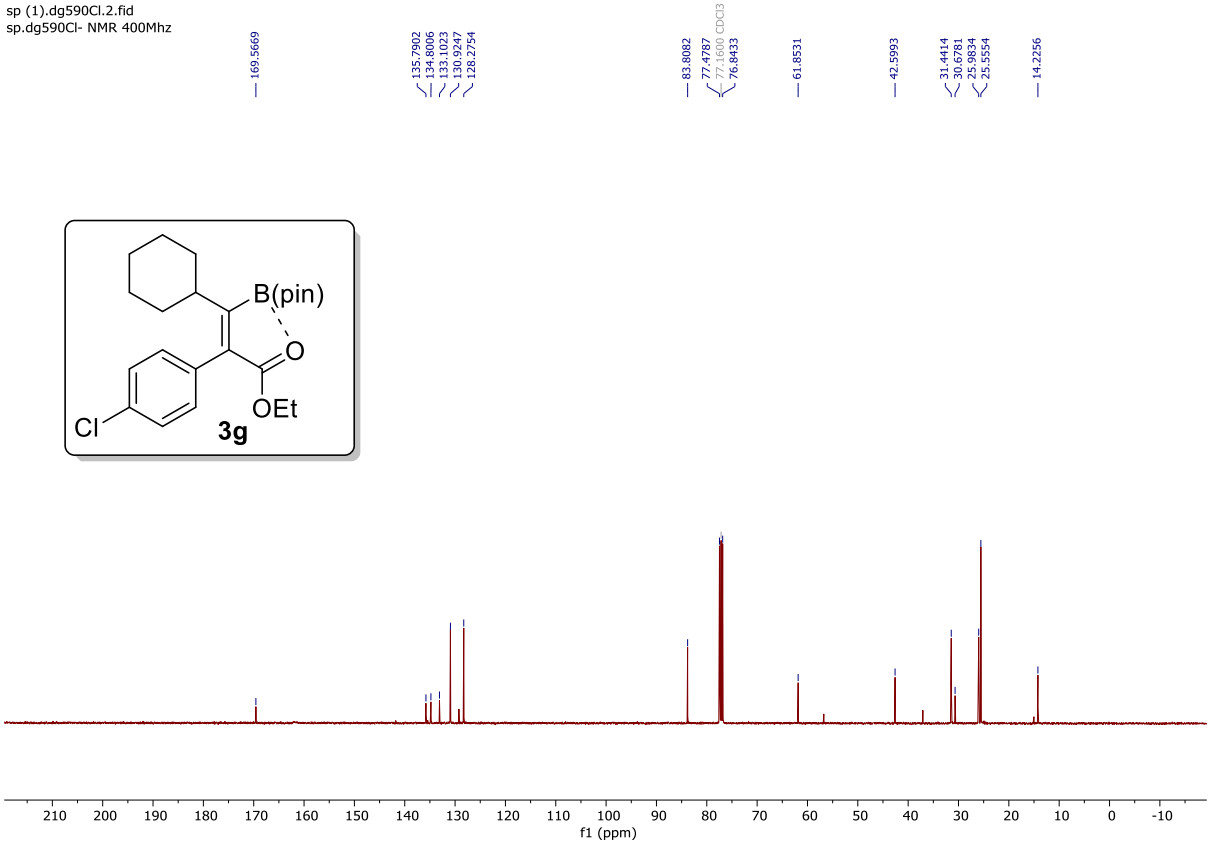
sp.dg590Cl- NMR 400Mhz

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7.2447
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7.1864
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7.1635
7.1450
7.1314
7.1161
7.1105
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7.0072
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6.8537
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6.8293
6.8195
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3.7348
3.7255
3.7077
2.8406
2.8201
2.7999
2.7790
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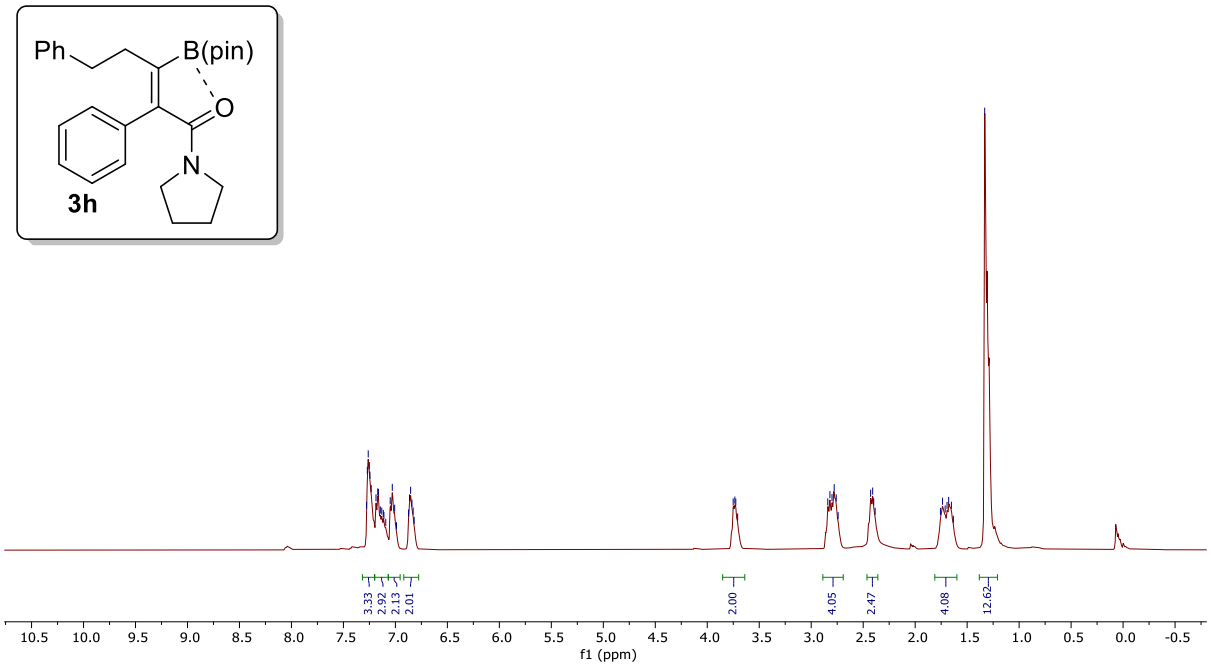
1.6326
1.3311


Ph
B(pin)
O
N
3h
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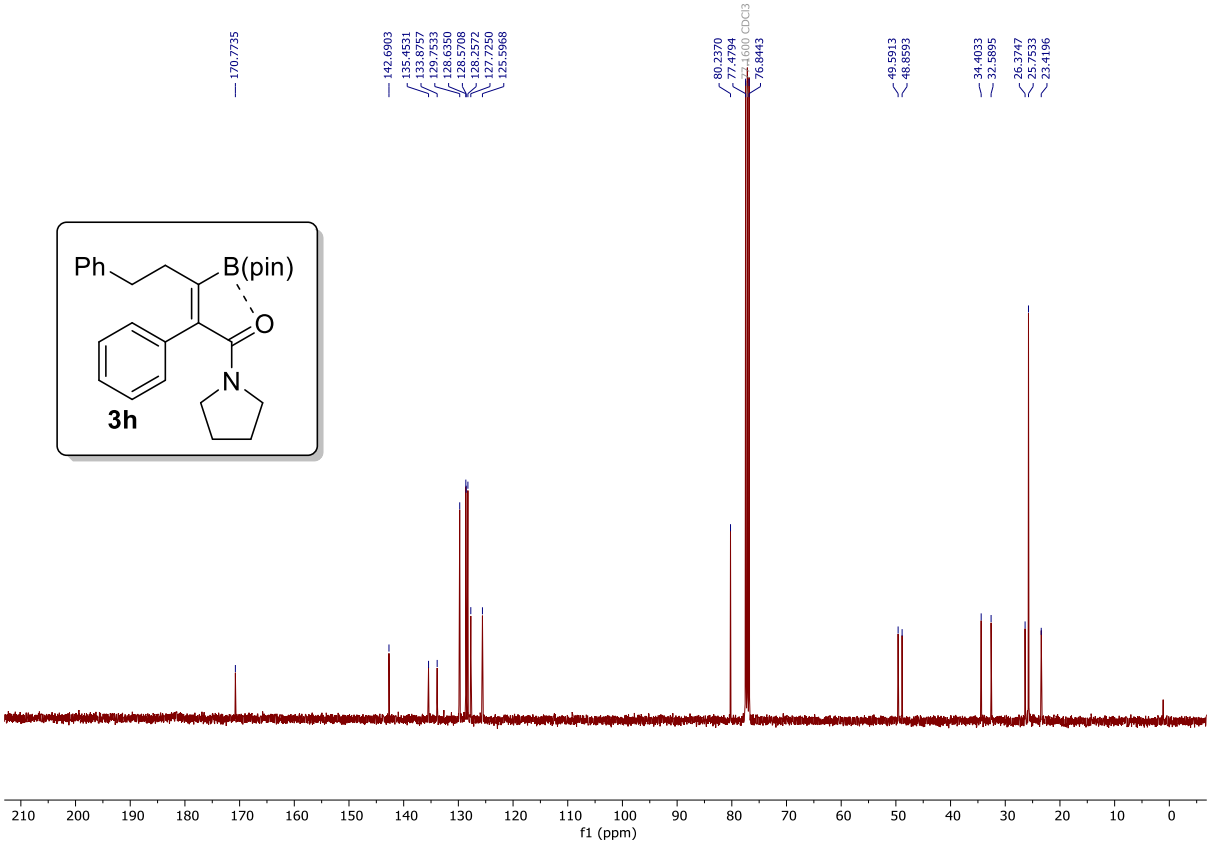
2.00
4.05
2.47
4.08
12.62
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.5708
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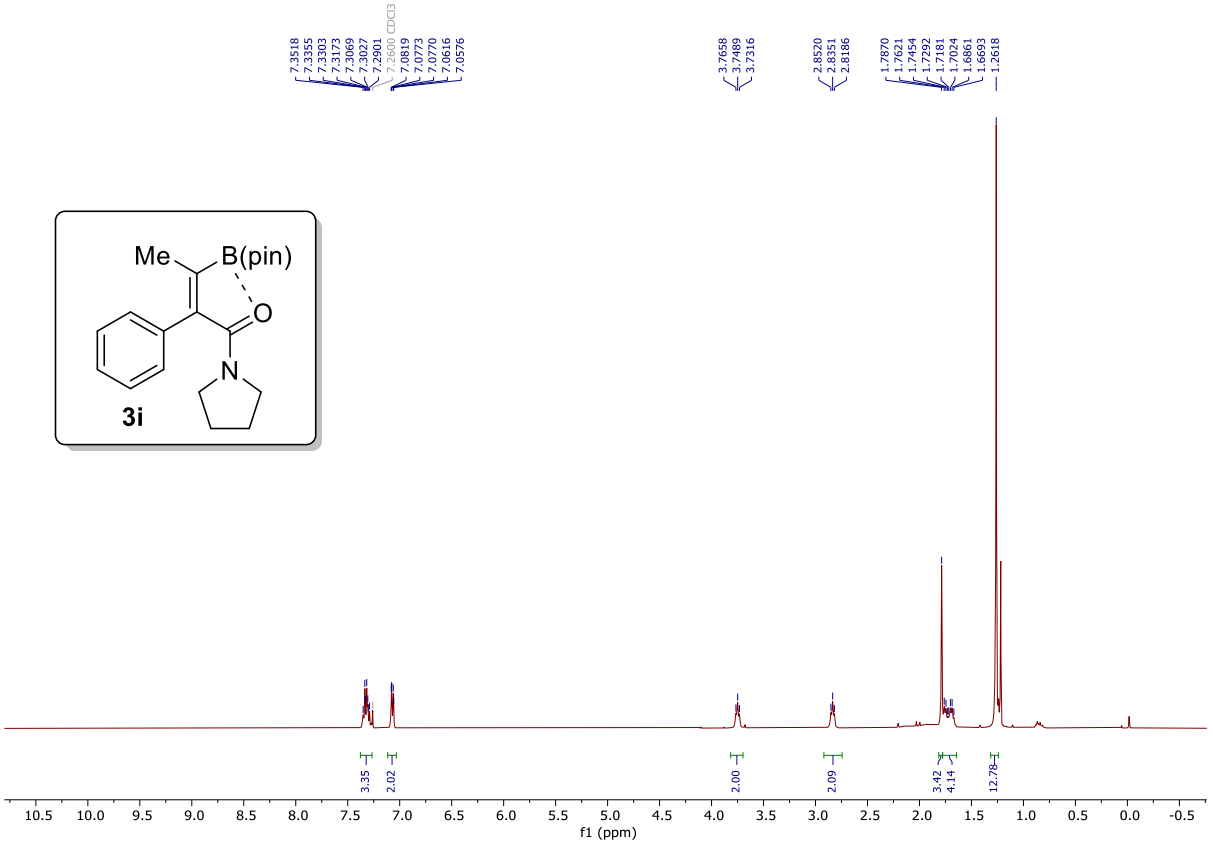
127.7250
125.5968
80.2370
77.4794
77.1600 CDCl3
76.8443
49.5913
48.8593
34.4033
32.5895
26.3747
25.7533
23.4196
Ph
B(pin)
O
N
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.0819
7.0773
7.0770
7.0616
7.0576
3.7658
3.7489
3.7316
2.8520
2.8351
2.8186
1.7870
1.7621
1.7454
1.7292
1.7181
1.7024
1.6861
1.6693
1.2618
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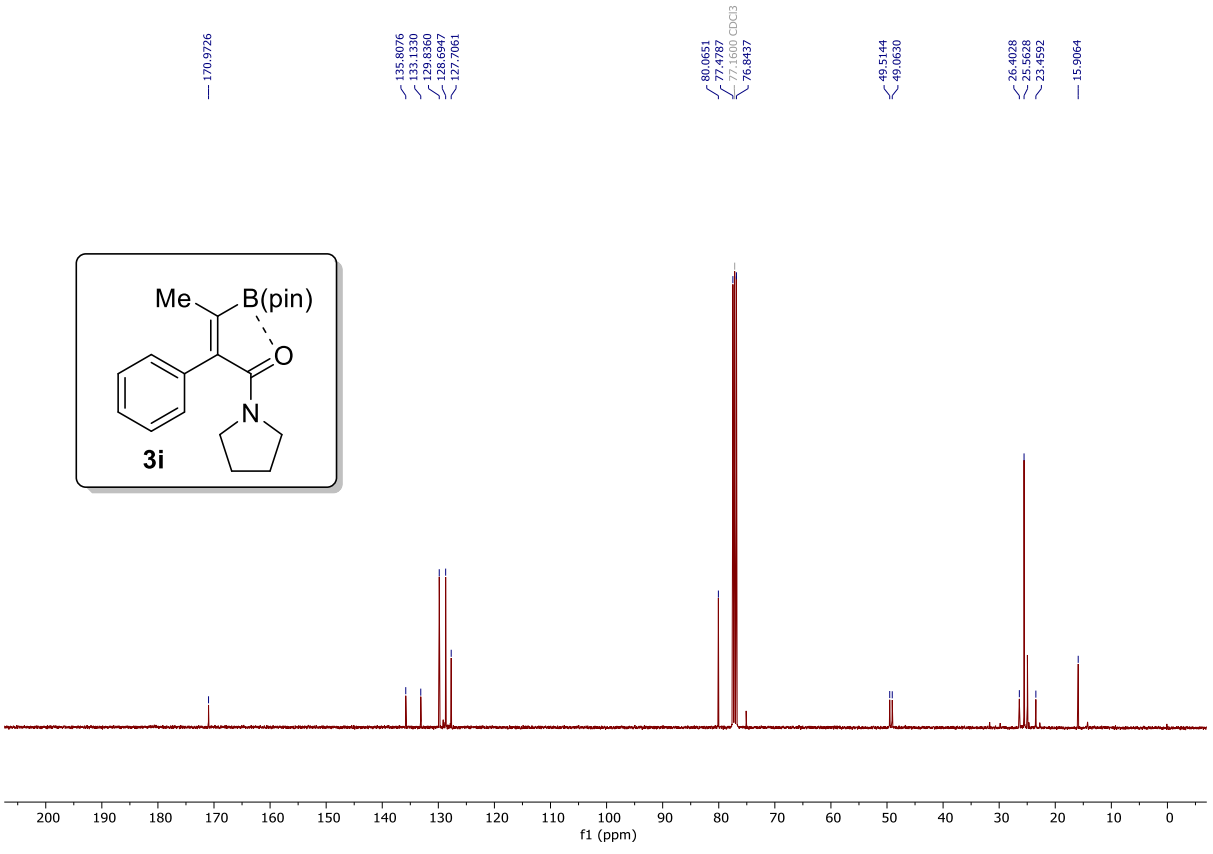
12.78
f1 (ppm)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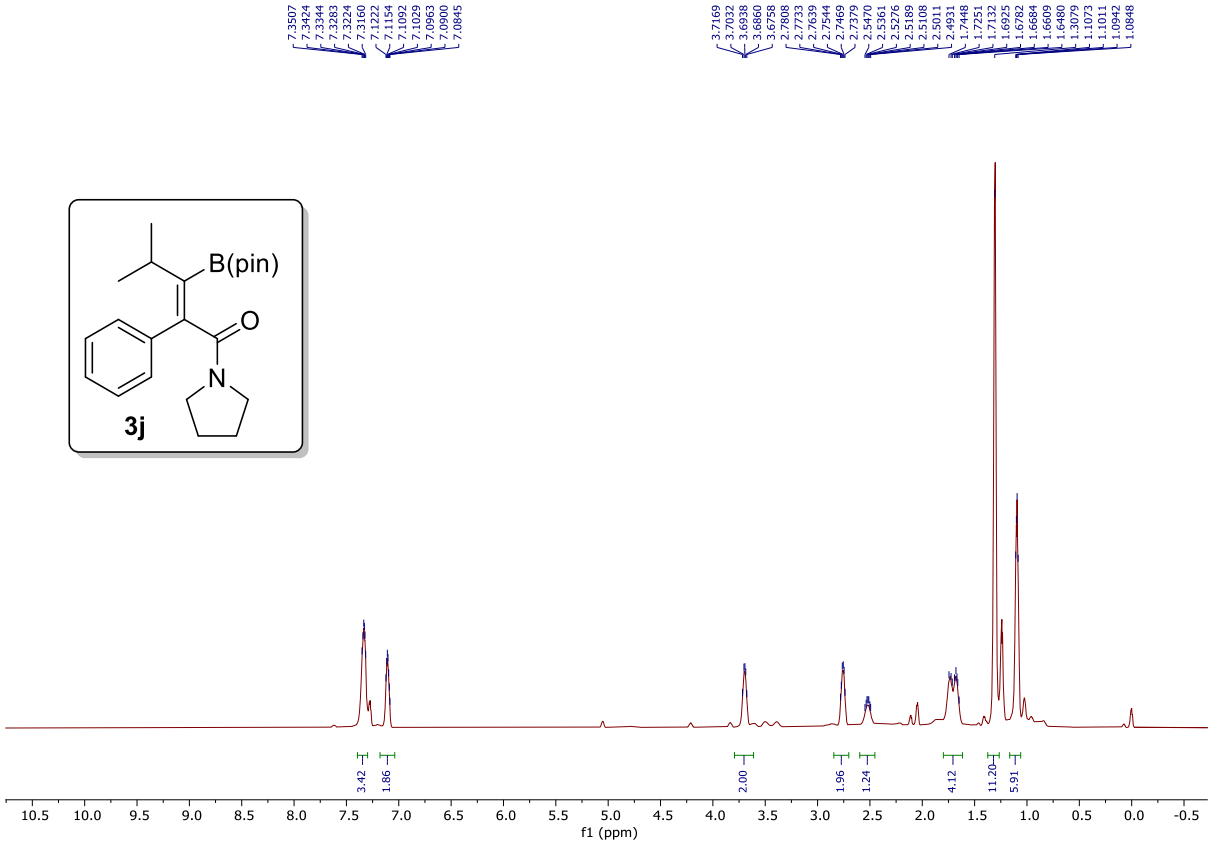
15.9064
Me
B(pin)
O
N
3i
f1 (ppm)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7.1029
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7.0900
7.0845
3.7169
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2.7469
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1.6684
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1.1011
1.0942
1.0848
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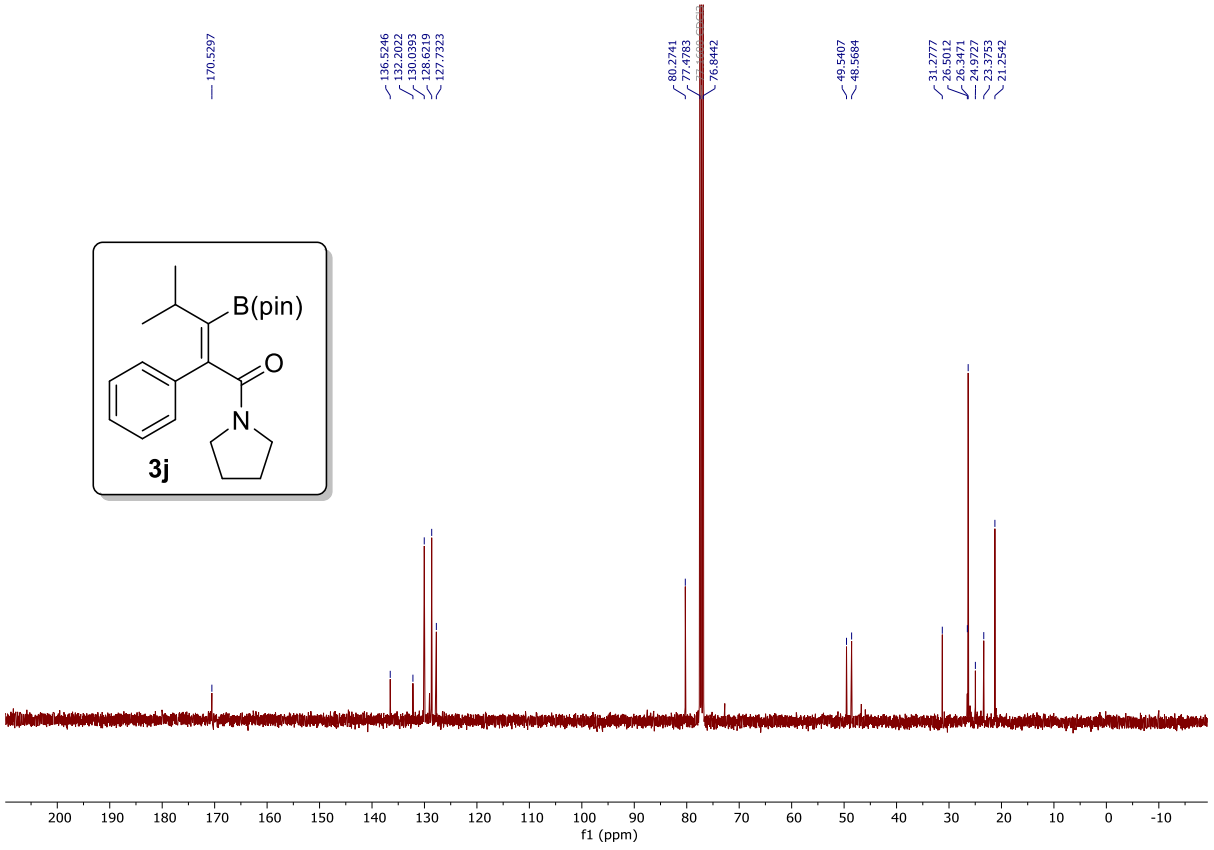
5.91
f1 (ppm)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130.0393
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80.2741
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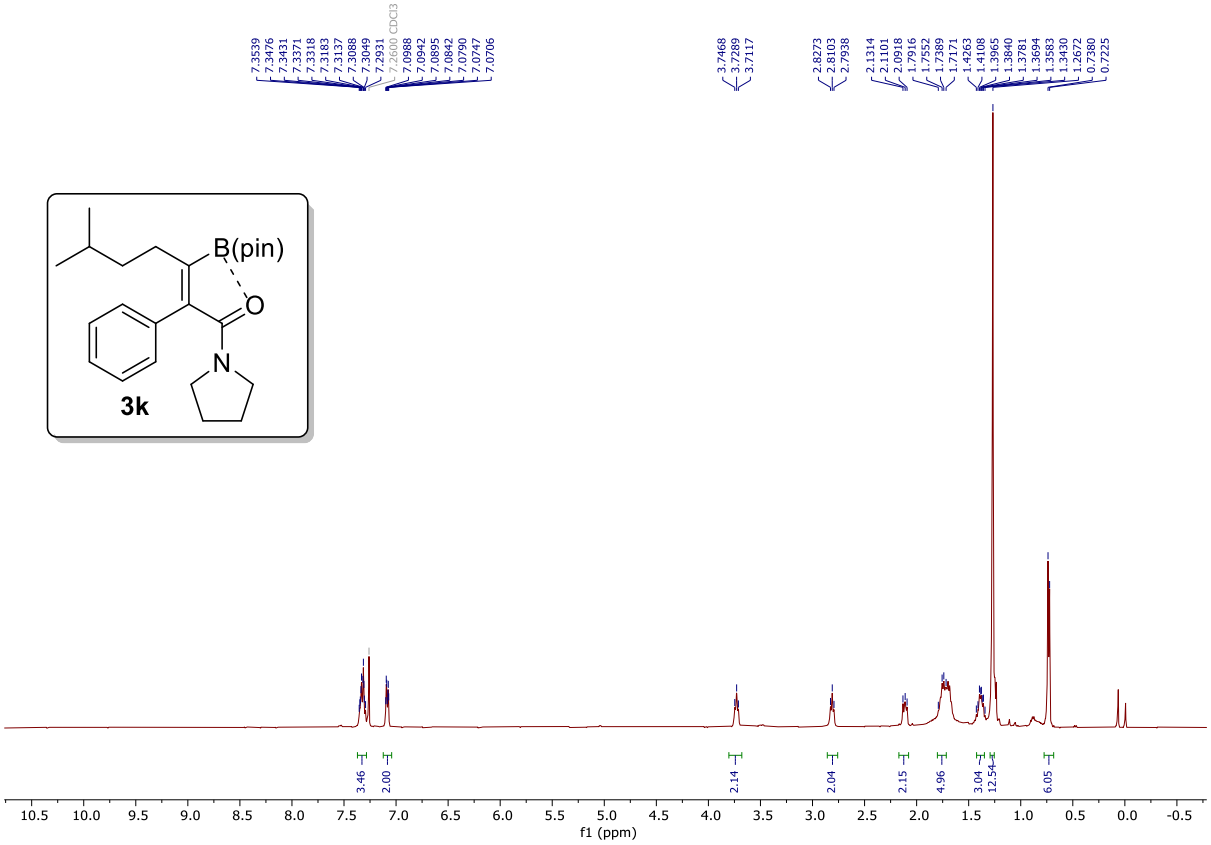
B(pin)
O
N
3j
f1 (ppm)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7.0706
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3.7299
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1.4108
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1.2672
0.7380
0.7225
B(pin)
O
N
3k
3.46
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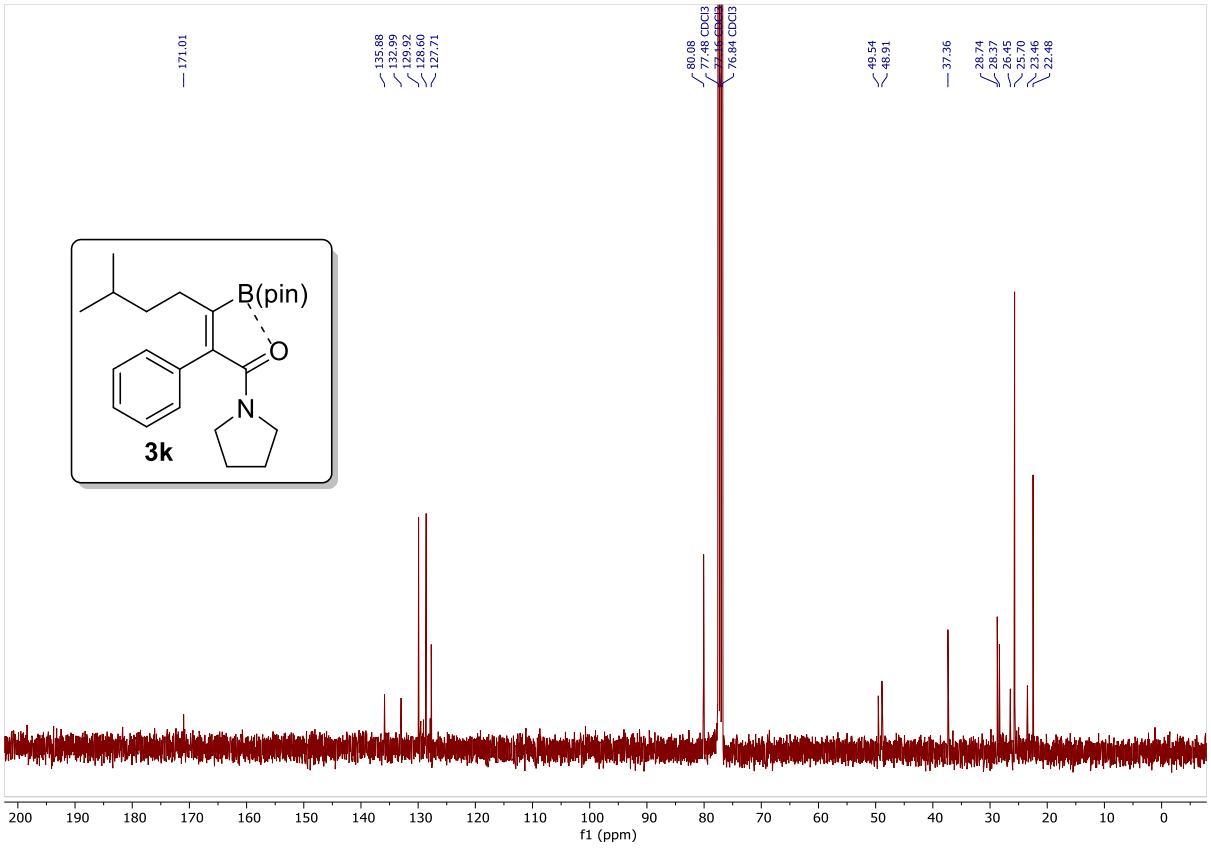
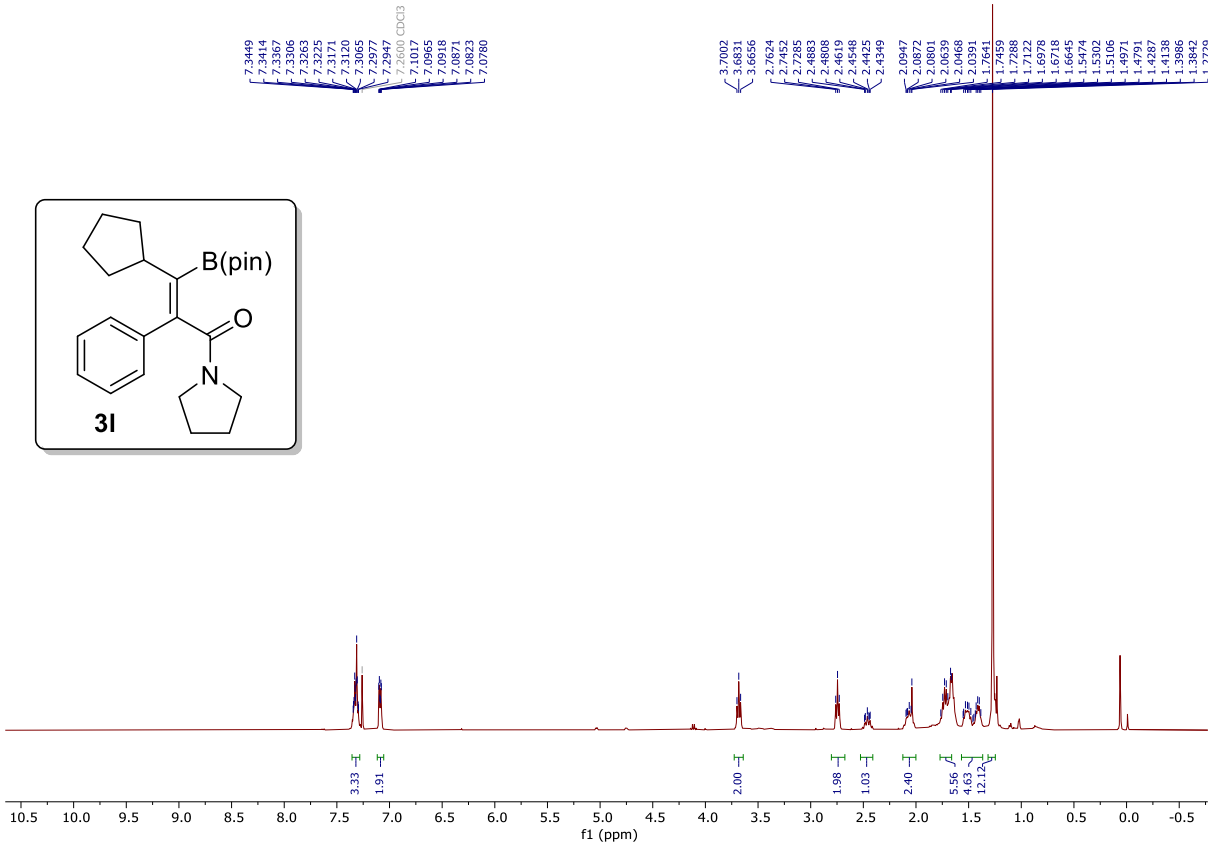
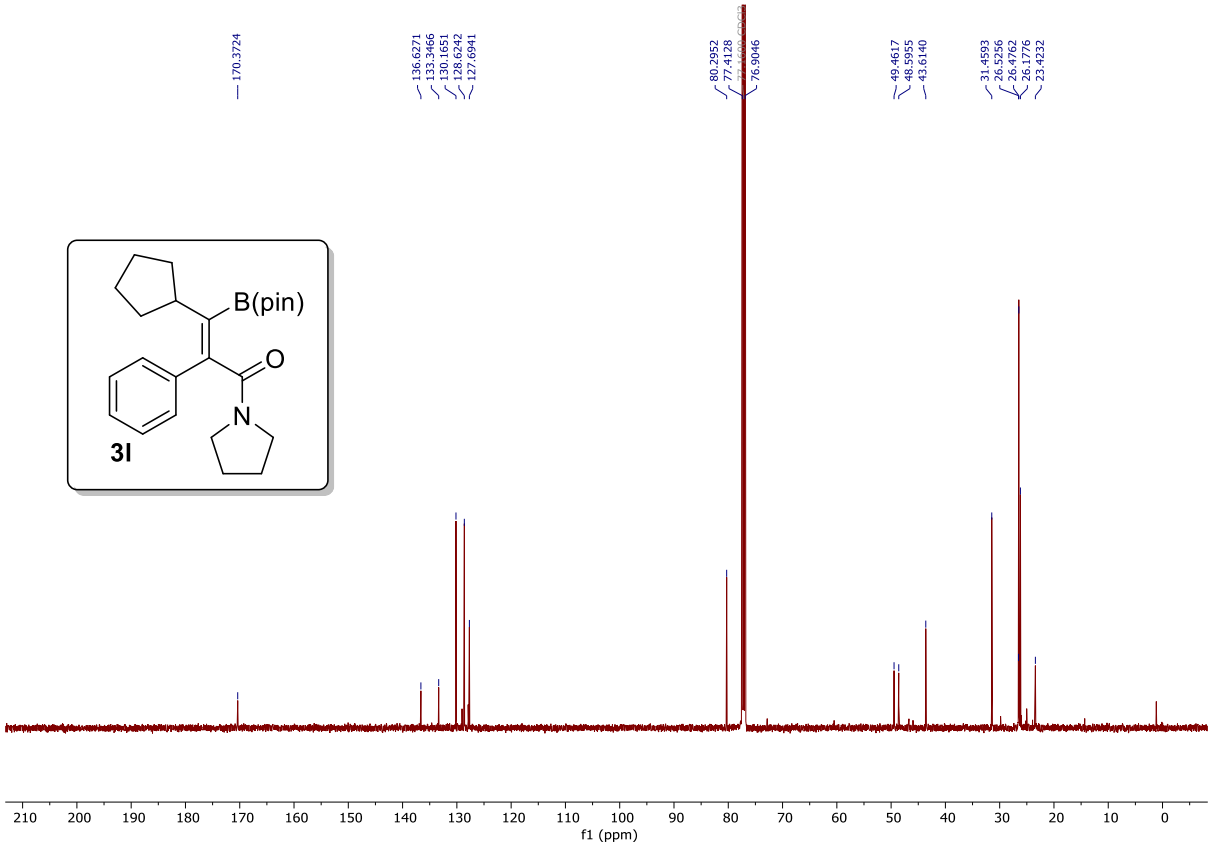
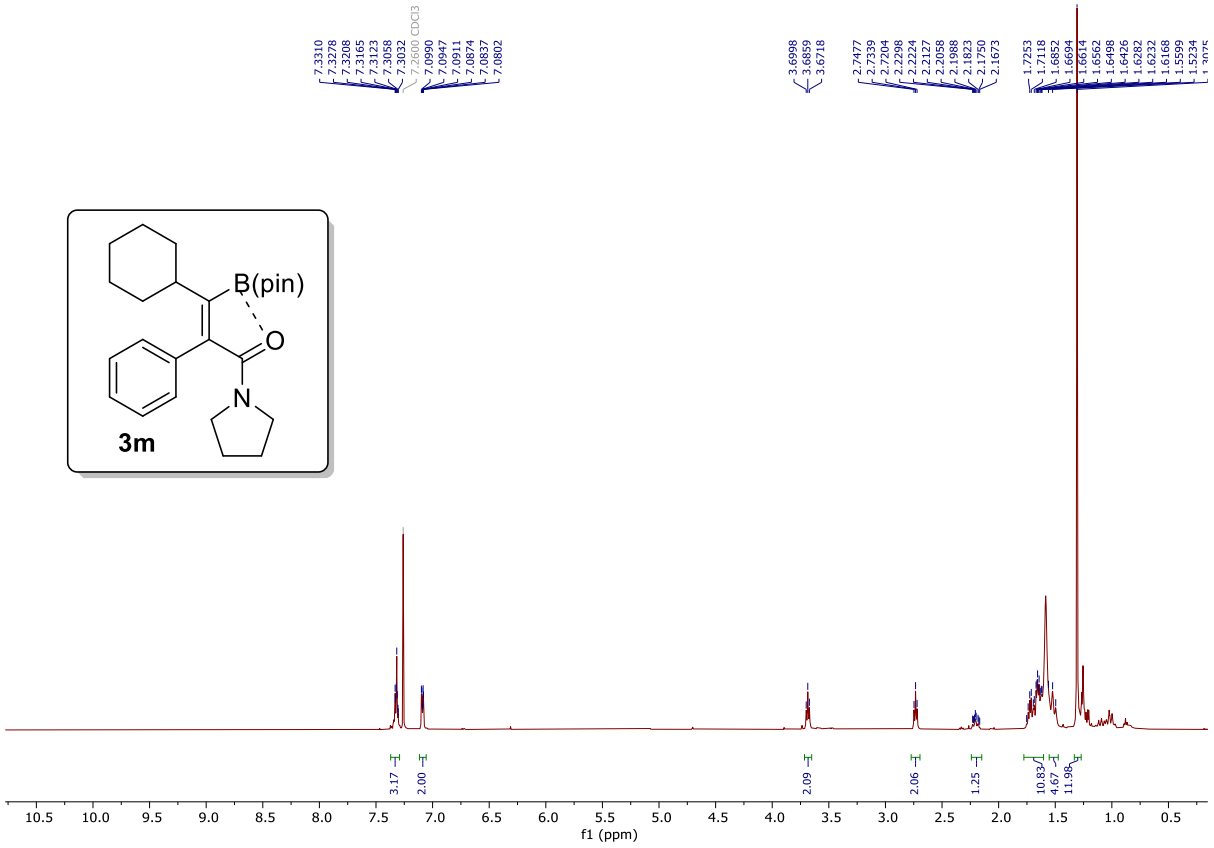
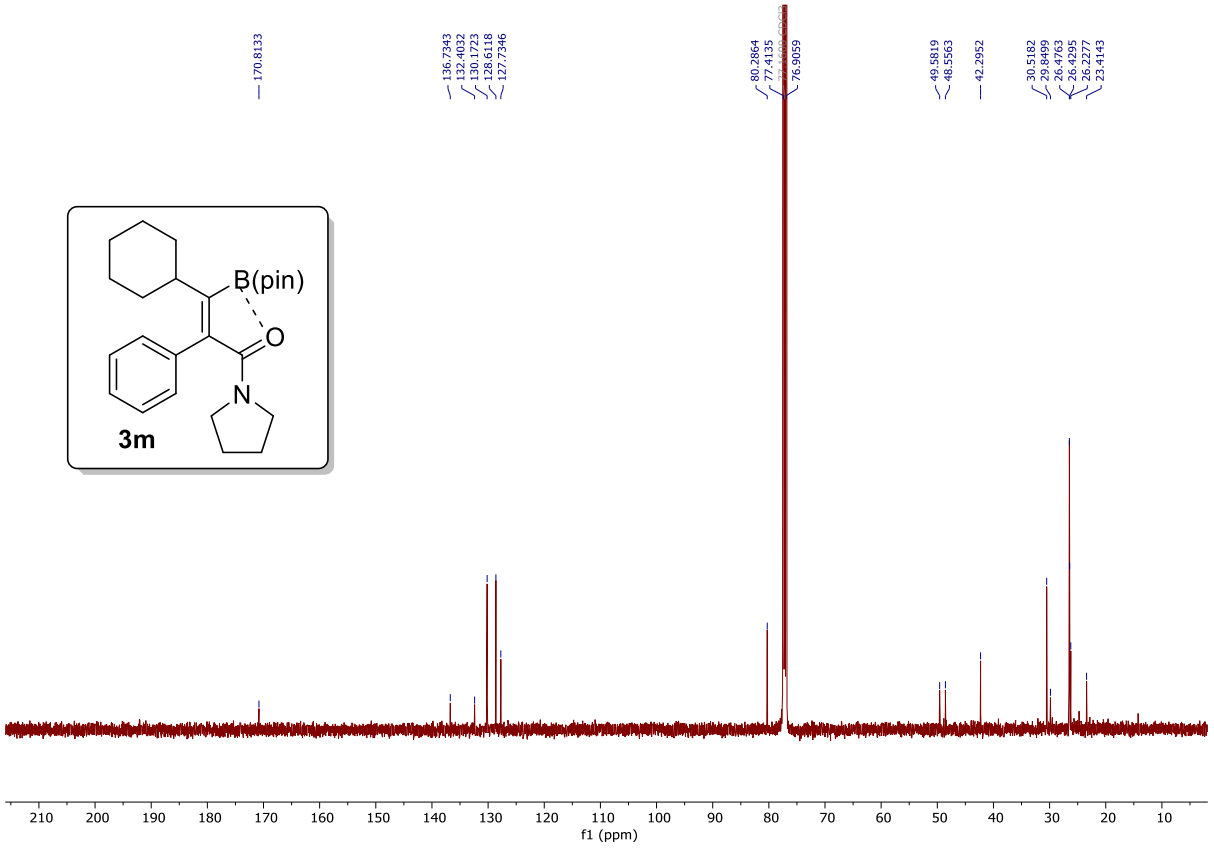
2.14
2.04
2.15
4.96
3.04
12.54
6.05
f1 (ppm)


171.01
135.88
132.99
129.92
128.60
127.71
80.08
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
49.54
48.91
37.36
28.74
28.37
26.45
25.70
23.46
22.48
B(pin)
O
N
3k
f1 (ppm)

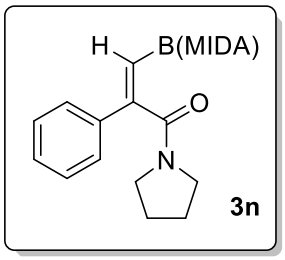

B(pin)
O
N
3l
f1 (ppm)

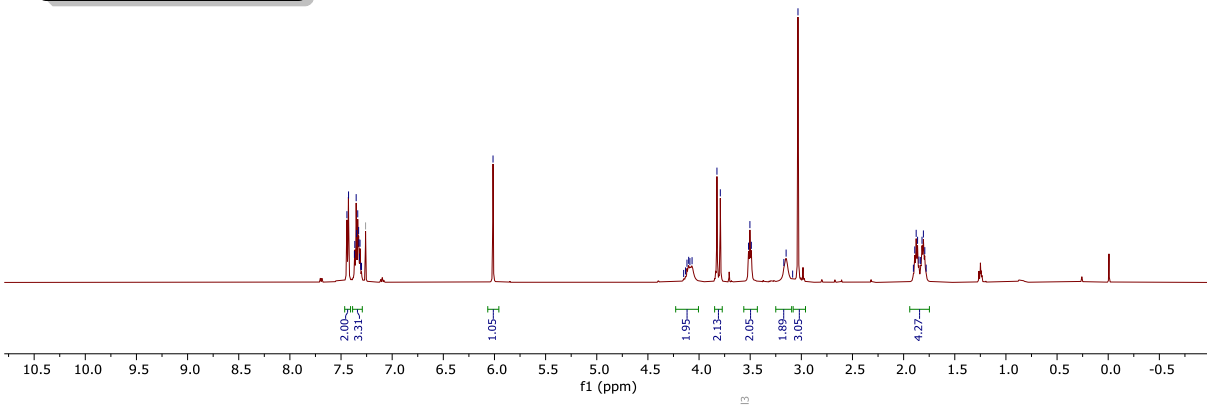

B(pin)
O
N
3l
f1 (ppm)

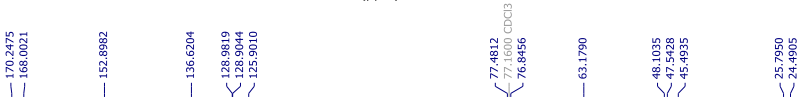

B(pin)
O
N
3m
f1 (ppm)

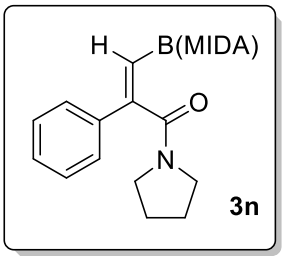

B(pin)
O
N
3m
f1 (ppm)


7.4423
7.4265
7.3693
7.3654
7.3520
7.3479
7.3367
7.3279
7.3251
7.3197
7.3142
7.3068
7.2998
7.2600 CDCl3
6.0141
4.1505
4.1323
4.1180
4.1014
4.0893
4.0683
3.8250
3.7920
3.5162
3.5027
3.4887
3.1711
3.1488
3.0850
3.0328
1.9044
1.8912
1.8774
1.8637
1.8505
1.8336
1.8203
1.8068
1.7931
1.7795


H
B(MIDA)
O
N
3n

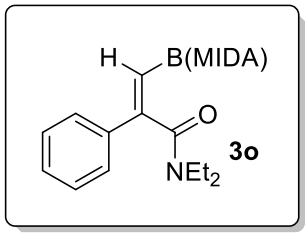

2.00
3.31
1.05
1.95
2.13
2.05
1.89
3.05
4.27
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

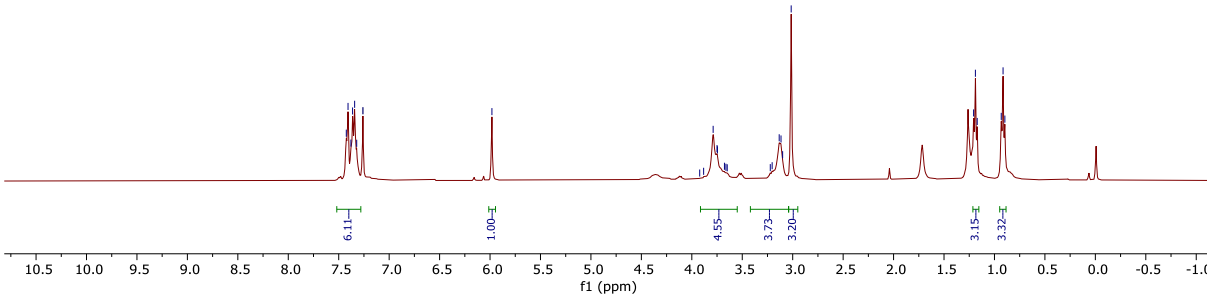

170.2475
168.0021
152.8982
136.6204
128.9819
128.9044
125.9010
77.4812
77.1600 CDCl3
76.8456
63.1790
48.1035
47.5428
45.4935
25.7950
24.4905

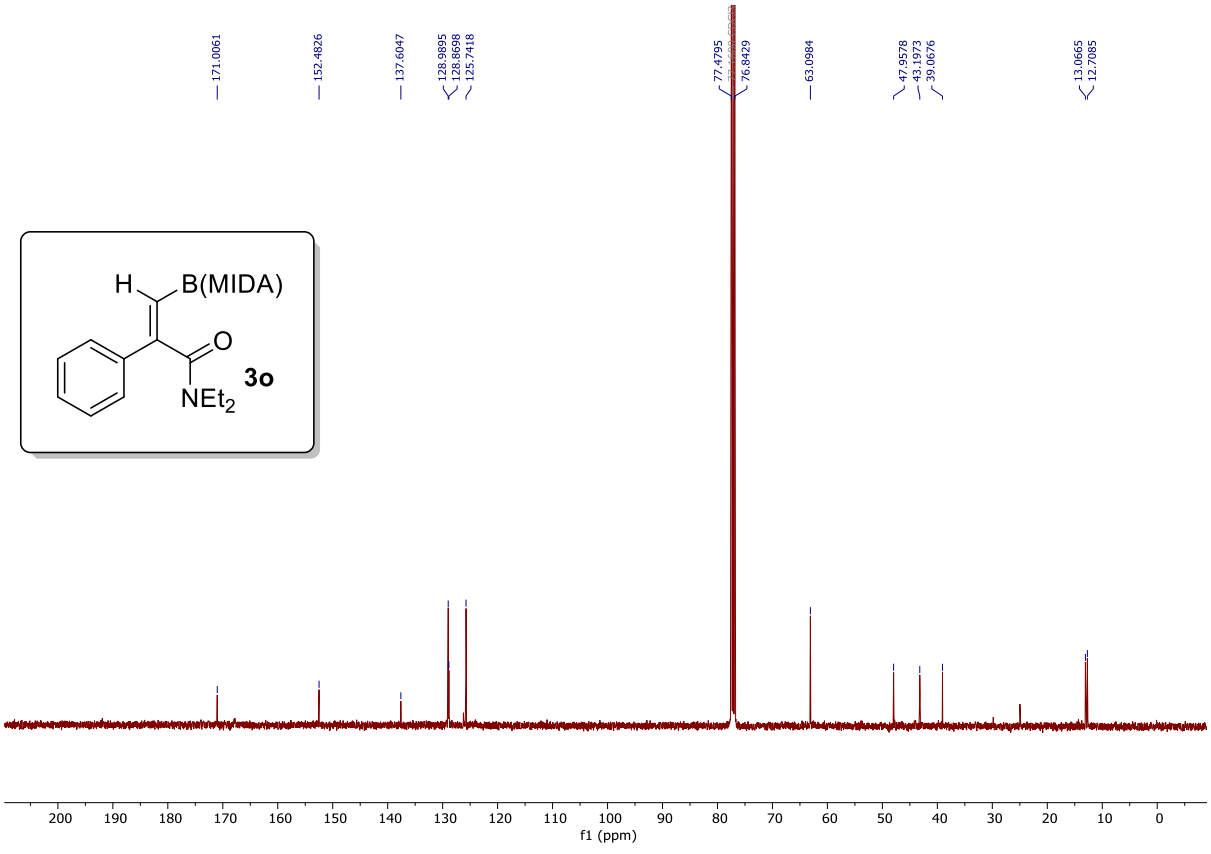

H
B(MIDA)
O
N
3n

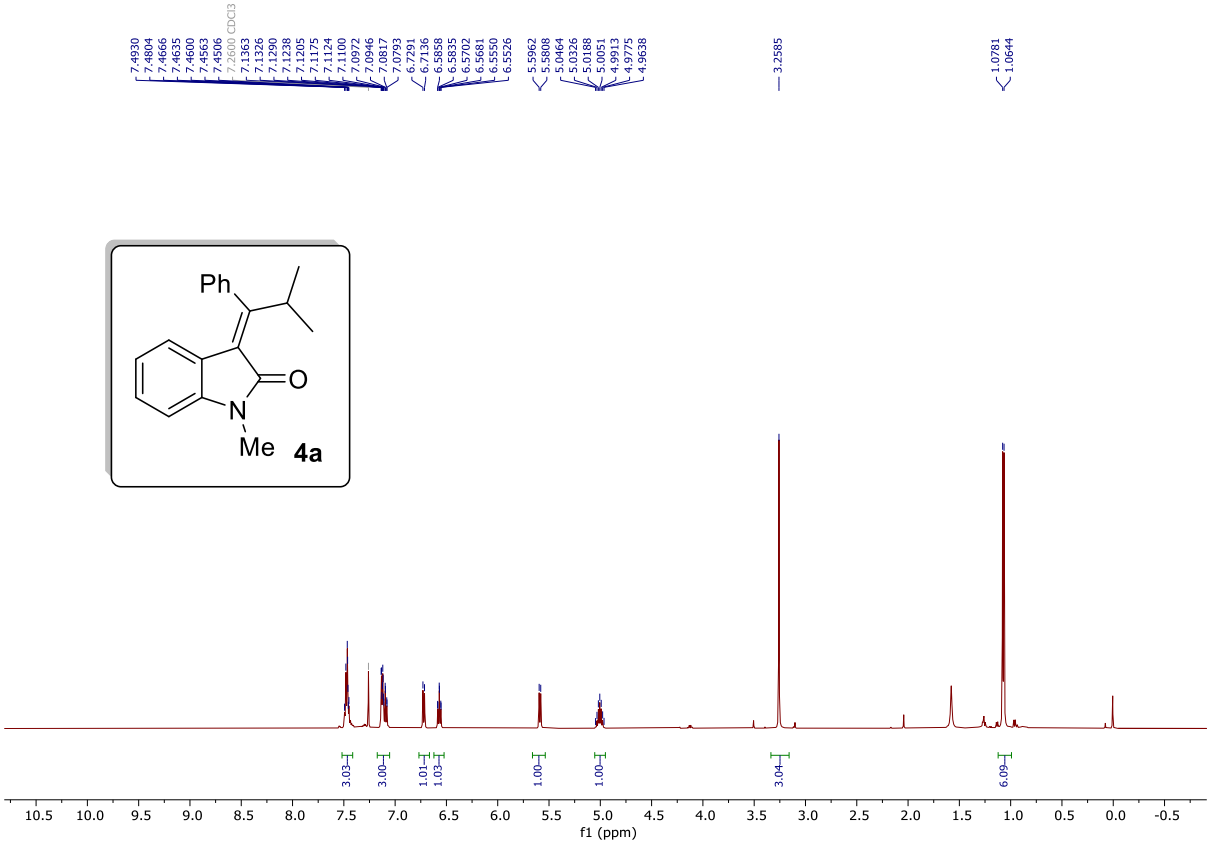
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

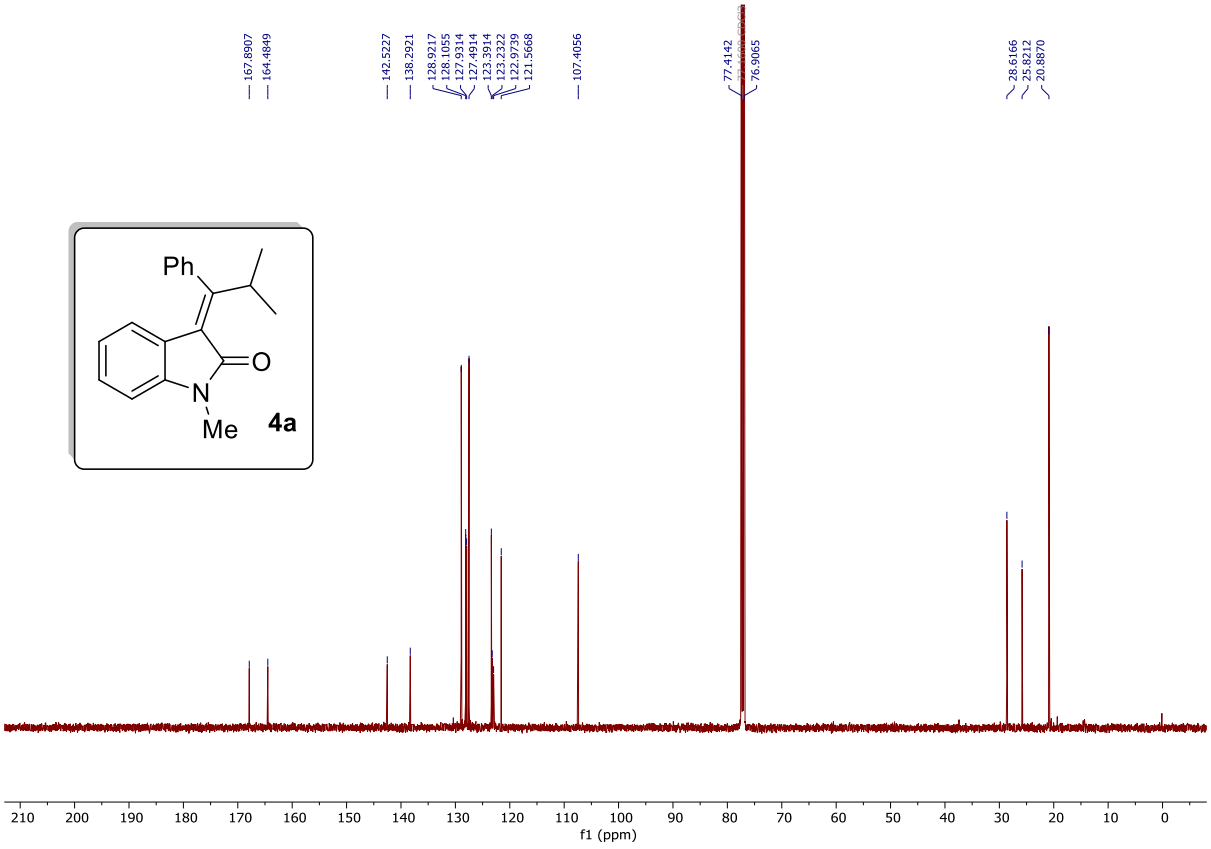
sp.dg481r.1.fid
sp.dg481r-400 mhz

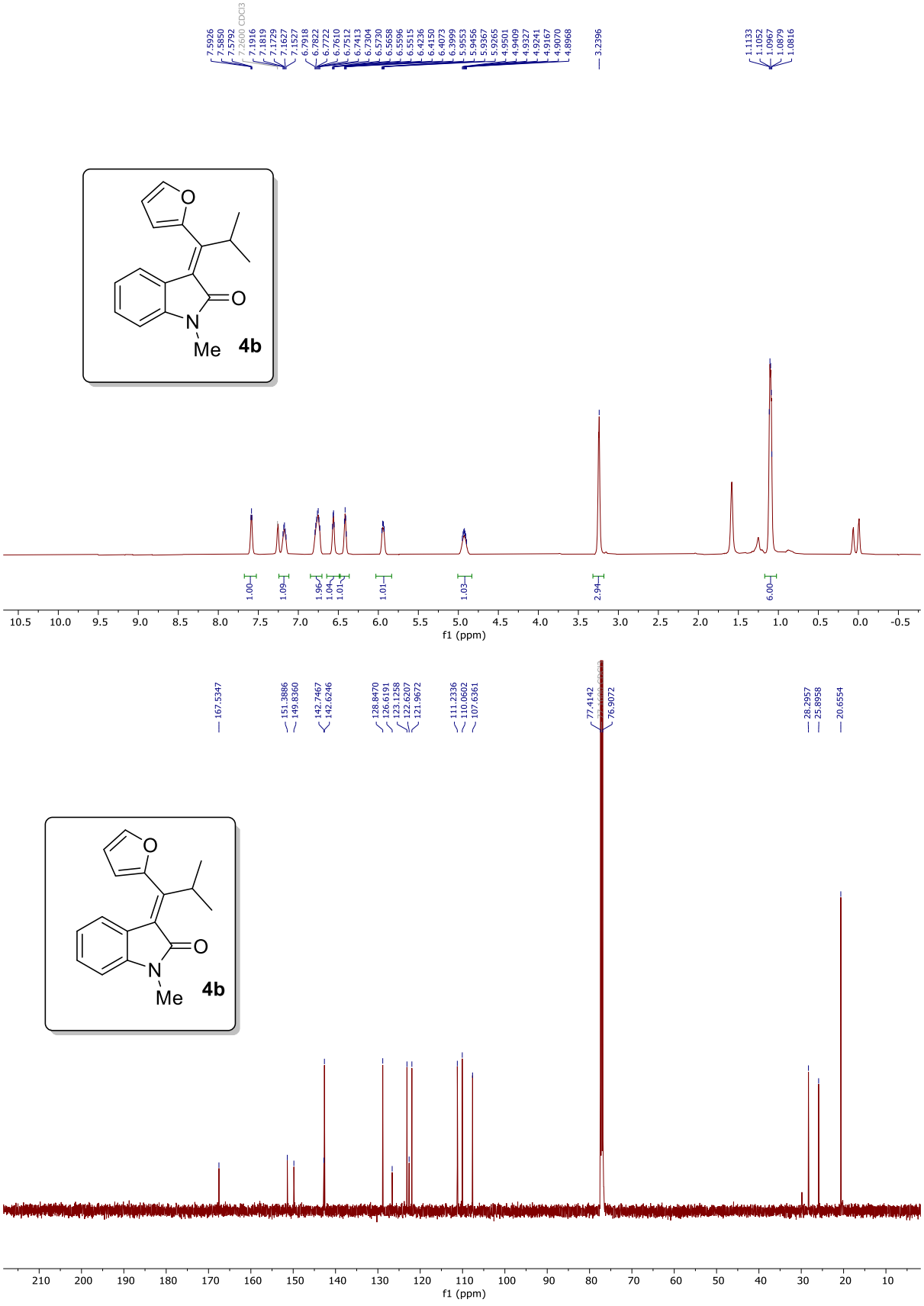


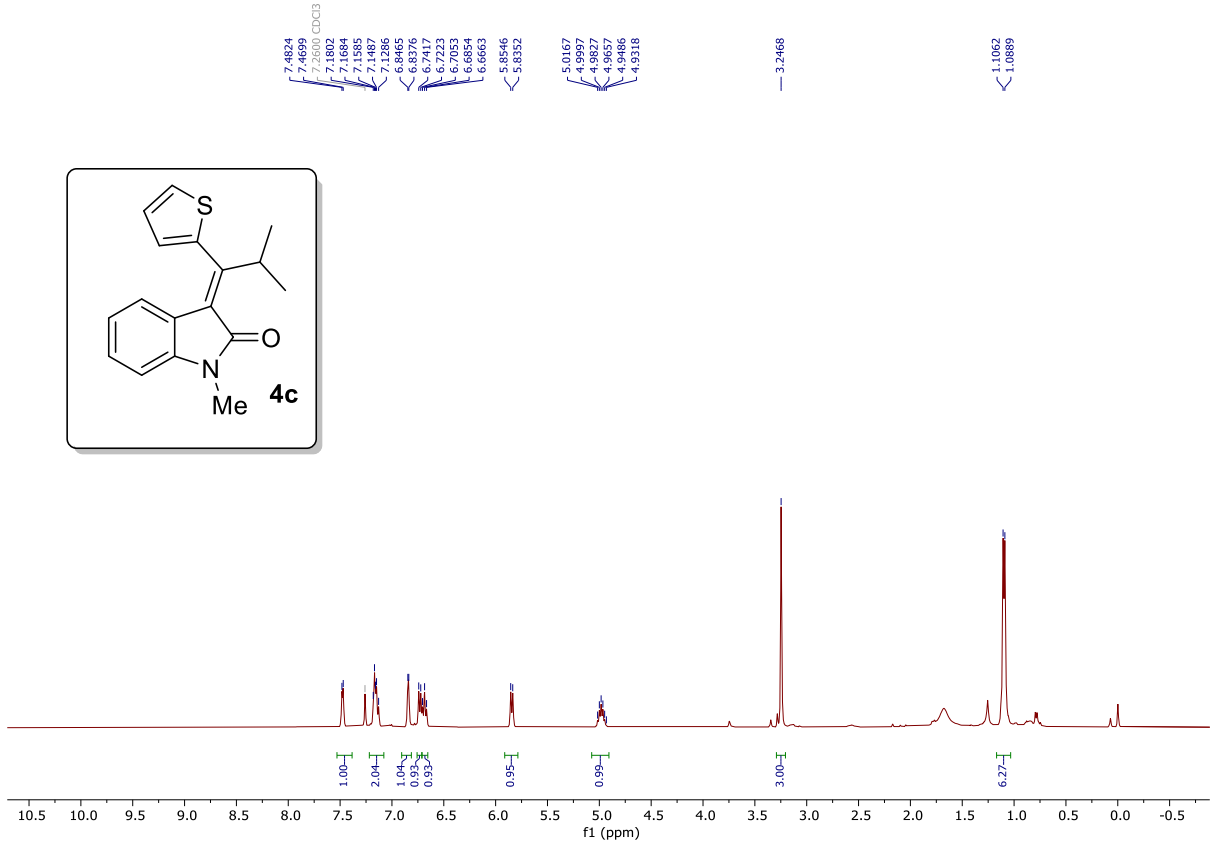


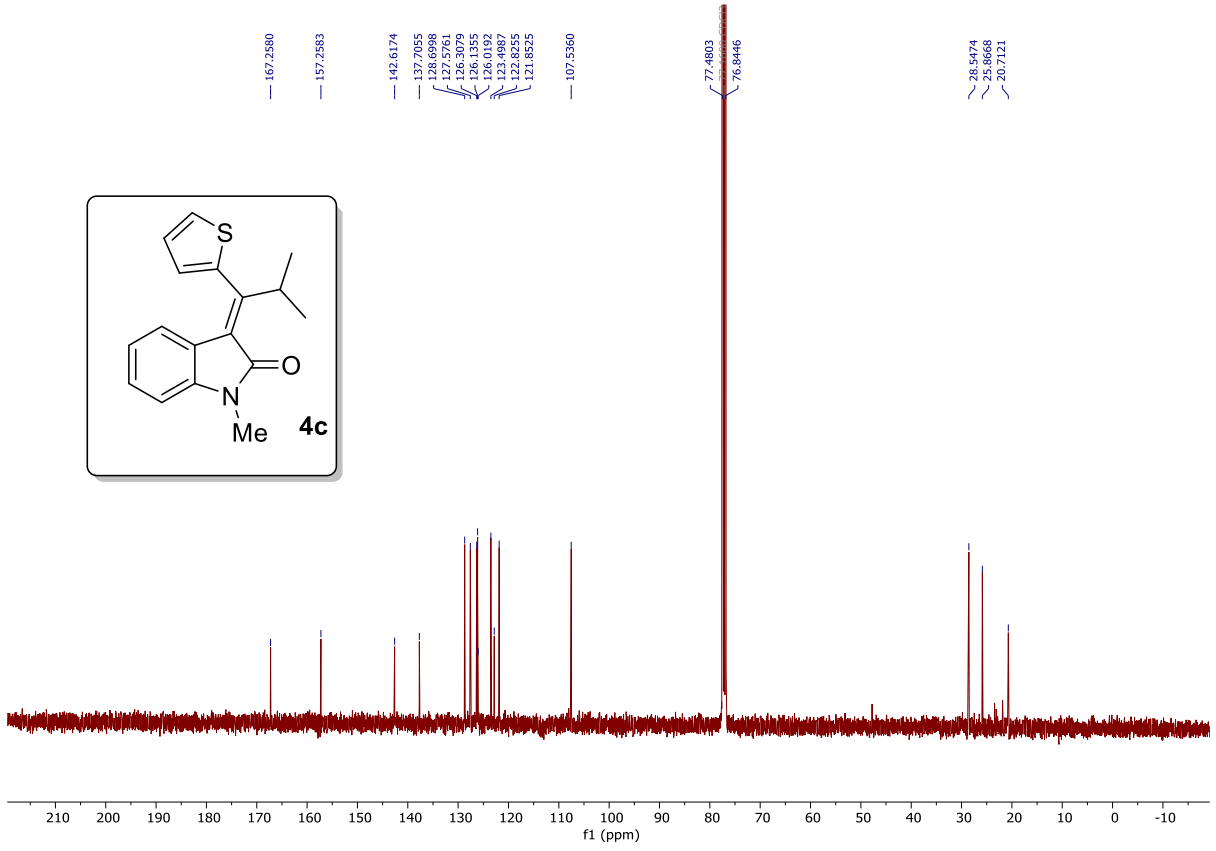


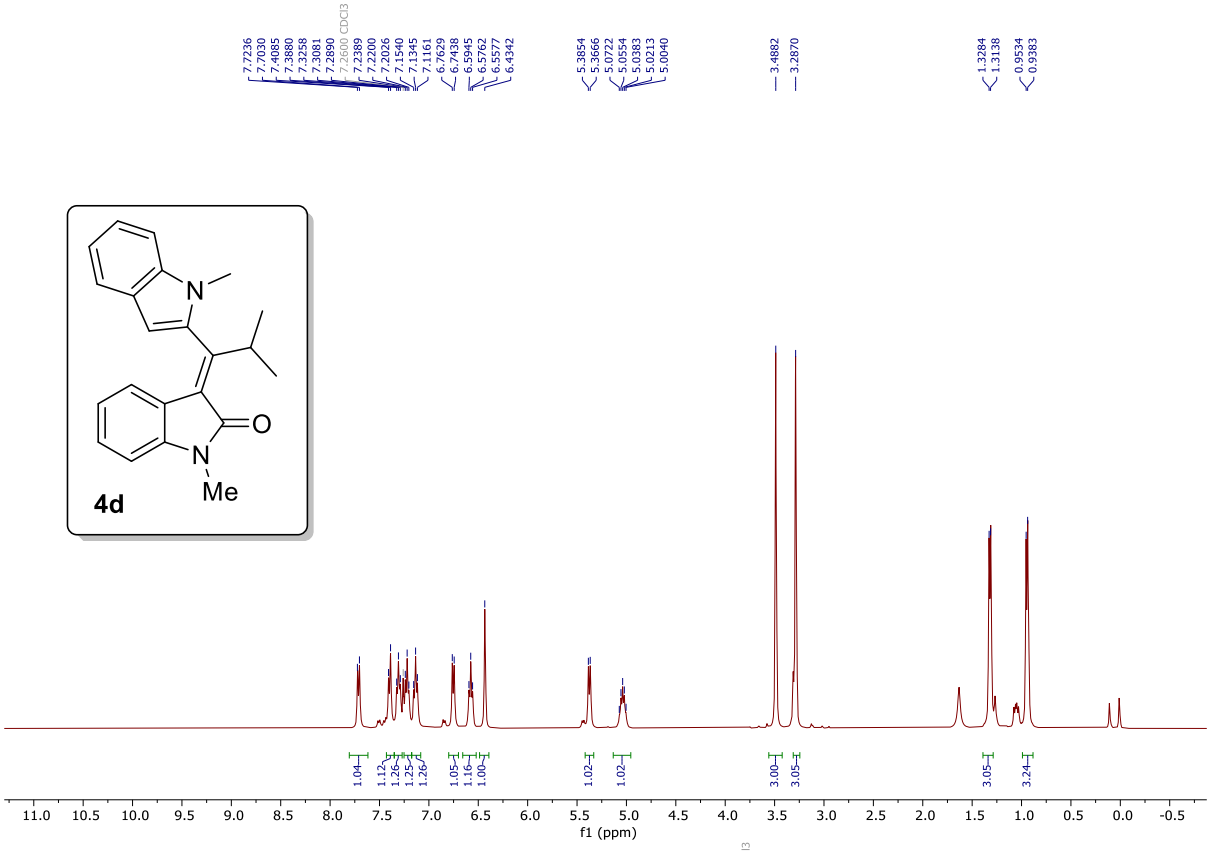

7.4930
7.4804
7.4666
7.4655
7.4600
7.4563
7.4506
7.3660
CDCl3
7.1363
7.1326
7.1290
7.1238
7.1205
7.1175
7.1124
7.1100
7.0972
7.0946
7.0817
7.0793
6.7291
6.7136
6.5858
6.5835
6.5702
6.5681
6.5550
6.5526
5.5962
5.5808
5.0464
5.0326
5.0188
5.0051
4.9913
4.9775
4.9638
3.2585
1.0781
1.0644
Ph
O
N
Me
4a
3.03
3.00
1.01
1.03
1.00
1.00
3.04
6.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

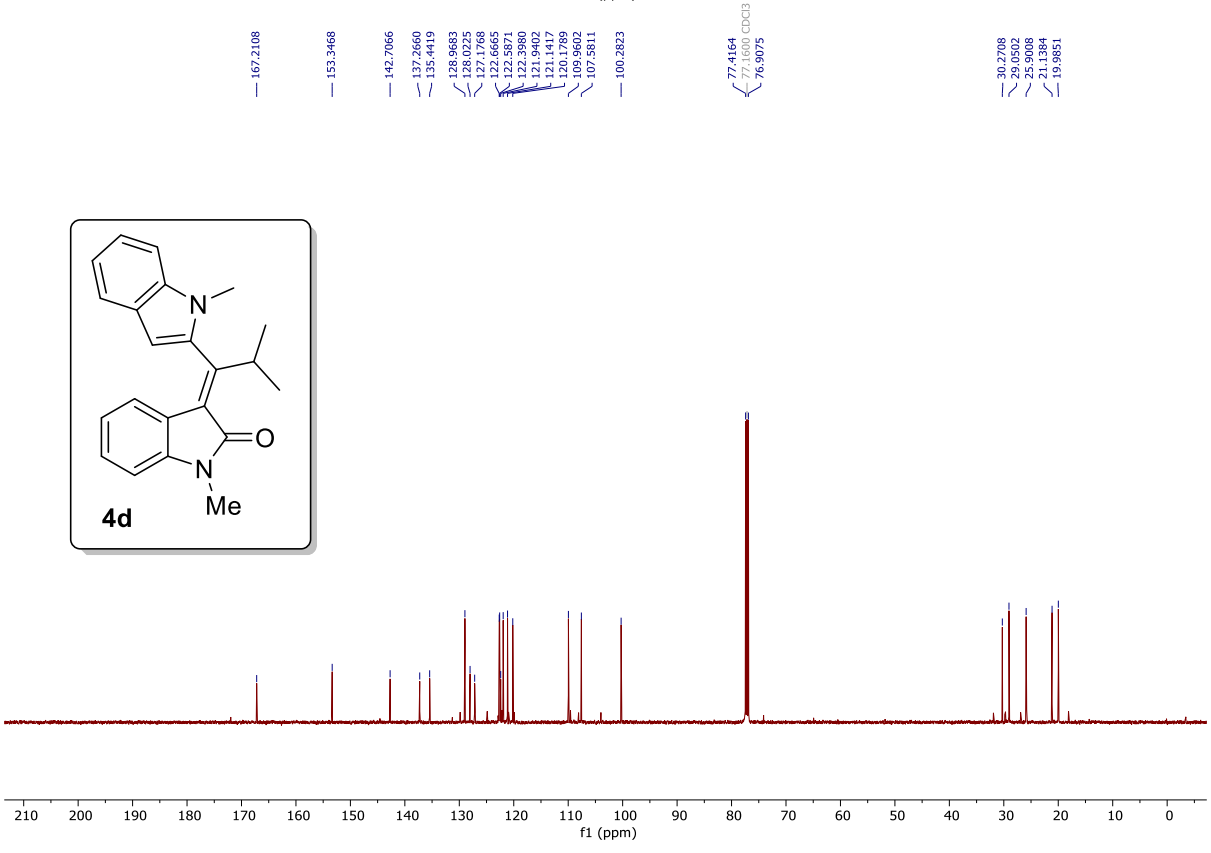

167.8907
164.4849
142.5227
138.2921
128.9217
128.1055
127.9314
127.4914
123.3914
123.2322
122.9739
121.5668
107.4056
77.4142
76.9065
28.6166
25.8212
20.8870
Ph
O
N
Me
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.5926
7.5850
7.5792
7.2600 CDCl3
7.1916
7.1819
7.1729
7.1627
7.1527
6.7918
6.7822
6.7722
6.7610
6.7512
6.7413
6.7304
6.5730
6.5658
6.5596
6.5515
6.4236
6.4150
6.4073
6.3999
5.9553
5.9456
5.9367
5.9265
4.9501
4.9409
4.9327
4.9241
4.9167
4.9070
4.8968
3.2396
1.1133
1.1052
1.0967
1.0879
1.0816
4b
1.00
1.09
1.96
1.04
1.01
1.01
1.03
2.94
6.00
f1 (ppm)
167.5347
151.3886
149.8360
142.7467
142.6246
128.8470
126.6191
123.1258
122.6207
121.9672
111.2336
110.0602
107.6361
77.4142
76.9072
28.2957
25.8958
20.6554
4b
f1 (ppm)


7.4824
7.4699
7.2600 CDCl3
7.1802
7.1684
7.1585
7.1487
7.1286
6.8465
6.8376
6.7417
6.7223
6.7053
6.6854
6.6663
5.8546
5.8352
5.0167
4.9997
4.9827
4.9657
4.9486
4.9318
3.2468
1.1062
1.0889
S
O
N
Me
4c
1.00
2.04
1.04
0.93
0.93
0.95
0.99
3.00
6.27
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.2580
157.2583
142.6174
137.7055
128.6998
127.5761
126.3079
126.1355
126.0192
123.4987
122.8555
121.8525
107.5360
77.4803
76.8446
28.5474
25.8668
20.7121
S
O
N
Me
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.7236
7.7030
7.4085
7.3880
7.3258
7.3081
7.2890
7.2680 CDCl3
7.2589
7.2200
7.2026
7.1540
7.1345
7.1161
6.7629
6.7438
6.5945
6.5762
6.5577
6.4342
5.3854
5.3666
5.0722
5.0554
5.0383
5.0213
5.0040
3.4882
3.2870
1.3284
1.3138
0.9534
0.9383
4d
N
O
N
Me
1.04
1.12
1.26
1.25
1.26
1.05
1.16
1.00
1.02
1.02
3.00
3.05
3.05
3.24
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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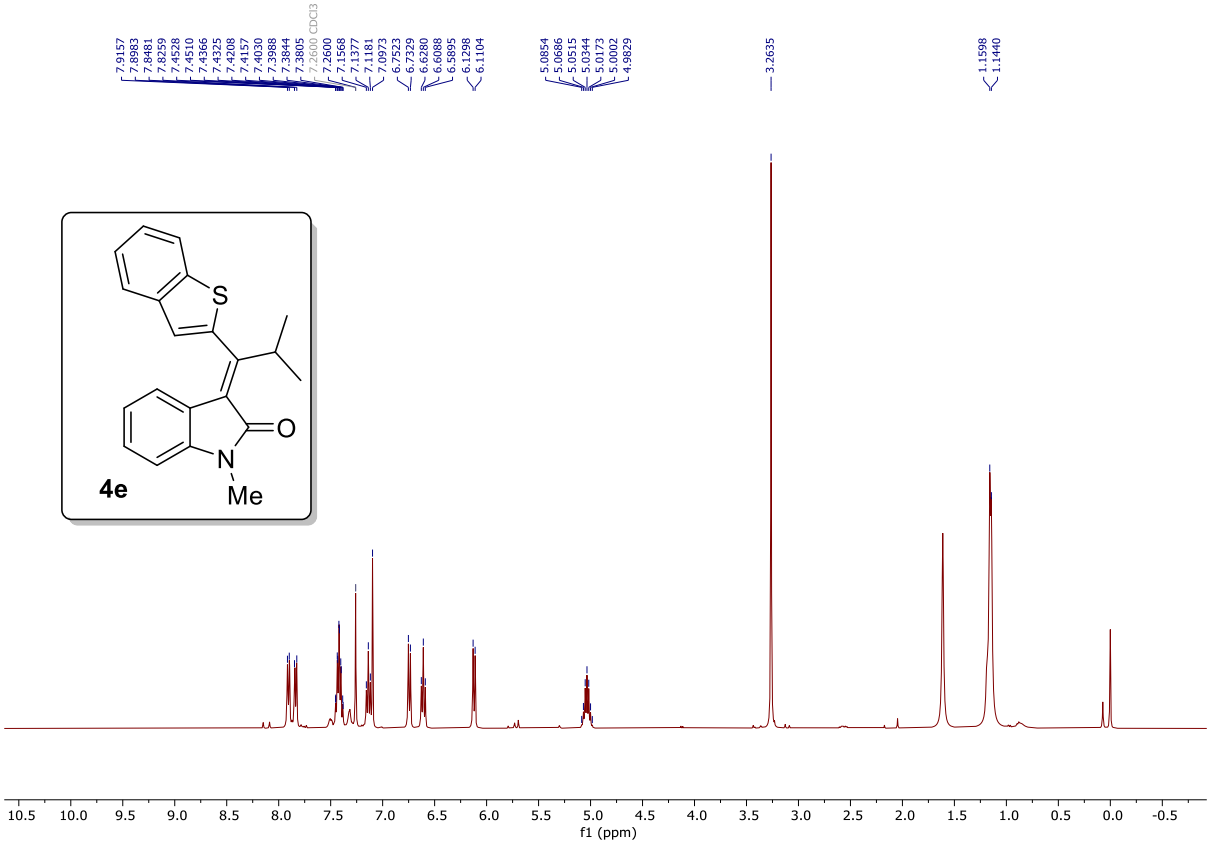
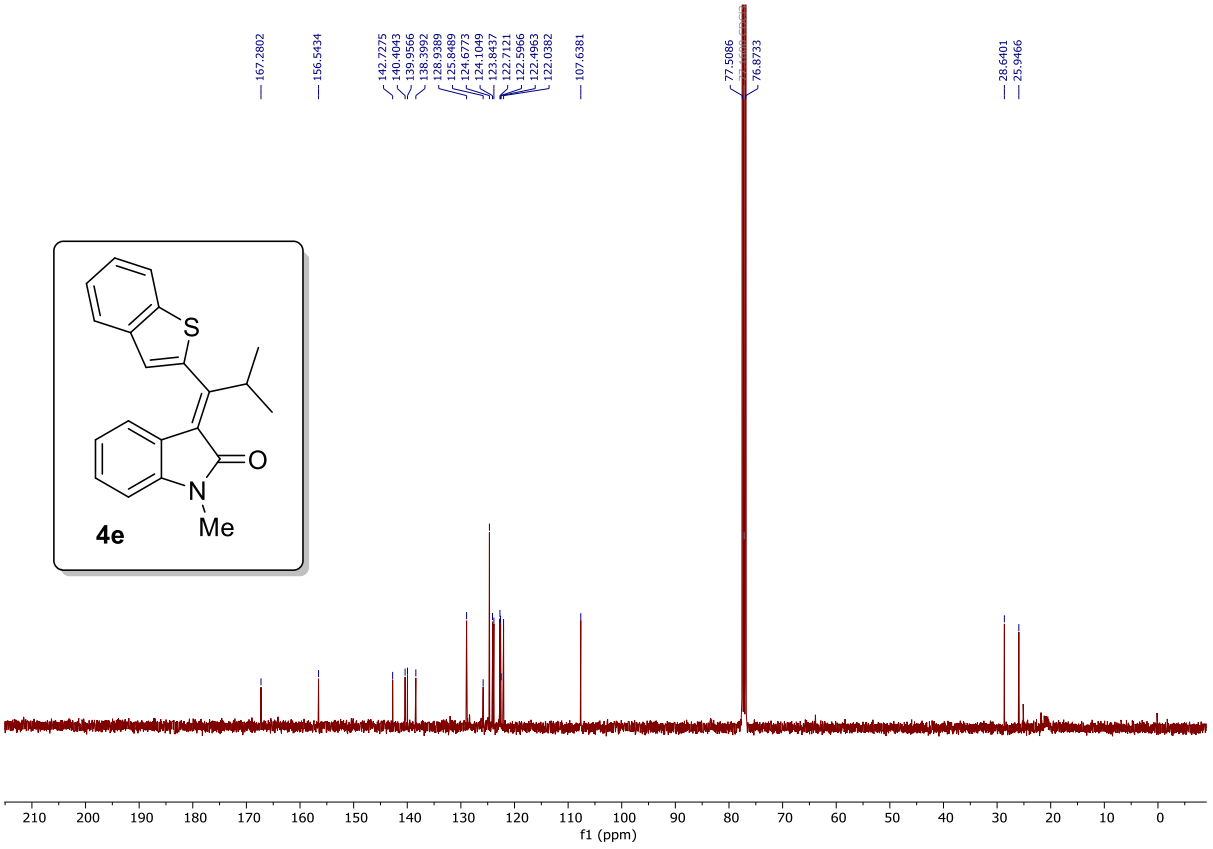
142.7066
137.2660
135.4419
128.9683
128.0225
127.1768
122.6665
122.5871
122.3980
121.9402
121.1417
120.1789
109.9602
107.5811
100.2823
77.4164
77.1600 CDCl3
76.9075
30.2708
29.0502
25.9008
21.1384
19.9851
4d
N
O
N
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.9157
7.8983
7.8461
7.8259
7.4528
7.4510
7.4366
7.4325
7.4208
7.4157
7.4030
7.3988
7.3844
7.3805
7.2600 CDCl3
7.2600
7.1568
7.1377
7.1181
7.0973
6.7523
6.7329
6.6280
6.6088
6.5895
6.1298
6.1104
5.0854
5.0686
5.0515
5.0344
5.0173
5.0002
4.9829
3.2635
1.1598
1.1440
S
O
N
Me
4e
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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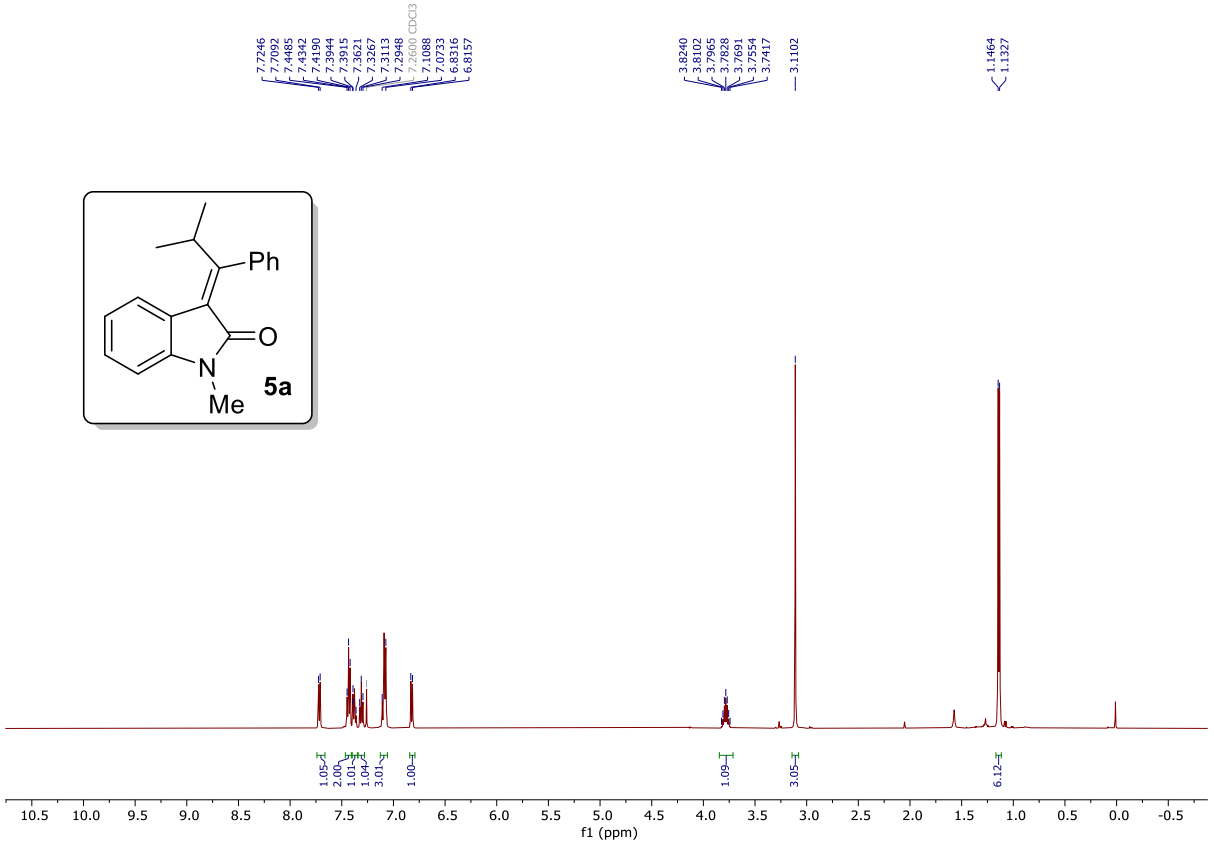
142.7275
140.4043
139.9566
138.3992
128.9389
125.8489
124.6773
124.1049
123.8437
122.7121
122.5966
122.4963
122.0382
107.6381
77.5086
76.8733
28.6401
25.9466
S
O
N
Me
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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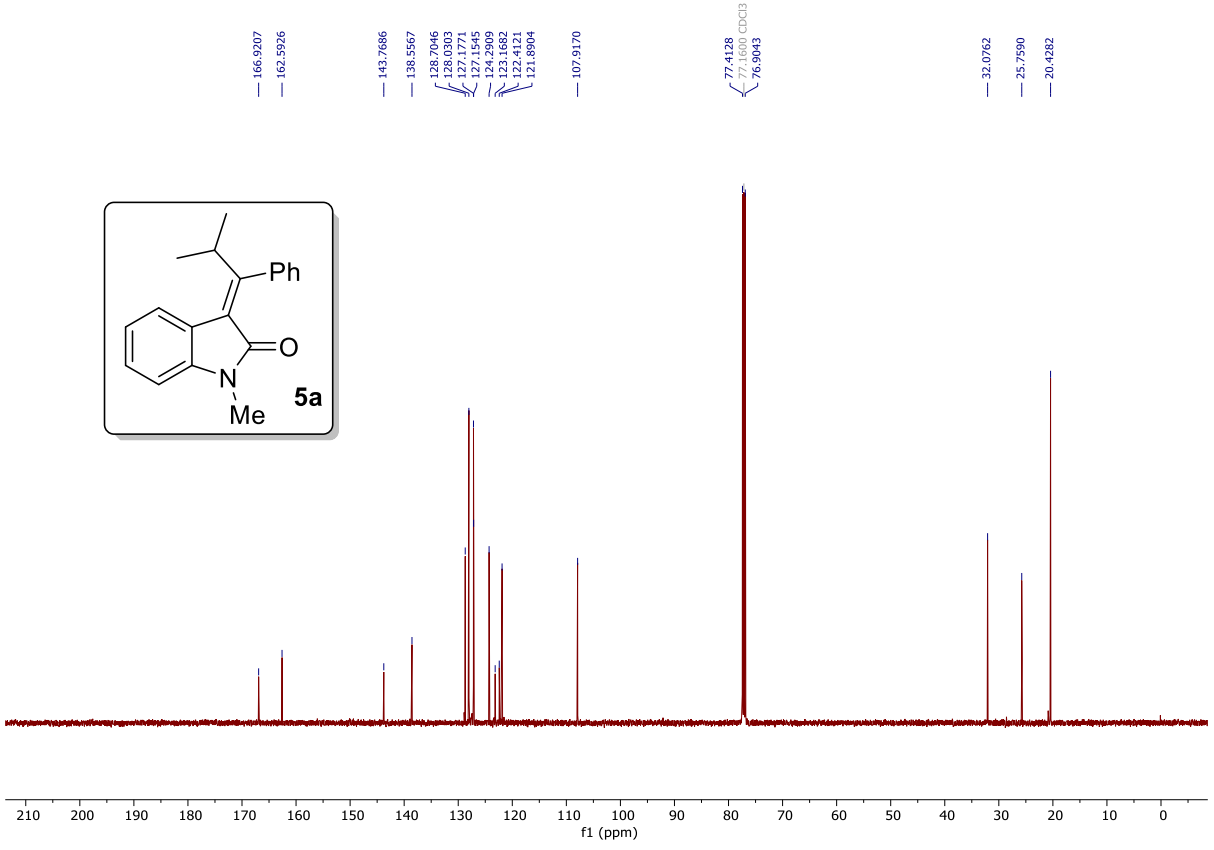
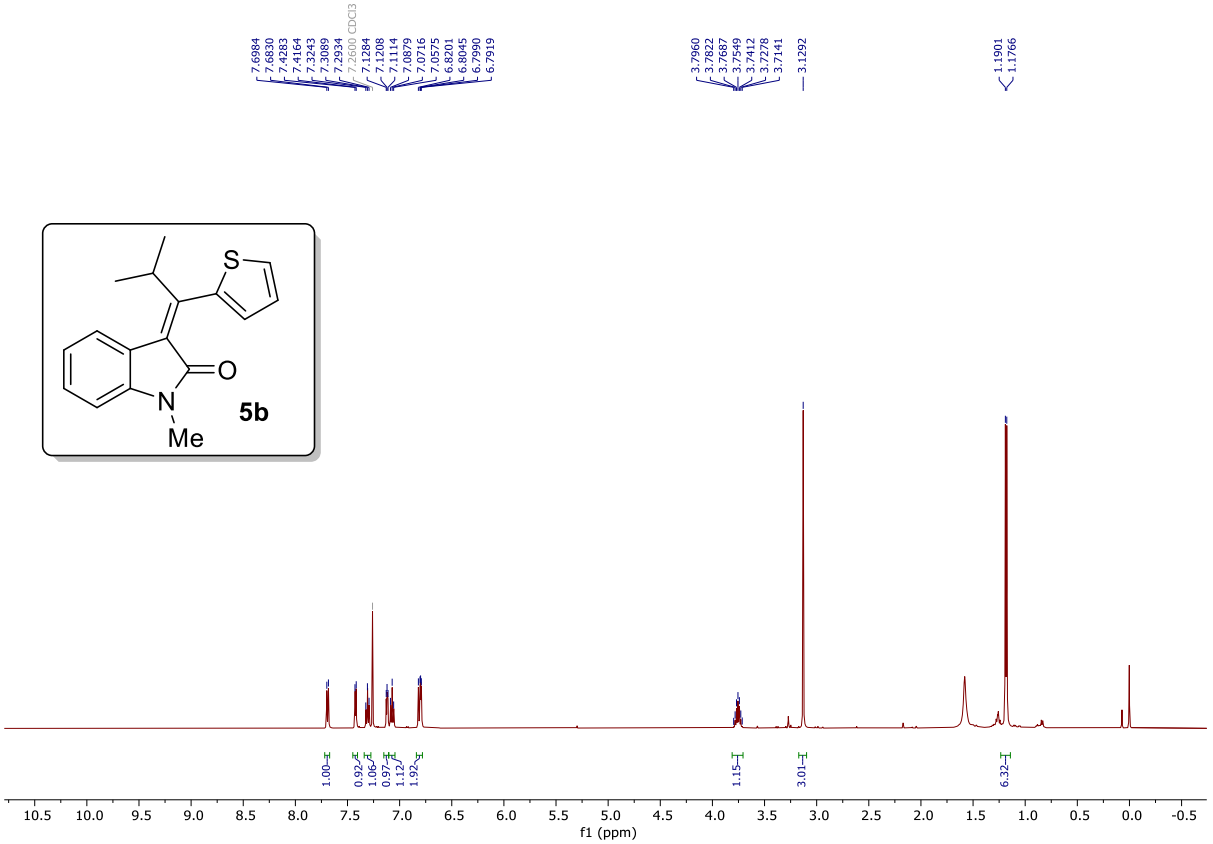
7.4342
7.4190
7.3944
7.3915
7.3621
7.3267
7.3113
7.2948
7.2600 CDCl3
7.1088
7.0733
6.8316
6.8157
3.8240
3.8102
3.7965
3.7828
3.7691
3.7554
3.7417
3.1102
1.1464
1.1327
Ph
O
N
Me
5a
1.05
2.00
1.01
1.04
3.01
1.00
1.09
3.05
6.12
f1 (ppm)


166.9207
162.5926
143.7686
138.5567
128.7046
128.0303
127.1771
127.1545
124.2909
123.1682
122.4121
121.8904
107.9170
77.4128
77.1600 CDCl3
76.9043
32.0762
25.7590
20.4282
Ph
O
N
Me
5a
f1 (ppm)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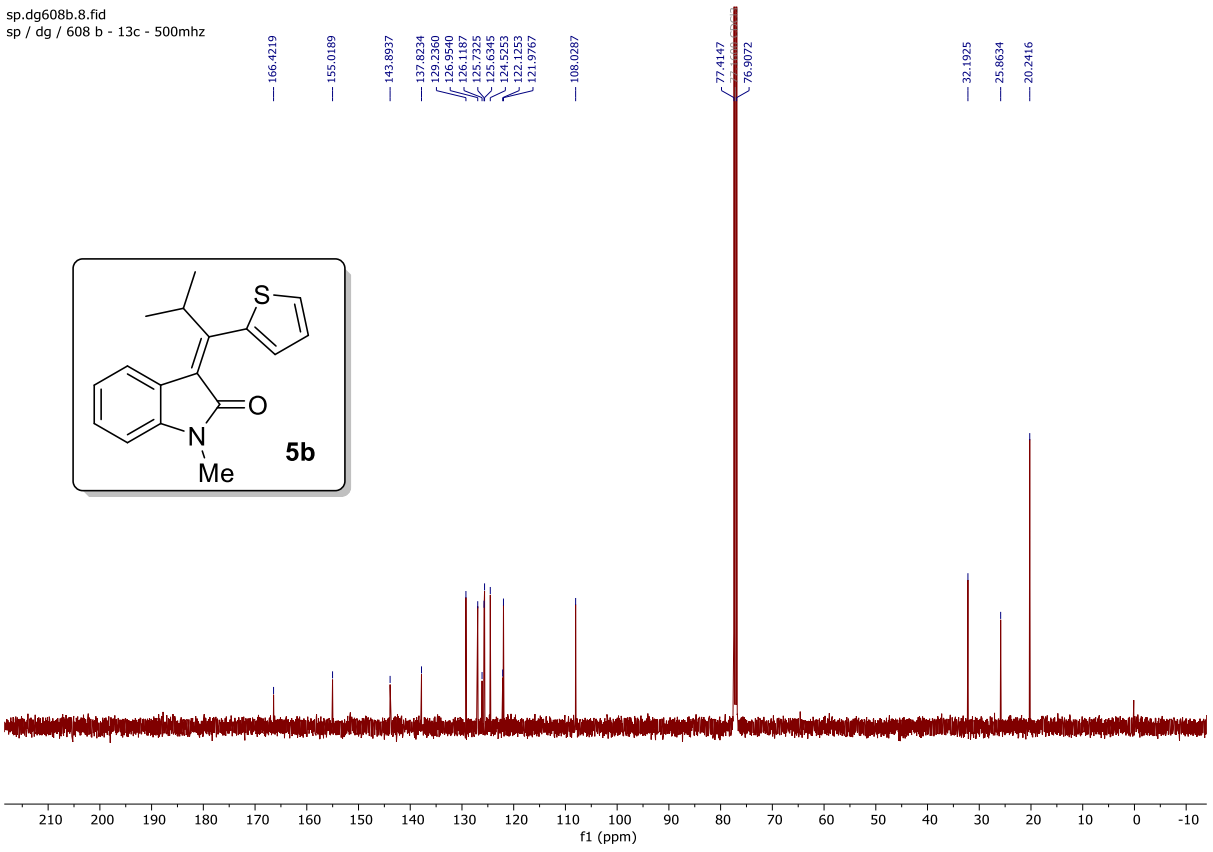
7.6830
7.4283
7.4164
7.3243
7.3089
7.2934
7.2600 CDCl3
7.1284
7.1208
7.1114
7.0879
7.0716
7.0575
6.8201
6.8045
6.7990
6.7919
3.7960
3.7822
3.7687
3.7549
3.7412
3.7278
3.7141
3.1292
1.1901
1.1766
S
O
N
Me
5b
1.00
0.92
1.06
0.97
1.12
1.92
1.15
3.01
6.32
f1 (ppm)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sp / dg / 608 b - 13c - 500mhz
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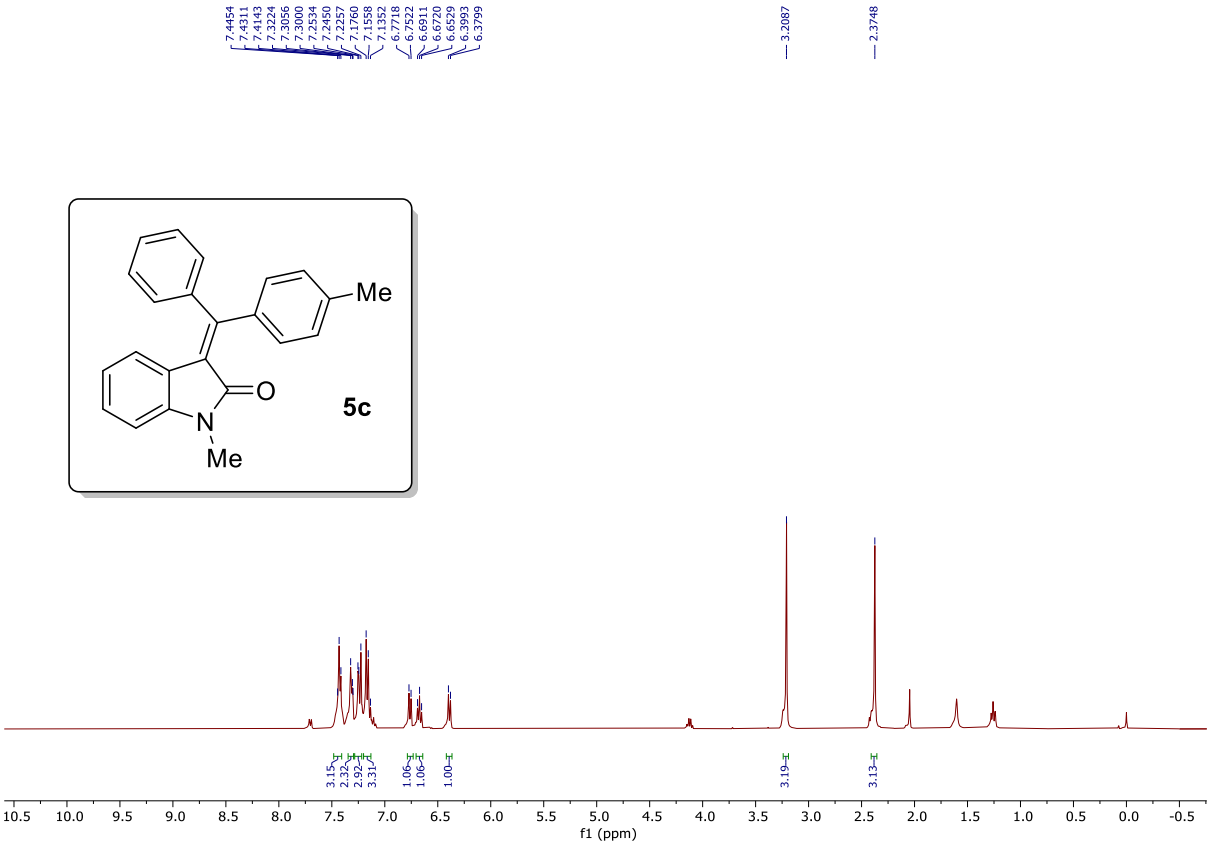
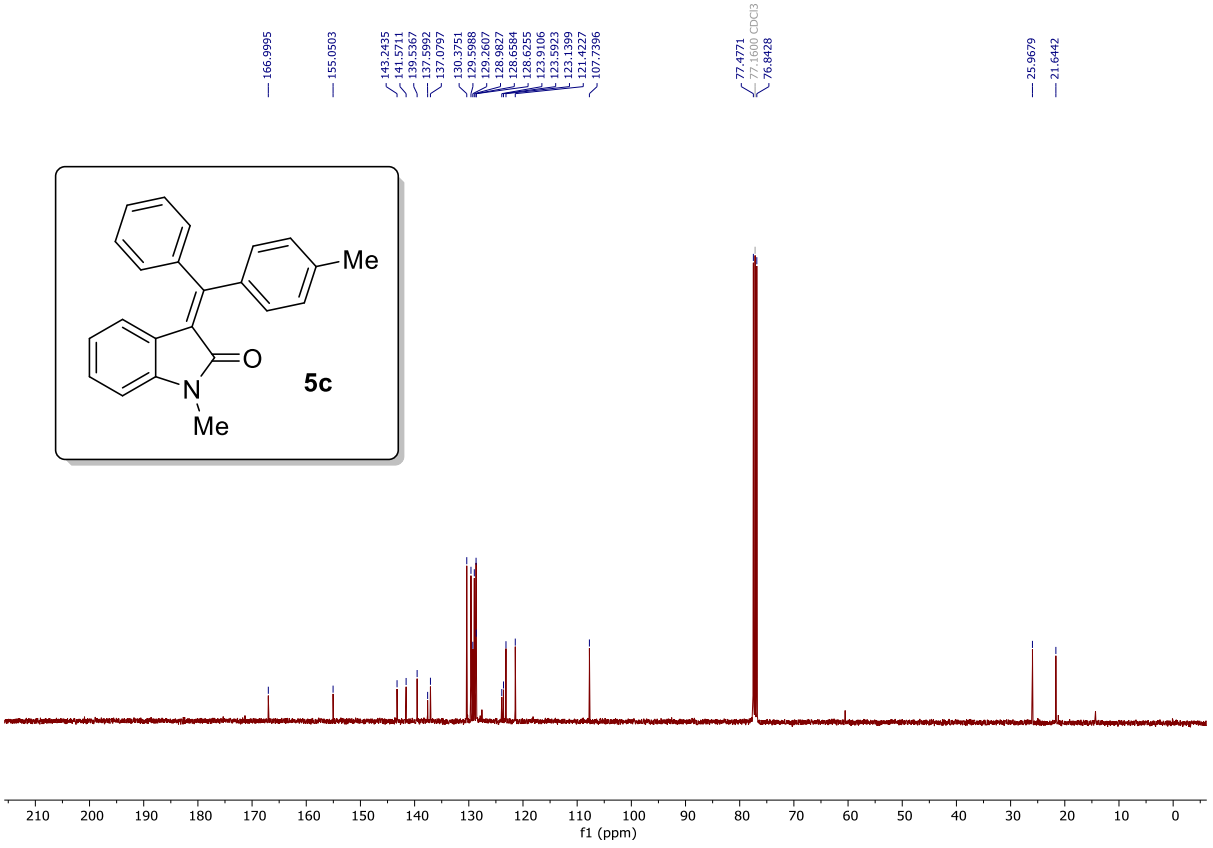
137.8234
129.2360
126.9540
126.1187
125.7325
125.6345
124.5253
122.1253
121.9767
108.0287
77.4147
76.9072
32.1925
25.8634
20.2416
S
O
N
Me
5b
f1 (ppm)


7.4454
7.4311
7.4143
7.3224
7.3056
7.3000
7.2534
7.2450
7.2257
7.1760
7.1558
7.1352
6.7718
6.7522
6.6911
6.6720
6.6529
6.3993
6.3799
3.2087
2.3748
Me
O
N
Me
5c
3.15
2.32
2.92
3.31
1.06
1.06
1.00
3.19
3.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.9995
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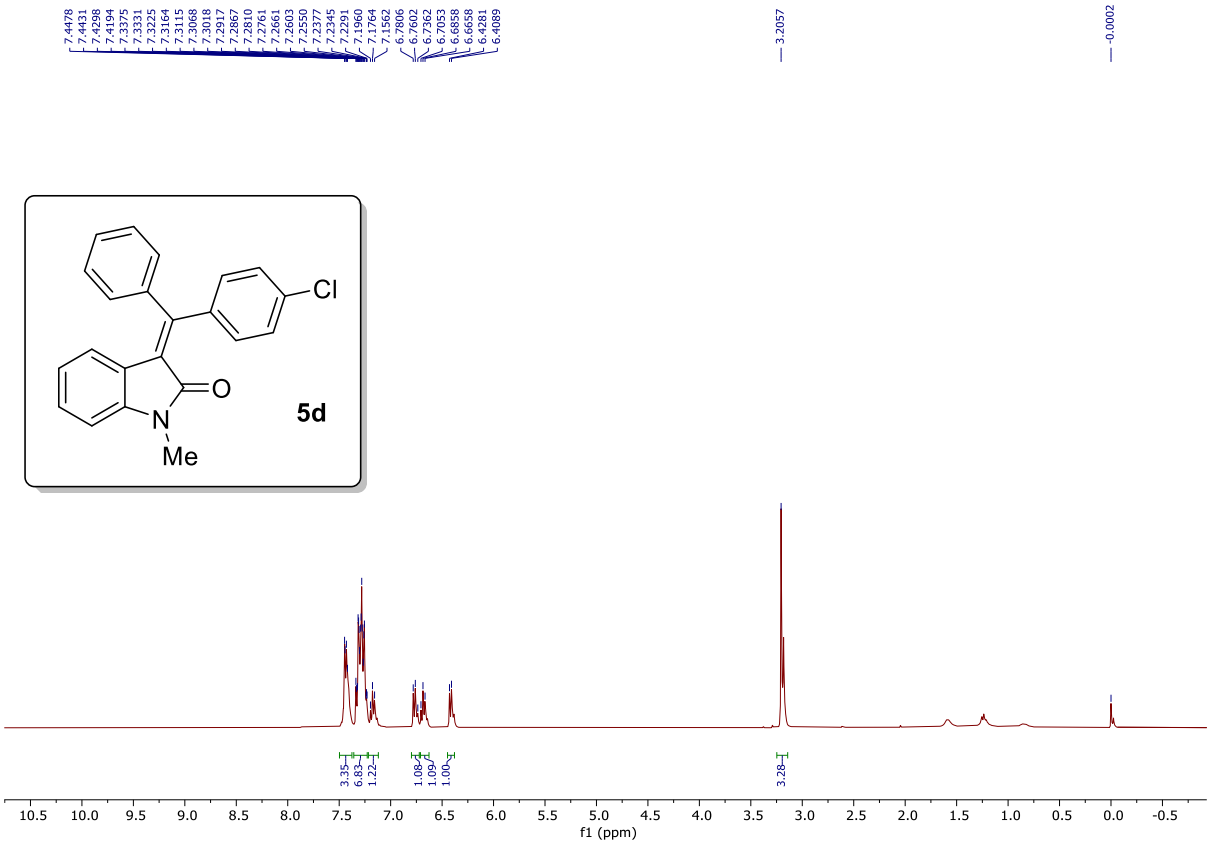
141.5711
139.5367
137.5992
137.0797
130.3751
129.5988
129.2607
128.9827
128.6584
128.6255
123.9106
123.5923
123.1399
121.4227
107.7396
77.4771
77.1600 CDCl3
76.8428
25.9679
21.6442
Me
O
N
Me
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.4478
7.4431
7.4298
7.4194
7.3375
7.3331
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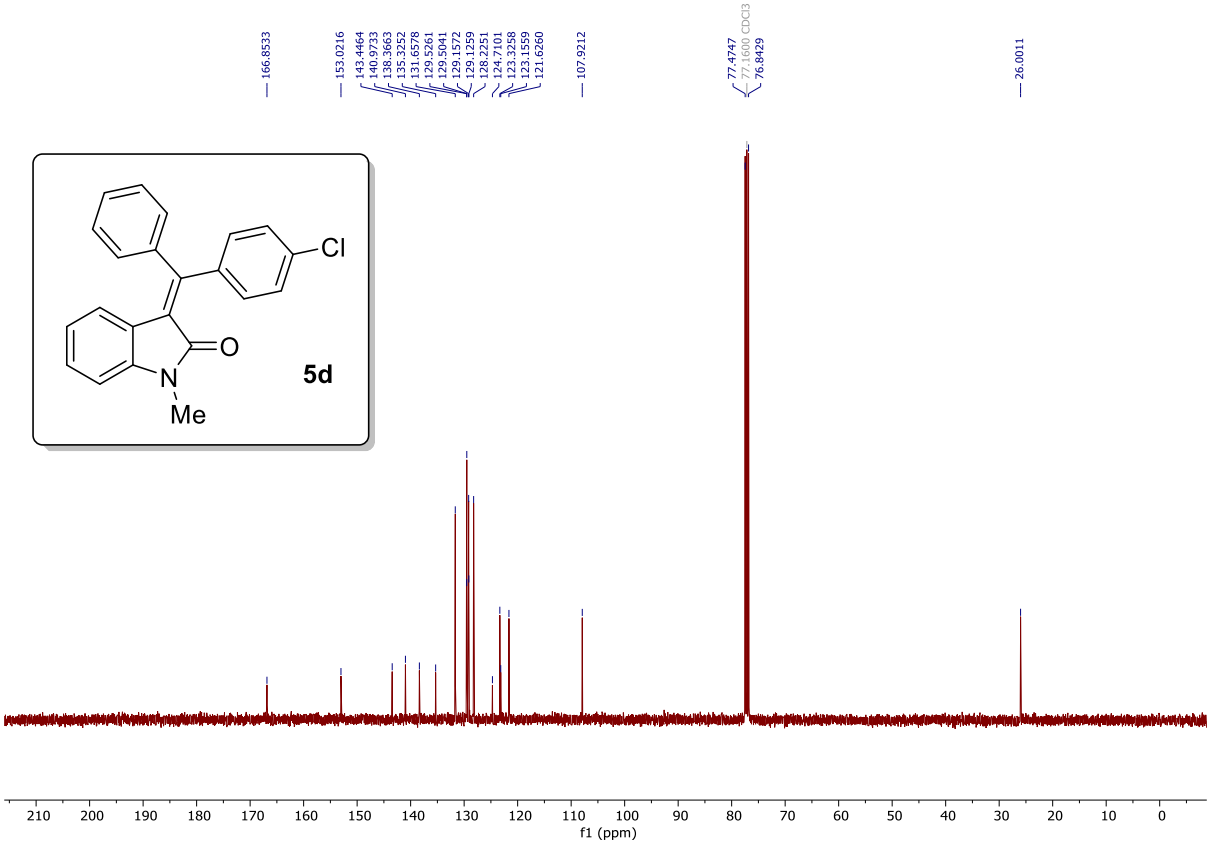
7.3115
7.3068
7.3018
7.2917
7.2867
7.2810
7.2761
7.2661
7.2603
7.2550
7.2377
7.2345
7.2291
7.1960
7.1764
7.1562
7.1366
6.7600
6.7362
6.7053
6.6858
6.6658
6.4281
6.4089
3.2057
-0.0002
Cl
O
N
Me
5d
3.35
6.83
1.22
1.08
1.09
1.00
3.28
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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135.3252
131.6578
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129.1572
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128.2251
124.7101
123.3258
123.1559
121.6260
107.9212
77.4747
77.1600 CDCl3
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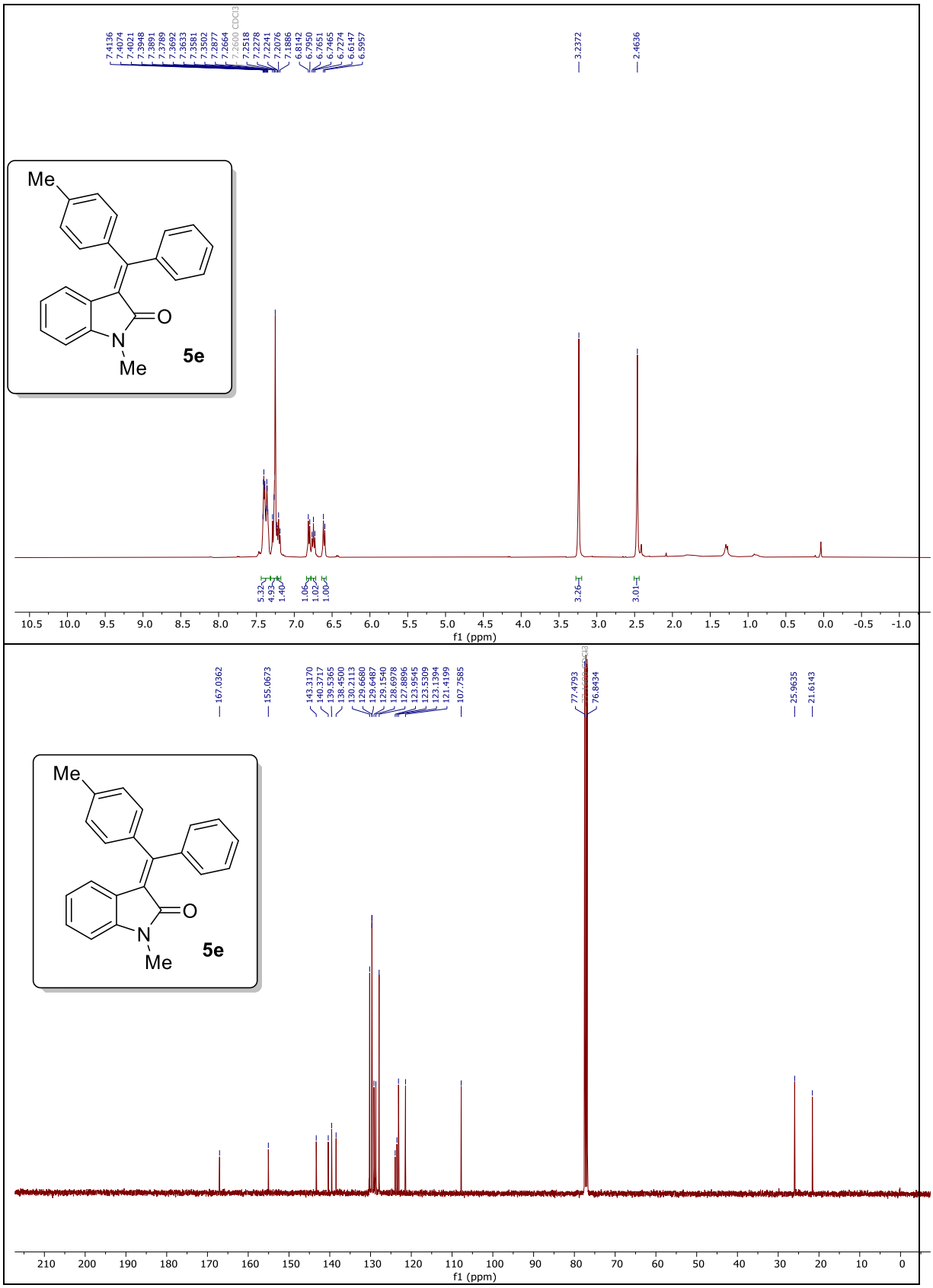
Cl
O
N
Me
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2664
7.2600 CDCl3
7.2518
7.2278
7.2241
7.2076
7.1886
6.8142
6.7950
6.7651
6.7465
6.7274
6.6147
6.5957
3.2372
2.4636
Me
O
N
Me
5e
5.32
4.93
1.40
1.06
1.02
1.00
3.26
3.01
f1 (ppm)
167.0362
155.0673
143.3170
140.3717
139.5365
138.4500
130.2113
129.6680
129.6487
129.1540
128.6978
127.8896
123.9545
123.5309
123.1394
121.4199
107.7585
77.4793
76.8434
25.9635
21.6143
Me
O
N
Me
5e
f1 (ppm)


7.2864
7.2830
7.2656
7.2555
7.2464
7.2418
7.2389
7.2121
7.1992
7.1957
7.1775
7.1742
7.1707
7.1585
7.1550
7.1516
7.1393
7.1359
7.1325
6.9312
6.9277
6.9119
6.9091
6.9055
6.9021
6.8890
6.8852
6.8820
6.8133
6.8033
6.7985
6.7934
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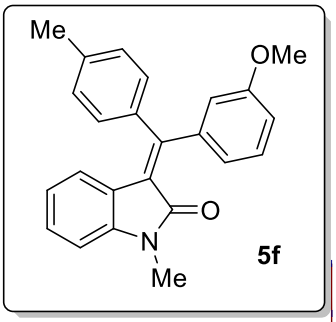
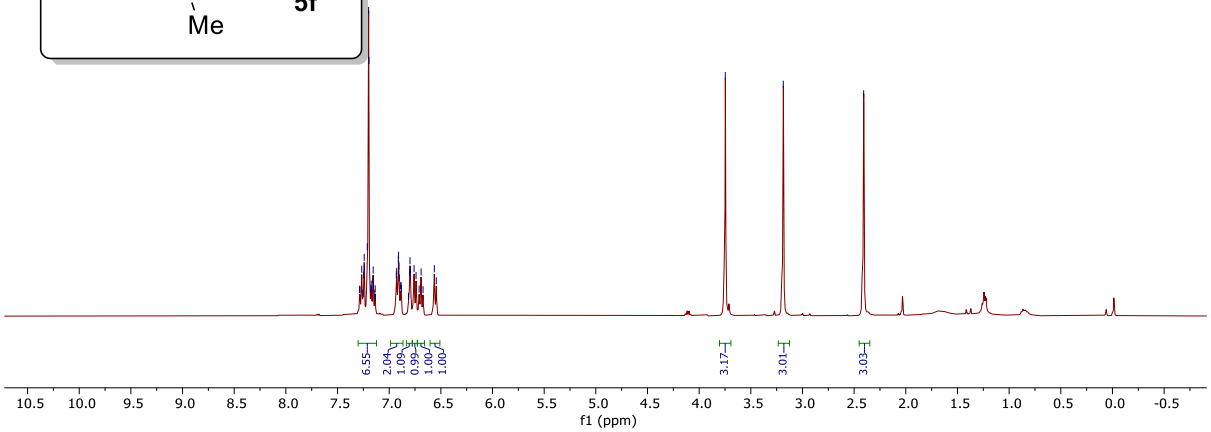
2.4079


Me
OMe
O
N
Me
5f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1.09
0.99
1.00
1.00
3.17
3.01
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.9094
159.2090
154.6809
143.3732
141.8337
139.5140
138.2488
129.6718
129.5088
128.8655
128.7604
124.1252
123.4621
123.1743
122.6029
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114.3689
107.7506
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77.1600 CDCl3
76.8447
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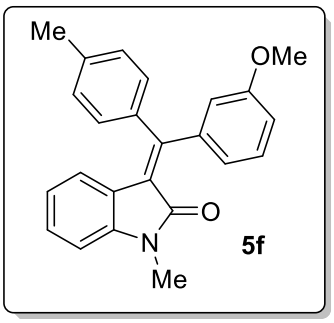
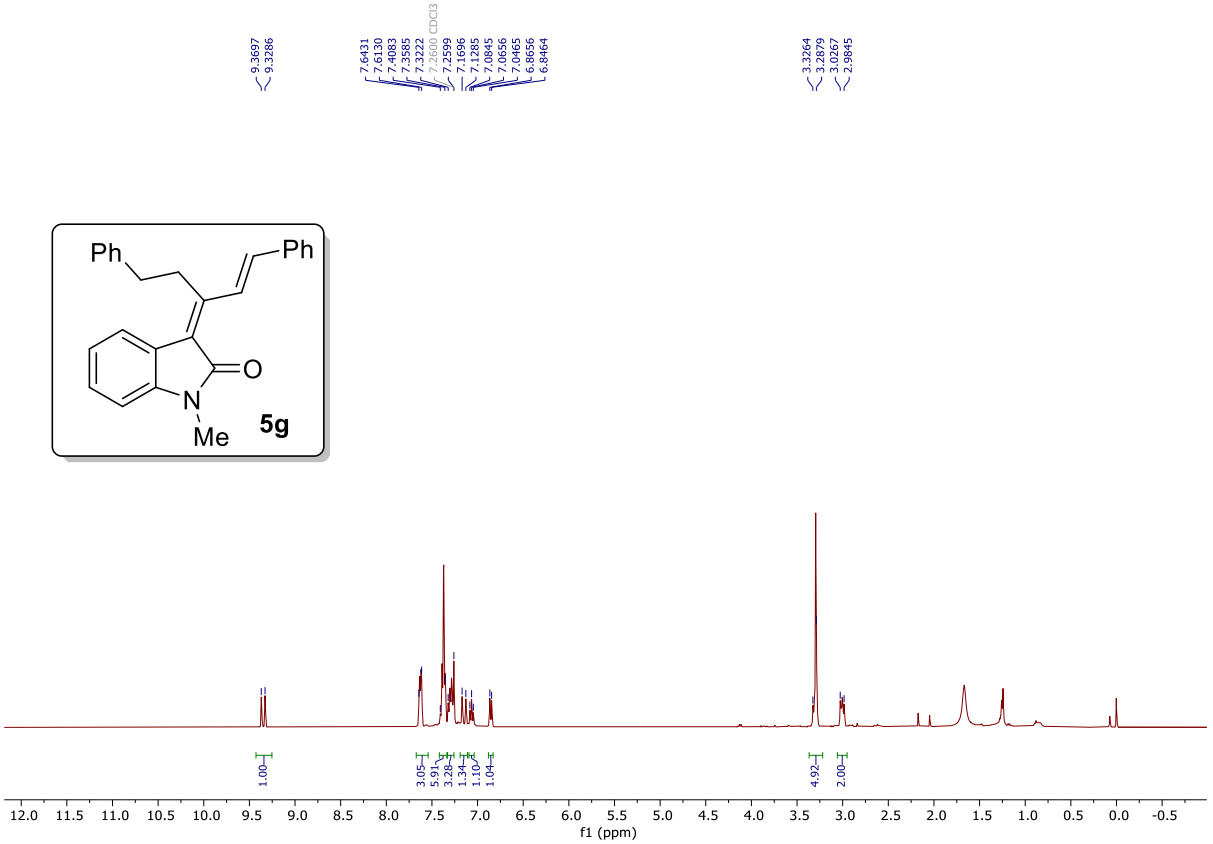
25.9786
21.6101


Me
OMe
O
N
Me
5f

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.3222
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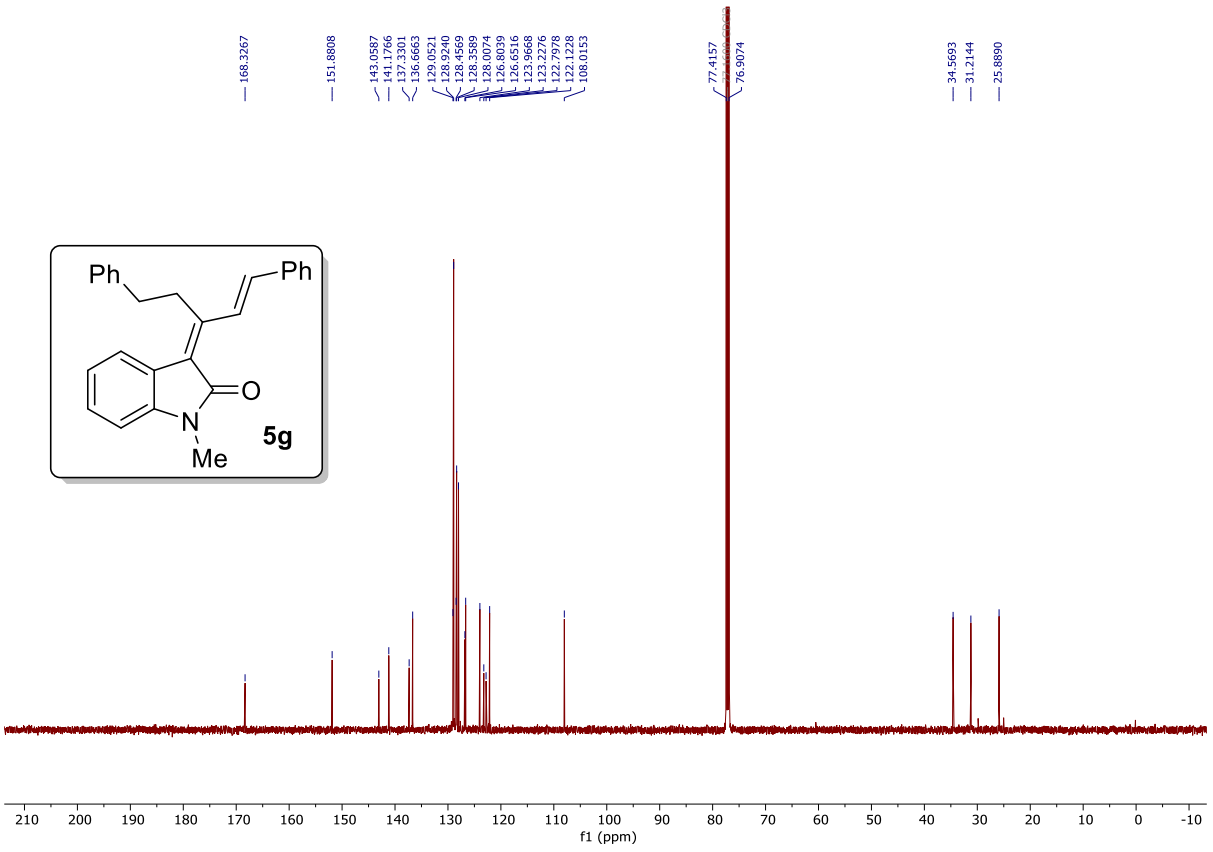
7.0845
7.0656
7.0465
6.8656
6.8464
3.3264
3.2879
3.0267
2.9845
Ph
Ph
O
N
Me
5g
1.00
3.05
5.91
3.28
1.34
1.10
1.04
4.92
2.00
f1 (ppm)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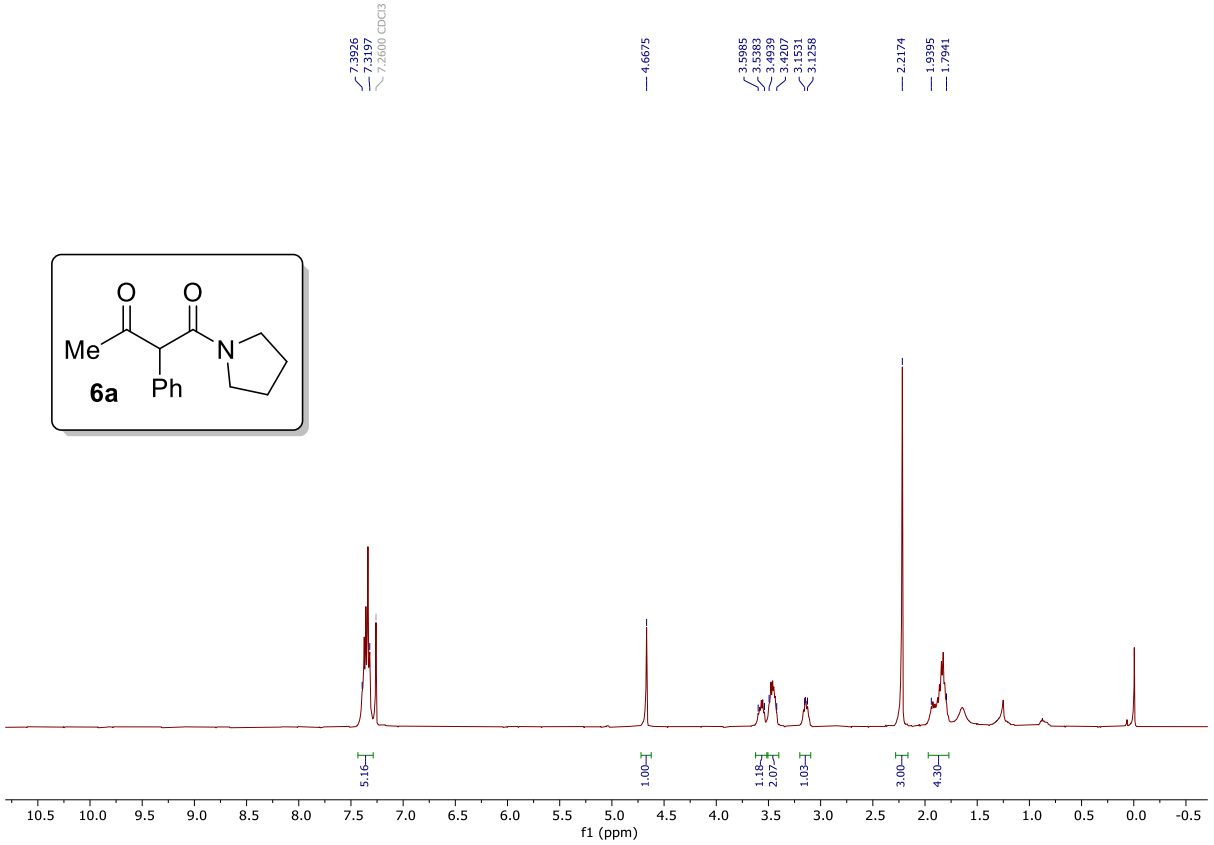
143.0587
141.1766
137.3301
136.6663
129.0521
128.9240
128.4569
128.3589
128.0074
126.8039
126.6516
123.9668
123.2276
122.7978
122.1228
108.0153
77.4157
76.9074
34.5693
31.2144
25.8890
Ph
Ph
O
N
Me
5g
f1 (ppm)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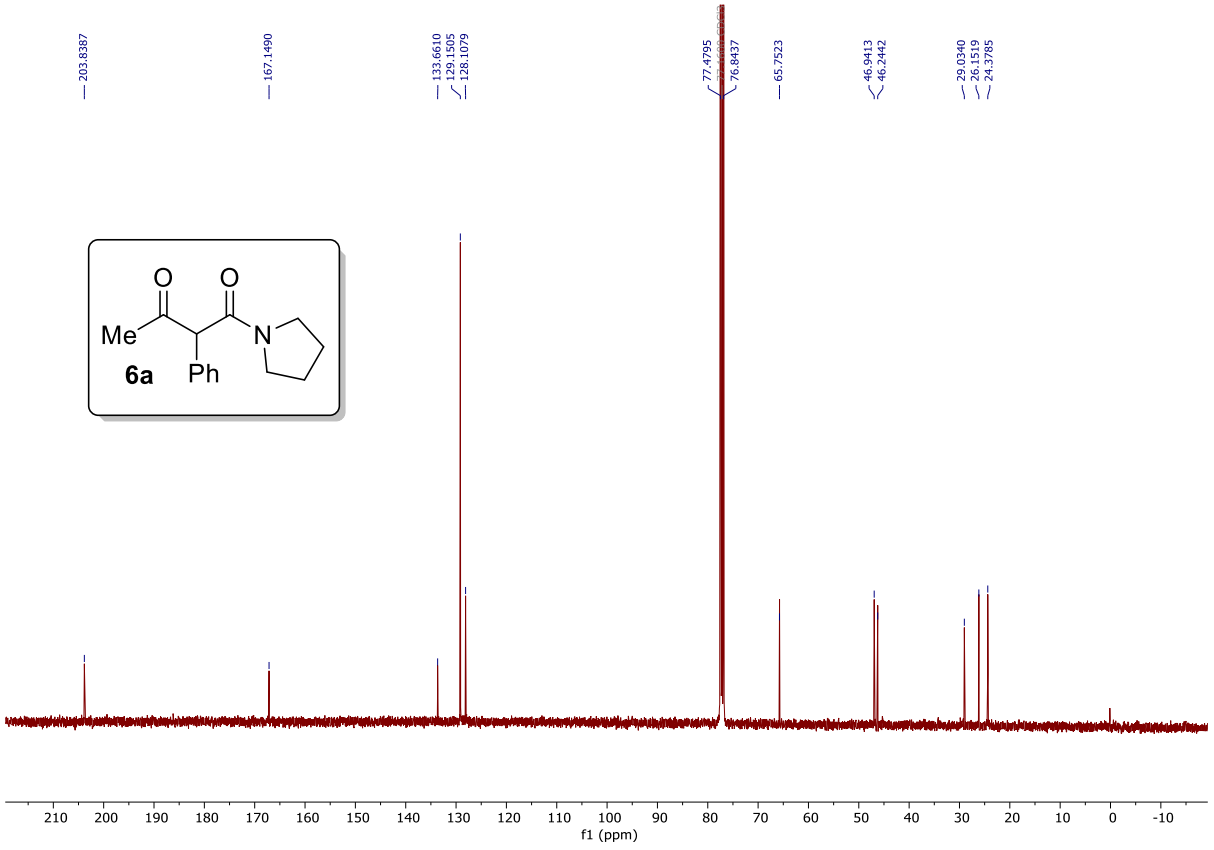
7.3197
7.2600 CDCl3
4.6675
3.5985
3.5383
3.4939
3.4207
3.1531
3.1258
2.2174
1.9395
1.7941
O
O
Me
N
Ph
6a
5.16
1.00
1.18
2.07
1.03
3.00
4.30
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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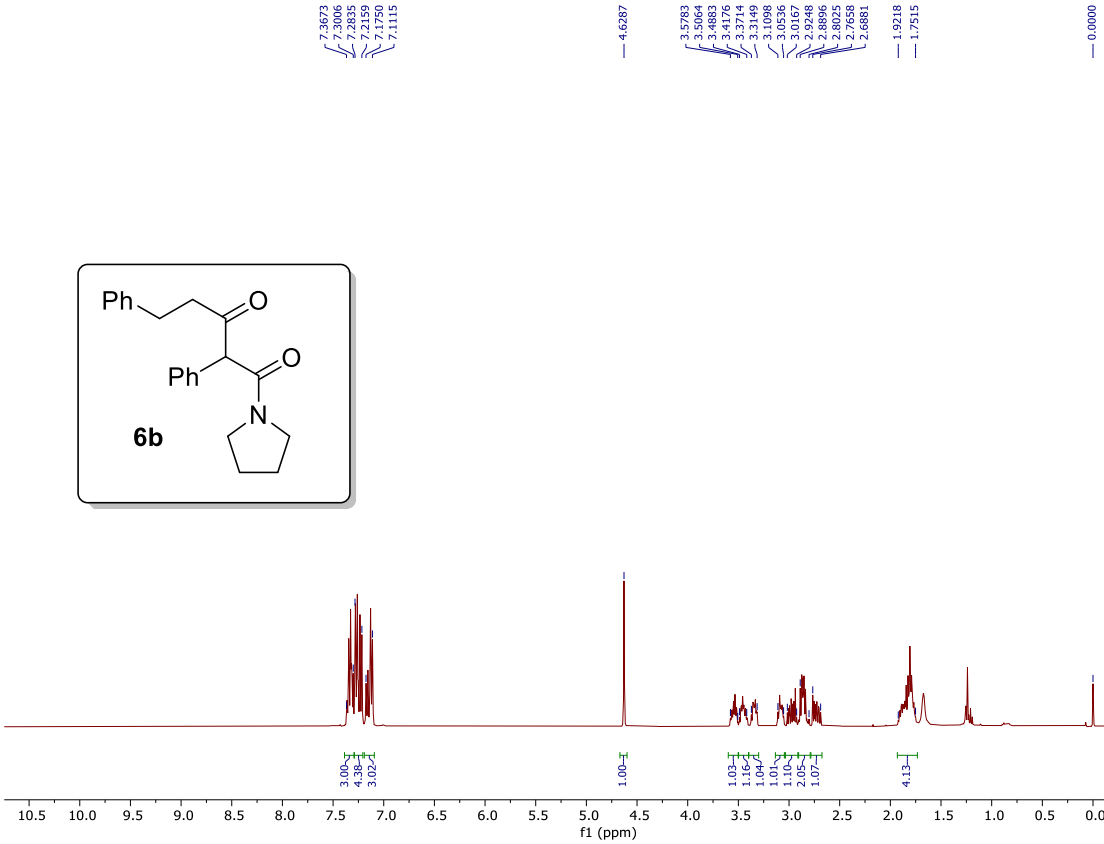
128.1079
77.4795
76.8437
65.7523
46.9413
46.2442
29.0340
26.1519
24.3765
O
O
Me
N
Ph
6a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.2159
7.1750
7.1115
4.6287
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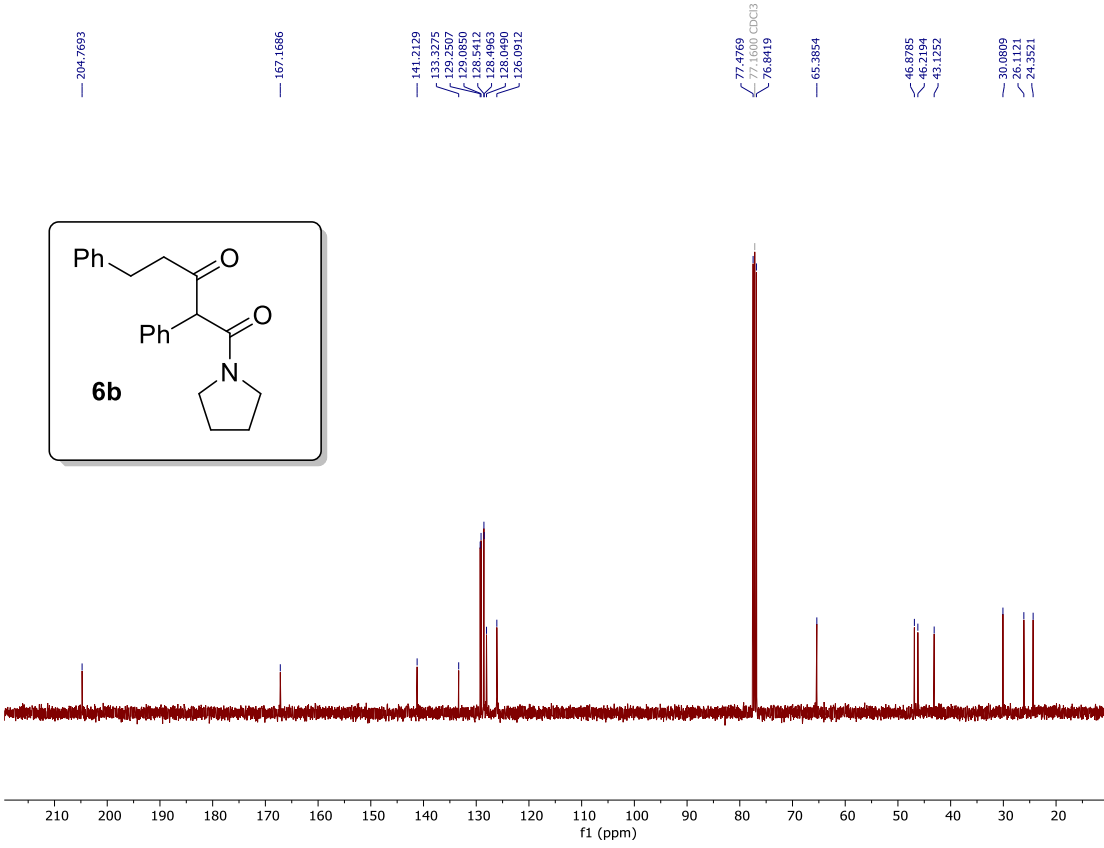
3.5064
3.4883
3.4176
3.3714
3.3149
3.1098
3.0536
3.0167
2.9248
2.8896
2.8025
2.7658
2.6881
1.9218
1.7515
0.0000
Ph
O
Ph
O
N
6b
3.00
4.38
3.02
1.00
1.03
1.16
1.04
1.01
1.10
2.05
1.07
4.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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77.1600 CDCl3
76.8419
65.3854
46.8785
46.2194
43.1252
30.0809
26.1121
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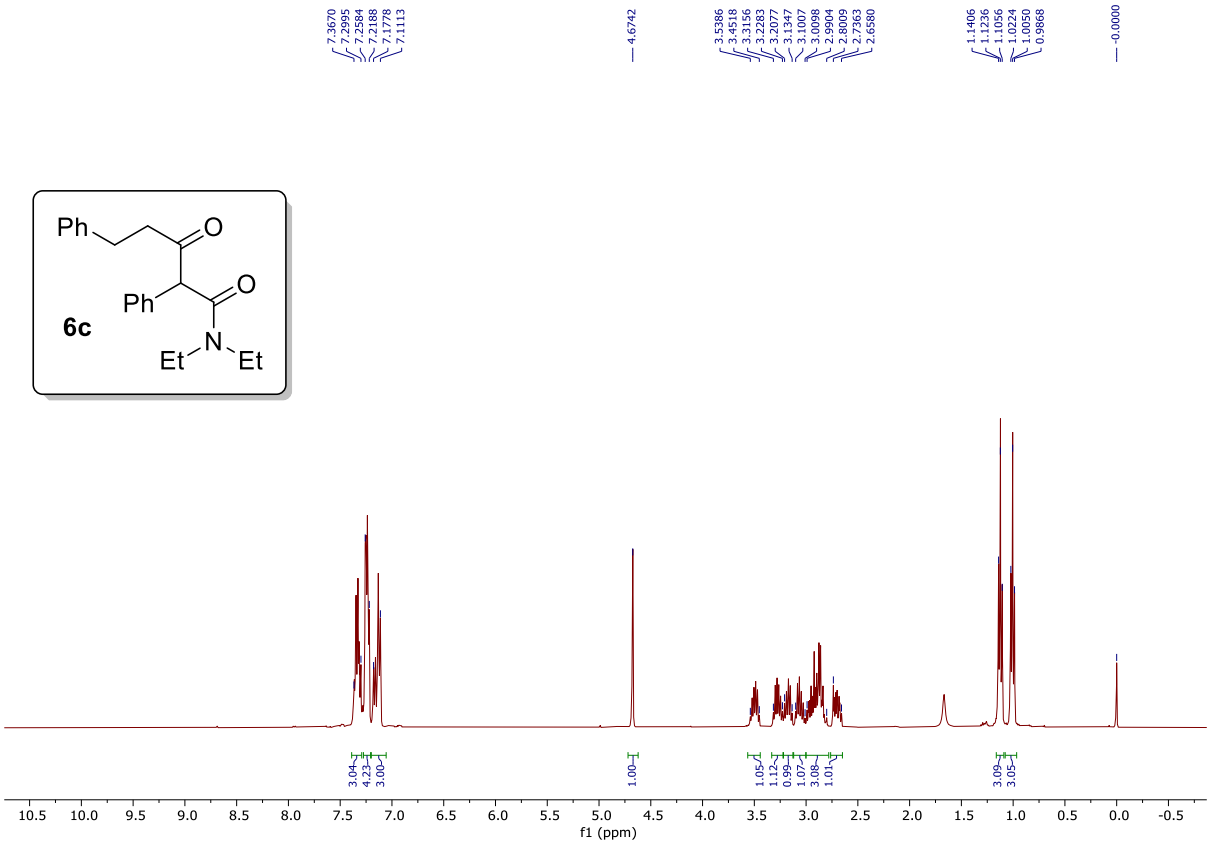
Ph
O
Ph
O
N
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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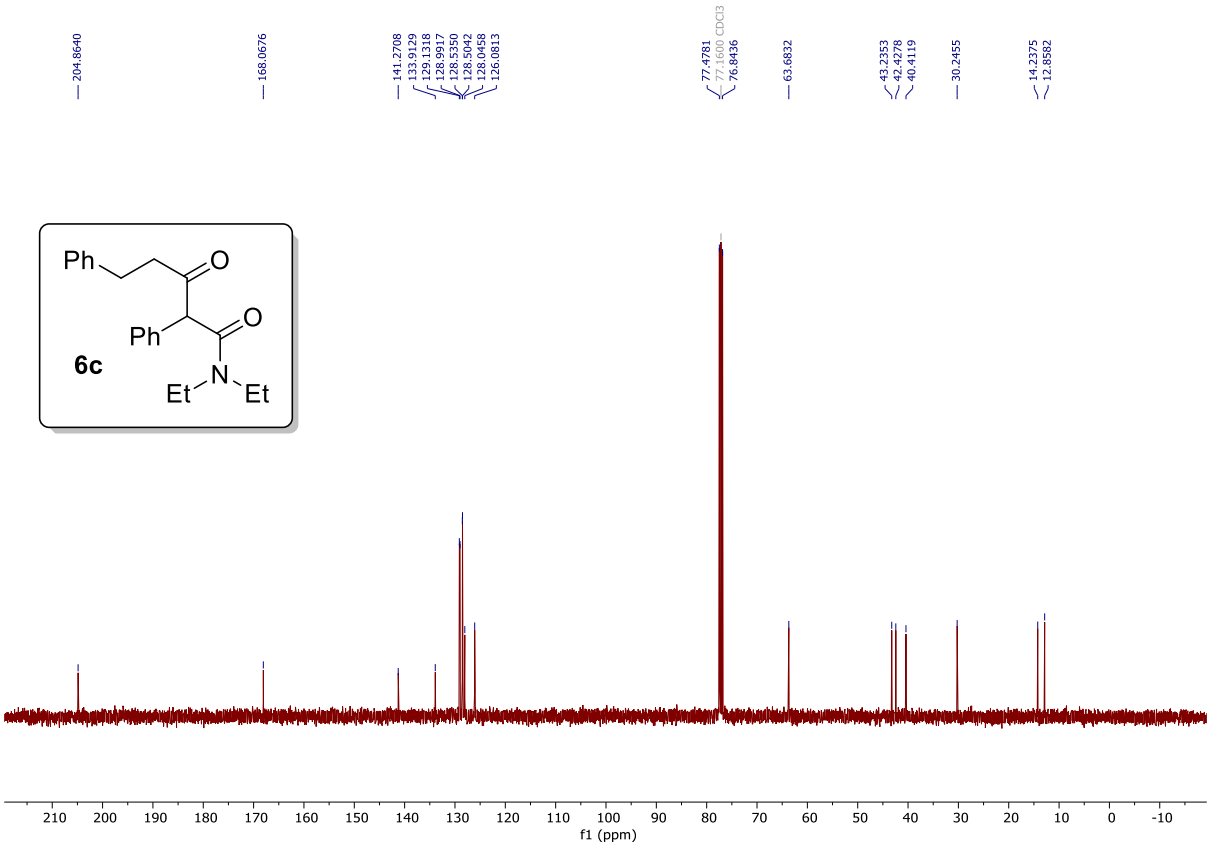
7.2188
7.1778
7.1113
4.6742
3.5386
3.4518
3.3156
3.2283
3.2077
3.1347
3.1007
3.0098
2.9904
2.8009
2.7363
2.6580
1.1406
1.1236
1.1056
1.0224
1.0050
0.9868
-0.0000
Ph
O
Ph
O
6c
N
Et
Et
3.04
4.23
3.00
1.00
1.05
1.12
0.99
1.07
3.08
1.01
3.09
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.1600 CDCl3
76.8436
63.6832
43.2353
42.4278
40.4119
30.2455
14.2375
12.8582
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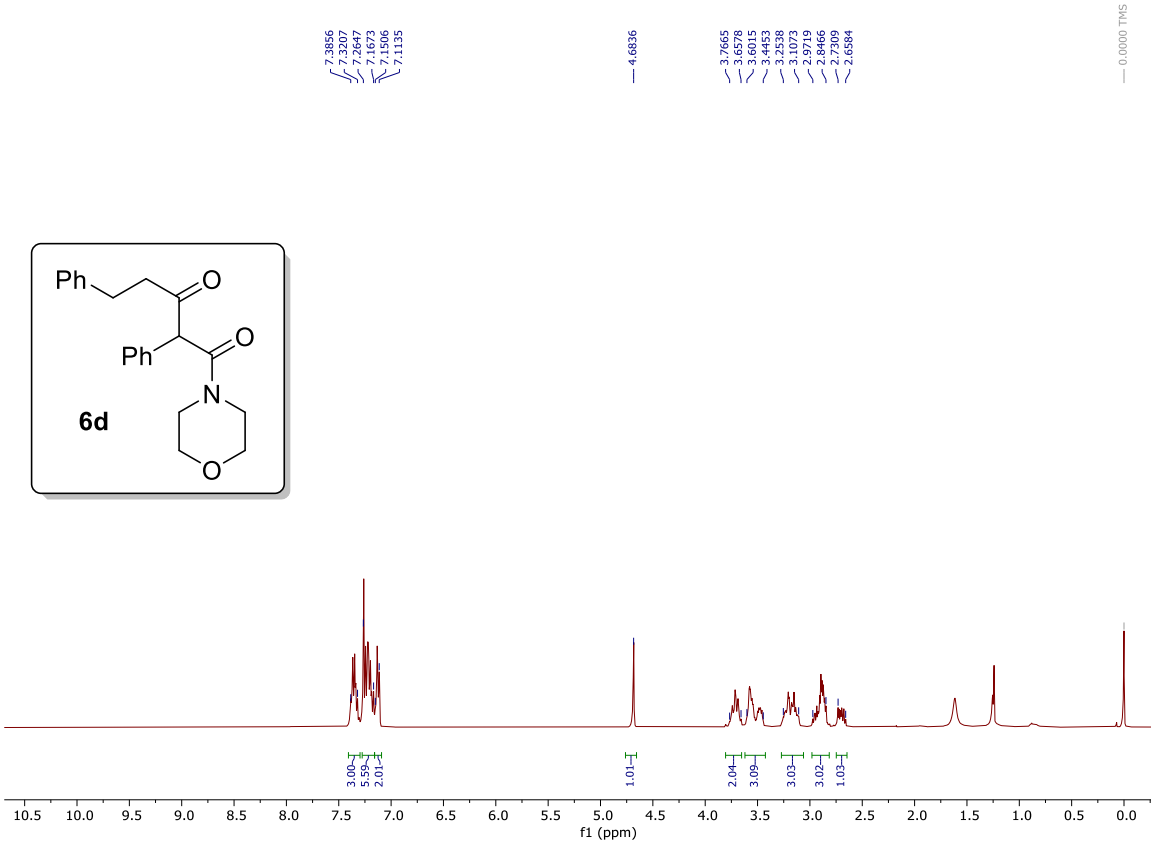
O
Ph
O
6c
N
Et
Et
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.1506
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4.6836
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3.6578
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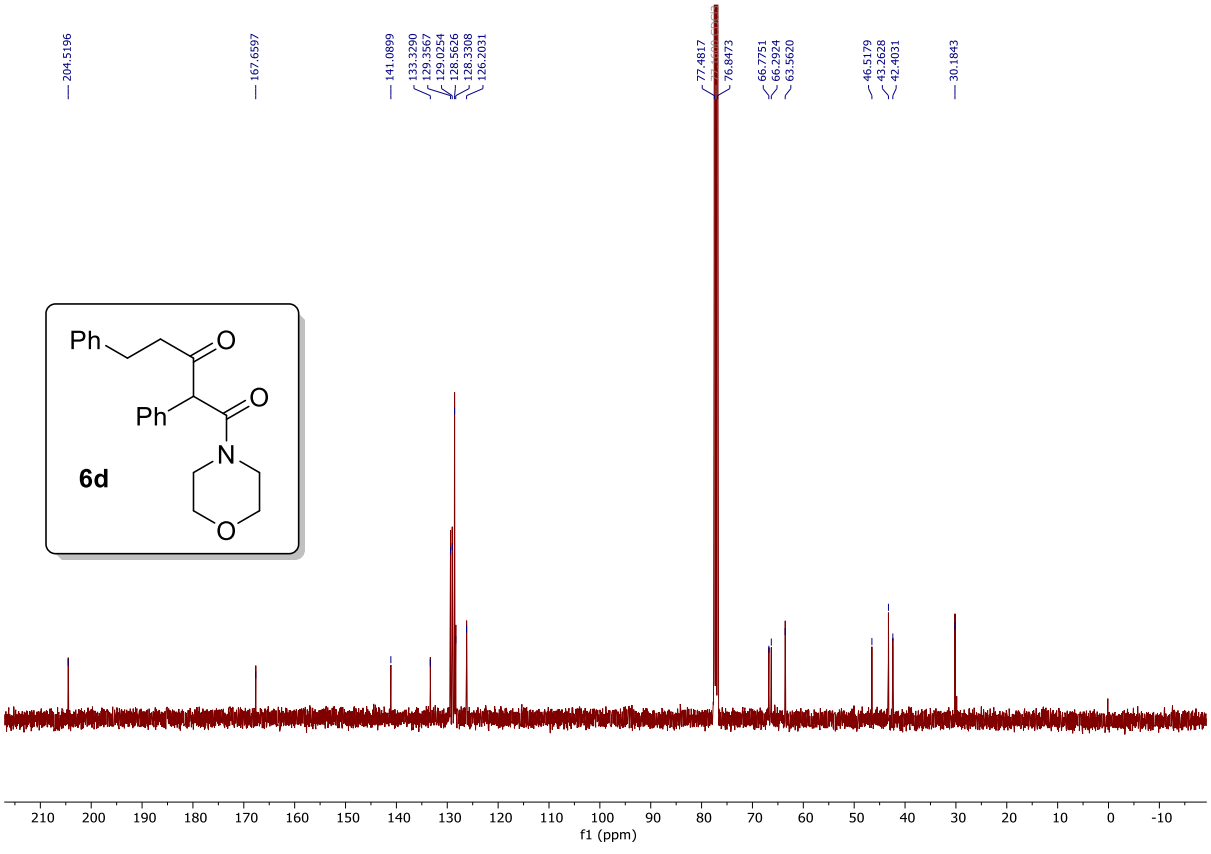
3.4453
3.2538
3.1073
2.9719
2.8466
2.7309
2.6584
0.0000 TMS
Ph
O
Ph
O
N
O
6d
3.00
5.59
2.01
1.01
2.04
3.09
3.03
3.02
1.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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76.8473
66.7751
66.2924
63.5620
46.5179
43.2628
42.4031
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Ph
O
Ph
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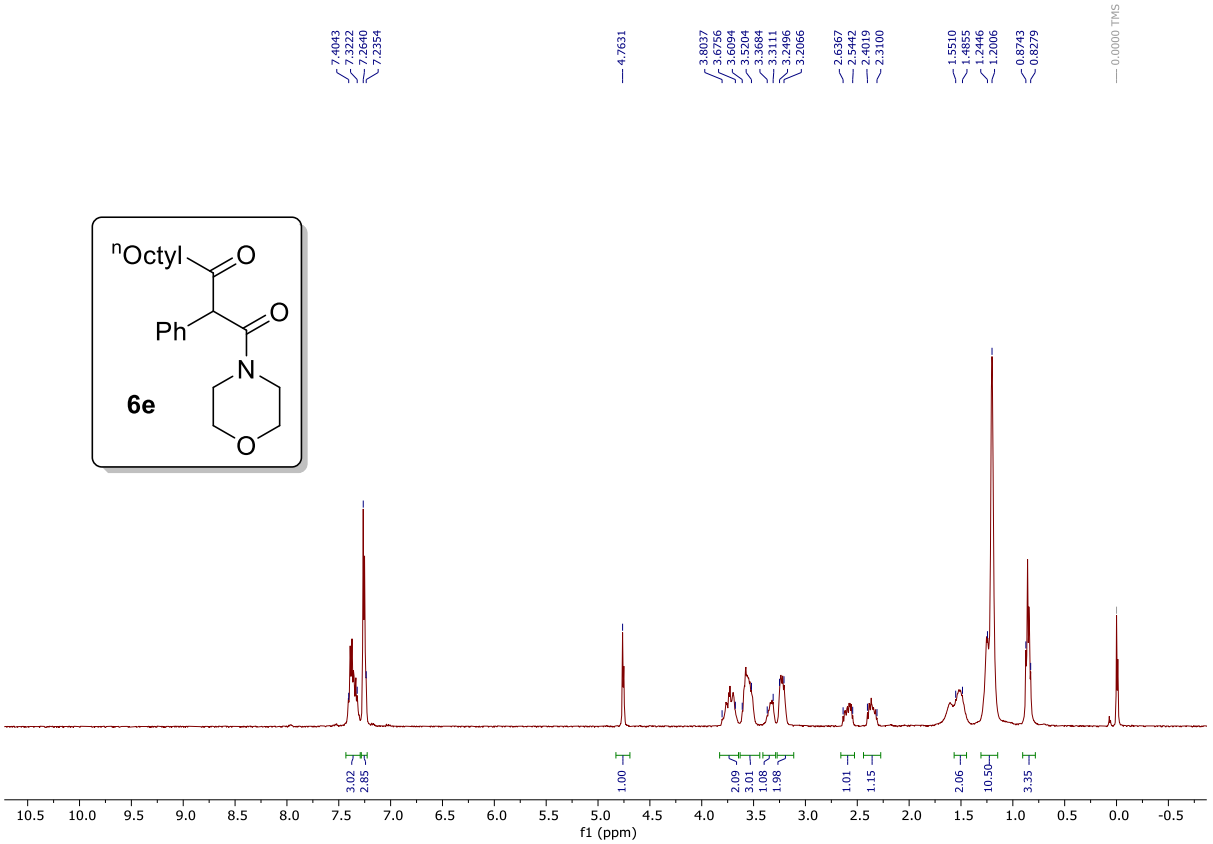
f1 (ppm)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3.6756
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3.5204
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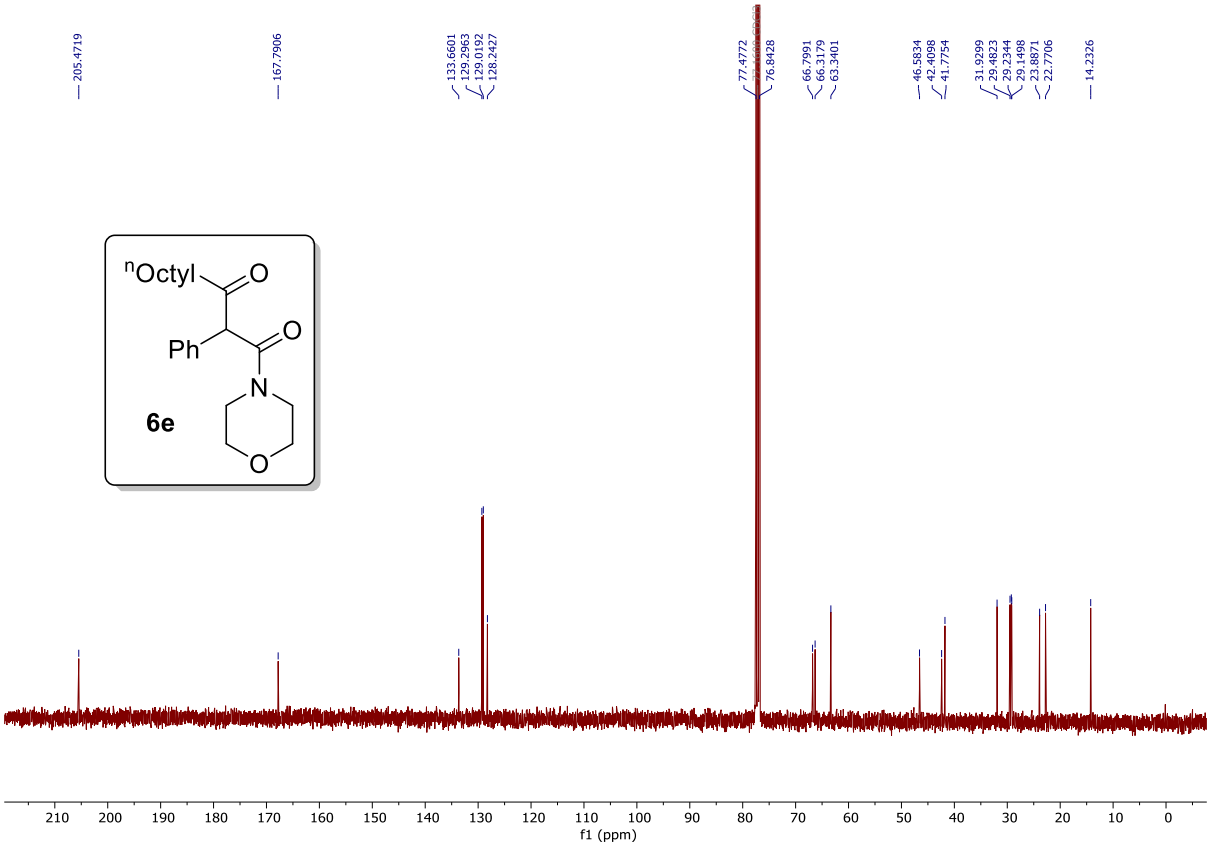
3.3111
3.2496
3.2066
2.6367
2.5442
2.4019
2.3100
1.5510
1.4855
1.2446
1.2006
0.8743
0.8279
0.0000 TMS
nOctyl
O
Ph
O
N
O
6e
3.02
2.85
1.00
2.09
3.01
1.08
1.98
1.01
1.15
2.06
10.50
3.35
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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31.9299
29.4823
29.2344
29.1498
23.8871
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Ph
O
N
O
6e
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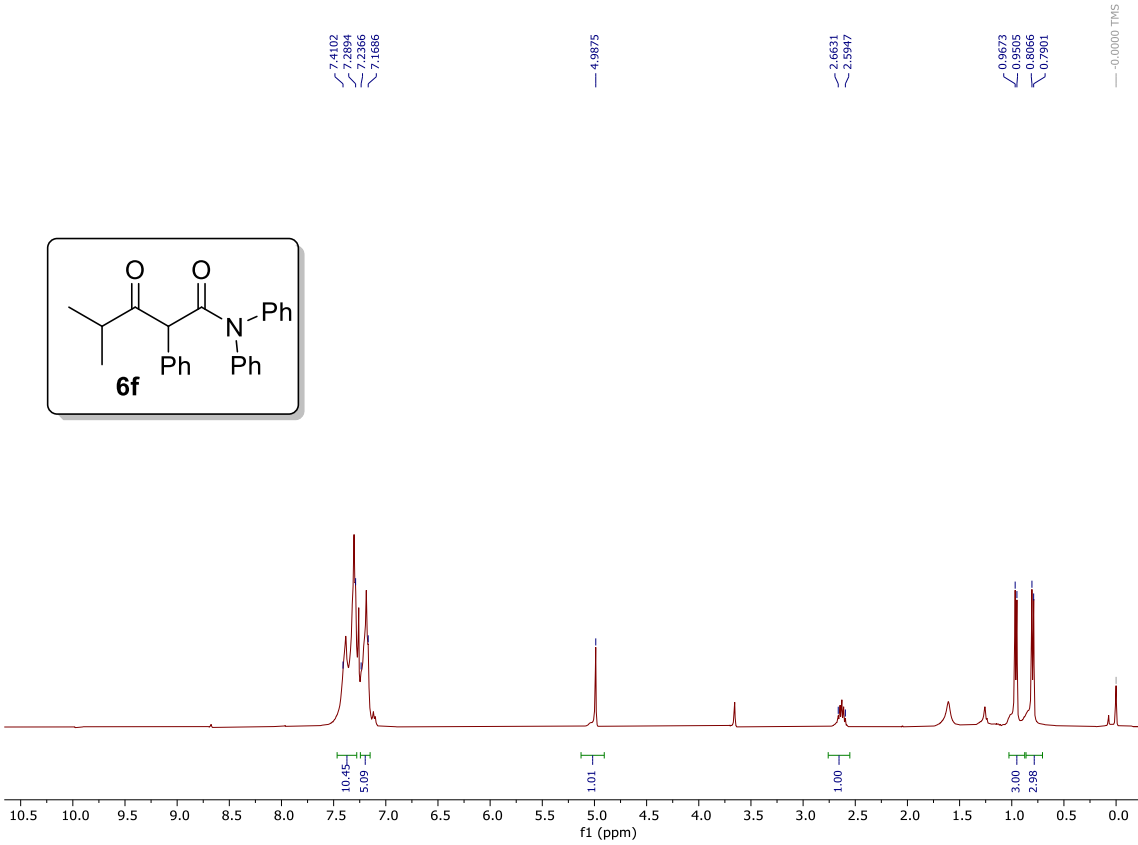
f1 (ppm)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0.7901
-0.0000 TMS
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O
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Ph
Ph
Ph
6f
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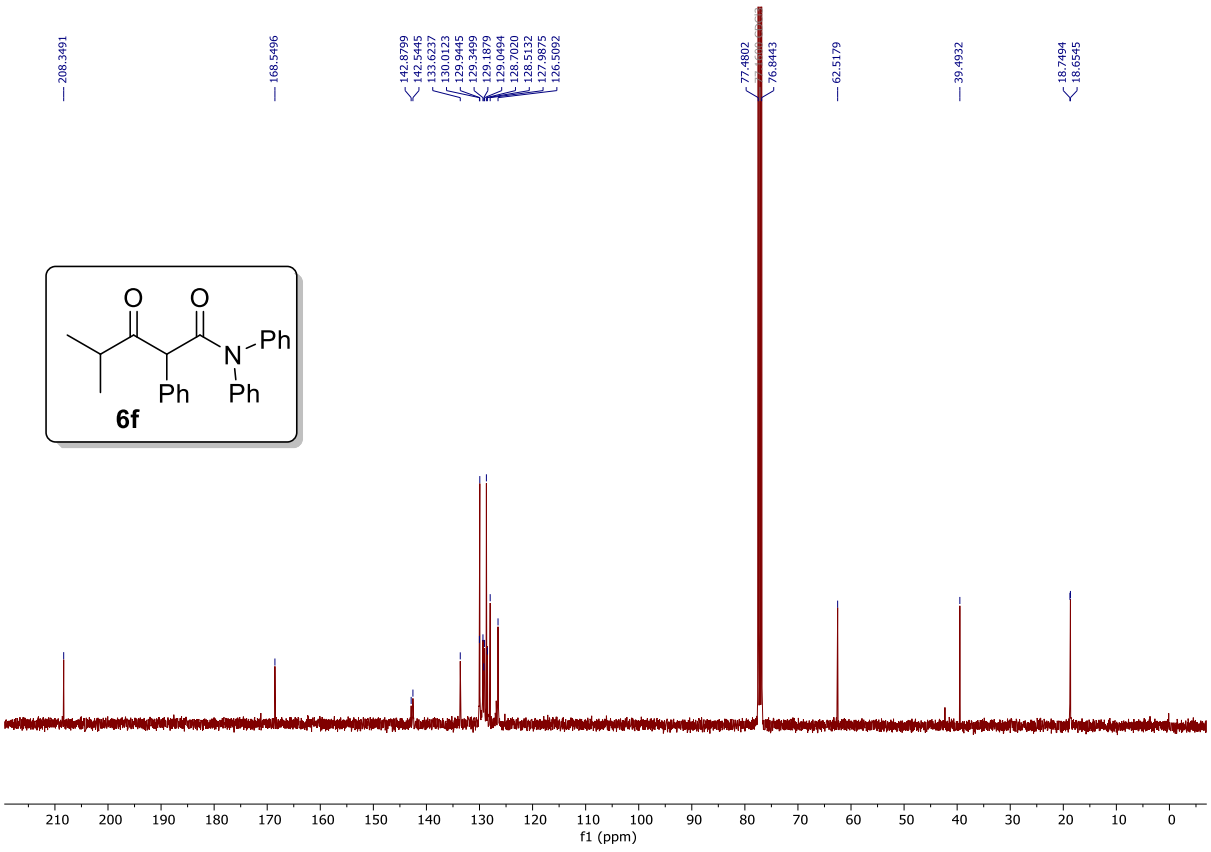
1.00
3.00
2.98
f1 (ppm)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127.9875
126.5092
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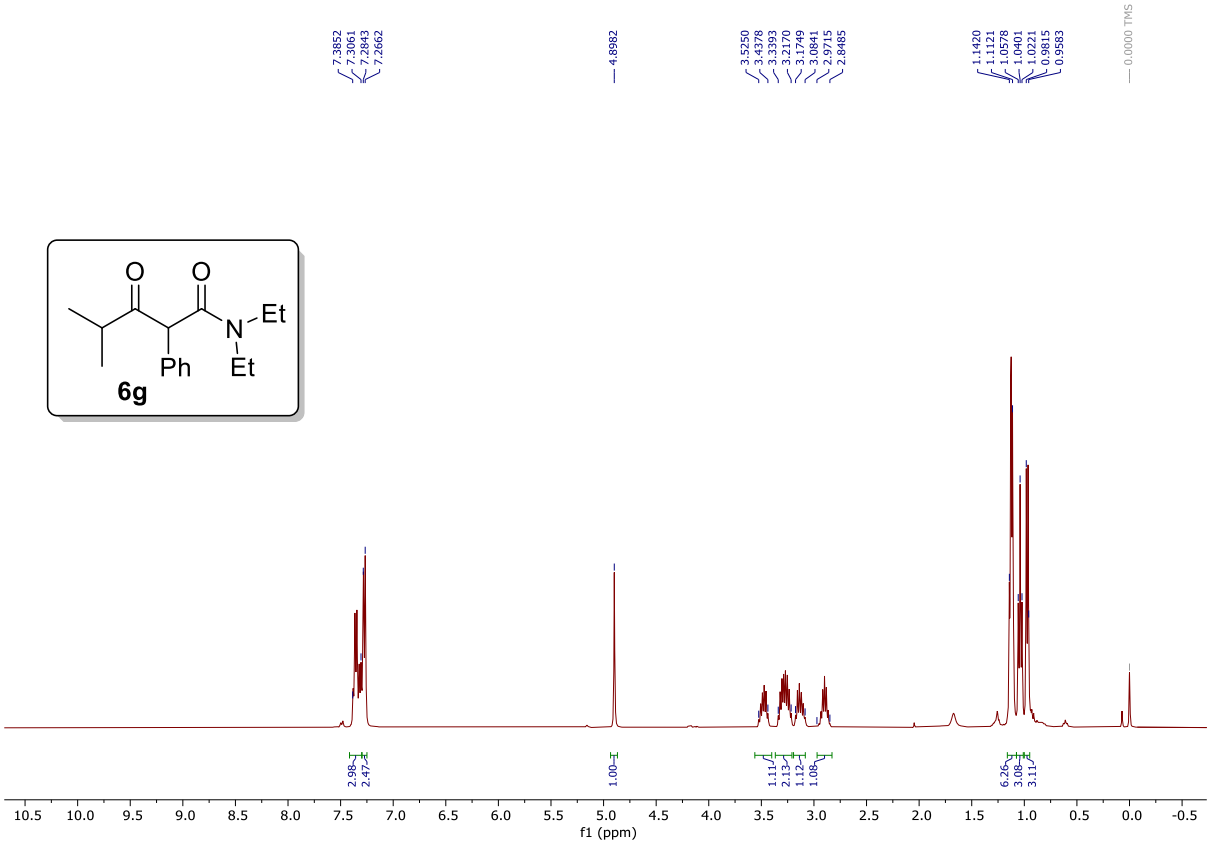
O
N
Ph
Ph
Ph
6f
f1 (ppm)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O
N
Et
Et
Ph
6g
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1.00
1.11
2.13
1.12
1.08
6.26
3.08
3.11
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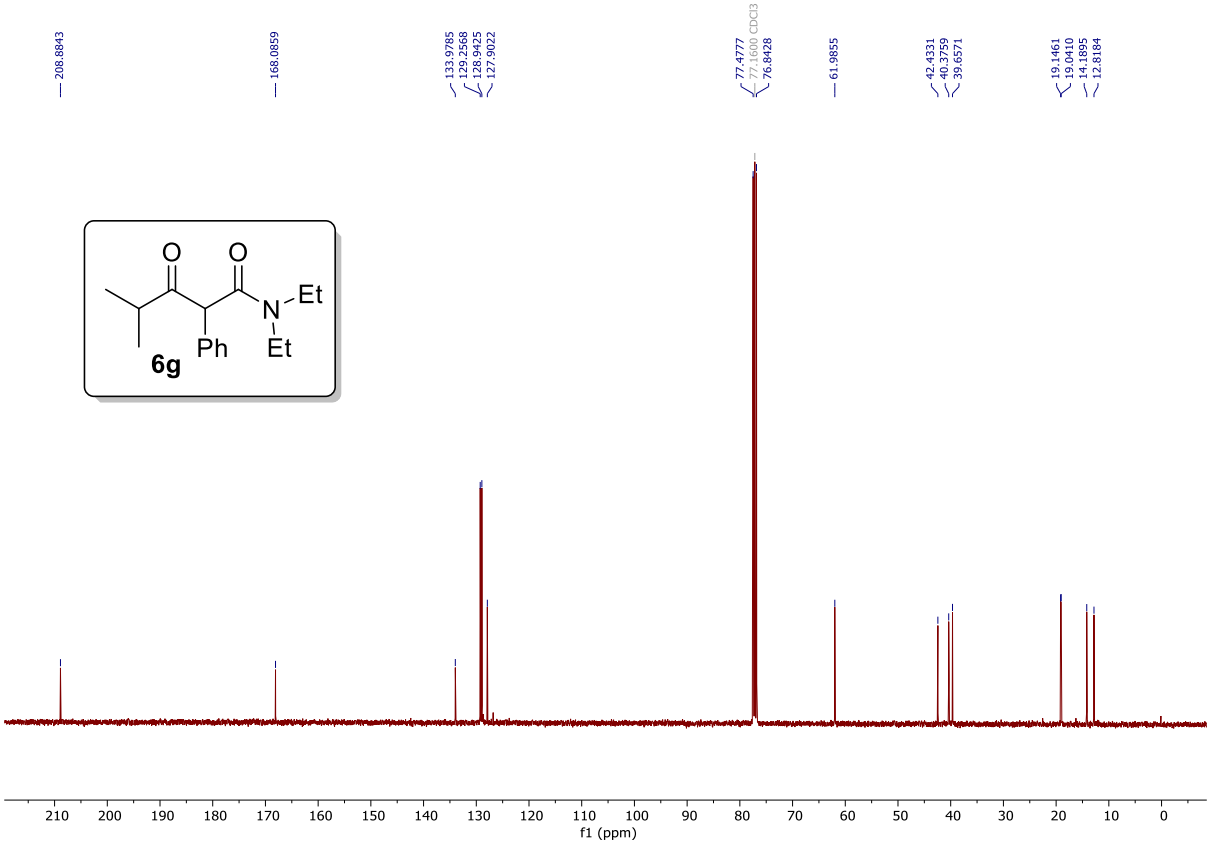
f1 (ppm)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61.9855
42.4331
40.3759
39.6571
19.1461
19.0410
14.1895
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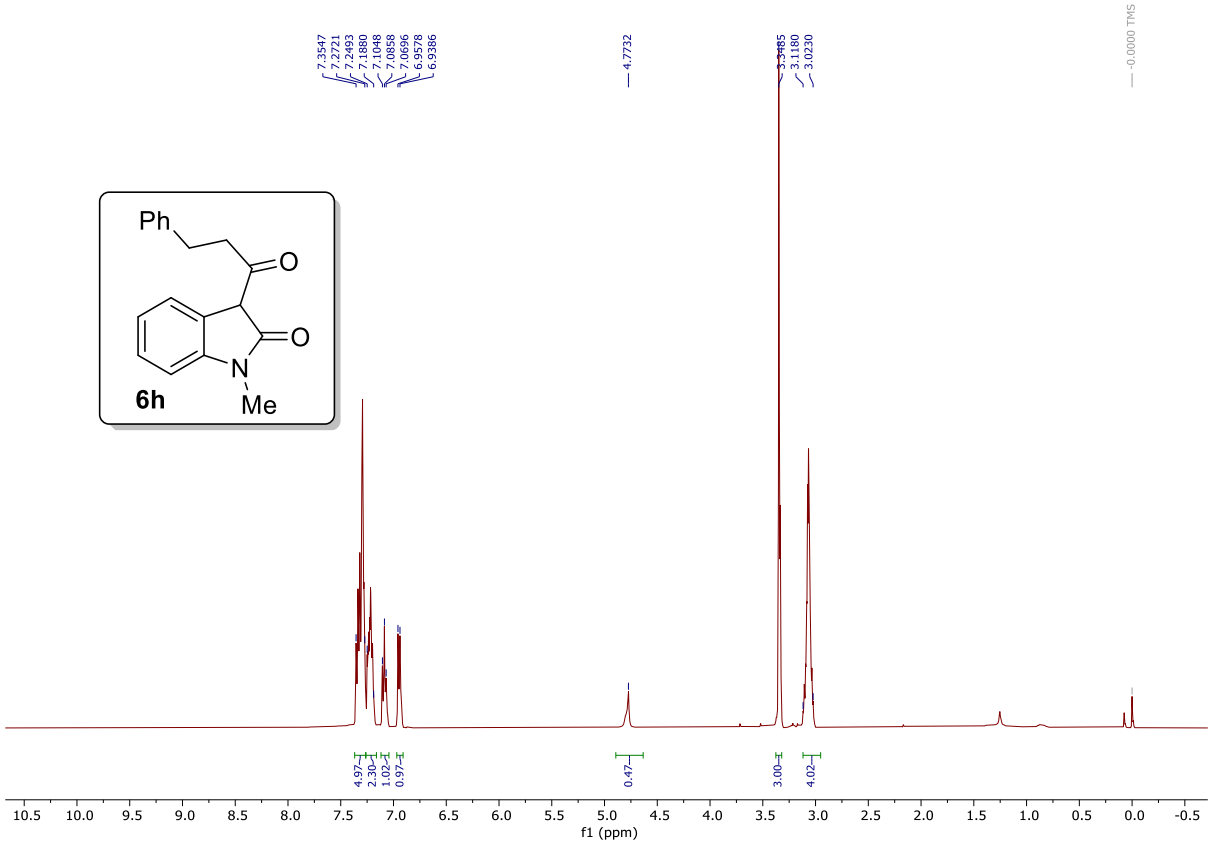
O
N
Et
Et
Ph
6g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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3.1180
3.0230
0.0000 TMS
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Me
6h
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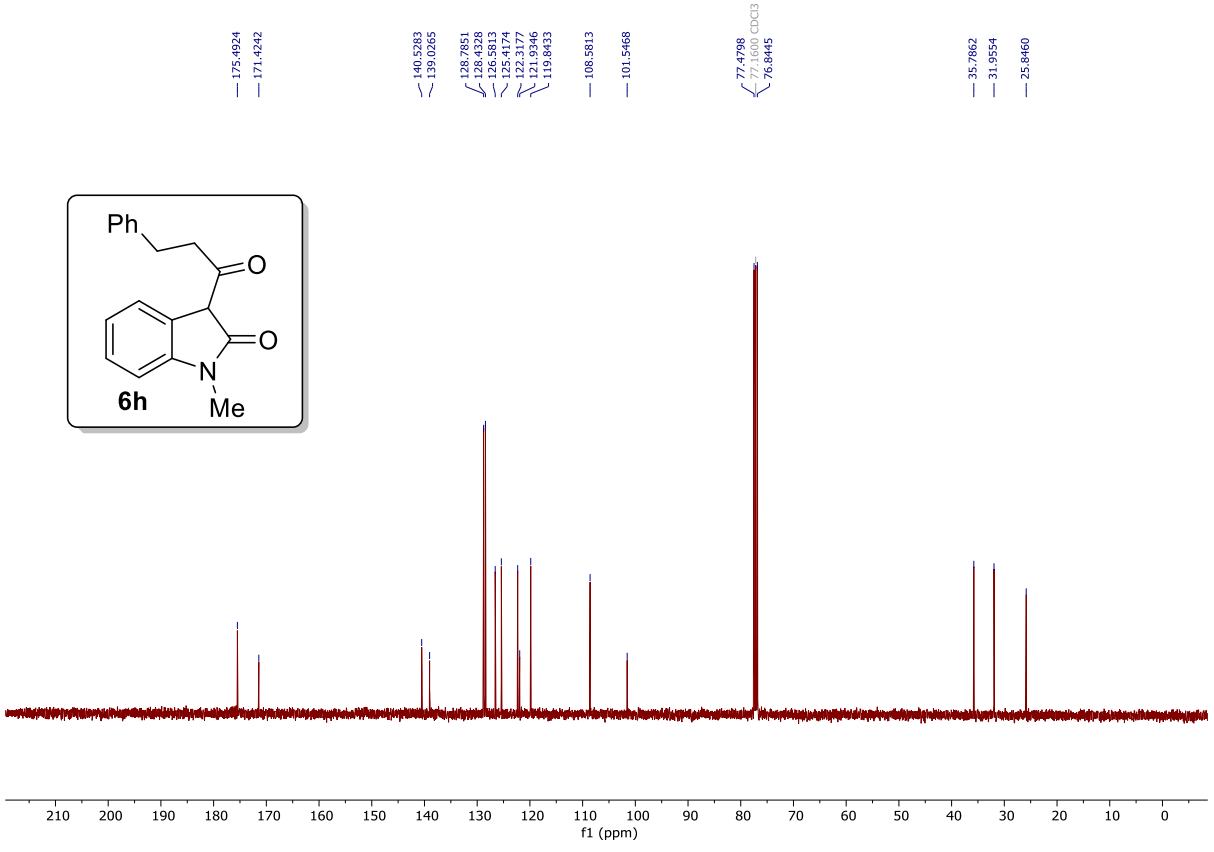
0.47
3.00
4.02
f1 (ppm)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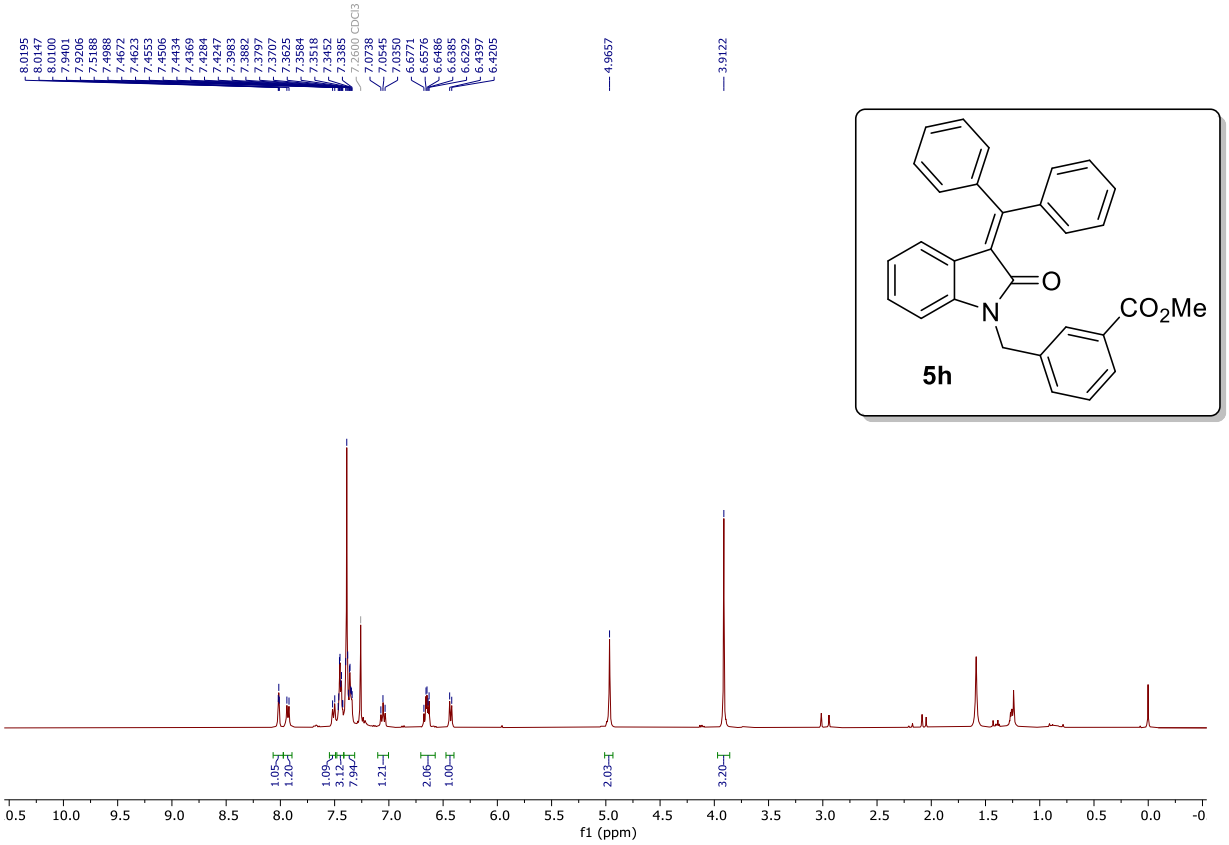
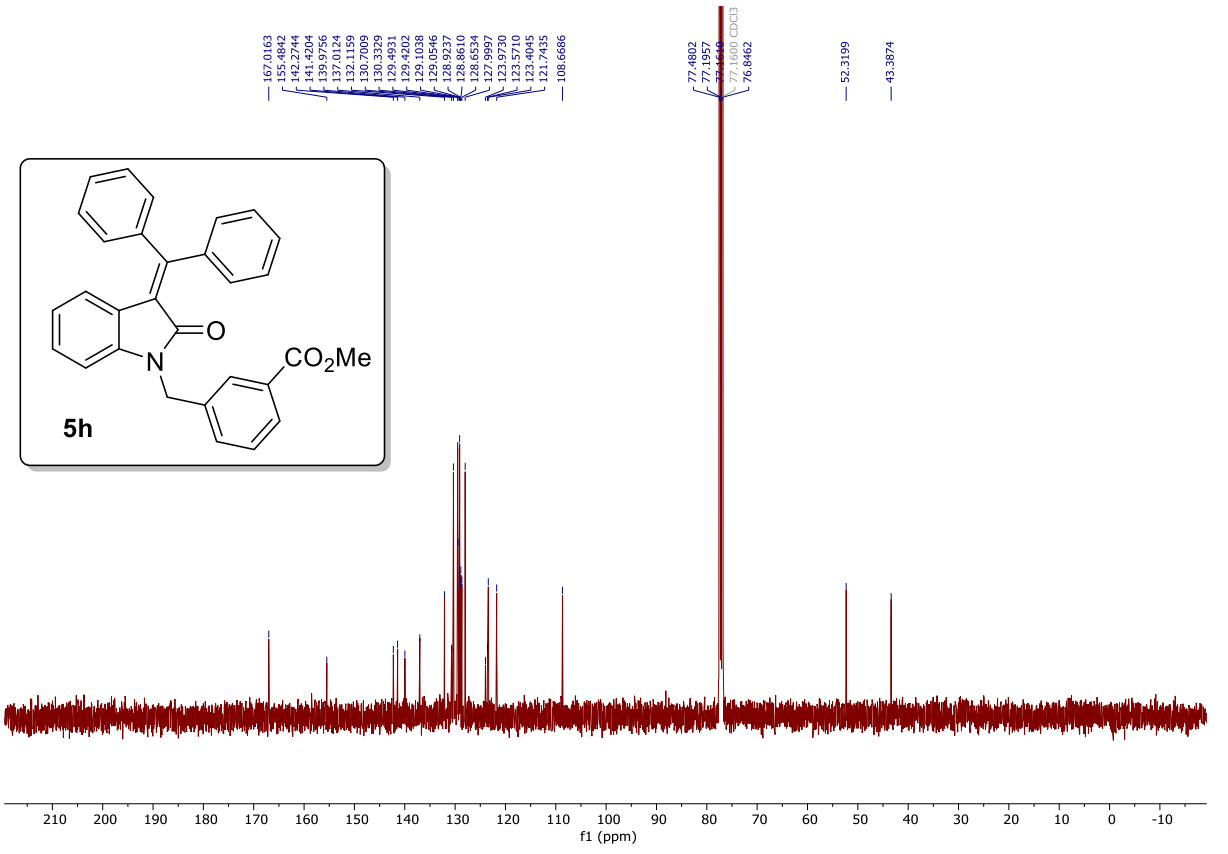
119.8433
108.5813
101.5468
77.4798
77.1600 CDCl3
76.8445
35.7862
31.9554
25.8460
Ph
O
O
N
Me
6h
f1 (ppm)


8.0195
8.0147
8.0100
7.9401
7.9206
7.5188
7.4988
7.4672
7.4623
7.4553
7.4506
7.4444
7.4369
7.4284
7.4247
7.3983
7.3882
7.3797
7.3707
7.3625
7.3584
7.3518
7.3452
7.3385
7.2600 CDCl3
7.0738
7.0545
7.0350
6.6771
6.6576
6.6486
6.6385
6.6292
6.4397
6.4205
4.9657
3.9122
O
N
CO2Me
5h
1.05
1.20
1.09
3.12
7.94
1.21
2.06
1.00
2.03
3.20
f1 (ppm)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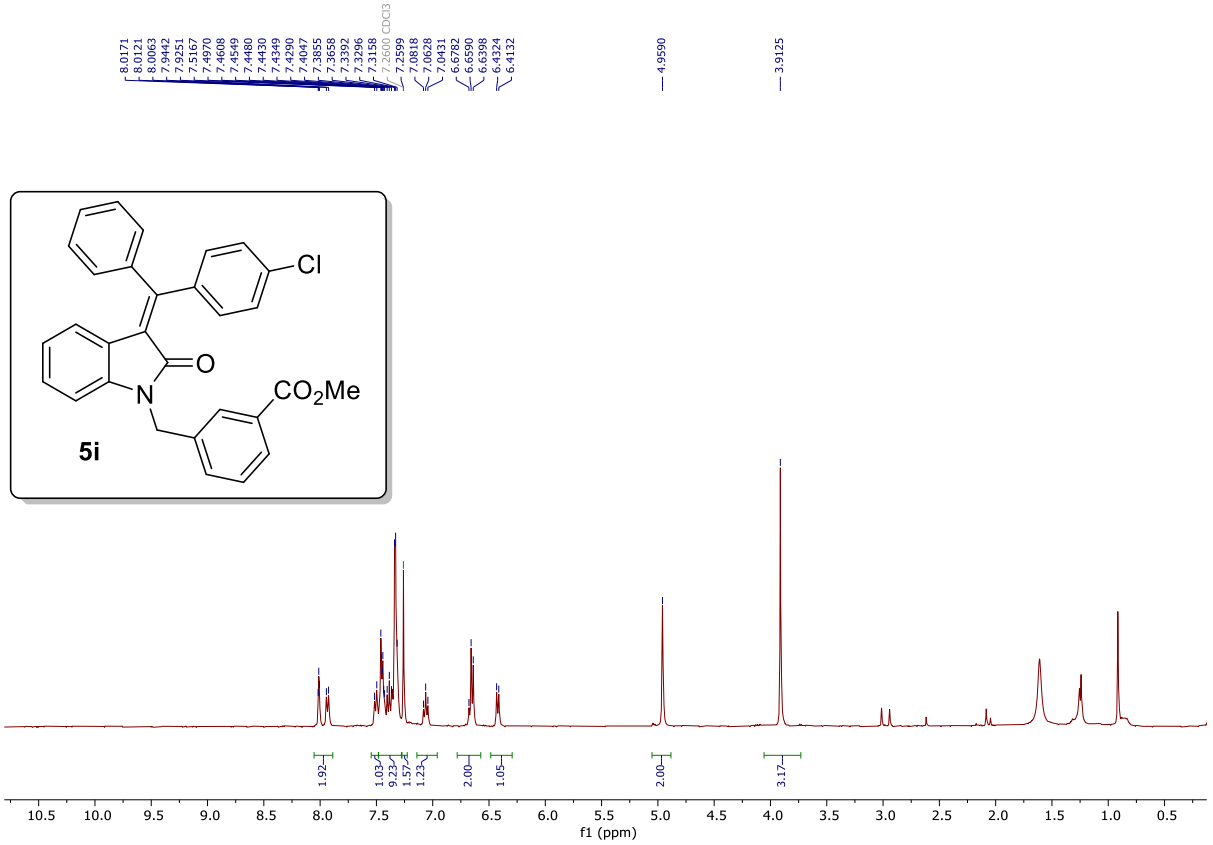
155.4842
142.2744
141.4204
139.9756
137.0124
132.1159
130.7009
130.3329
129.4931
129.4202
129.1038
129.0546
128.9237
128.8610
128.6534
127.9997
123.9730
123.5710
123.4045
121.7435
108.6686
77.4802
77.1957
77.1600 CDCl3
76.8462
52.3199
43.3874
O
N
CO2Me
5h
f1 (ppm)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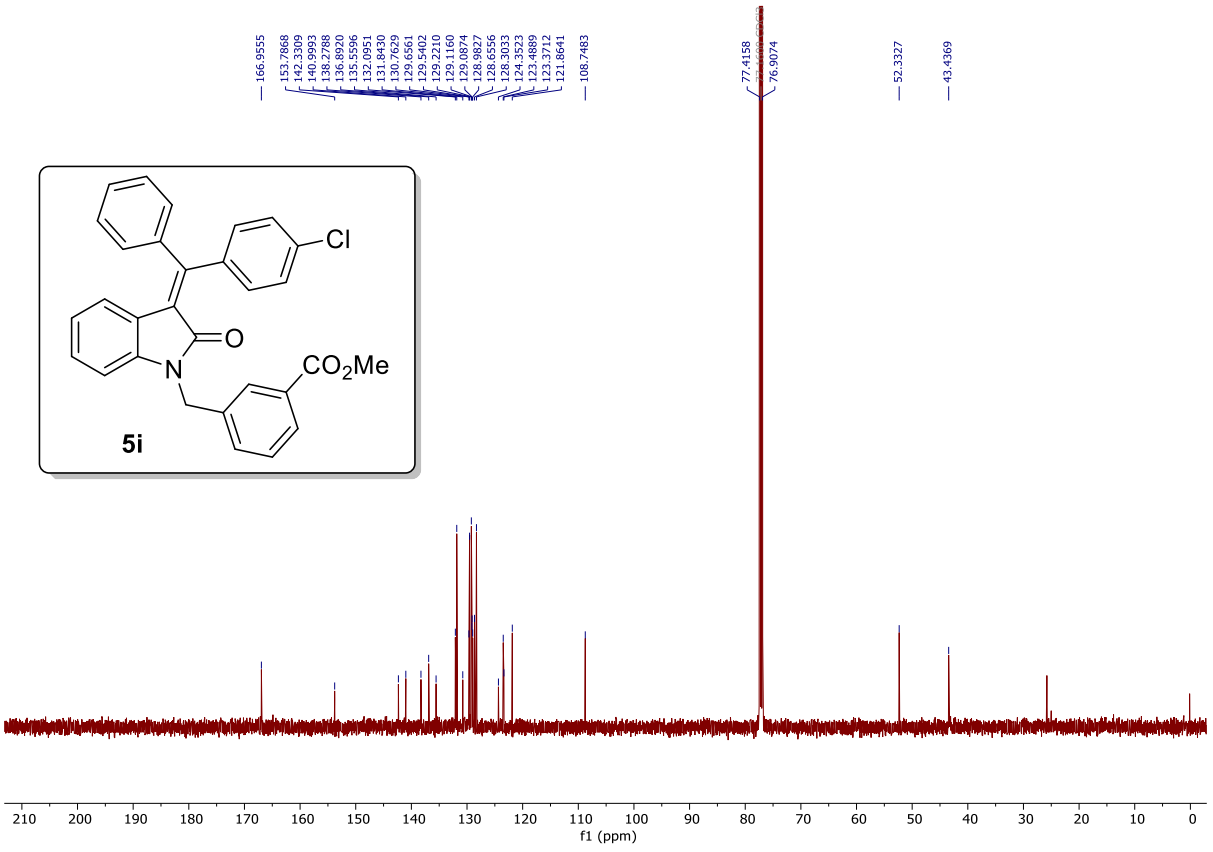
8.0121
8.0063
7.9442
7.9251
7.5167
7.4970
7.4608
7.4549
7.4480
7.4430
7.4349
7.4290
7.4047
7.3855
7.3658
7.3392
7.3296
7.3158
7.2599
7.0818
7.0628
7.0431
6.6782
6.6590
6.6398
6.4324
6.4132
4.9590
3.9125
CDCl3
Cl
O
N
CO2Me
5i
1.92
1.03
9.23
1.57
1.23
2.00
1.05
2.00
3.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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153.7868
142.3309
140.9993
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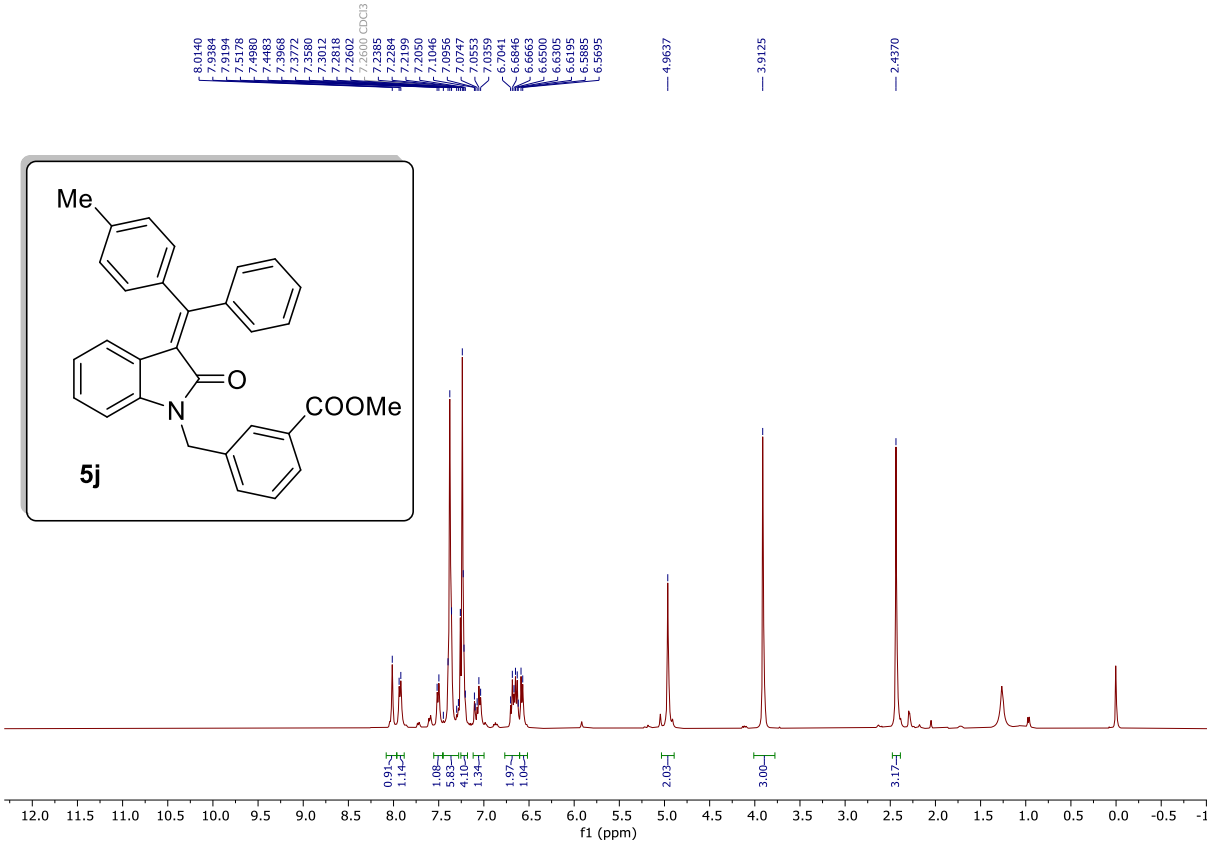
136.8920
135.5596
132.0951
131.8430
130.7629
129.6561
129.5402
129.2210
129.1160
129.0874
128.9827
128.6556
128.3033
124.3523
123.4889
123.3712
121.8641
108.7483
77.4158
76.9074
52.3327
43.4369
Cl
O
N
CO2Me
5i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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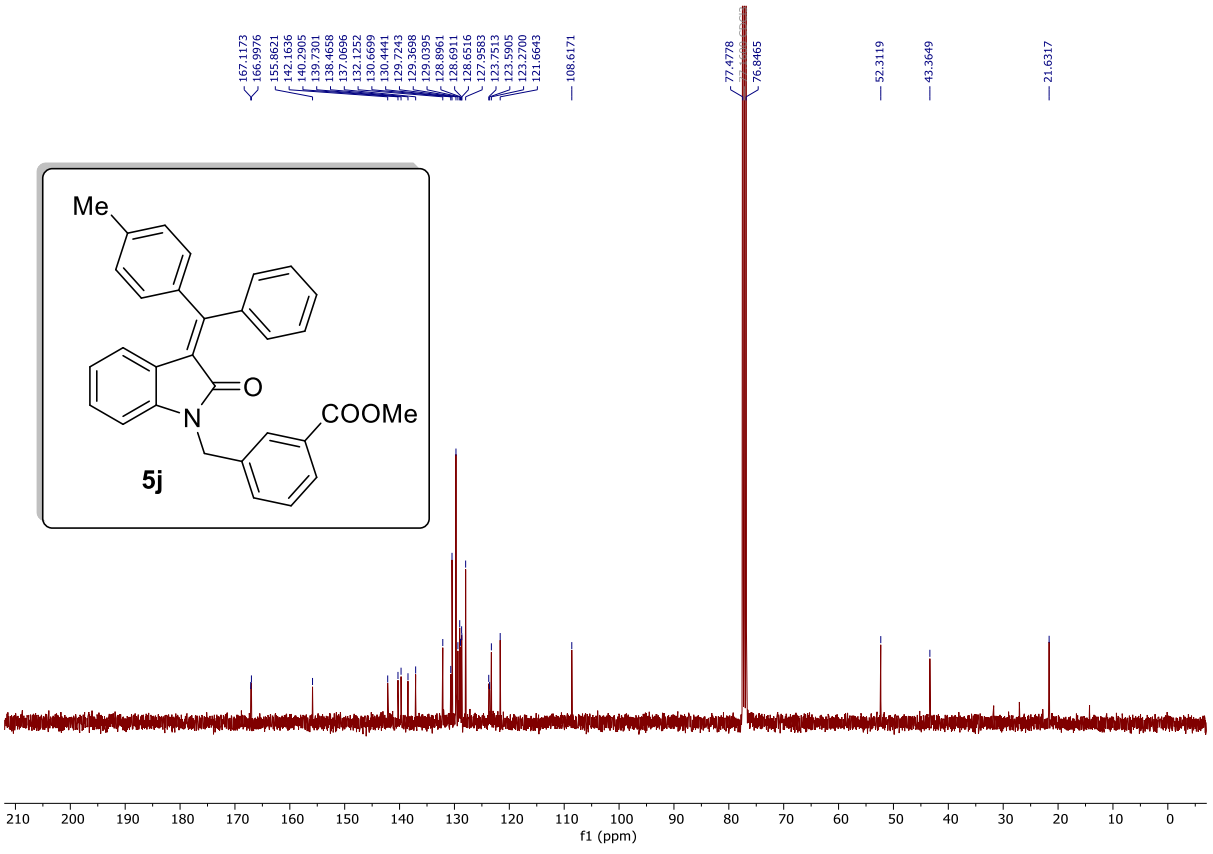
7.9194
7.5178
7.4980
7.4483
7.3968
7.3772
7.3580
7.3012
7.2818
7.2602
7.2600 CDCl3
7.2385
7.2284
7.2199
7.2050
7.1046
7.0956
7.0747
7.0553
7.0359
6.7041
6.6846
6.6663
6.6500
6.6305
6.6195
6.5885
6.5695
4.9637
3.9125
2.4370
Me
O
N
COOMe
5j
0.91
1.14
1.08
5.83
4.10
1.34
1.97
1.04
2.03
3.00
3.17
f1 (ppm)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155.8621
142.1636
140.2095
139.7201
138.4658
137.0696
132.1252
130.6699
130.4441
129.7243
129.3698
129.0395
128.8961
128.6911
128.6516
127.9583
123.7513
123.5905
123.2700
121.6643
108.6171
77.4778
76.8465
52.3119
43.3649
21.6317
Me
O
N
COOMe
5j
f1 (ppm)


7.9480
7.9119
7.8928
7.6377
7.6184
7.4656
7.4628
7.4462
7.4440
7.4394
7.4292
7.4247
7.4116
7.4075
7.4054
7.3999
7.3942
7.3897
7.3745
7.3709
7.3553
7.3398
7.3359
7.3208
7.3165
7.3120
7.2999
7.2959
7.2918
7.2600 CDCl3
7.1887
7.1693
7.1502
7.0728
7.0535
7.0346
6.6723
6.6527
4.8958
3.8948
2.9867
2.9828
2.9722
2.9633
2.9532
2.9439
2.9401
1.7373
1.7207
1.7040
1.6873
1.6708
1.5468
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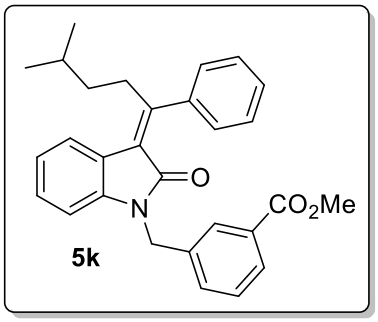
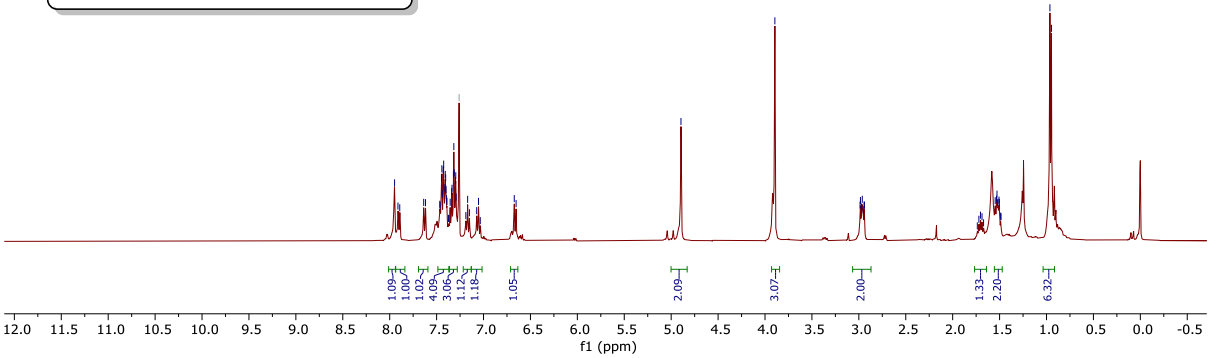
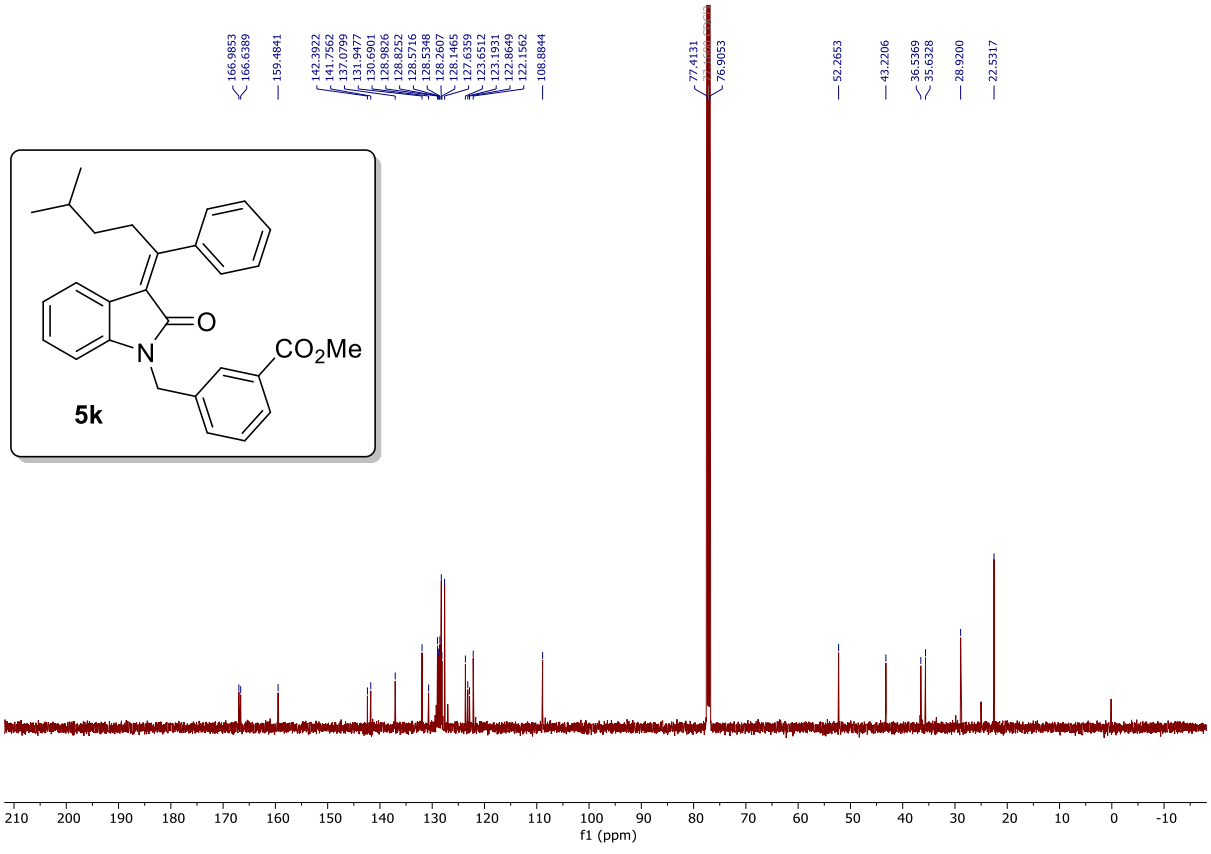
1.5175
1.5065
1.5024
1.4889
1.4853
0.9636
0.9471


O
N
CO2Me
5k


1.09
1.00
1.02
4.09
3.06
1.12
1.18
1.05
2.09
3.07
2.00
1.33
2.20
6.32
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.9853
166.6389
159.4841
142.3922
141.7562
137.0799
131.9477
130.6901
128.9826
128.8252
128.5716
128.5348
128.2607
128.1465
127.6359
123.6512
123.1931
122.8649
122.1562
108.8844
77.4131
77.0000 CDCl3
76.9053
52.2653
43.2206
36.5369
35.6328
28.9200
22.5317
O
N
CO2Me
5k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5. References:

1. a) H. Li, X. Shangguan, Z. Zhang, S. Huang, Y. Zhang, and J. Wang, *Org. Lett*. **2014**, 16, 448-451. b) K. Hong, X. Liu, and J. P. Morken, *J. Am. Chem. Soc.* **2014**, 136, 10581-10584. c) E. K. Edelstein, A. C. Grote, M. D. Palkowitz, and J. P. Morken, *Synlett*, **2018**, 29, 1749-1752. d) Y. Zhou, T. Xiong, L.-Y Zhou; H.-Y. Li, Y. C. Xiao, and F.-Er. Chen, *Org. Lett*., **2022**, 24, 791-796.
2. a) C. Feng, and T.-P. Loh, *Angew. Chem. Int. Ed.* **2013**, 52, 12414-12417. b) A. Muthukumar, G. N. Rao, and G. Sekar, *Org. Biomol. Chem.*, **2019**, 17, 3921-3933.
3. H. Qu, Y. Chen, X. Ceng, P. Tang, H. Wang, F. Chen, *Asian J. Org. Chem*., 2022, 11, e202200188.
4. R. Shintani, T. Yamagami, T. Hayashi, *Org. Lett*., **2006**, 8, 4799-4801.
5. S. Park, J. Lee, K. J. Shin, E. Oh, J. H. Seo, *Molecules*, **2017**, 22, 503.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SP_DG_222

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: SP_DG_222

```
Bond precision:   C-C = 0.0045 A          Wavelength=0.71073

Cell:             a=8.6631(4)     b=13.5282(6)     c=35.3230(15)
                  alpha=90        beta=90          gamma=90
Temperature:      296 K
```

	Calculated	Reported
Volume	4139.7(3)	4139.7(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C20 H28 B N O4	C20 H28 B N O4
Sum formula	C20 H28 B N O4	C20 H28 B N O4
Mr	357.24	357.24
Dx,g cm-3	1.146	1.146
Z	8	8
Mu (mm-1)	0.078	0.078
F000	1536.0	1536.0
F000'	1536.71	
h,k,lmax	10,16,42	10,16,42
Nref	3861	3861
Tmin,Tmax	0.977,0.988	0.652,0.745
Tmin'	0.973	

```
Correction method= # Reported T Limits: Tmin=0.652 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 25.497

R(reflections)= 0.0677( 2894)                    wR2(reflections)=
                                                 0.1817( 3861)
S = 1.122                  Npar= 244
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00453 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         32 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     10.548 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.479 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
```

Alert level G

```
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O3       .      107.6 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O4       .      107.4 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       51.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

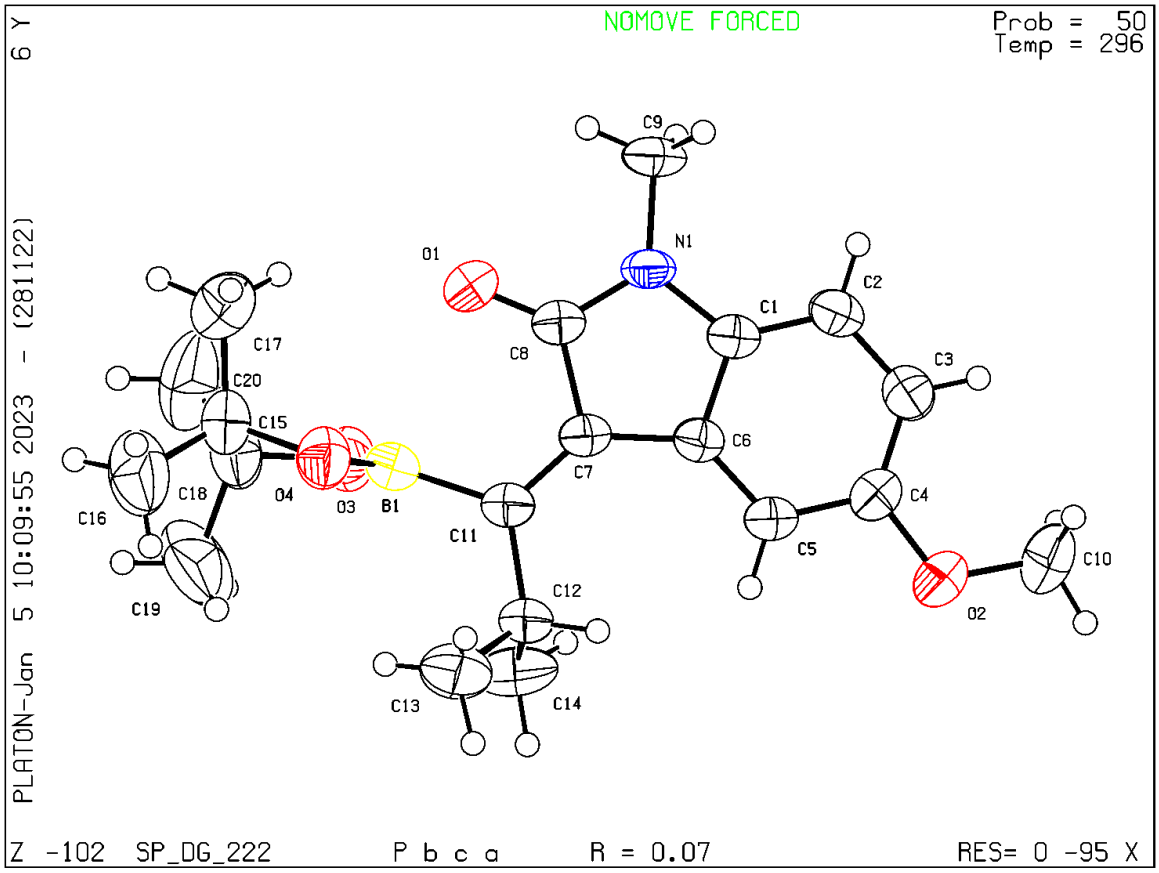
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock SP_DG_222 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SP_DG_325

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: SP_DG_325

```
Bond precision:   C-C = 0.0048 A          Wavelength=0.71073

Cell:          a=8.867(3)          b=11.445(4)       c=12.457(4)
               alpha=102.292(11)   beta=95.249(14)   gamma=98.197(11)
Temperature:   296 K
```

	Calculated	Reported
Volume	1212.8(7)	1212.8(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H34 B N O3	?
Sum formula	C27 H34 B N O3	C27 H34 B N O3
Mr	431.36	431.36
Dx,g cm-3	1.181	1.181
Z	2	2
Mu (mm-1)	0.075	0.075
F000	464.0	464.0
F000'	464.19	
h,k,lmax	10,13,14	10,13,14
Nref	4271	4267
Tmin,Tmax	0.985,0.989	0.614,0.745
Tmin'	0.985	

```
Correction method= # Reported T Limits: Tmin=0.614 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 24.998

R(reflections)= 0.0633( 2295)                    wR2(reflections)=
                                                 0.1658( 4267)
S = 1.010                  Npar= 293
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.131
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00485 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H9B      ..H9B      .       2.14 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -0.679 Report
```

Alert level G

```
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.131 Report
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O1       .      108.5 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O2       .      107.4 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O3       .      109.1 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.0 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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9 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

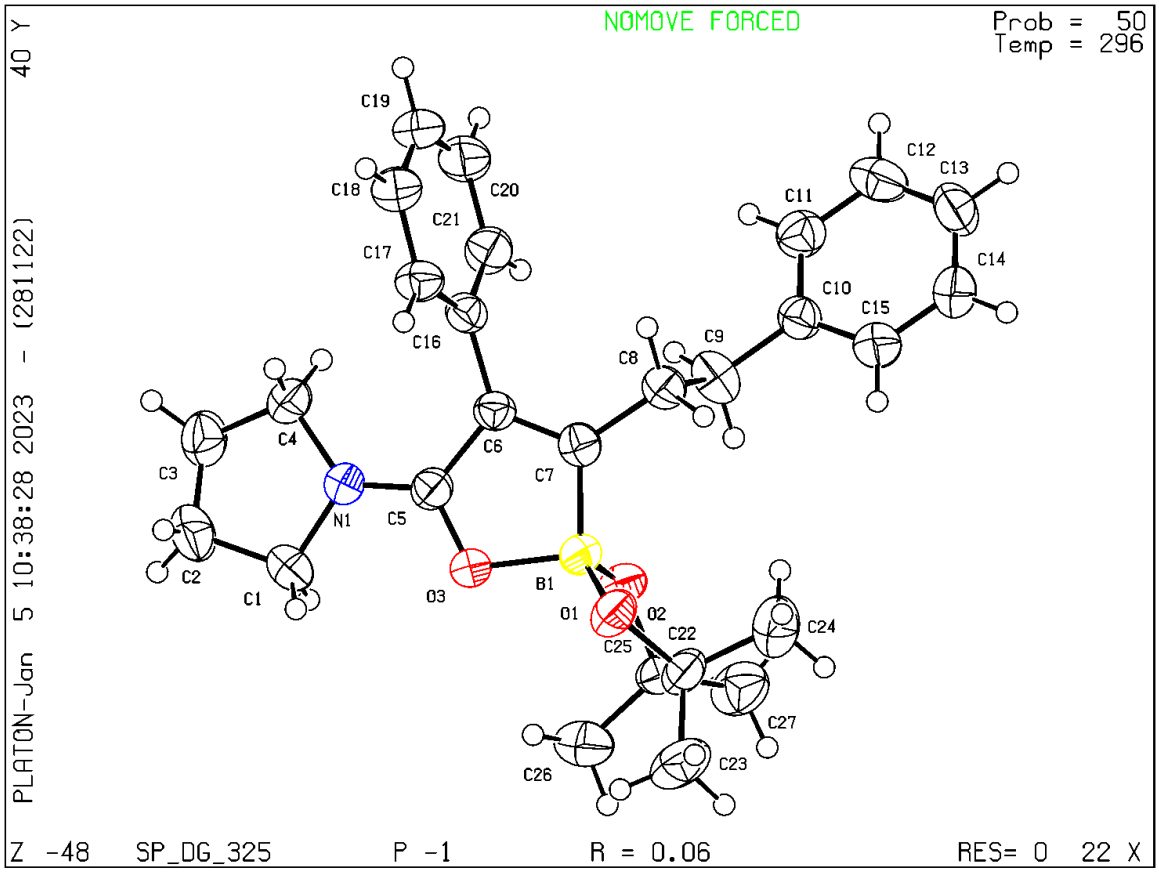
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock SP_DG_325 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SP_DG_108

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: SP_DG_108

```
Bond precision:   C-C = 0.0034 A          Wavelength=0.71073

Cell:             a=11.7963(7)    b=8.2830(4)         c=15.9743(10)
                  alpha=90        beta=105.775(2)     gamma=90
Temperature:      296 K

                 Calculated                Reported
Volume           1502.04(15)               1502.04(15)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C19 H19 N O               C19 H19 N O
Sum formula      C19 H19 N O               C19 H19 N O
Mr               277.35                    277.35
Dx,g cm-3        1.227                     1.226
Z                4                         4
Mu (mm-1)        0.075                     0.075
F000             592.0                     592.0
F000'            592.23
h,k,lmax         14,10,19                  14,10,19
Nref             2796                      2795
Tmin,Tmax        0.987,0.993               0.976,0.982
Tmin'            0.981

Correction method= # Reported T Limits: Tmin=0.976 Tmax=0.982
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.499

R(reflections)= 0.0605( 2033)                wR2(reflections)=
                                             0.1937( 2795)
S = 1.042                 Npar= 194
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.088 Report

Alert level G

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 51.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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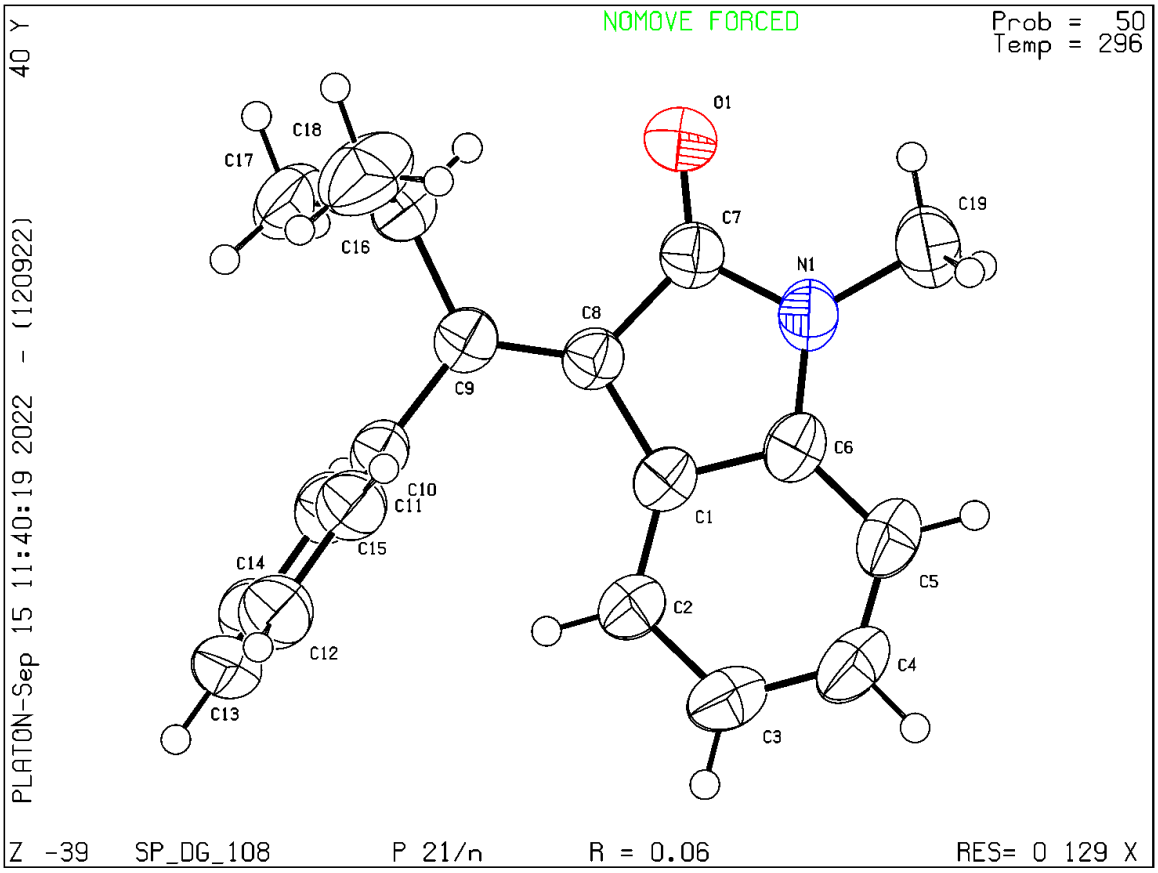
PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock SP_DG_108 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

```
Bond precision:   C-C = 0.0034 A          Wavelength=0.71073

Cell:               a=9.004(12)      b=9.504(11)         c=18.11(2)
                    alpha=90         beta=94.20(3)       gamma=90
Temperature:        296 K

                 Calculated                  Reported
Volume           1546(3)                     1546(3)
Space group      P 21/n                      P 21/n
Hall group       -P 2yn                      -P 2yn
Moiety formula   C19 H19 N O                 ?
Sum formula      C19 H19 N O                 C19 H19 N O
Mr               277.35                      277.35
Dx,g cm-3        1.192                       1.192
Z                4                           4
Mu (mm-1)        0.073                       0.073
F000             592.0                       592.0
F000'            592.23
h,k,lmax         12,12,24                    12,12,24
Nref             3831                        3823
Tmin,Tmax        0.992,0.994                 0.991,0.993
Tmin'            0.991

Correction method= # Reported T Limits: Tmin=0.991 Tmax=0.993
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 28.292

R(reflections)= 0.0558( 2358)                wR2(reflections)=
                                             0.1661( 3823)
S = 1.048                  Npar= 193
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
PLAT410_ALERT_2_B Short Intra H...H Contact  H00A     ..H00I     .       1.89 Ang.
                                                     x,y,z  =      1_555 Check
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT148_ALERT_3_C s.u. on the      a    - Axis is (Too) Large ....      0.012 Ang.
PLAT148_ALERT_3_C s.u. on the      b    - Axis is (Too) Large ....     0.0110 Ang.
PLAT148_ALERT_3_C s.u. on the      c    - Axis is (Too) Large ....      0.020 Ang.
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C00G     --C00K     .        5.5 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C00G Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.078 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
```

Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         40 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

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```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY02_shelx
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT410_shelx
;
PROBLEM: Short Intra H...H Contact  H00A     ..H00I     .       1.89 Ang.
RESPONSE: ...
;
_vrf_PLAT148_shelx
;
PROBLEM: s.u. on the      a    - Axis is (Too) Large ....      0.012 Ang.
RESPONSE: ...
;
_vrf_PLAT220_shelx
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.6 Ratio
RESPONSE: ...
;
_vrf_PLAT230_shelx
;
PROBLEM: Hirshfeld Test Diff for    C00G     --C00K     .        5.5 s.u.
RESPONSE: ...
;
_vrf_PLAT242_shelx
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of       C00G Check
RESPONSE: ...
;
_vrf_PLAT767_shelx
;
PROBLEM: INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
RESPONSE: ...
;
_vrf_PLAT906_shelx
;
PROBLEM: Large K Value in the Analysis of Variance ......      5.078 Check
RESPONSE: ...
;
_vrf_PLAT911_shelx
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
RESPONSE: ...
;
_vrf_PLAT934_shelx
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock shelx - ellipsoid plot