Supporting Information

An Indole-Amide-Based Phosphine Ligand Enabling a General Palladium-Catalyzed Sterically Hindered Suzuki-Miyaura Cross-Coupling Reaction

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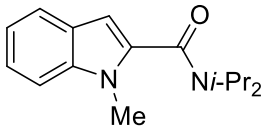
1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All Suzuki-Miyaura reactions were performed in a resealable screw-cap Schlenk tube (approx. 20 mL volume) in the presence of a Teflon coated magnetic stirrer bar (5 mm × 10 mm). Dioxane and toluene were freshly distilled from sodium under nitrogen.[1] Tetrahydrofuran (THF) was freshly distilled from sodium benzophenone ketyl under nitrogen.[1] Hexane was freshly distilled from anhydrous calcium hydride under nitrogen.[1] Water was freshly distilled under nitrogen.[1]New bottle of *n*-butyllithium was used (*Note*: since the concentration of *n*-BuLi from old bottle may vary, we recommend performing a titration prior to use). 4-Chloro-3,5-dimethylanisole, [2] 2-chloro-1,3,5-triethylbenzene, [3] 4-chloro-3,5-dimethylphenyl dimethylsulfamate, [4] 2-chloro-4-methoxytoluene [5] and 4-chloro-3-methoxybenzaldehyde[6] were synthesized according to the literature methods. 2,4,6-Tris(2-methylphenyl)boroxine was prepared according to the literature methods.[7] Thin layer chromatography was performed on precoated silica gel 60 F_{254} plates. Silica gel (230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Stuart Melting Point SMP30 instrument. NMR spectra were recorded on a Bruker spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C, 376 MHz for ^{19}F and 162 MHz for ^{31}P). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). ^{31}P NMR spectra were referenced to 85% H_3PO_4 externally. Coupling constants (J) were reported in Hertz (Hz). Mass spectra (EI-MS) was recorded on a HP 5977A MSD Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on an Agilent 6540 ESI-QToF-MS or APPI-QToF-MS and a Waters GCT Premier EI-ToF-MS. GC-MS analysis was conducted on a HP 7890B GC system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 7890 GC-FID system. All yields reported refer to the isolated yield of compounds. Compounds described in the literature were characterized by comparison of their ^{1}H, ^{13}C and/or ^{19}F NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

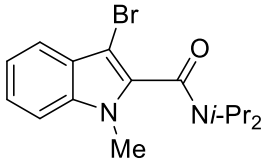
2. Ligand synthesis and characterization

N,*N*-Diisopropyl-1-methyl-1*H*-indole-2-carboxamide (P1)



1-Methylindole (2.50 mL, 20.0 mmol) was dissolved in freshly distilled THF (30 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *t*-BuLi (20 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at room temperature, *N*,*N*-diisopropylcarbamoyl chloride (3.93 g, 24.0 mmol) was added at -78 °C. The reaction temperature was then increased to room temperature and the reaction was stirred for 1 h. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the concentrated mixture was diluted with ethyl acetate and washed with water and brine. The organic layer was dried over Na_2SO_4, and then concentrated. The concentrated mixture was then subjected to column chromatography and eluted with ethyl acetate/hexane (1:9 and 2:8) mixture. The eluent was evaporated to yield *N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide as the light yellow solid (4.62 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13–1.70 (br m, 12H), 3.48–4.27 (br m, 2H) superimposed to 3.76 (s, 3H), 6.47 (s, 1H), 7.12 (t, J = 7.8 Hz, 1H), 7.23–7.27 (m, 1H), 7.33 (d, J = 8.2 Hz, 1H), 7.60 (d, J = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 30.8, 99.9, 109.6, 120.0, 121.2, 122.5, 126.8, 134.8, 137.1, 163.9. The data are in agreement with those previously reported in the literature.[8]

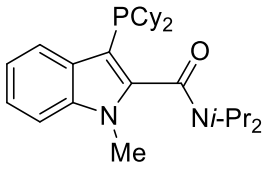
3-Bromo-*N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide (P1')



N-Bromosuccinimide (3.02 g, 17.0 mmol) was added to a solution of *N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide (4.38 g, 17.0 mmol) in anhydrous chloroform (25 mL) in portion at room temperature. After stirring for 30 min, water was added to the reaction mixture. The organic layer was washed with water and brine, and then concentrated. The concentrated solution was filtered over a pad of silica and eluted with dichloromethane. The eluent was then concentrated. The solid was subjected to recrystallization from dichloromethane/hexane. The white solid was collected, washed with hexane and dried over vacuum to afford 3-bromo-*N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide (4.00 g, 70%). M.p.= 134.9-136.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.11 (d, J = 6.7 Hz, 3H), 1.31 (d, J = 6.6 Hz, 3H), 1.62 (d, J = 6.8 Hz, 6H), 3.56–3.65 (m, 1H), 3.73 (s, 3H), 3.85–3.95 (m, 1H), 7.20–7.24 (m, 1H), 7.29–7.34 (m, 2H), 7.57 (d, J = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 20.6, 21.1, 21.5, 31.1, 46.4, 51.6, 87.3, 109.7, 119.6, 120.7, 123.2, 126.4, 133.6, 135.9, 162.0; HRMS (ESI): calcd.

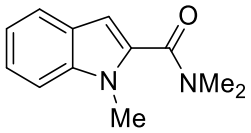
for $C_{16}H_{22}BrN_2O^+$: 337.0910, found 337.0914.

3-(Dicyclohexylphosphanyl)-*N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide (L1)



3-Bromo-*N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide (1.00 g, 3.0 mmol) was dissolved in freshly distilled THF (10 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (3.3 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.73 mL, 3.3 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was successively washed with ethanol and methanol. The off-white solid was collected by filtration and dried over vacuum to afford 3-(dicyclohexylphosphanyl)-*N*,*N*-diisopropyl-1-methyl-1*H*-indole-2-carboxamide (1.13 g, 83%). M.p.= 180.4-184.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.93–1.32 (m, 15H), 1.39–1.97 (m, 18H), 2.66–2.74 (m, 1H), 3.52–3.59 (m, 1H), 3.69 (s, 3H), 3.84–3.90 (m, 1H), 7.16 (t, *J* = 7.1 Hz, 1H), 7.26 (t, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.0, 20.4, 21.2, 21.4, 21.5, 26.1, 26.6, 27.0, 27.15, 27.24, 27.3, 27.4, 27.5, 27.6, 29.87, 29.89, 30.1, 30.2, 30.8, 31.1, 31.3, 31.6, 31.7, 31.8, 32.0, 35.6, 35.7, 46.0, 51.0, 102.0, 102.2, 109.7, 120.0, 121.8, 122.4, 130.35, 130.43, 137.8, 144.6, 145.1, 163.7; ^{31}P NMR (162 MHz, CD_2Cl_2) δ -17.1; HRMS (ESI): calcd. for $C_{28}H_{44}N_2OP^+$: 455.3186, found 455.3185.

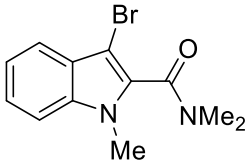
***N*,*N*,1-Trimethyl-1*H*-indole-2-carboxamide (P2)**



1-Methylindole (6.24 mL, 50.0 mmol) was dissolved in freshly distilled THF (100 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *t*-BuLi (55.0 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at room temperature, *N*,*N*-dimethylcarbamoyl chloride (5.06 mL, 55.0 mmol) was added. The reaction temperature was then increased to room temperature and the reaction was stirred for 1 h. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the concentrated mixture was diluted with ethyl acetate and washed with water and brine. The organic layer was dried over Na_2SO_4, and then concentrated. The concentrated mixture was then subjected to column chromatography and eluted with ethyl acetate/hexane

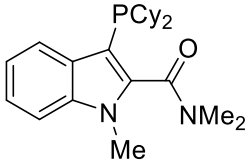
(1:9 - 2:8) mixture. The eluent was evaporated. The solid product was generated after addition of hexane. The light yellow solid was collected by filtration and dried over vacuum to afford *N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (5.67 g, 56%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (s, 6H), 3.85 (s, 3H), 6.64 (s, 1H), 7.13–7.17 (m, 1H), 7.28–7.32 (m, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.1, 103.9, 109.8, 120.1, 121.5, 123.2, 126.4, 132.0, 137.8, 164.4. The data are in agreement with those previously reported in the literature.[9]

3-Bromo-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (P2')



N-Bromosuccinimide (0.51 g, 2.75 mmol) was added to a solution of *N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (4.38 g, 2.5 mmol) in anhydrous chloroform (25 mL) in portion at 0 °C. After stirring for 1 h at room temperature, water was added to the reaction mixture. The organic layer was washed with water and brine, and then concentrated. The concentrated solution was subjected to column chromatography and eluted with ethyl acetate/hexane (1:1) mixture. The eluent was then concentrated under reduced pressure. The final product was dried over vacuum to afford 3-bromo-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide as brown liquid (0.68 g, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.10 (s, 3H), 3.20 (s, 3H), 3.77 (s, 3H), 7.20–7.24 (m, 1H), 7.32–7.34 (m, 2H), 7.56–7.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.6, 31.4, 34.9, 38.4, 67.9, 90.1, 109.8, 119.8, 120.8, 123.9, 126.3, 131.3, 136.6, 162.8; HRMS (ESI): calcd. for $C_{12}H_{13}BrN_2NaO^+$: 303.0103, found 303.0103.

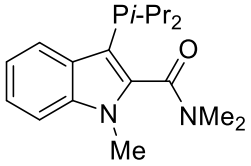
3-(Dicyclohexylphosphanyl)-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (L2)



3-Bromo-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (0.99 g, 3.27 mmol) was dissolved in freshly distilled THF (10 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (3.3 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.79 mL, 3.6 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was successively washed with methanol. The white solid was collected by filtration and dried over vacuum to afford 3-(dicyclohexylphosphanyl)-*N*,*N*,1-

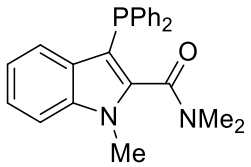
trimethyl-1*H*-indole-2-carboxamide (0.30 g, 76%). M.p.= 204.1-205.7 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.98–1.97 (m, 21H), 2.61–2.69 (m, 1H), 2.93 (s, 3H), 3.19 (s, 3H), 3.68 (s, 3H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.27 (t, *J* = 7.1Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.1, 26.5, 26.9, 27.1, 27.2, 27.4, 27.5, 30.0, 30.5, 30.6, 30.9, 31.2, 31.4, 31.6, 31.8, 32.0, 34.7, 35.2, 35.3, 38.7, 103.3, 103.4, 109.9, 120.2, 122.3, 122.5, 130.1, 138.2, 142.8, 143.2, 164.8; ^{31}P NMR (162 MHz, $CDCl_3$) δ -15.2; HRMS (ESI): calcd. for $C_{24}H_{36}N_2OP^+$: 399.2560, found 399.2559.

3-(Diisopropylphosphanyl)-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (L8)



3-Bromo-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (1.61 g, 8.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 ºC. Titrated *n*-BuLi (9.6 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 ºC, chlorodiisopropylphosphine (1.53 mL, 9.6 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the concentrated mixture was dissolved in dichloromethane and filter through celite. The solution was evaporated and subjected to column chromatography and eluted with ethyl acetate/hexane (2:8 and 1:1) mixture. The eluent was evaporated and washed with hexane. The light orange solid was collected by filtration and dried over vacuum to afford 3-(diisopropylphosphanyl)-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (1.6 g, 63%). M.p.= 159.2-160.1 ºC; ^{1}H NMR (400 MHz, C_6D_6) δ 0.95-1.04 (m, 6H), 1.14-1.21 (m, 6H), 2.08-2.15 (m, 1H), 2.45 (s, 3H), 2.73-2.79 (m, 1H), 2.81 (s, 3H), 3.15 (s, 3H), 7.01-7.03 (m, 1H), 7.16-7.23 (m, 2H), 7.81-7.83 (m, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 20.5, 20.6, 21.3, 21.4, 21.5, 21.67, 21.69, 21.9, 22.6, 22.7, 26.1, 26.2, 30.4, 34.1, 37.9, 38.0, 104.1, 104.2, 110.4, 120.6, 122.6, 122.7, 130.4, 130.5, 138.7, 143.7, 144.1, 164.4; ^{31}P NMR (162 MHz, C_6D_6) δ -5.34; HRMS (ESI): calcd. for $C_{18}H_{28}N_2OP^+$: 319.1934, found 319.1936.

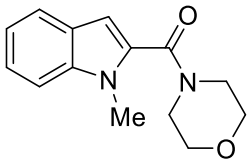
3-(Diphenylphosphanyl)-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (L9)



3-Bromo-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (2.47 g, 8.8 mmol) was dissolved in freshly distilled THF (30 mL) at room temperature under nitrogen atmosphere. The solution

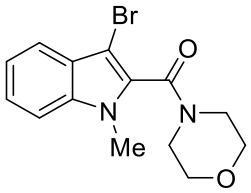
was cooled to -78 °C. Titrated *n*-BuLi (9.68 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodiphenylphosphine (1.95 mL, 10.56 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was successively washed with ethanol. The light orange solid was collected by filtration and dried over vacuum to afford 3-(diphenylphosphanyl)-*N*,*N*,1-trimethyl-1*H*-indole-2-carboxamide (1.88 g, 55%). M.p.= 178.5-179.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.84 (s, 3H), 3.12 (s, 3H), 3.76 (s, 3H), 6.95 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.23–7.50 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.0, 34.6, 38.69, 38.73, 103.5, 109.9, 120.5, 122.3, 122.8, 127.8, 127.98, 128.03, 128.1, 128.2, 128.3, 129.1, 132.5, 132.6, 132.7, 132.8, 136.7, 136.9, 137.0, 138.3, 141.8, 142.2, 164.1; ^{31}P NMR (162 MHz, $CDCl_3$) δ -29.2; HRMS (ESI): calcd. for $C_{24}H_{24}N_2OP^+$: 387.1621, found 387.1624.

(1-Methyl-1*H*-indol-2-yl)(morpholino)methanone (P3)



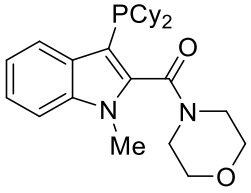
1-Methylindole (6.24 mL, 50.0 mmol) was dissolved in freshly distilled THF (125 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *t*-BuLi (55 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at room temperature, *N*,*N*-morpholinecarbonyl chloride (7.00 mL, 60.0 mmol) was added at -78 °C. The reaction temperature was then increased to room temperature and the reaction was stirred for 1 h. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the concentrated mixture was diluted with ethyl acetate and washed with water and brine. The organic layer was dried over Na_2SO_4, and then concentrated. The concentrated mixture was then subjected to recrystallization from ethyl acetate/hexane. The solid was collected, washed with hexane and dried over vacuum to afford (1-methyl-1*H*-indol-2-yl)(morpholino)methanone as the light yellow solid (8.73 g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.73–3.75 (m, 4H), 3.79–3.82 (m, 4H), 3.86 (s, 3H), 6.60 (s, 1H), 7.14–7.18 (m, 1H), 7.29–7.33 (m, 1H), 7.36–7.38 (m, 1H), 7.63 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.1, 66.9, 103.8, 109.8, 120.3, 121.5, 123.4, 126.2, 131.0, 137.9, 163.1. The data are in agreement with those previously reported in the literature.[10]

(3-Bromo-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (P3')



N-Bromosuccinimide (5.61 g, 31.5 mmol) was added to a solution of (1-methyl-1*H*-indol-2-yl)(morpholino)methanone (7.32 g, 30.0 mmol) in anhydrous chloroform (100 mL) in portion at room temperature. After stirring for 10 min, water was added to the reaction mixture. The organic layer was washed with water and brine, and then concentrated. The concentrated solution was filtered over a pad of silica and eluted with dichloromethane. The concentrated solution was evaporated to give a solid product. The solid was subjected to recrystallization from ethyl acetate/hexane. The white solid was collected and dried over vacuum to afford (3-bromo-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (8.29 g, 86%). M.p.= 159.4-160.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.40–3.46 (m, 1H), 3.55–3.68 (m, 2H), 3.78 (s, 3H), 3.80–3.89 (m, 5H), 7.19–7.26 (m, 1H), 7.33–7.34 (m, 2H), 7.57 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.4, 42.5, 47.7, 66.8, 67.3, 90.2, 109.8, 119.9, 120.9, 124.2, 126.1, 130.2, 136.7, 161.4; HRMS (ESI): calcd. for $C_{14}H_{16}BrN_2O_2^+$: 323.0390, found 323.0389.

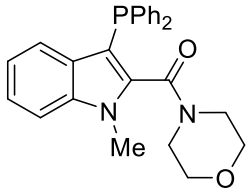
(3-(Dicyclohexylphosphanyl)-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (L3)



(3-Bromo-1-methyl-1H-indol-2-yl)(morpholino)methanone (1.61 g, 5.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (6.0 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -90 °C, chlorodicyclohexylphosphine (1.32 mL, 6.0 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was washed with methanol and collected by filtration. The white solid was subjected to recrystallization from dichloromethane/methanol. The off-white solid was collected by filtration and dried over vacuum to afford (3-(dicyclohexylphosphanyl)-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (1.26 g, 57%). M.p.= 203.1-205.8 °C; ^{1}H NMR (400 MHz, C_6D_6) δ 0.80–1.45 (m, 11H), 1.50–2.04 (m, 10H), 2.73–2.83 (m, 2H), 3.06–3.12 (m, 1H), 3.16–3.33 (m, 5H), 3.45–3.73 (m, 4H), 7.02–7.08 (m, 1H), 7.18–7.22 (m, 2H), 7.90–7.93 (m, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 26.4, 26.9, 27.2, 27.3, 27.5, 27.55, 27.61,

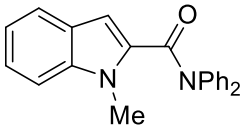
27.8, 30.4, 30.5, 30.6, 31.0, 31.1, 31.9, 32.1, 32.2, 32.4, 32.5, 36.0, 36.1, 42.2, 47.40, 47.44, 66.7, 67.06, 67.09, 104.0, 104.1, 110.4, 120.9, 122.66, 122.73, 130.66, 130.73, 138.7, 142.8, 143.3, 163.0; ^{31}P NMR (162 MHz, C_6D_6) δ -16.0; HRMS (ESI): calcd. for $C_{26}H_{38}N_2O_2P^+$: 441.2665, found 441.2669.

(3-(Diphenylphosphanyl)-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (L10)



(3-Bromo-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (0.65 g, 2.0 mmol) was dissolved in freshly distilled THF (10 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (2.2 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodiphenylphosphine (0.44 mL, 2.4 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was washed with methanol and collected by filtration. The white solid was subjected to recrystallization from dichloromethane/methanol. The white solid was collected by filtration and dried over vacuum to afford (3-(diphenylphosphanyl)-1-methyl-1*H*-indol-2-yl)(morpholino)methanone (0.59 g, 69%). M.p.= 155.7-156.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.25–3.34 (m, 3H) 3.45–3.49 (m, 1H), 3.74–3.92 (m, 7H), 6.96 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 7.25–7.41 (m, 10H), 7.46–7.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.2, 42.3, 47.6, 66.7, 66.8, 104.0, 104.1, 110.1, 120.8, 122.5, 123.1, 127.9, 128.18, 128.25, 128.46, 128.52, 128.9, 129.0, 132.3, 132.5, 132.7, 132.8, 136.4, 137.0, 138.5, 141.0, 141.5, 162.9; ^{31}P NMR (162 MHz, $CDCl_3$) δ -29.6; HRMS (ESI): calcd. for $C_{26}H_{26}N_2O_2P^+$: 429.1726, found 429.1728.

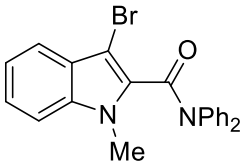
1-Methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide (P4)



1-Methylindole (2.50 mL, 20.0 mmol) was dissolved in freshly distilled THF (100 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (20 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at room temperature, *N*,*N*-diphenylcarbamoyl chloride (5.56 g, 24.0 mmol) was added at -78 °C. The reaction temperature was then increased to room temperature and the reaction was stirred for 1 h. The solvent was removed under reduced pressure. After the solvent was removed

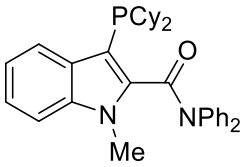
under vacuum, the concentrated mixture was filtered through a short silica pad and eluted with ethyl acetate/hexane (2:8) mixture. The eluent was collected and concentrated under reduced pressure. Hexane (10 mL) was added into the crude product and the crude product was stirred vigorously to generate white solid at 0 °C. The solid was collected through filtration. The white solid was further purified by recrystallization using ethanol and filtered to yield 1-methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide (4.84 g, 74%) was obtained. M.p.= 122.1-123.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.07 (s, 3H), 6.30 (s, 1H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.25–7.31 (m, 6H), 7.33–7.41 (m, 6H), 7.48 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.6, 108.7, 109.8, 120.0, 122.0, 123.9, 125.9, 126.4, 127.2, 129.2, 132.1, 138.1, 143.8, 163.7; HRMS (ESI): calcd. for $C_{22}H_{19}N_2O^+$: 327.1492, found 327.1495.

3-Bromo-1-methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide (P4')



N-Bromosuccinimide (0.89 g, 5.0 mmol) was added to a solution of 1-methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide (1.63 g, 5.0 mmol) in anhydrous chloroform (25 mL) in portion at room temperature. After stirring for 1 h, water was added to the reaction mixture. The organic layer was washed with water and brine, and then concentrated. The concentrated solution was filtered over a pad of silica and eluted with dichloromethane. The eluent was then concentrated and dried over vacuum to afford 3-bromo-1-methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide as off-white solid (1.21 g, 60%). M.p.= 163.6-164.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.96 (s, 3H), 7.17–7.34 (m, 13H), 7.49 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.5, 91.3, 109.7, 120.0, 120.6, 124.2, 126.1, 126.8, 128.9, 132.1, 136.8, 142.4, 163.0; HRMS (ESI): calcd. for $C_{22}H_{18}BrN_2O^+$: 405.0597, found 405.0602.

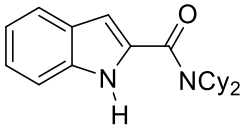
3-(Dicyclohexylphosphanyl)-1-methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide (L4)



3-Bromo-1-methyl-*N*,*N*-diphenyl-1H-indole-2-carboxamide (1.21 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C in a dry ice/acetone bath. Titrated *n*-BuLi (3.0 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.73 mL, 3.3 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced

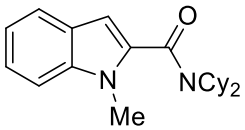
pressure. After the solvent was removed under vacuum, the solid product was washed with methanol and collected by filtration. The white solid was subjected to recrystallization from dichloromethane/methanol. The white solid was collected and dried over vacuum to afford 3-(dicyclohexylphosphanyl)-1-methyl-*N*,*N*-diphenyl-1*H*-indole-2-carboxamide (1.16 g, 74%). M.p.= 211.2-213.3 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.96–1.93 (m, 21H), 2.34–2.51 (m, 1H), 3.92 (s, 3H), 7.03–7.14 (m, 6H), 7.26–7.36 (m, 3H), 7.39–7.53 (m, 4H), 7.68 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.2, 26.3, 27.2, 27.4, 28.6, 30.3, 31.5, 32.0, 36.3, 105.3, 109.9, 120.1, 122.6, 122.8, 126.1, 126.7, 127.3, 128.7, 129.2, 130.0, 130.1, 138.4, 143.1, 164.6; ^{31}P NMR (162 MHz, $CDCl_3$) δ -16.9; HRMS (ESI): calcd. for $C_{34}H_{40}N_2OP^+$: 523.2873, found 523.2875.

_N_,_N_-Dicyclohexyl-1_H_-indole-2-carboxamide (P5)



To a stirred suspension of 1*H*-indole-2-carboxylic acid (8.05 g, 50.0 mmol) in anhydrous dichloromethane (100 mL) at room temperature was added DMF (5 drops) and followed by oxalyl chloride (6.5 mL, 75 mmol). The mixture was stirred at room temperature for 2 h. The solvent was removed under reduced pressure, the residue was dissolved in anhydrous dichloromethane (100 mL). *N*,*N*-Dicyclohexylamine (29.8 mL, 150 mmol) was added at 0 ºC. The resulting mixture was stirred at room temperature for 30 min. The reaction was then quenched with water (200 mL) and extracted with DCM for three times. The combined organic layers were washed with water, brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The brown oil was obtained. Ethanol (30 mL) was added and the mixture was stirred at 0 ºC for 1 h. The solid was generated and washed ethanol/water mixture. The light yellow solid and dried under vacuum to yield *N*,*N*-dicyclohexyl-1*H*-indole-2-carboxamide (8.74 g, 54%). M.p.= 184.6-187.5 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14–1.42 (m, 8H), 1.55–2.18 (m, 14H), 6.68 (s, 1H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.25–7.29 (m, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 9.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.3, 26.1, 31.0, 57.8, 103.4. 111.8. 120.1. 121.5. 123.7. 127.4. 131.4. 135.5. 163.1; HRMS (ESI): calcd. for $C_{21}H_{29}N_2O^+$: 325.2274, found 325.2277.

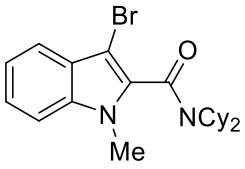
_N_,_N_-Dicyclohexyl-1-methyl-1_H_-indole-2-carboxamide (P5')



N,*N*-Dicyclohexyl-1H-indole-2-carboxamide (5 mmol) was dissolved in 20 ml THF in dropping funnel and added dropwise to the 20 mL THF solution contained 1.5 equiv. NaH

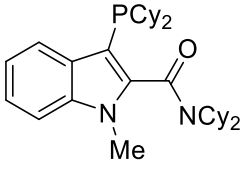
(60% in mineral oil, 7.5 mmol) at room temperature. NaH was washed with dry hexane under N_2. The mixture stirred for 30 min at room temperature. Dimethylsulfate (5.5 mmol) was then added to the mixture dropwise. The mixture was stirred at room temperature for 2 h. Solvent was removed by vacuum. Ethyl acetate and water were added to the mixture and the organic phase was separated. The combined organic phase was washed with brine several times and concentrated. The concentrated mixture was applied to silica pad and eluted with ethyl acetate. The organic solvent was dried over Na_2SO_4 and evaporated in vacuum. *N*,*N*-Dicyclohexyl-1-methyl-1*H*-indole-2-carboxamide (1.39 g, 82%) as yellow solid was obtained. M.p.=159.5-161.5 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (br, 6H), 1.62–1.80 (m, 12H), 2.62 (br, 2H), 3.17 (br, 1H), 3.78–3.87 (m, 4H), 6.48 (s, 1H), 7.13–7.17 (m, 1H), 7.26–7.30 (m, 1H), 7.36 (d, *J* = 8,0 Hz, 1H), 7.63 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.2, 25.9 (br), 30.6 (br), 30.8, 100.0, 109.6, 119.8, 121.3, 122.4, 126.8, 134.8, 137.3, 164.0; HRMS (ESI): calculated for $C_{22}H_{31}N_2O^+$ $[M+H]^+$: 339.2431, found: 339.2434.

3-Bromo-*N*,*N*-dicyclohexyl-1-methyl-1*H*-indole-2-carboxamide (P5")



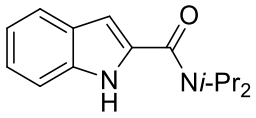
N-Bromosuccinimide (0.71 g, 4.0 mmol) was added to a solution of *N*,*N*-dicyclohexyl-1-methyl-1*H*-indole-2-carboxamide (1.35 g, 4.0 mmol) in anhydrous chloroform (20 mL) in portion at room temperature. After stirring for 30 min, water was added to the reaction mixture. The organic layer was washed with water and brine, and then concentrated. The concentrated solution was subjected to column chromatography and eluted with ethyl acetate/hexane (1:4) mixture. The eluent was then concentrated and dried over vacuum to afford 3-bromo-*N*,*N*-dicyclohexyl-1-methyl-1*H*-indole-2-carboxamide (1.31 g, 80%) as white solid. M.p.=158.2-160.0 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02–1.18 (m, 3H), 1.26–1.39 (m, 3H), 1.48–1.60 (m, 4H), 1.62–1.79 (m, 5H), 1.84–1.93 (m, 2H), 2.14–2.17 (m, 1H), 2.56–2.90 (m, 2H), 3.12–3.18 (m, 1H), 3.44–3.51 (m, 1H), 3.71 (s, 3H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.29–7.34 (m, 2H), 7.57 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 25.3, 25.4, 25.5, 26.5, 26.6, 29.5, 29.9, 31.1, 31.6, 32.1, 56.6, 60.4, 87.3, 109.7, 119.7, 120.5, 123.1, 126.5, 133.7, 136.0, 162.2; HRMS (ESI): calcd. for $C_{22}H_{30}BrN_2O^+$: 417.1536, found 417.1540.

***N*,*N*-Dicyclohexyl-3-(dicyclohexylphosphanyl)-1-methyl-1*H*-indole-2-carboxamide (L5)**



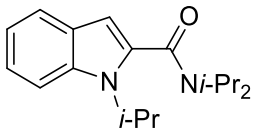
3-Bromo-*N*,*N*-dicyclohexyl-1-methyl-1*H*-indole-2-carboxamide (1.25 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (3.3 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.80 mL, 3.6 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was successively washed with methanol. The white solid was collected and dried over vacuum to afford *N*,*N*-dicyclohexyl-3-(dicyclohexylphosphanyl)-1-methyl-1*H*-indole-2-carboxamide (1.14 g, 72%). M.p.= 223.9-229.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.95–1.37 (m, 15H), 1.46–1.89 (m, 22H), 1.94–1.97 (m, 1H), 2.20–2.23 (m, 1H), 2.63–2.80 (m, 3H), 3.06–3.11 (m, 1H), 3.26–3.32 (m, 1H), 3.66 (s, 3H), 7.14–7.17 (m, 1H), 7.24–7.28 (m, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0, 25.1, 25.2, 25.5, 26.1, 26.5, 26.6, 26.7, 27.1, 27.2, 27.3, 27.36, 27.41, 27.46, 27.5, 27.7, 29.3, 29.7, 29.9, 30.6, 30.7, 30.89, 30.97, 31.03, 31.2, 31.4, 31.5, 31.59, 31.64, 31.8, 32.0, 35.7, 35.8, 56.2, 59.7, 101.9, 102.1, 109.7, 119.9, 121.7, 122.5, 130.5, 130.6, 137.8, 145.0, 145.4, 163.8; ^{31}P NMR (162 MHz, CD_2Cl_2) δ -16.3; HRMS (ESI): calcd. for $C_{34}H_{52}N_2OP^+$: 535.3812, found 535.3817.

_N_,_N_-Diisopropyl-1_H_-indole-2-carboxamide (P6)



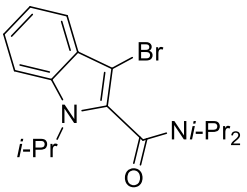
To a stirred suspension of 1*H*-indole-2-carboxylic acid (5.0 g, 31.0 mmol) in anhydrous chloroform (250 mL) at room temperature was added DMF (5 drops), followed by oxalyl chloride (4.42 mL, 52.3 mmol). The mixture was refluxed at 80 °C for 1 h. The solvent was removed under reduced pressure, the residue was dissolved in anhydrous chloroform (100 mL). *N*,*N*-Diisopropylamine (100 mmol) was added. The resulting mixture was stirred at room temperature for 30 min. The reaction was then quenched with water (350 mL) and extracted with DCM for three times. The combined organic layers were washed with water, brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The solid was subjected to recrystallization from hot ethanol/water. The solid was generated and washed by ethanol/water mixture. The light yellow solid and dried under vacuum to yield *N*,*N*-diisopropyl-1*H*-indole-2-carboxamide (4.3 g, 56%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.40–1.50 (m, 12H), 4.32 (br, 2H), 6.71 (s, 1H), 7.10–7.14 (m, 1H), 7.23–7.27 (m, 1H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 9.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.9, 103.3, 111.6. 120.2. 121.5. 123.8. 127.4. 131.3. 135.3, 162.7. The data are in agreement with those previously reported in the literature.[11]

_N_,_N_-Diisopropyl-1-isopropyl-1_H_-indole-2-carboxamide (P6')



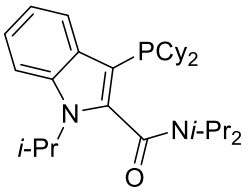
N,*N*-Diisopropyl-1*H*-indole-2-carboxamide (2.4 g, 10 mmol) was dissolved in a freshly distillated DMF (100 mL) at room temperature under a nitrogen atmosphere. KOH (5.6 g, 100 mmol) was then added into the reaction mixture and kept stirring at 0 ℃ for 15 min. 2-Bromopropane (9.4 mL, 100 mmol) was added dropwise at 0 ℃. The reaction mixture was stirred at 0 ℃ for overnight. After completion of reaction, water was added to the reaction mixture. The mixture was then extracted with DCM and the organic later was washed with large amount of water, and then concentrated. The concentrated was subjected to column chromatography and eluted with ethyl acetate/hexane (1: 9). The solution was evaporated to give a white solid. The final product *N*,*N*-diisopropyl-1-isopropyl-1*H*-indole-2-carboxamide (1.56 g, 54%) was dried under vacuum. M.p. = 92.7-93.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18–1.33 (m, 6H), 1.52–1.64 (m, 6H), 1.70–1.72 (m, 6H), 3.51–3.61 (m, 1H), 4.07–4.28 (m, 1H), 4.71–4.79 (m, 1H), 6.45 (s, 1H), 7.16 (t, *J*= 7.5 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J*= 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 21.6, 45.9, 48.9, 49.0, 51.0, 99.4, 111.5, 119.6, 121.4, 121.8, 127.7, 134.7, 134.9, 164.7; HRMS: calcd. for $C_{18}H_{27}N_2O^+$: 287.2118, found 287.2121.

3-Bromo-_N_,_N_,1-triisopropyl-1_H_-indole-2-carboxamide (P6")



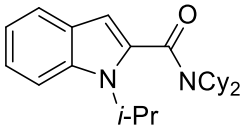
N-Bromosuccinimide (0.53 g, 3.0 mmol) was added to a solution of *N*,*N*,1-triisopropyl-1*H*-indole-2-carboxamide (0.85 g, 3.0 mmol) in anhydrous chloroform (10 mL) in portion at 0 ºC. After stirring for 30 min, the reaction mixture was concentrated. The concentrated solution was subjected to gel filtration and eluted with ethyl acetate/hexane (1:9) mixture. The solution was evaporated to give a white solid. The final product of 3-bromo-*N*,*N*,1-triisopropyl-1*H*-indole-2-carboxamide (1.06 g, 97%) was dried under vacuum. M.p. = 89.7-90.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16 (d, *J* = 6.5 Hz, 3H), 1.35 (d, *J* = 6.4 Hz, 3H), 1.63–1.70 (m, 12H), 3.57–3.65 (m, 1H), 3.92–3.99 (m, 1H), 4.53–4.61 (m, 1H), 7.20–7.30 (m, 2H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.60 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.1, 20.5, 21.0, 21.5, 21.6, 21.9, 46.3, 50.3, 51.5, 87.0, 112.1, 119.9, 120.3, 122.6, 127.5, 133.3, 133.6, 162.4; HRMS: calcd. for $C_{18}H_{26}BrN_2O^+$: 365.1223, found 365.1225.

3-(Dicyclohexylphosphanyl)-*N*,*N*,1-triisopropyl-1*H*-indole-2-carboxamide (L6)



3-Bromo-*N*,*N*,1-triisopropyl-1*H*-indole-2-carboxamide (1.97 g, 5.4 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (5.4 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (1.32 mL, 6.0 mmol) was added. The reaction was allowed to warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was washed with methanol and collected by filtration. The white solid was subjected to recrystallization from dichloromethane/methanol. The white solid was collected and dried over vacuum to afford 3-(dicyclohexylphosphanyl)-*N*,*N*,1-triisopropyl-1*H*-indole-2-carboxamide (0.98 g, 38%). M.p.= 173.7-174.9 °C; ^{1}H NMR (400 MHz, C_6D_6) δ 0.80 (d, *J* = 6.7 Hz, 3H), 0.83–0.91 (m, 1H), 0.94–1.05 (m, 1H), 1.10–1.29 (m, 8H), 1.30–1.40 (m, 10H), 1.42–1.59 (m, 6H), 1.68–1.73 (m, 5H), 1.83–2.08 (m, 5H), 2.72–2.79 (m, 1H), 3.15–3.22 (m, 1H), 3.92–4.02 (m, 1H), 4.43–4.54 (m, 1H), 7.14–7.21 (m, 2H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 20.2, 20.8, 21.2, 21.4, 21.5, 21.6, 26.4, 27.1, 27.4, 27.5, 27.6, 27.7, 27.8, 27.9, 30.60, 30.64, 30.7, 30.8, 31.8, 32.0, 32.6, 32.7, 32.9, 33.1, 36.7, 36.8, 46.1, 49.9, 50.8, 101.9, 113.2, 120.3, 121.9, 123.0, 132.37, 132.44, 136.1, 145.2, 145.7, 164.2; ^{31}P NMR (162 MHz, C_6D_6) δ -19.3; HRMS (ESI): calcd. for $C_{30}H_{48}N_2OP^+$: 483.3499, found 483.3502.

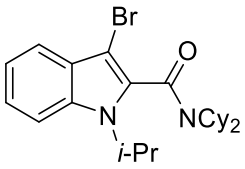
***N*,*N*-Dicyclohexyl-1-isopropyl-1*H*-indole-2-carboxamide (P7)**



N,*N*-Dicyclohexyl-1*H*-indole-2-carboxamide (6.49 g, 20 mmol) was dissolved in a freshly distillated DMF (100 mL) at room temperature under a nitrogen atmosphere. KOH (11.22 g, 200 mmol) was then added into the reaction mixture and kept stirring at 0 °C. 2-Bromopropane (18.78 mL, 200 mmol) in a freshly distillated DMF (20 mL) was added dropwise at 0 °C. The reaction mixture was stirred at 0 °C for 24 h. After stirring for overnight, water was added to the reaction mixture. The mixture was then extracted with DCM and the organic layer was washed with water, and then concentrated. Hexane was added and the mixture was allowed to stir for 10 min to give a white solid. The white solid was filtered and dried under vacuum to afford the final product *N*,*N*-dicyclohexyl-1-isopropyl-1*H*-indole-2-carboxamide (5.4 g, 74%).

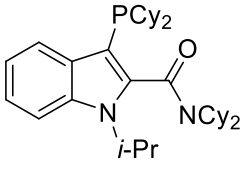
M.p.= 154.8-155.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.10–1.32 (m, 6H), 1.57–1.89 (m, 18H), 2.58–2.81 (m, 2H), 3.05–3.23 (m, 1H), 3.70–3.93 (m, 1H), 4.47–4.77 (m, 1H), 6.40 (s, 1H), 7.14 (t, *J* = 7.2 Hz, 1H), 7.24 (t, *J* = 7.3 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.7, 25.1, 26.5, 29.8, 31.4, 49.0, 56.2, 59.9, 99.3, 111.6, 119.5, 121.56, 121.64, 128.0, 135.0, 135.1, 165.0; HRMS (ESI): calcd. for $C_{24}H_{35}N_2O^+$: 367.2744, found 367.2747.

3-Bromo-*N*,*N*-dicyclohexyl-1-isopropyl-1*H*-indole-2-carboxamide (P7')



N-Bromosuccinimide (1.77 g, 10.0 mmol) was added to a solution of *N*,*N*-dicyclohexyl-1-isopropyl-1*H*-indole-2-carboxamide (3.66 g, 10.0 mmol) in anhydrous chloroform (30 mL) in portion at room temperature. After stirring for 30 min, water was added to the reaction mixture. The organic layer was washed with water and brine, and then concentrated. The concentrated solution was filtered over a pad of silica and eluted with dichloromethane. The eluent was then concentrated. The solid was subjected to recrystallization from dichloromethane/hexane. The white solid was collected, washed with hexane and dried over vacuum to afford 3-bromo-*N*,*N*-dicyclohexyl-1-isopropyl-1*H*-indole-2-carboxamide (1.93 g, 44%). M.p.= 148.1-149.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.04–1.15 (m, 3H), 1.24–1.39 (m, 3H), 1.53–1.70 (m, 12H), 1.75–1.78 (m, 3H), 1.86–1.95 (m, 2H), 2.22–2.25 (m, 1H), 2.68–2.82 (m, 2H), 3.12–3.18 (m, 1H), 3.45–3.52 (m, 1H), 4.49–4.59 (m, 1H), 7.20–7.29 (m, 2H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 21.8, 25.1, 25.2, 25.3, 25.5, 26.50, 26.54, 29.3, 29.9, 31.4, 32.2, 50.3, 56.5, 60.5, 86.8, 112.2, 120.0, 120.2, 122.5, 127.7, 133.6, 162.6; HRMS (ESI): calcd. for $C_{24}H_{34}BrN_2O^+$: 445.1849, found 445.1848.

***N*,*N*-Dicyclohexyl-3-(dicyclohexylphosphanyl)-1-isopropyl-1*H*-indole-2-carboxamide (L7)**



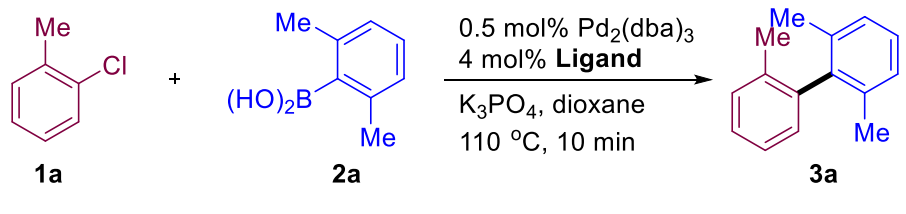
3-Bromo-*N*,*N*-dicyclohexyl-1-isopropyl-1*H*-indole-2-carboxamide (0.89 g, 2.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 °C. Titrated *n*-BuLi (2.2 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.53 mL, 2.4 mmol) was added. The reaction was allowed to

warm to room temperature and stirred overnight. The solvent was removed under reduced pressure. After the solvent was removed under vacuum, the solid product was washed with ethanol. The white solid was collected and dried over vacuum to afford 3-(dicyclohexylphosphanyl)-*N*,*N*,1-triisopropyl-1*H*-indole-2-carboxamide (0.72 g, 64%). M.p.= 229.1-230.5 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.99–1.32 (m, 16H), 1.53–1.75 (m, 22H), 1.81–1.90 (m, 5H), 1.96–1.99 (m, 1H), 2.33–2.36 (m, 1H), 2.61–2.82 (m, 3H), 3.07–3.13 (m, 1H), 3.36–3.42 (m, 1H), 4.44–4.54 (m, 1H), 7.14 (t, *J* = 7.3 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 21.7, 25.1, 25.2, 25.3, 25.6, 26.2, 26.6, 26.7, 27.1, 27.2, 27.4, 27.5, 27.7, 29.1, 29.9, 30.0, 30.6, 30.8, 30.9, 31.3, 31.5, 32.0, 32.3, 32.6, 36.1, 36.2, 49.7, 56.3, 59.7, 112.6, 119.5, 121.1, 122.9, 135.3, 145.5, 164.1; ^{31}P NMR (162 MHz, $CDCl_3$) δ -16.4; HRMS (ESI): calcd. for $C_{36}H_{56}N_2OP^+$: 563.4125, found 563.4129.

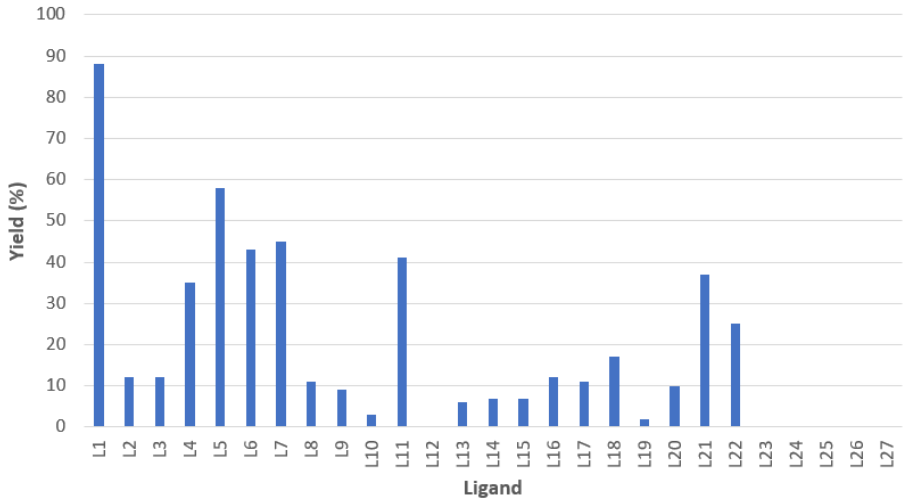
3. General procedure and data of ligand and reaction condition screenings

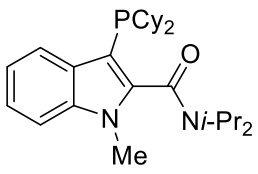
An array of Schlenk tubes were equipped with a Teflon-coated magnetic stir bar (5 mm × 10 mm) and fitted with a screw cap. Pd source (1.0 mol%, 0.005 mmol), ligand (4.0 mol%, 0.02 mmol), 2,6-dimethylphenyl boronic acid (1.0 mmol) and base (1.5 mmol) were added to the Schlenk tubes. The tubes were carefully evacuated and backfilled with nitrogen for three cycles. 2-Chlorotoluene (58.4 μL, 0.5 mmol) followed by the corresponding solvent (1.5 mL) were added by micropipette and syringe respectively. The tubes were then placed into a preheated oil bath (110 °C) and stirred for 10 minutes. After completion of reaction, the reaction tube was allowed to reach room temperature. Ethyl acetate (~3 mL), dodecane (113 μL, internal standard), and water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

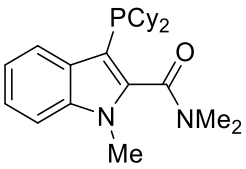
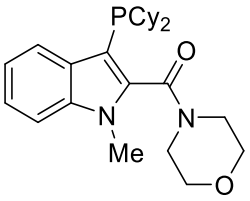
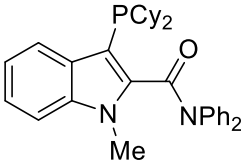
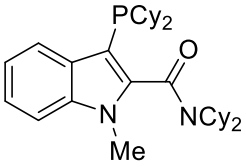
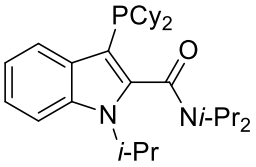
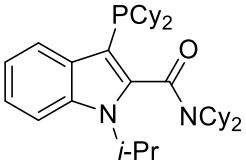
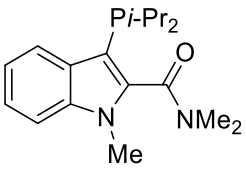
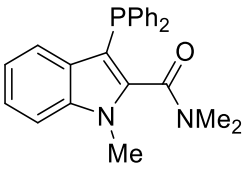
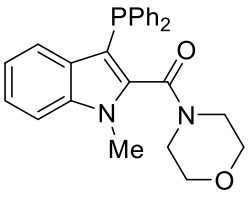
Table S1. Ligand screening of Pd-catalyzed Suzuki-Miyaura coupling reaction of 2-chlorotoluene with (2,6-dimethylphenyl)boronic acid[a]

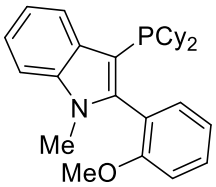
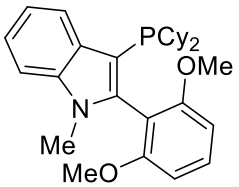
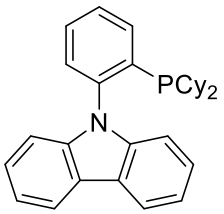


1a 2a 3a



Code	Ligands	Yield of **3a** (%)
L1		88

L2		12
L3		12
L4		35
L5		58
L6		43
L7		45
L8		11
L9		9
L10		3

L11	PCy_3	41
L12	PPh_3	0
L13	P*t*-Bu_3•HBF_4	6
L14	cataCXium®A	7
L15	cataCXium®PinCy	7
L16	SPhos	12
L17	XPhos	11
L18	BrettPhos	17
L19	CyJohnPhos	2
L20		10
L21		37
L22		25
L23	MorDalPhos	0
L24[b]	*rac*-BINAP	0
L25[b]	DPEPhos	0
L26[b]	XantPhos	0
L27[b]	dppf	0

[a]Reaction conditions: 2-chlorotoluene **1a** (0.5 mmol), (2,6-dimethylphenyl)boronic acid **2a** (1.0 mmol), $Pd_2(dba)_3$ (0.5 mol%), ligand (Pd:L = 1:4), K_3PO_4 (1.5 mmol), and dioxane (1.5 mL) were stirred under N_2 at 110 °C for 10 min. Calibrated GC yields were reported using dodecane as the internal standard. [b]2 mol% Ligand (Pd: P = 1: 4) was used instead.

4. General procedures for Suzuki coupling of aryl chlorides

General procedure for Suzuki-Miyaura coupling of aryl chlorides (0.05-0.1 mol % Pd catalysts loading)

$Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol) and **L1** (9.1 mg, 0.02 mmol) were charged in 10.0 mL freshly distilled dioxane (0.1 mol% Pd per 1.0 mL Pd complex stock solution) or in 5.0 mL freshly distilled toluene (0.2 mol% Pd per 1.0 mL Pd complex stock solution) under nitrogen. Arylboronic acid (1.0 mmol), aryl chloride (if solid, 0.5 mmol), and K_3PO_4 (318 mg, 1.5 mmol) were loaded into an array of Schlenk tubes equipped with a Teflon-coated magnetic stir bar (4 mm × 10 mm). The tube was evacuated and flushed with nitrogen for three times. Aryl chloride (if liquid, 0.5 mmol) was added by micropipette afterwards. The corresponding volume of stock solution and solvent were then immediately added to the Schlenk tubes by syringes (final volume: 1.5 mL). The tubes were placed into a preheated oil bath (110 °C) and stirred for 10 minutes to 2 hours. After completion of reaction, the reaction tube was allowed to cool down to room temperature. Before GC or TLC analysis, ethyl acetate (~3 mL) and water (~2 mL) were added for extraction. The organic layer was separated and the aqueous layer was washed with ethyl acetate. The filtrate was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

General procedure for Suzuki-Miyaura coupling of aryl chlorides (0.005 mol % Pd catalysts loading)

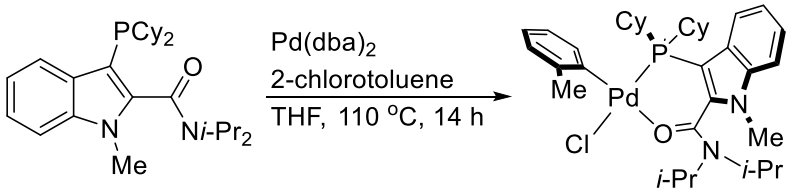
$Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol) and **L1** (9.1 mg, 0.02 mmol) were charged in 10.0 mL freshly distilled dioxane (0.1 mol% Pd per 1.0 mL Pd complex stock solution) under nitrogen. The stock solution was then further diluted by taking 0.5 mL of it to 5.0 mL freshly distilled dioxane (0.01 mol% Pd per 1.0 mL Pd complex stock solution) under nitrogen. Tri-arylboroxine (0.3 mmol), aryl chloride (if solid, 0.5 mmol), and K_3PO_4 (318 mg, 1.5 mmol) were loaded into an array of Schlenk tubes equipped with a Teflon-coated magnetic stir bar (4 mm × 10 mm). The tube was evacuated and flushed with nitrogen for three times. Aryl chloride (if liquid, 0.5 mmol) was added by micropipette afterwards. Further diluted stock solution (0.5 mL) and 1.0 mL of freshly distilled dioxane were then immediately added to the Schlenk tubes by syringes (final volume: 1.5 mL). The tubes were placed into a preheated oil bath (110 °C) and stirred for 24 hours. After completion of reaction, the reaction tube was allowed to reach room temperature. Before GC or TLC analysis, ethyl acetate (~3 mL) and water (~2 mL) were added. The organic layer was separated and the aqueous layer was washed with ethyl acetate. The filtrate was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

5. General procedure for gram-scale Suzuki coupling of aryl chloride

$Pd_2(dba)_3$ (2.3 mg, 0.0025 mmol), **L1** (9.1 mg, 0.02 mmol), 2-fluorophenylboronic acid (2.8 g, 20 mmol), and K_3PO_4 (6.4 g, 30 mmol) were charged into a 100 mL round-bottom Schlenk flask equipped with a Teflon-coated magnetic stir bar (6 mm × 30 mm). The flask was evacuated and flushed with nitrogen for three times. 2-Chloro-1,3-dimethylbenzene (1.4 g, 10 mmol) and dioxane (30 mL) were added by syringes afterwards. The flask was placed into a preheated oil bath (110 °C) and stirred for 30 minutes. Ethyl acetate and water were added to the flask and the mixture was transferred to separating funnel and subjected to extraction. The organic layers were combined and concentrated. The crude product was purified by column chromatography on silica gel (230-400 mesh) to afford the desired product (1.7 g, 85%).

6. Preparation of the oxidative addition adduct of C1

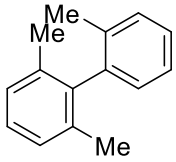
$Pd(dba)_2$ (0.575 g, 1.0 mmol) and **L1** (0.9080 g, 2.0 mmol) were loaded into a Schlenk tube (100 mL) equipped with a screw cap and Teflon-coated magnetic stir bar. The tube was carefully evacuated and back-filled with nitrogen for three cycles. 2-Chlorotoluene (1.89 g, 15.0 mmol) and subsequently THF (30 mL) were added by syringe. The solution was stirred at room temperature for 5 min. The tube was placed into a preheated oil bath (110 °C) and stirred for 14 h. After completion of the reaction, the reaction tube was warmed to room temperature. The unreacted palladium was filtered through Celite, and the solvent was removed. The crude product was washed successively with hexane. The product was further recrystallized from DCM and hexane. The product was then then dried under to give the palladium complex C1 as a grey green solid. A single crystal of C1 suitable for X-ray diffraction was obtained by vapor diffusion of hexane into a dichloromethane solution containing C1.



L1 **C1**

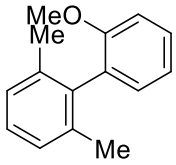
7. Characterization data for coupling products

2,2',6-Trimethyl-1,1'-biphenyl (Table 3, 4 and 5, product 3a)[12]



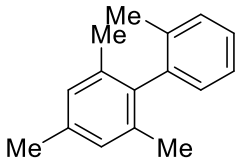
Eluents (Hexane, R_f= 0.52) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.07 (s, 6H), 2.09 (s, 3H), 7.12–7.14 (m, 1H), 7.21–7.23 (m, 2H), 7.26–7.30 (m, 1H), 7.35–7.40 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.4, 20.3, 126.0, 126.9, 127.0, 127.2, 128.8, 129.9, 135.5, 135.8, 140.5, 141.0.

2'-Methoxy-2,6-dimethyl-1,1'-biphenyl (Table 3 and 4, product 3b)[13]



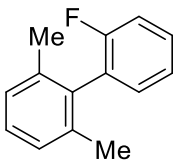
Eluents (Ethyl acetate: Hexane= 1: 50, R_f= 0.31) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.20 (s, 6H), 3.87 (s, 3H), 7.13–7.22 (m, 3H), 7.27–7.35 (m, 3H), 7.48–7.52 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 55.3, 110.8, 120.6, 126.96, 126.99, 128.3, 129.5, 130.6, 136.5, 138.2, 156.4.

2,2',4,6-Tetramethyl-1,1'-biphenyl (Table 3 and 4, product 3c)[14]



Eluents (Hexane, R_f= 0.64) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.11 (s, 6H), 2.16 (s, 3H), 2.51 (s, 3H), 7.12 (s, 2H), 7.18–7.20 (m, 1H), 7.38–7.43 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.4, 20.2, 21.0, 126.0, 126.9, 128.0, 129.1, 129.9, 135.6, 135.8, 136.2, 138.2, 140.5.

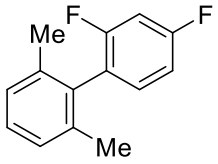
2'-Fluoro-2,6-dimethyl-1,1'-biphenyl (Table 3 and 4, product 3d)[13]



Eluents (Hexane, R_f= 0.59) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.17 (s, 6H), 7.22–7.32 (m, 6H), 7.41–7.46 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

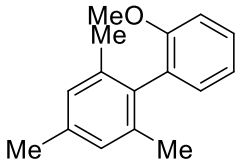
20.4, 115.7 (d, J = 22.4 Hz), 124.1 (d, J = 3.5 Hz), 127.3, 127.7, 128.0 (d, J = 17.7 Hz), 128.9 (d, J = 7.9 Hz), 131.3 (d, J = 4.0 Hz), 135.3, 136.6, 159.5 (d, J = 242.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.0 (s).

2,4-Difluoro-2',6'-dimethyl-1,1'-biphenyl (Table 3 and 4, product 3e)[15]



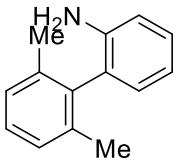
Eluents (Hexane, R_f= 0.50) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.14 (s, 6H), 6.97–7.05 (m, 2H), 7.15–7.22 (m, 3H), 7.27–7.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 104.1 (dd, J = 25.2 Hz, J = 26.2 Hz), 111.4 (dd, J = 20.7 Hz, J = 3.7 Hz), 124.0 (dd, J = 18.1 Hz, J = 4.1 Hz), 127.4, 128.0, 131.9 (dd, J = 5.4 Hz, J = 9.3 Hz), 134.3, 136.8, 159.5 (dd, J = 245.5 Hz, J = 11.7 Hz), 162.3 (dd, J = 246.4 Hz, J = 11.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.6 (m, 1F), -110.5 (m, 1F).

2'-Methoxy-2,4,6-trimethyl-1,1'-biphenyl (Table 3, product 3f)[16]



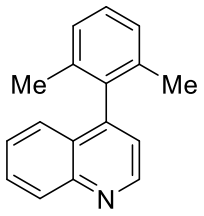
Eluents (Dichloromethane: Hexane= 1: 20, R_f= 0.31) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.02 (s, 6H), 2.36 (s, 3H), 3.77 (s, 3H), 6.97–7.08 (m, 5H), 7.34–7.38 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.3, 21.1, 55.4, 110.8, 120.6, 127.9, 128.2, 129.5, 130.9, 135.2, 136.4, 136.5, 156.7.

2',6'-Dimethyl-[1,1'-biphenyl]-2-amine (Table 3, product 3g)[17]



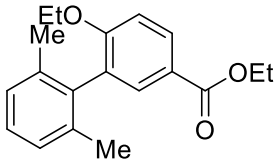
Eluents (Ethyl acetate: Hexane= 1: 9, R_f= 0.57) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.08 (s, 6H), 3.40 (br, 2H), 6.79–6.86 (m, 2H), 6.94 (d, J = 7.4 Hz, 1H), 7.15–7.22 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 115.0, 118.5, 126.1, 127.5, 127.6, 128.1, 129.7, 137.2, 137.8, 143.3.

4-(2,6-Dimethylphenyl)quinoline (Table 3, product 3h)



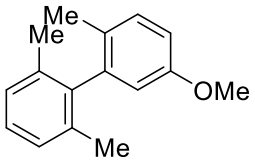
Eluents (Ethyl acetate: Hexane= 1: 4, R_f= 0.35) was used for flash column chromatography. Light yellow solid; m.p.= 96.5 - 98.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.92 (s, 6H), 7.19–7.23 (m, 3H), 7.29–7.32 (m, 1H), 7.39–7.43 (m, 2H), 7.72 (t, *J* = 7.5 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 8.95 (d, *J* = 4.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.1, 121.4, 125.2, 126.7, 127.0, 127.4, 128.0, 129.4, 129.7, 135.9, 136.8, 147.9, 148.4, 150.2; HRMS (ESI): calcd. for $C_{17}H_{16}N^+$: 234.1277, found 234.1282.

Ethyl 6-ethoxy-2',6'-dimethyl-[1,1'-biphenyl]-3-carboxylate (Table 3, product 3i)



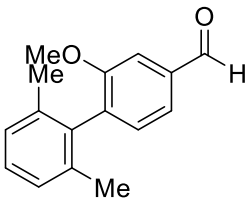
Eluents (Ethyl acetate: Hexane= 1: 4, R_f= 0.68) was used for flash column chromatography. Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.27 (t, *J* = 7.0 Hz, 3H), 1.40 (t, *J* = 7.1 Hz, 3H), 2.06 (s, 6H), 4.07–4.12 (m, 2H), 4.35–4.41 (m, 2H), 7.03 (d, *J* = 8.7 Hz, 1H), 7.13–7.15 (m, 2H), 7.18–7.22 (m, 1H), 7.84 (s, 1H), 8.11 (d, *J* = 8.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.3, 20.2, 60.4, 63.6, 111.0, 122.6, 126.9, 127.0, 129.5, 130.5, 132.3, 136.2, 137.2, 159.4, 166.2; HRMS (ESI): calcd. for $C_{19}H_{23}O_3^+$: 299.1642, found 299.1645.

5-Methoxy-2,2',6'-trimethyl-1,1'-biphenyl (Table 3, product 3j)



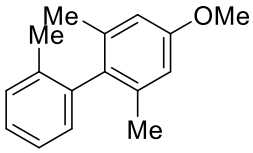
Eluents (Dichloromethane: Hexane= 1: 20, R_f= 0.37) was used for flash column chromatography. Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.03 (s, 3H), 2.11 (s, 6H), 3.89 (s, 3H), 6.74 (s, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 7.22-7.32 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.3, 20.2, 55.1, 112.5, 114.0, 126.9, 127.2, 127.5, 130.8, 135.7, 141.0, 141.5, 157.9; HRMS (APPI): calcd. for $C_{16}H_{18}O$: 226.1352, found 226.1352.

2-Methoxy-2',6'-dimethyl-[1,1'-biphenyl]-4-carbaldehyde (Table 3, product 3k)



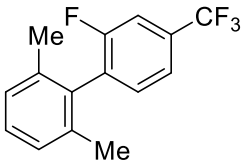
Eluents (Ethyl acetate: Hexane= 1: 9, R_f= 0.34) was used for flash column chromatography. Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.05 (s, 6H), 3.86 (s, 3H), 7.16–7.29 (m, 4H), 7.57–7.60 (m, 2H), 10.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 55.6, 109.2, 124.4, 127.1, 127.6, 131.2, 135.9, 136.7, 136.9, 137.0, 157.3, 191.8; HRMS (ESI): calcd. for $C_{16}H_{17}O_2^+$: 241.1223, found 241.1224.

4-Methoxy-2,2',6-trimethyl-1,1'-biphenyl (Table 3, product 3l)[18]



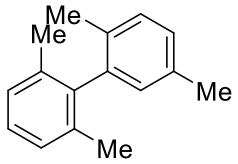
Eluents (Ethyl acetate: Hexane= 1: 50, R_f= 0.45) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 6H), 2.02 (s, 3H), 3.87 (s, 3H), 6.72 (s, 2H), 7.05–7.06 (m, 2H), 7.27-7.31 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.4, 20.6, 55.0, 112.5, 125.9, 126.9, 129.5, 129.9, 133.7, 136.2, 137.2, 140.3, 158.2.

2-Fluoro-2',6'-dimethyl-4-(trifluoromethyl)-1,1'-biphenyl (Table 4, product 3m)



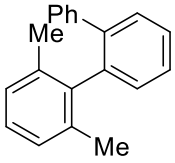
Eluents (Hexane, R_f= 0.69) was used for flash column chromatography. Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.04 (s, 6H), 7.13 (d, J = 7.6 Hz, 2H), 7.20-7.28 (m, 2H), 7.45-7.47 (m, 1H), 7.61-7.65 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 116.4 (d, J = 24.0 Hz), 123.8 (q, J = 270.4 Hz), 126.4-126.6 (m), 126.8 (d, J = 3.2 Hz), 127.1 (d, J = 3.6 Hz), 127.5, 128.4, 128.9-129.1 (m), 133.7, 136.5, 161.4 (d, J = 148.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.4 (s, 1F), -61.8 (s, 3F); HRMS (EI): calcd. for $C_{15}H_{12}F_4^+$: 268.0870, found 268.0879.

2,2',5,6'-Tetramethyl-1,1'-biphenyl (Table 4, product 3n)[13]



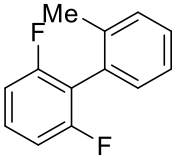
Eluents (Hexane, R_f= 0.50) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.07 (s, 3H), 2.10 (s, 6H), 2.47 (s, 3H), 6.98 (s, 1H), 7.19–7.31 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.9, 20.3, 21.0, 126.8, 127.1, 127.7, 129.4, 129.8, 132.3, 135.3, 135.8, 140.4, 141.2.

2,6-Dimethyl-1,1':2',1''-terphenyl (Table 4, product 3o)[13]



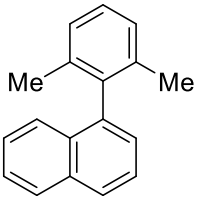
Eluents (Hexane, R_f= 0.48) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.98 (s, 6H), 6.99–7.00 (m, 2H), 7.08–7.22 (m, 7H), 7.41–7.53 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 126.5, 126.9, 127.1, 127.3, 127.4, 127.6, 128.8, 130.1, 130.3, 136.1, 138.9, 140.75, 140.78, 141.3.

2,6-Difluoro-2'-methyl-1,1'-biphenyl (Table 4 and 5, product 3p)[19]



Eluents (Hexane, R_f= 0.52) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 6.99–7.05 (m, 2H), 7.26–7.40 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 111.2–111.4 (m), 117.9–118.3 (m), 125.5, 128.6, 128.8, 129.0-129.2 (m), 130.1, 130.6, 137.3, 160.2 (dd, J = 245.9 Hz, J = 7.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.3 (s).

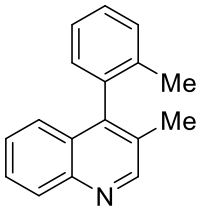
1-(2,6-Dimethylphenyl)naphthalene (Table 4, product 3q)[20]



Eluents (Hexane, R_f= 0.61) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.01 (s, 6H), 7.27–7.29 (m, 2H), 7.34–7.38 (m, 2H), 7.43–7.45 (m, 2H), 7.54–7.58

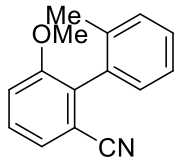
(m, 1H), 7.61–7.65 (m, 1H), 7.94–8.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 125.4, 125.68, 125.75, 126.0, 126.4, 127.2, 127.25, 127.31, 128.3, 131.7, 133.7, 137.0, 138.7, 139.6.

3-Methyl-4-(*o*-tolyl)quinoline (Table 4, product 3r)[21]



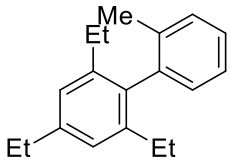
Eluents (Ethyl acetate: Hexane= 1: 4, R_f= 0.40) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.92 (s, 3H), 2.17 (s, 3H), 7.06 (d, *J* = 7.4 Hz, 1H), 7.27–7.38 (m, 5H), 7.61 (t, *J* = 7.6 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.88 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.0, 19.3, 125.4, 125.9, 126.4, 127.2, 128.0, 128.07, 128.08, 128.8, 129.3, 130.1, 135.7, 136.2, 145.8, 146.7, 152.5.

6-Methoxy-2'-methyl-[1,1'-biphenyl]-2-carbonitrile (Table 4, product 3s)[18]



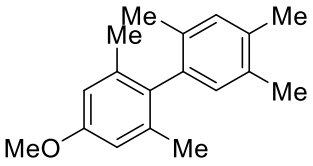
Eluents (Ethyl acetate: Hexane= 1: 9, R_f= 0.33) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.12 (s, 3H), 3.78 (s, 3H), 7.18–7.20 (m, 2H), 7.28–7.37 (m, 4H), 7.43 (t, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.5, 55.8, 114.3, 115.0, 117.7, 124.5, 125.7, 128.6, 129.2, 129.6, 129.9, 134.2, 134.6, 136.6, 157.0.

2,4,6-Triethyl-2'-methyl-1,1'-biphenyl (Table 4, product 3t)[22]



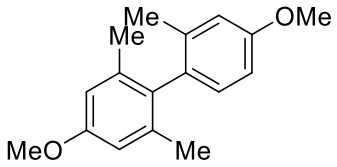
Eluents (Hexane, R_f= 0.60) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.11 (t, *J* = 7.6 Hz, 6H), 1.40 (t, *J* = 7.6 Hz, 3H), 2.07 (s, 3H), 2.24–2.41 (m, 4H), 2.75–2.81 (m, 2H), 7.09 (s, 2H), 7.17–7.21 (m, 1H), 7.28–7.35 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.2, 15.4, 19.9, 26.5, 28.7, 125.1, 125.5, 126.9, 129.7, 130.1, 136.3, 137.1, 140.0, 141.7, 143.0.

4'-Methoxy-2,2',4,5,6'-pentamethyl-1,1'-biphenyl (Table 4, product 3u)



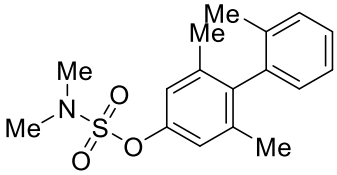
Eluents (Ethyl acetate: Hexane= 1: 9, R_f= 0.79) was used for flash column chromatography. Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.00 (s, 3H), 2.04 (s, 6H), 2.33 (s, 3H), 2.36 (s, 3H), 3.89 (s, 3H), 6.76 (s, 2H), 6.87 (s, 1H), 7.13 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.8, 19.2, 19.4, 20.7, 54.9, 112.4, 130.6, 131.2, 133.2, 133.7, 133.8, 134.8, 137.3, 137.6, 158.1; HRMS (ESI): calcd. for $C_{18}H_{23}O^+$: 255.1743, found 255.1744.

4,4'-Dimethoxy-2,2',6-trimethyl-1,1'-biphenyl (Table 4, product 3v)



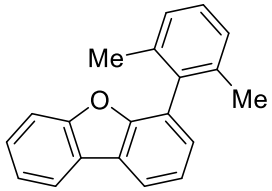
Eluents (Ethyl acetate: Hexane= 1:9, R_f= 0.69) was used for flash column chromatography. Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.00 (s, 6H), 2.01 (s, 3H), 3.86 (s, 3H), 3.87 (s, 3H), 6.73 (s, 2H), 6.83–6.85 (m, 1H), 6.89–6.90 (m, 1H), 6.97 (d, J = 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 20.6, 54.9, 55.0, 111.1, 112.4, 115.3, 130.3, 132.6, 133.3, 137.5, 137.7, 158.1, 158.4; HRMS (ESI): calcd. for $C_{17}H_{21}O_2^+$: 257.1536, found 257.1536.

2,2',6-Trimethyl-[1,1'-biphenyl]-4-yl dimethylsulfamate (Table 4, product 3w)



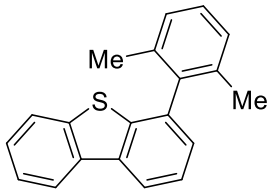
Eluents (Ethyl acetate: Hexane= 1: 9, R_f= 0.46) was used for flash column chromatography. Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.99 (s, 9H), 3.05 (s, 6H), 7.00–7.02 (m, 1H), 7.09 (s, 2H), 7.26–7.33 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.2, 20.3, 38.7, 119.9, 126.1, 127.2, 128.7, 130.0, 135.4, 137.8, 139.3, 139.5, 148.7; HRMS (ESI): calcd. for $C_{17}H_{22}NO_3S^+$: 320.1315, found 320.1315.

4-(2,6-Dimethylphenyl)dibenzo[*b,d*]furan (Table 4, product 3x)



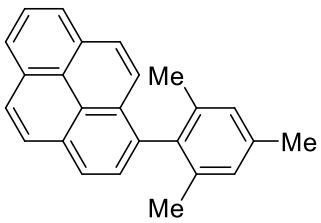
Eluents (Ethyl acetate: Hexane= 1: 50, R_f= 0.61) was used for flash column chromatography. Colorless gel; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.17 (s, 6H), 7.30–.45 (m, 5H), 7.49–7.53 (m, 2H), 7.60 (d, *J* = 8.2 Hz, 1H), 8.04–8.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 111.9, 119.5, 120.6, 122.6, 122.9, 124.3, 124.4, 124.9, 127.1, 127.4, 127.9, 128.2, 135.9, 136.9, 153.6, 156.2; HRMS (APPI): calcd. for $C_{20}H_{16}O$: 272.1196, found 272.1201.

4-(2,6-Dimethylphenyl)dibenzo[*b,d*]thiophene (Table 4, product 3y)



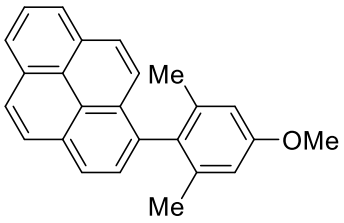
Eluents (Ethyl acetate: Hexane= 1: 20, R_f= 0.63) was used for flash column chromatography. White solid; m.p.= 86.9-87.7°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.16 (s, 6H), 7.28–7.41 (m, 4H), 7.51–7.58 (m, 2H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 7.3 Hz, 1H), 8.25–8.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.0, 120.1, 121.7, 122.8, 124.3, 125.0, 126.6, 126.9, 127.5, 128.0, 135.7, 135.97, 136.03, 136.3, 139.4, 139.7, 139.8; HRMS (ESI): calcd. for $C_{20}H_{16}S$: 288.0973, found 288.0973.

1-Mesitylpyrene (Table 4, product 3z)



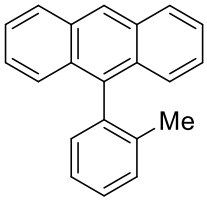
Eluents (Hexane, R_f= 0.58) was used for flash column chromatography. White solid; m.p.= 140.6-141.4°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.01 (s, 6H), 2.54 (s, 3H), 7.18 (s, 2H), 7.74 (d, *J* = 9.1 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 8.03–8.09 (m, 2H), 8.15–8.28 (m, 4H), 8.33 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 21.2, 124.8, 124.9, 125.9, 127.1, 127.3, 127.4, 127.5, 128.2, 128.9, 130.3, 131.1, 131.3, 136.5, 137.0, 137.1; HRMS (ESI): calcd. for $C_{25}H_{20}$: 320.1565, found 320.1565.

1-(4-Methoxy-2,6-dimethylphenyl)pyrene (Table 4, product 3aa)[23]



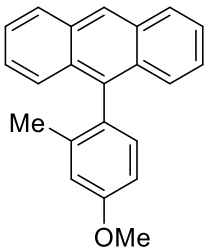
Eluents (Ethyl acetate: Hexane= 1: 20, R_f= 0.58) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 6H), 3.95 (s, 3H), 6.87 (s, 2H), 7.68 (d, *J* = 9.2 Hz, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.98–8.05 (m, 2H), 8.11–8.19 (m, 3H), 8.23 (d, *J* = 7.6 Hz, 1H), 8.27 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 55.2, 112.7, 124.86, 124.91, 124.95, 124.97, 125.9, 127.1, 127.4, 127.5, 127.7, 129.3, 130.3, 131.1, 131.3, 132.6, 136.3, 138.5, 158.8.

9-(*o*-Tolyl)anthracene (Table 4 and 5, product 3ab)[24]



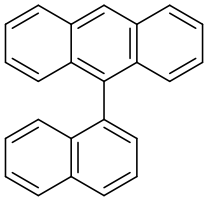
Eluents (Hexane, R_f= 0.65) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 3H), 7.35–7.55 (m, 8H), 7.54–7.64 (m, 2H), 8.11–8.13 (m, 2H), 8.56 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 125.1, 125.4, 125.8, 126.4, 126.5, 127.8, 128.4, 129.9, 130.0, 131.2, 131.4, 136.4, 137.8, 138.1.

9-(4-Methoxy-2-methylphenyl)anthracene (Table 4, product 3ac)[25]



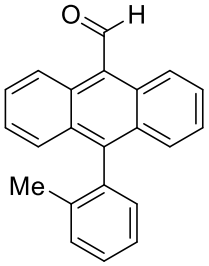
Eluents (Ethyl acetate: Hexane= 1: 9, R_f= 0.70) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.87 (s, 3H), 3.95 (s, 3H), 6.95–7.03 (m, 2H), 7.19 (d, *J* = 8.3 Hz, 1H), 7.35–7.38 (m, 2H), 7.46–7.49 (m, 2H), 7.57–7.59 (m, 2H), 8.06–8.08 (m, 2H), 8.50 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.0, 55.3, 111.1, 115.4, 125.1, 125.3, 126.2, 126.6, 128.4, 130.35, 130.41, 131.4, 132.1, 136.2, 139.2, 159.2.

9-(Naphthalen-1-yl)anthracene (Table 4, product 3ad)[26]



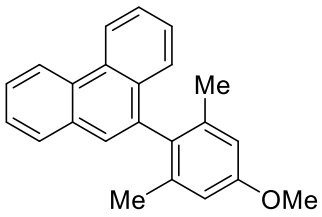
Eluents (Hexane, R_f= 0.55) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18–7.33 (m, 4H), 7.50–7.62 (m, 6H), 7.76 (t, *J* = 7.5 Hz, 1H), 8.07–8.18 (m, 4H), 8.66 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 125.1, 125.47, 125.51, 125.9, 126.2, 126.5, 126.9, 128.1, 128.2, 128.4, 129.1, 131.0, 131.4, 133.5, 133.7, 134.9, 136.5.

10-(*o*-Tolyl)anthracene-9-carbaldehyde (Table 4 and 5, product 3ae)[18]



Eluents (Ethyl acetate: Hexane= 1: 4, R_f= 0.57) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.85 (s, 3H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.39–7.51 (m, 5H), 7.57–7.60 (m, 2H), 7.65–7.69 (m, 2H), 9.02–9.05 (m, 2H), 11.60 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.6, 123.6, 125.0, 125.7, 125.9, 127.5, 128.4, 128.7, 129.6, 130.2, 130.4, 131.7, 137.2, 137.6, 145.2, 193.4.

9-(4-Methoxy-2,6-dimethylphenyl)phenanthrene (Table 4, product 3af)[27]



Eluents (Ethyl acetate: Hexane= 1:20, R_f= 0.54) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 6H), 3.90 (s, 3H), 6.79 (s, 2H), 7.44–7.51 (m, 2H), 7.56 (s, 1H), 7.61–7.71 (m, 3H), 7.89 (d, *J* = 7.6 Hz, 1H), 8.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.7, 55.2, 112.7, 122.6, 122.9, 126.1, 126.36, 126.43, 126.6, 126.7, 127.6, 128.5, 130.0, 130.6, 131.6, 131.98, 132.01, 137.1, 138.5, 158.7.

8. X-ray crystallographic data of C1

Table S2. Crystal data and structure refinement for SCM2105.

Identification code	SCM2105
Empirical formula	C36 H52 Cl3 N2 O P Pd
Formula weight	772.52
Temperature	297(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.0002(5) A alpha = 93.8303(14) deg. b = 12.8129(5) A beta = 97.7328(14) deg. c = 14.2811(6) A gamma = 110.1124(13) deg.
Volume	1859.03(14) A^3
Z, Calculated density	2, 1.380 Mg/m^3
Absorption coefficient	0.788 mm^-1
F(000)	804
Crystal size	0.68 x 0.36 x 0.28 mm
Theta range for data collection	2.00 to 27.74 deg.
Limiting indices	-14<=h<=14, -16<=k<=16, -18<=l<=18
Reflections collected / unique	96713 / 8667 [R(int) = 0.0230]
Completeness to theta = 27.74	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8096 and 0.6164
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8667 / 0 / 403
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0647
R indices (all data)	R1 = 0.0275, wR2 = 0.0663
Largest diff. peak and hole	0.753 and -0.788 e.A^-3

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for SCM2105.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1)	7107(1)	8403(1)	2740(1)	27(1)
O(1)	5627(1)	6048(1)	1451(1)	38(1)
Pd(1)	7601(1)	6960(1)	2120(1)	29(1)
Cl(1)	8049(1)	5393(1)	1524(1)	47(1)
Cl(2)	7931(1)	4868(1)	4729(1)	123(1)
Cl(3)	8079(2)	3231(1)	3294(1)	146(1)
N(1)	3857(1)	7743(1)	822(1)	32(1)
N(2)	3517(1)	5472(1)	1623(1)	30(1)
C(1)	9449(2)	7606(2)	2778(1)	38(1)
C(2)	9738(2)	7553(2)	3753(2)	47(1)
C(3)	11028(3)	7906(2)	4218(2)	65(1)
C(4)	12032(2)	8328(2)	3718(2)	73(1)
C(5)	11769(2)	8377(2)	2768(2)	67(1)
C(6)	10476(2)	8001(2)	2269(2)	51(1)
C(7)	10252(3)	8005(3)	1209(2)	71(1)
C(8)	6803(2)	8270(1)	3970(1)	31(1)
C(9)	6198(2)	9084(2)	4355(1)	43(1)
C(10)	5926(2)	8892(2)	5364(2)	54(1)
C(11)	5079(2)	7689(2)	5417(2)	58(1)
C(12)	5690(2)	6886(2)	5047(2)	51(1)
C(13)	5951(2)	7059(2)	4038(1)	40(1)
C(14)	8252(2)	9849(1)	2753(1)	36(1)
C(15)	9491(2)	10192(2)	3511(2)	45(1)
C(16)	10366(2)	11396(2)	3468(2)	65(1)
C(17)	10721(3)	11561(3)	2500(3)	88(1)
C(18)	9500(3)	11238(2)	1739(2)	79(1)
C(19)	8599(2)	10032(2)	1765(2)	52(1)
C(20)	5592(2)	8390(1)	2035(1)	29(1)

C(21)	5185(2)	9312(1)	1777(1)	32(1)
C(22)	5540(2)	10447(2)	2126(2)	44(1)
C(23)	4918(2)	11086(2)	1676(2)	54(1)
C(24)	3942(2)	10637(2)	875(2)	54(1)
C(25)	3537(2)	9528(2)	531(1)	44(1)
C(26)	4147(2)	8876(1)	1003(1)	33(1)
C(27)	2993(2)	7051(2)	-26(1)	44(1)
C(28)	4706(2)	7453(1)	1455(1)	28(1)
C(29)	4621(2)	6271(1)	1506(1)	28(1)
C(30)	2300(2)	5661(2)	1792(1)	39(1)
C(31)	2083(2)	5527(2)	2816(2)	59(1)
C(32)	1100(2)	4893(2)	1089(2)	56(1)
C(33)	3501(2)	4306(1)	1674(1)	38(1)
C(34)	4431(3)	4212(2)	2527(2)	61(1)
C(35)	3720(3)	3806(2)	744(2)	57(1)
C(36)	8535(4)	4612(3)	3728(2)	105(1)

Table S4. Bond lengths [A] and angles [deg] for SCM2105.

P(1)-C(20)	1.8214(16)
P(1)-C(8)	1.8396(16)
P(1)-C(14)	1.8453(17)
P(1)-Pd(1)	2.2575(4)
O(1)-C(29)	1.2457(19)
O(1)-Pd(1)	2.1304(12)
Pd(1)-C(1)	1.9815(17)
Pd(1)-Cl(1)	2.3600(4)
Cl(2)-C(36)	1.713(4)
Cl(3)-C(36)	1.710(4)
N(1)-C(28)	1.372(2)
N(1)-C(26)	1.373(2)
N(1)-C(27)	1.458(2)
N(2)-C(29)	1.331(2)
N(2)-C(30)	1.487(2)
N(2)-C(33)	1.494(2)
C(1)-C(6)	1.392(3)
C(1)-C(2)	1.398(3)
C(2)-C(3)	1.387(3)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.370(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.359(4)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.404(3)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.501(4)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-C(9)	1.528(2)
C(8)-C(13)	1.529(2)
C(8)-H(8A)	0.9800
C(9)-C(10)	1.529(3)

C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.515(3)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.514(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.523(3)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(19)	1.522(3)
C(14)-C(15)	1.533(2)
C(14)-H(14A)	0.9800
C(15)-C(16)	1.522(3)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.495(4)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.524(4)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.528(3)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(28)	1.387(2)
C(20)-C(21)	1.453(2)
C(21)-C(22)	1.405(2)
C(21)-C(26)	1.406(2)
C(22)-C(23)	1.374(3)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.396(3)
C(23)-H(23A)	0.9300

C(24)-C(25)	1.368(3)
C(24)-H(24A)	0.9300
C(25)-C(26)	1.394(2)
C(25)-H(25A)	0.9300
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-C(29)	1.492(2)
C(30)-C(31)	1.525(3)
C(30)-C(32)	1.528(3)
C(30)-H(30A)	0.9800
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-C(35)	1.520(3)
C(33)-C(34)	1.521(3)
C(33)-H(33A)	0.9800
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700

C(20)-P(1)-C(8)	106.79(7)
C(20)-P(1)-C(14)	103.43(7)
C(8)-P(1)-C(14)	105.96(8)
C(20)-P(1)-Pd(1)	108.25(5)
C(8)-P(1)-Pd(1)	112.10(5)
C(14)-P(1)-Pd(1)	119.37(6)
C(29)-O(1)-Pd(1)	128.93(10)
C(1)-Pd(1)-O(1)	172.07(6)
C(1)-Pd(1)-P(1)	92.81(5)

O(1)-Pd(1)-P(1)	93.48(3)
C(1)-Pd(1)-Cl(1)	88.16(5)
O(1)-Pd(1)-Cl(1)	85.32(3)
P(1)-Pd(1)-Cl(1)	177.002(17)
C(28)-N(1)-C(26)	108.14(13)
C(28)-N(1)-C(27)	126.79(14)
C(26)-N(1)-C(27)	123.81(14)
C(29)-N(2)-C(30)	124.84(14)
C(29)-N(2)-C(33)	119.06(14)
C(30)-N(2)-C(33)	115.90(13)
C(6)-C(1)-C(2)	119.12(18)
C(6)-C(1)-Pd(1)	121.04(15)
C(2)-C(1)-Pd(1)	119.46(15)
C(3)-C(2)-C(1)	120.9(2)
C(3)-C(2)-H(2A)	119.6
C(1)-C(2)-H(2A)	119.6
C(4)-C(3)-C(2)	119.6(2)
C(4)-C(3)-H(3A)	120.2
C(2)-C(3)-H(3A)	120.2
C(5)-C(4)-C(3)	120.3(2)
C(5)-C(4)-H(4A)	119.9
C(3)-C(4)-H(4A)	119.9
C(4)-C(5)-C(6)	121.7(2)
C(4)-C(5)-H(5A)	119.1
C(6)-C(5)-H(5A)	119.1
C(1)-C(6)-C(5)	118.3(2)
C(1)-C(6)-C(7)	122.48(19)
C(5)-C(6)-C(7)	119.1(2)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(9)-C(8)-C(13)	110.86(15)
C(9)-C(8)-P(1)	114.35(12)
C(13)-C(8)-P(1)	109.20(11)
C(9)-C(8)-H(8A)	107.4

C(13)-C(8)-H(8A)	107.4
P(1)-C(8)-H(8A)	107.4
C(8)-C(9)-C(10)	111.26(16)
C(8)-C(9)-H(9A)	109.4
C(10)-C(9)-H(9A)	109.4
C(8)-C(9)-H(9B)	109.4
C(10)-C(9)-H(9B)	109.4
H(9A)-C(9)-H(9B)	108.0
C(11)-C(10)-C(9)	111.86(18)
C(11)-C(10)-H(10A)	109.2
C(9)-C(10)-H(10A)	109.2
C(11)-C(10)-H(10B)	109.2
C(9)-C(10)-H(10B)	109.2
H(10A)-C(10)-H(10B)	107.9
C(12)-C(11)-C(10)	111.07(18)
C(12)-C(11)-H(11A)	109.4
C(10)-C(11)-H(11A)	109.4
C(12)-C(11)-H(11B)	109.4
C(10)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-C(13)	111.28(17)
C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12B)	109.4
C(13)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-C(8)	111.82(15)
C(12)-C(13)-H(13A)	109.3
C(8)-C(13)-H(13A)	109.3
C(12)-C(13)-H(13B)	109.3
C(8)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	107.9
C(19)-C(14)-C(15)	111.25(16)
C(19)-C(14)-P(1)	109.91(13)
C(15)-C(14)-P(1)	114.41(12)
C(19)-C(14)-H(14A)	107.0
C(15)-C(14)-H(14A)	107.0
P(1)-C(14)-H(14A)	107.0

C(16)-C(15)-C(14)	110.42(17)
C(16)-C(15)-H(15A)	109.6
C(14)-C(15)-H(15A)	109.6
C(16)-C(15)-H(15B)	109.6
C(14)-C(15)-H(15B)	109.6
H(15A)-C(15)-H(15B)	108.1
C(17)-C(16)-C(15)	111.6(2)
C(17)-C(16)-H(16A)	109.3
C(15)-C(16)-H(16A)	109.3
C(17)-C(16)-H(16B)	109.3
C(15)-C(16)-H(16B)	109.3
H(16A)-C(16)-H(16B)	108.0
C(16)-C(17)-C(18)	111.3(2)
C(16)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
C(17)-C(18)-C(19)	110.8(2)
C(17)-C(18)-H(18A)	109.5
C(19)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
C(19)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	108.1
C(14)-C(19)-C(18)	111.3(2)
C(14)-C(19)-H(19A)	109.4
C(18)-C(19)-H(19A)	109.4
C(14)-C(19)-H(19B)	109.4
C(18)-C(19)-H(19B)	109.4
H(19A)-C(19)-H(19B)	108.0
C(28)-C(20)-C(21)	105.18(13)
C(28)-C(20)-P(1)	123.30(12)
C(21)-C(20)-P(1)	130.18(12)
C(22)-C(21)-C(26)	117.16(15)
C(22)-C(21)-C(20)	136.09(16)
C(26)-C(21)-C(20)	106.70(14)
C(23)-C(22)-C(21)	119.48(19)
C(23)-C(22)-H(22A)	120.3

C(21)-C(22)-H(22A)	120.3
C(22)-C(23)-C(24)	121.60(19)
C(22)-C(23)-H(23A)	119.2
C(24)-C(23)-H(23A)	119.2
C(25)-C(24)-C(23)	120.83(18)
C(25)-C(24)-H(24A)	119.6
C(23)-C(24)-H(24A)	119.6
C(24)-C(25)-C(26)	117.41(19)
C(24)-C(25)-H(25A)	121.3
C(26)-C(25)-H(25A)	121.3
N(1)-C(26)-C(25)	127.76(16)
N(1)-C(26)-C(21)	108.89(14)
C(25)-C(26)-C(21)	123.35(16)
N(1)-C(27)-H(27A)	109.5
N(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(1)-C(28)-C(20)	110.86(14)
N(1)-C(28)-C(29)	122.87(14)
C(20)-C(28)-C(29)	126.24(14)
O(1)-C(29)-N(2)	120.20(14)
O(1)-C(29)-C(28)	117.99(14)
N(2)-C(29)-C(28)	121.80(14)
N(2)-C(30)-C(31)	111.22(16)
N(2)-C(30)-C(32)	111.69(16)
C(31)-C(30)-C(32)	110.88(17)
N(2)-C(30)-H(30A)	107.6
C(31)-C(30)-H(30A)	107.6
C(32)-C(30)-H(30A)	107.6
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5

C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(2)-C(33)-C(35)	111.81(15)
N(2)-C(33)-C(34)	113.06(15)
C(35)-C(33)-C(34)	112.16(18)
N(2)-C(33)-H(33A)	106.4
C(35)-C(33)-H(33A)	106.4
C(34)-C(33)-H(33A)	106.4
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
Cl(3)-C(36)-Cl(2)	115.4(2)
Cl(3)-C(36)-H(36A)	108.4
Cl(2)-C(36)-H(36A)	108.4
Cl(3)-C(36)-H(36B)	108.4
Cl(2)-C(36)-H(36B)	108.4
H(36A)-C(36)-H(36B)	107.5

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters (A^2 x 10^3) for SCM2105.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
P(1)	25(1)	26(1)	28(1)	2(1)	3(1)	8(1)
O(1)	27(1)	33(1)	53(1)	-4(1)	4(1)	12(1)
Pd(1)	26(1)	32(1)	29(1)	1(1)	5(1)	12(1)
Cl(1)	45(1)	50(1)	49(1)	-13(1)	1(1)	27(1)
Cl(2)	133(1)	112(1)	115(1)	22(1)	62(1)	16(1)
Cl(3)	221(2)	91(1)	154(1)	31(1)	54(1)	80(1)
N(1)	33(1)	30(1)	31(1)	4(1)	0(1)	12(1)
N(2)	30(1)	27(1)	36(1)	5(1)	7(1)	11(1)
C(1)	30(1)	37(1)	46(1)	-3(1)	1(1)	15(1)
C(2)	48(1)	43(1)	49(1)	-3(1)	-5(1)	21(1)
C(3)	67(2)	60(1)	63(1)	-13(1)	-24(1)	33(1)
C(4)	40(1)	66(2)	104(2)	-21(2)	-15(1)	23(1)
C(5)	34(1)	61(1)	101(2)	-13(1)	11(1)	14(1)
C(6)	35(1)	48(1)	69(1)	-3(1)	14(1)	14(1)
C(7)	62(2)	84(2)	72(2)	11(1)	35(1)	24(1)
C(8)	32(1)	32(1)	28(1)	2(1)	4(1)	11(1)
C(9)	53(1)	39(1)	40(1)	2(1)	14(1)	21(1)
C(10)	71(1)	60(1)	41(1)	1(1)	19(1)	33(1)
C(11)	64(1)	73(2)	47(1)	18(1)	27(1)	28(1)
C(12)	60(1)	49(1)	45(1)	17(1)	18(1)	17(1)
C(13)	47(1)	34(1)	38(1)	6(1)	10(1)	10(1)
C(14)	31(1)	29(1)	43(1)	6(1)	4(1)	6(1)
C(15)	36(1)	36(1)	54(1)	3(1)	-4(1)	5(1)
C(16)	45(1)	40(1)	91(2)	6(1)	-8(1)	-3(1)
C(17)	55(2)	68(2)	117(3)	31(2)	16(2)	-14(1)
C(18)	75(2)	64(2)	83(2)	39(1)	19(2)	0(1)
C(19)	50(1)	51(1)	49(1)	18(1)	11(1)	7(1)
C(20)	28(1)	27(1)	31(1)	3(1)	4(1)	10(1)

C(21)	33(1)	29(1)	36(1)	5(1)	7(1)	13(1)
C(22)	46(1)	32(1)	53(1)	-1(1)	2(1)	16(1)
C(23)	61(1)	32(1)	73(2)	4(1)	7(1)	23(1)
C(24)	59(1)	43(1)	69(1)	17(1)	5(1)	30(1)
C(25)	45(1)	44(1)	47(1)	14(1)	3(1)	21(1)
C(26)	34(1)	32(1)	35(1)	8(1)	7(1)	14(1)
C(27)	46(1)	43(1)	36(1)	1(1)	-7(1)	12(1)
C(28)	28(1)	28(1)	29(1)	4(1)	5(1)	11(1)
C(29)	28(1)	27(1)	27(1)	0(1)	2(1)	10(1)
C(30)	32(1)	39(1)	51(1)	8(1)	16(1)	14(1)
C(31)	59(1)	63(1)	58(1)	6(1)	31(1)	16(1)
C(32)	32(1)	66(1)	68(1)	8(1)	7(1)	14(1)
C(33)	41(1)	26(1)	47(1)	8(1)	7(1)	11(1)
C(34)	81(2)	47(1)	56(1)	19(1)	-1(1)	29(1)
C(35)	76(2)	36(1)	59(1)	-6(1)	6(1)	24(1)
C(36)	136(3)	90(2)	72(2)	18(2)	20(2)	16(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for SCM2105.

	x	y	z	U(eq)
H(2A)	9056	7276	4095	57
H(3A)	11210	7856	4865	78
H(4A)	12898	8581	4030	88
H(5A)	12463	8668	2440	81
H(7A)	9382	7999	1002	106
H(7B)	10347	7353	905	106
H(7C)	10883	8666	1044	106
H(8A)	7653	8426	4376	37
H(9A)	5383	8987	3940	51
H(9B)	6793	9846	4359	51
H(10A)	6753	9080	5794	65
H(10B)	5487	9384	5571	65
H(11A)	4972	7590	6072	70
H(11B)	4216	7524	5043	70
H(12A)	5105	6122	5054	61
H(12B)	6510	6998	5462	61
H(13A)	5121	6864	3611	48
H(13B)	6389	6564	3836	48
H(14A)	7780	10348	2898	43
H(15A)	9244	10121	4137	55
H(15B)	9971	9697	3407	55
H(16A)	9913	11894	3630	78
H(16B)	11162	11587	3932	78
H(17A)	11237	11109	2358	106
H(17B)	11256	12340	2493	106
H(18A)	9758	11315	1117	95
H(18B)	9029	11740	1843	95
H(19A)	7799	9863	1308	62
H(19B)	9032	9525	1583	62

H(22A)	6190	10762	2657	53
H(23A)	5153	11835	1910	65
H(24A)	3562	11097	572	65
H(25A)	2879	9221	2	53
H(27A)	2101	6970	12	66
H(27B)	3070	6326	-69	66
H(27C)	3238	7400	-581	66
H(30A)	2413	6435	1689	47
H(31A)	2835	6033	3244	89
H(31B)	1958	4771	2934	89
H(31C)	1318	5692	2914	89
H(32A)	1306	4902	456	84
H(32B)	382	5152	1113	84
H(32C)	858	4144	1255	84
H(33A)	2613	3853	1761	46
H(34A)	4317	4598	3089	91
H(34B)	5321	4540	2423	91
H(34C)	4241	3437	2606	91
H(35A)	3187	3957	220	85
H(35B)	3485	3011	741	85
H(35C)	4629	4133	684	85
H(36A)	8249	4999	3232	126
H(36B)	9486	4931	3869	126

Table S7. Torsion angles [deg] for SCM2105.

C(29)-O(1)-Pd(1)-C(1)	137.1(4)
C(29)-O(1)-Pd(1)-P(1)	-5.40(15)
C(29)-O(1)-Pd(1)-Cl(1)	171.84(15)
C(20)-P(1)-Pd(1)-C(1)	162.47(8)
C(8)-P(1)-Pd(1)-C(1)	-80.01(8)
C(14)-P(1)-Pd(1)-C(1)	44.68(9)
C(20)-P(1)-Pd(1)-O(1)	-22.36(7)
C(8)-P(1)-Pd(1)-O(1)	95.17(7)
C(14)-P(1)-Pd(1)-O(1)	-140.14(8)
C(20)-P(1)-Pd(1)-Cl(1)	-88.7(3)
C(8)-P(1)-Pd(1)-Cl(1)	28.8(3)
C(14)-P(1)-Pd(1)-Cl(1)	153.5(3)
O(1)-Pd(1)-C(1)-C(6)	105.8(5)
P(1)-Pd(1)-C(1)-C(6)	-111.65(15)
Cl(1)-Pd(1)-C(1)-C(6)	71.19(15)
O(1)-Pd(1)-C(1)-C(2)	-67.1(5)
P(1)-Pd(1)-C(1)-C(2)	75.40(14)
Cl(1)-Pd(1)-C(1)-C(2)	-101.76(14)
C(6)-C(1)-C(2)-C(3)	1.2(3)
Pd(1)-C(1)-C(2)-C(3)	174.24(16)
C(1)-C(2)-C(3)-C(4)	1.0(3)
C(2)-C(3)-C(4)-C(5)	-1.5(4)
C(3)-C(4)-C(5)-C(6)	-0.2(4)
C(2)-C(1)-C(6)-C(5)	-2.7(3)
Pd(1)-C(1)-C(6)-C(5)	-175.68(16)
C(2)-C(1)-C(6)-C(7)	175.3(2)
Pd(1)-C(1)-C(6)-C(7)	2.4(3)
C(4)-C(5)-C(6)-C(1)	2.3(4)
C(4)-C(5)-C(6)-C(7)	-175.8(2)
C(20)-P(1)-C(8)-C(9)	-49.83(14)
C(14)-P(1)-C(8)-C(9)	59.96(14)
Pd(1)-P(1)-C(8)-C(9)	-168.22(11)
C(20)-P(1)-C(8)-C(13)	75.03(13)
C(14)-P(1)-C(8)-C(13)	-175.18(12)

Pd(1)-P(1)-C(8)-C(13)	-43.37(13)
C(13)-C(8)-C(9)-C(10)	53.8(2)
P(1)-C(8)-C(9)-C(10)	177.81(14)
C(8)-C(9)-C(10)-C(11)	-54.9(2)
C(9)-C(10)-C(11)-C(12)	55.7(3)
C(10)-C(11)-C(12)-C(13)	-55.7(3)
C(11)-C(12)-C(13)-C(8)	55.6(2)
C(9)-C(8)-C(13)-C(12)	-54.5(2)
P(1)-C(8)-C(13)-C(12)	178.63(14)
C(20)-P(1)-C(14)-C(19)	-69.54(15)
C(8)-P(1)-C(14)-C(19)	178.30(13)
Pd(1)-P(1)-C(14)-C(19)	50.71(15)
C(20)-P(1)-C(14)-C(15)	164.47(14)
C(8)-P(1)-C(14)-C(15)	52.31(16)
Pd(1)-P(1)-C(14)-C(15)	-75.28(15)
C(19)-C(14)-C(15)-C(16)	55.0(2)
P(1)-C(14)-C(15)-C(16)	-179.74(17)
C(14)-C(15)-C(16)-C(17)	-56.5(3)
C(15)-C(16)-C(17)-C(18)	57.3(3)
C(16)-C(17)-C(18)-C(19)	-56.1(4)
C(15)-C(14)-C(19)-C(18)	-54.7(3)
P(1)-C(14)-C(19)-C(18)	177.53(18)
C(17)-C(18)-C(19)-C(14)	54.8(3)
C(8)-P(1)-C(20)-C(28)	-101.01(14)
C(14)-P(1)-C(20)-C(28)	147.44(14)
Pd(1)-P(1)-C(20)-C(28)	19.87(15)
C(8)-P(1)-C(20)-C(21)	94.26(16)
C(14)-P(1)-C(20)-C(21)	-17.29(17)
Pd(1)-P(1)-C(20)-C(21)	-144.85(14)
C(28)-C(20)-C(21)-C(22)	172.4(2)
P(1)-C(20)-C(21)-C(22)	-20.7(3)
C(28)-C(20)-C(21)-C(26)	-4.80(18)
P(1)-C(20)-C(21)-C(26)	162.01(13)
C(26)-C(21)-C(22)-C(23)	-3.3(3)
C(20)-C(21)-C(22)-C(23)	179.7(2)
C(21)-C(22)-C(23)-C(24)	-0.3(3)
C(22)-C(23)-C(24)-C(25)	2.4(4)
C(23)-C(24)-C(25)-C(26)	-0.8(3)

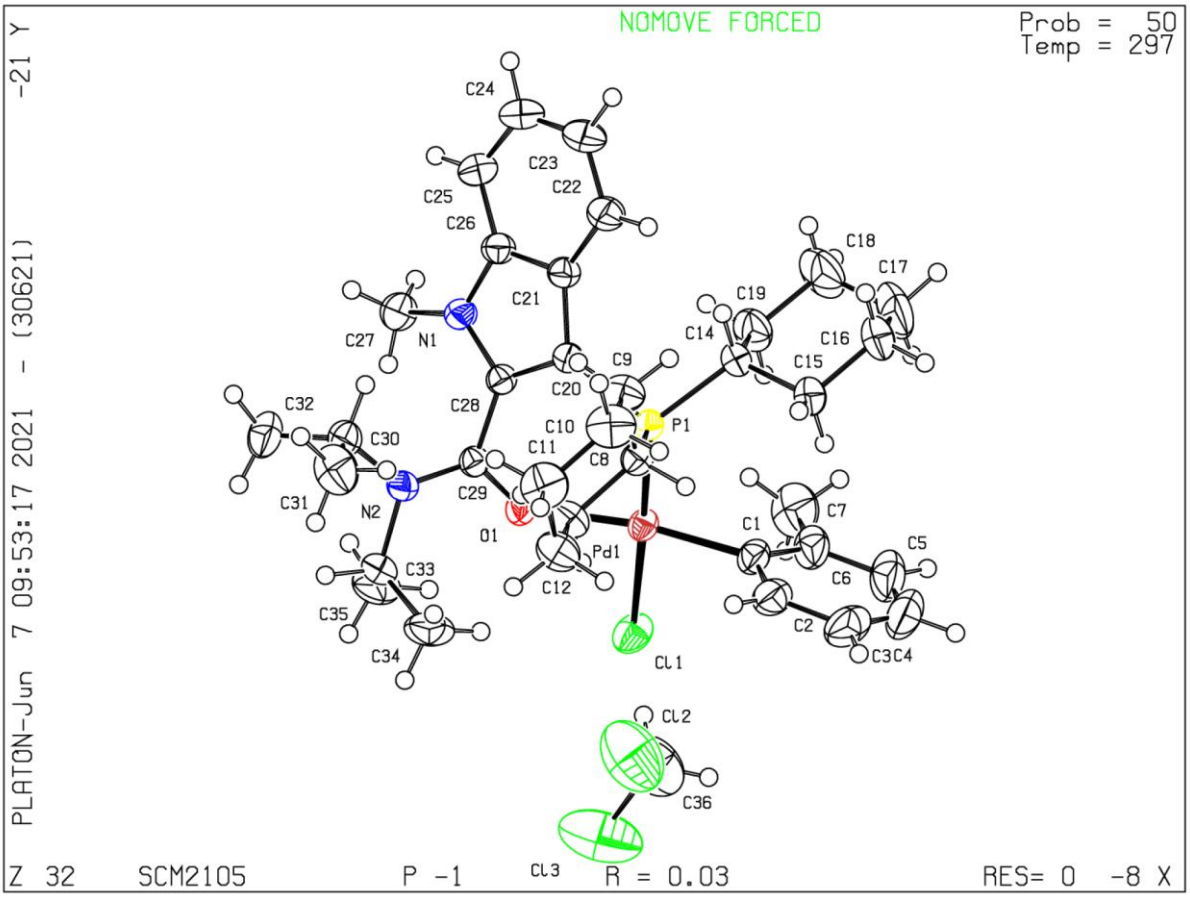
C(28)-N(1)-C(26)-C(25)	179.72(18)
C(27)-N(1)-C(26)-C(25)	11.8(3)
C(28)-N(1)-C(26)-C(21)	-1.08(19)
C(27)-N(1)-C(26)-C(21)	-169.03(16)
C(24)-C(25)-C(26)-N(1)	176.05(19)
C(24)-C(25)-C(26)-C(21)	-3.0(3)
C(22)-C(21)-C(26)-N(1)	-174.17(16)
C(20)-C(21)-C(26)-N(1)	3.68(19)
C(22)-C(21)-C(26)-C(25)	5.1(3)
C(20)-C(21)-C(26)-C(25)	-177.08(17)
C(26)-N(1)-C(28)-C(20)	-2.15(19)
C(27)-N(1)-C(28)-C(20)	165.34(16)
C(26)-N(1)-C(28)-C(29)	176.03(14)
C(27)-N(1)-C(28)-C(29)	-16.5(3)
C(21)-C(20)-C(28)-N(1)	4.31(18)
P(1)-C(20)-C(28)-N(1)	-163.65(12)
C(21)-C(20)-C(28)-C(29)	-173.78(15)
P(1)-C(20)-C(28)-C(29)	18.3(2)
Pd(1)-O(1)-C(29)-N(2)	-135.66(13)
Pd(1)-O(1)-C(29)-C(28)	43.2(2)
C(30)-N(2)-C(29)-O(1)	173.76(15)
C(33)-N(2)-C(29)-O(1)	-0.9(2)
C(30)-N(2)-C(29)-C(28)	-5.0(2)
C(33)-N(2)-C(29)-C(28)	-179.70(14)
N(1)-C(28)-C(29)-O(1)	126.73(17)
C(20)-C(28)-C(29)-O(1)	-55.4(2)
N(1)-C(28)-C(29)-N(2)	-54.4(2)
C(20)-C(28)-C(29)-N(2)	123.43(18)
C(29)-N(2)-C(30)-C(31)	-108.07(19)
C(33)-N(2)-C(30)-C(31)	66.7(2)
C(29)-N(2)-C(30)-C(32)	127.47(18)
C(33)-N(2)-C(30)-C(32)	-57.7(2)
C(29)-N(2)-C(33)-C(35)	-64.3(2)
C(30)-N(2)-C(33)-C(35)	120.59(18)
C(29)-N(2)-C(33)-C(34)	63.5(2)
C(30)-N(2)-C(33)-C(34)	-111.68(19)

Symmetry transformations used to generate equivalent atoms:

Table S8. Hydrogen bonds for SCM2105 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(27)-H(27B)...Cl(1)#1	0.96	2.74	3.4154(19)	127.8
C(30)-H(30A)...N(1)	0.98	2.42	3.155(2)	131.8
C(32)-H(32B)...Cl(1)#2	0.96	2.82	3.747(2)	162.9
C(34)-H(34B)...O(1)	0.96	2.41	2.919(3)	112.8
C(35)-H(35A)...Cl(1)#1	0.96	2.98	3.932(3)	170.4
C(35)-H(35C)...O(1)	0.96	2.43	2.927(3)	112.2
C(36)-H(36A)...Cl(1)	0.97	2.52	3.395(4)	150.1

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 x-1,y,z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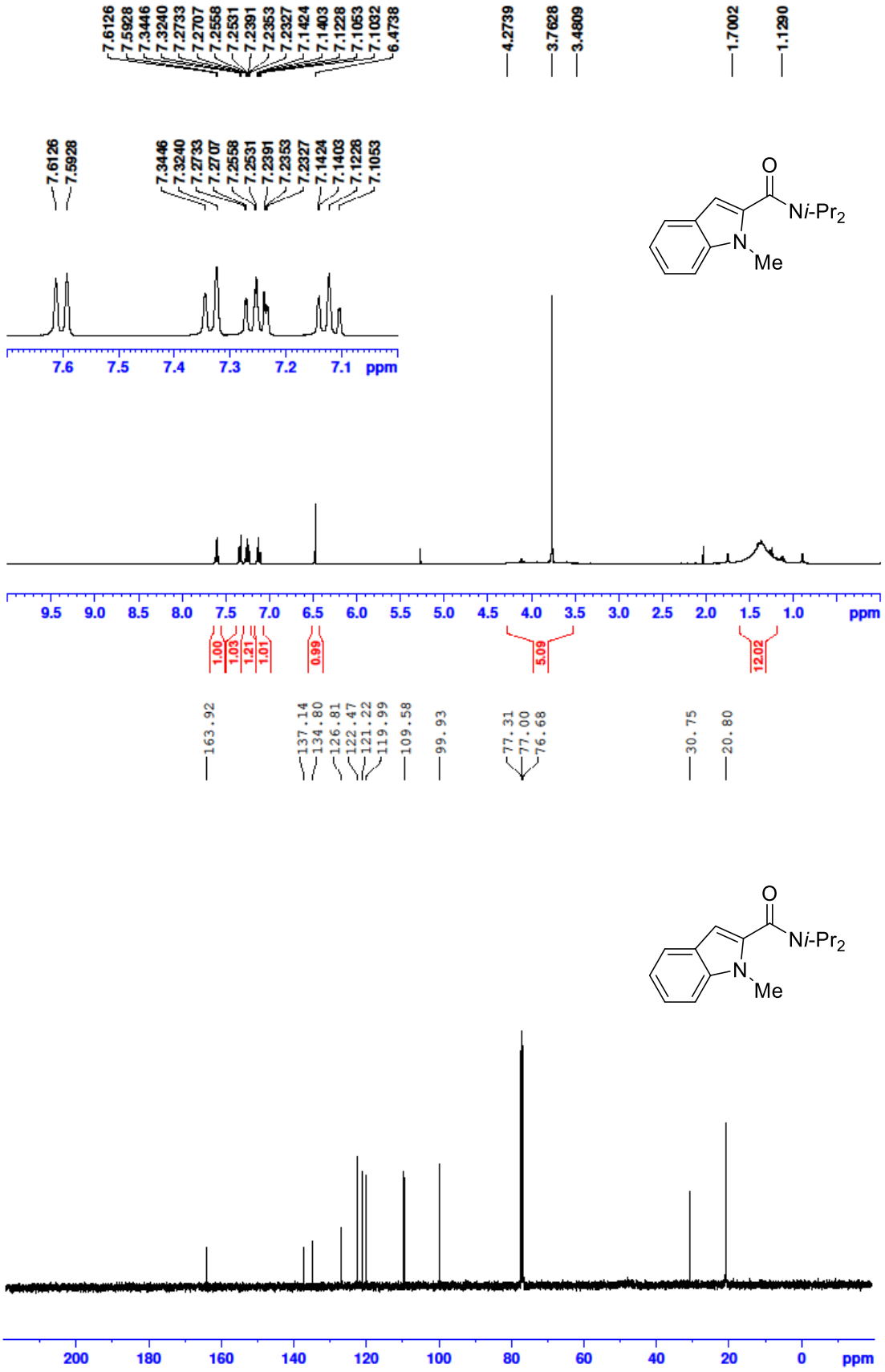
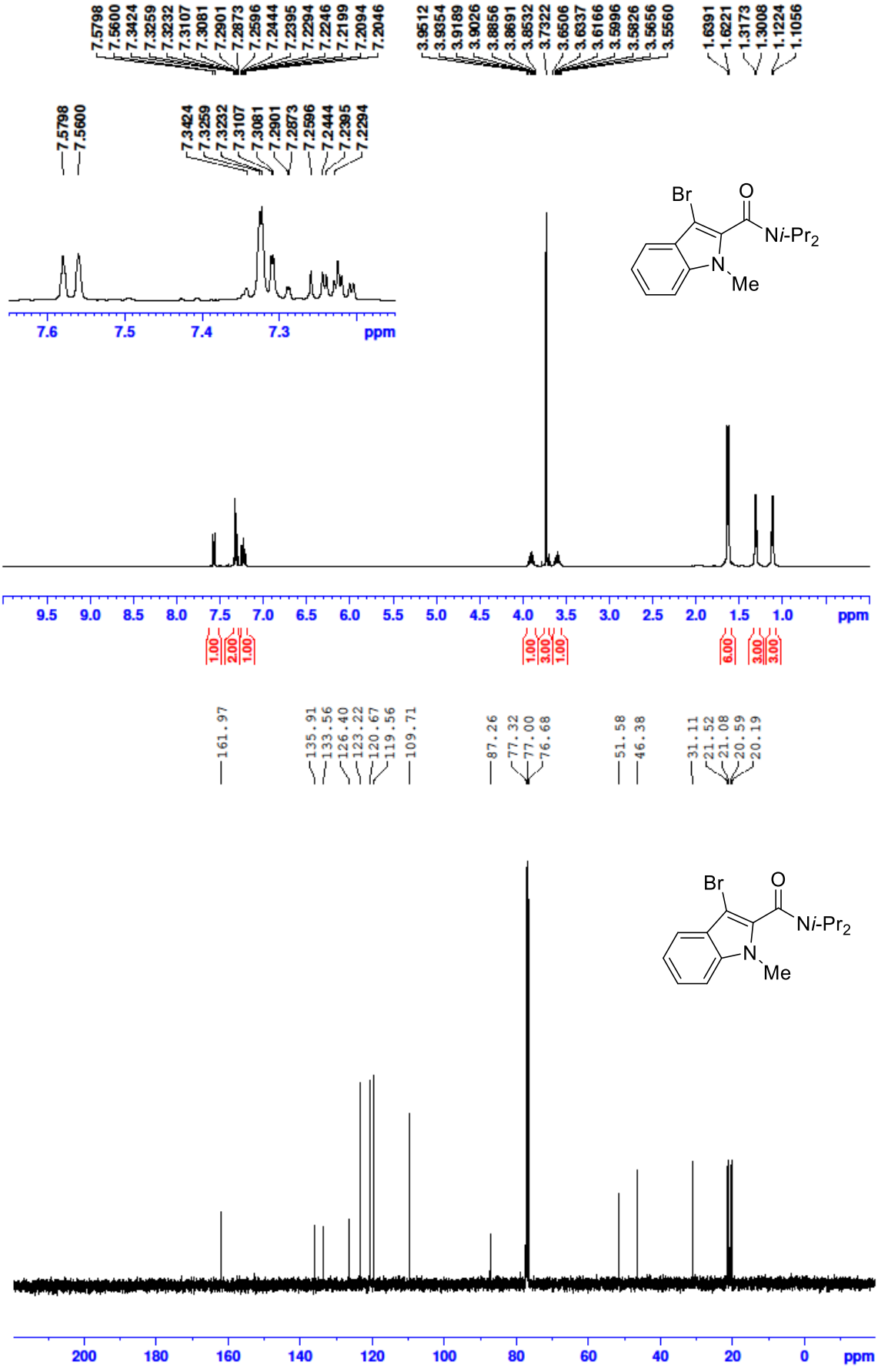
Prob = 50
Temp = 297
-21 Y
PLATON-Jun 7 09:53:17 2021 - (30621)
C24
C23
C22
C25
C26
C21
C27
N1
C18
C17
C19
C14
C16
C15
C9
C20
C28
C32
C30
C10
P1
C11
C8
C31
N2
C29
O1
Pd1
C12
C1
C7
C5
C6
C2
C3C4
C33
C35
C34
Cl1
Cl2
C36
Cl3
Z 32
SCM2105
P -1
R = 0.03
RES= 0 -8 X

9. ^{1}H, ^{13}C, ^{31}P, ^{19}F, NMR, MS, HRMS spectra

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7.3081
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7.2873
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7.2444
7.2395
7.2294
7.2246
7.2199
7.2094
7.2046
3.9512
3.9354
3.9189
3.9026
3.8856
3.8691
3.8532
3.7322
3.6506
3.6337
3.6166
3.5996
3.5826
3.5656
3.5560
1.6391
1.6221
1.3173
1.3008
1.1224
1.1056
Br
O
N*i*-Pr$_2$
N
Me
7.6
7.5
7.4
7.3
ppm
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
1.00
2.00
1.00
1.00
3.00
1.00
6.00
3.00
3.00
161.97
135.91
133.56
126.40
123.22
120.67
119.56
109.71
87.26
77.32
77.00
76.68
51.58
46.38
31.11
21.52
21.08
20.59
20.19
200
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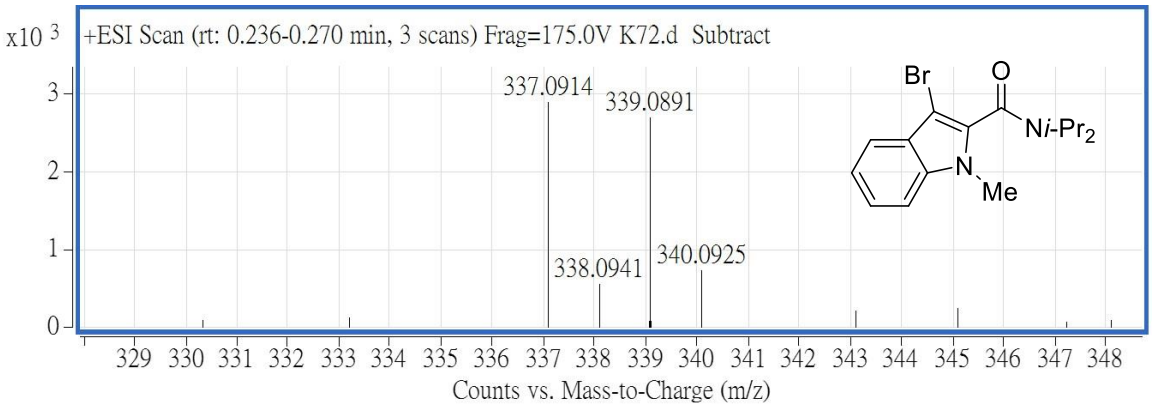
140
120
100
80
60
40
20
0
ppm



Mass	Calc. Mass	mDa	PPM	Formula
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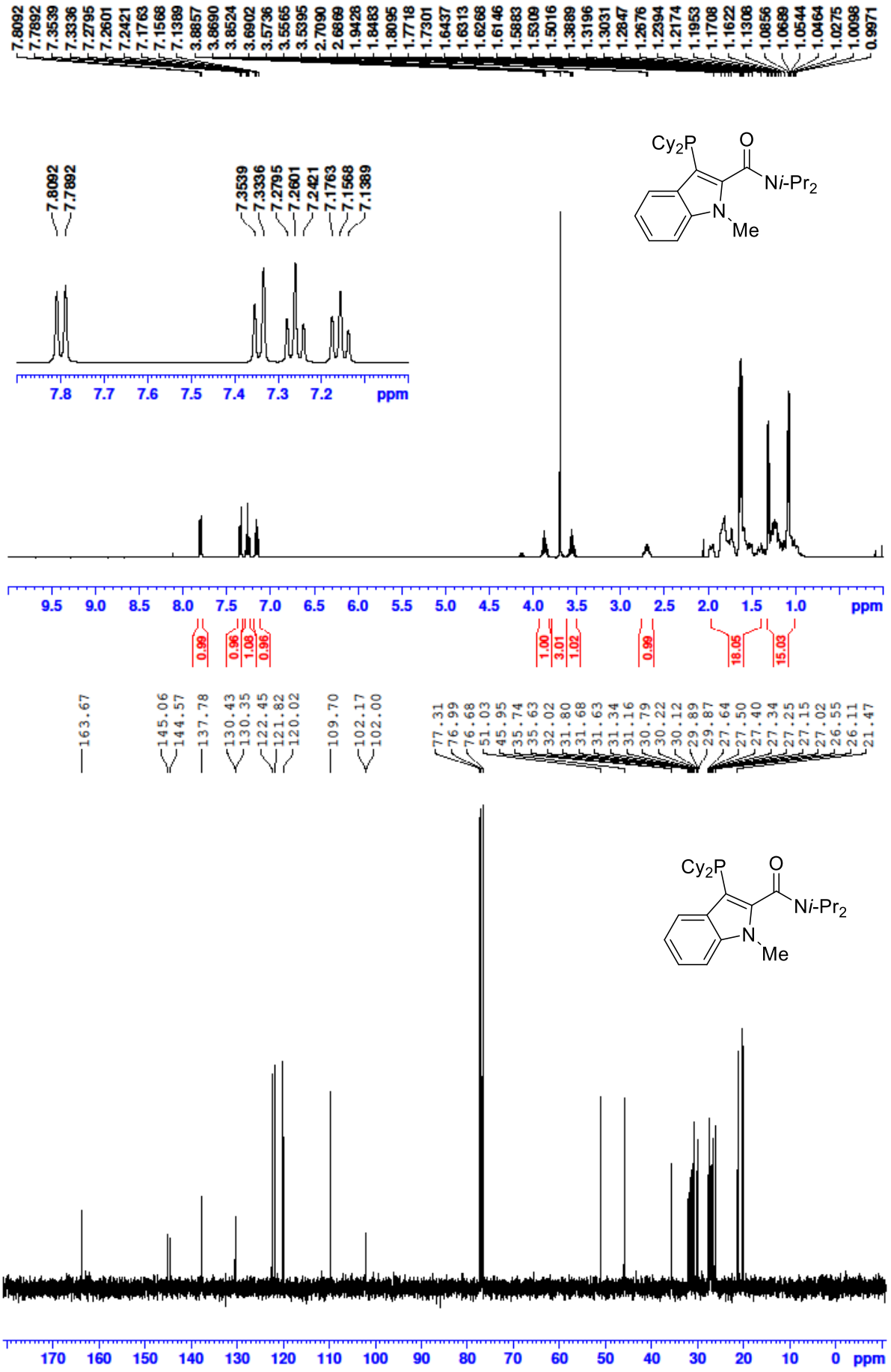
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7.3539
7.3336
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7.1568
7.1389
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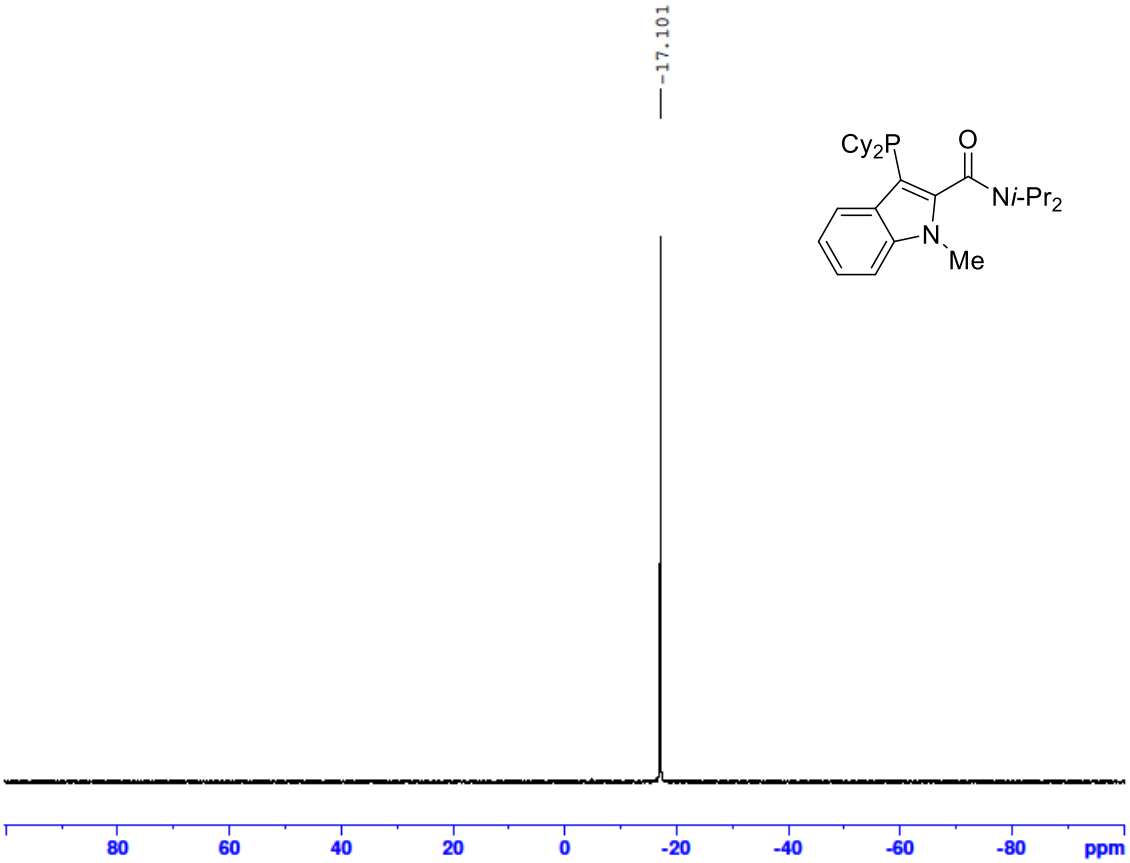
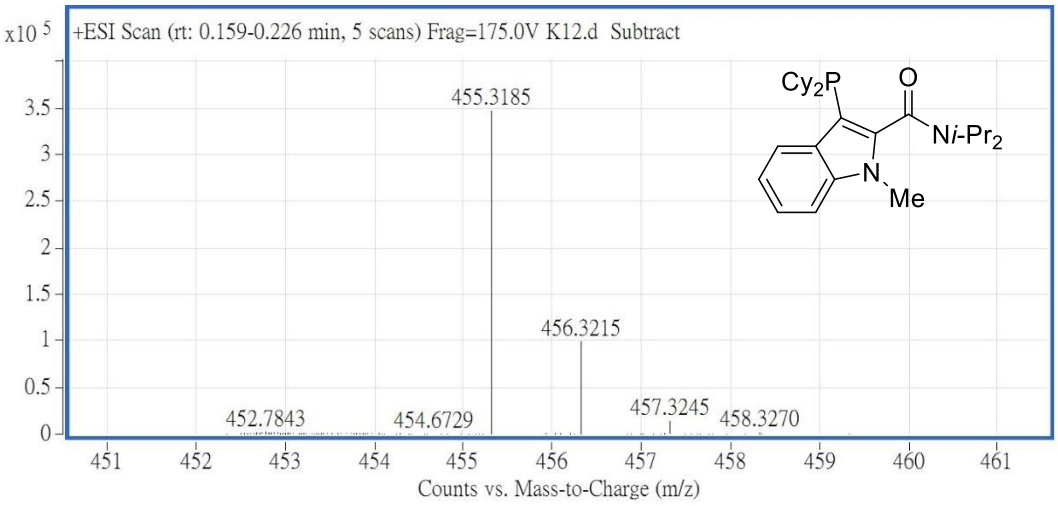
3.8524
3.6902
3.5736
3.5565
3.5395
2.7090
2.6869
1.9428
1.8483
1.8095
1.7718
1.7301
1.6437
1.6313
1.6268
1.6146
1.5883
1.5309
1.5016
1.3889
1.3196
1.3031
1.2847
1.2676
1.2394
1.2174
1.1953
1.1708
1.1622
1.1308
1.0856
1.0689
1.0544
1.0464
1.0275
1.0098
0.9971
Cy2P
O
N*i*-Pr2
N
Me
7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
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 ppm
0.99
0.96
1.08
0.96
1.00
3.01
1.02
0.99
18.05
15.03
163.67
145.06
144.57
137.78
130.43
130.35
122.45
121.82
120.02
109.70
102.17
102.00
77.31
76.99
76.68
51.03
45.95
35.74
35.63
32.02
31.80
31.68
31.63
31.34
31.16
30.79
30.22
30.12
29.89
29.87
27.64
27.50
27.40
27.34
27.25
27.15
27.02
26.55
26.11
21.47
Cy2P
O
N*i*-Pr2
N
Me
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm





Mass	Calc. Mass	mDa	PPM	Formula
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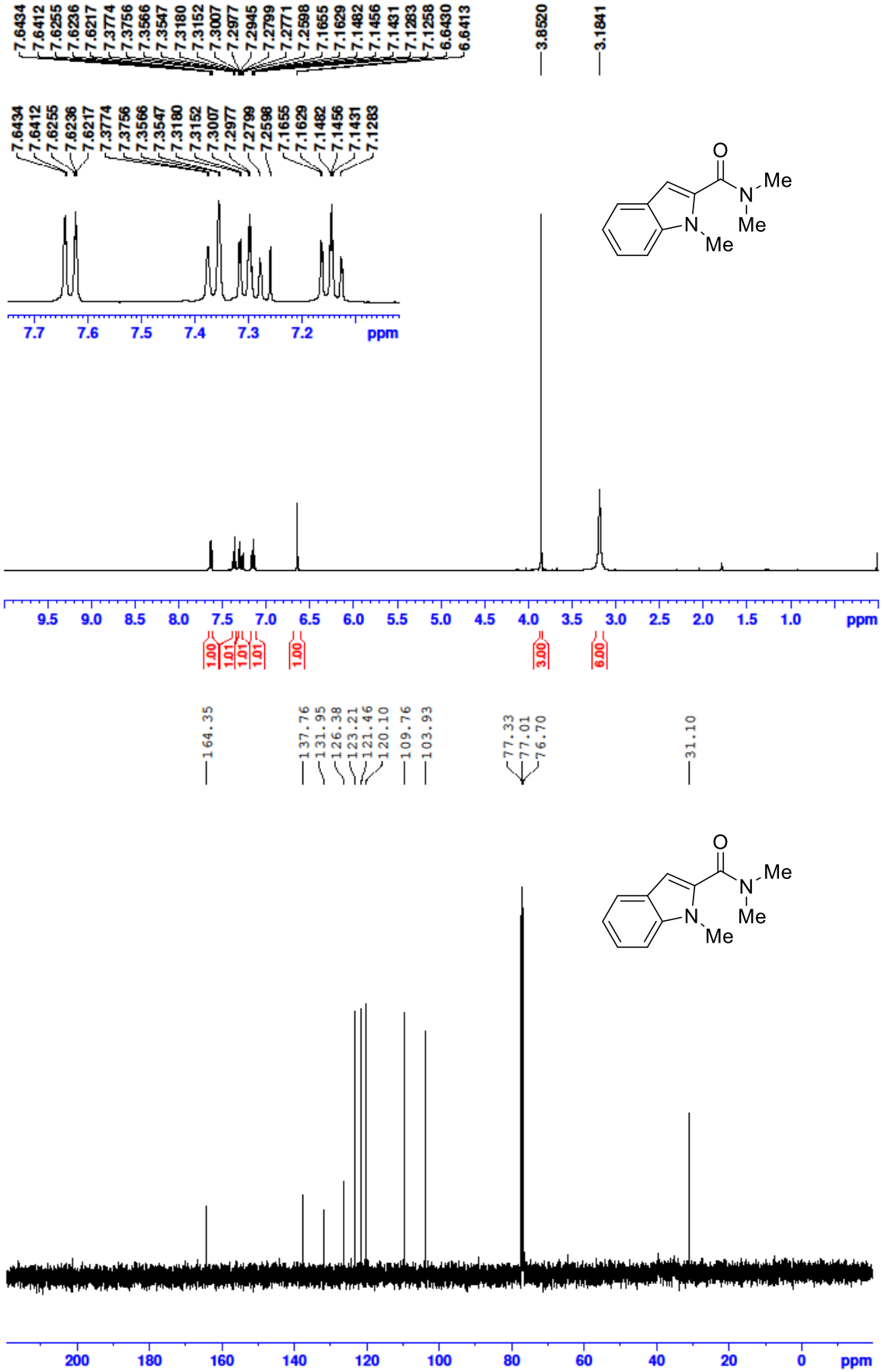
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7.6217
7.3774
7.3756
7.3566
7.3547
7.3180
7.3152
7.3007
7.2977
7.2945
7.2799
7.2771
7.2598
7.1655
7.1629
7.1482
7.1456
7.1431
7.1283
7.1258
6.6430
6.6413
3.8520
3.1841
O
N
Me
Me
N
Me
7.7
7.6
7.5
7.4
7.3
7.2
ppm
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9.0
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
ppm
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1.01
1.01
1.01
1.00
3.00
6.00
164.35
137.76
131.95
126.38
123.21
121.46
120.10
109.76
103.93
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200
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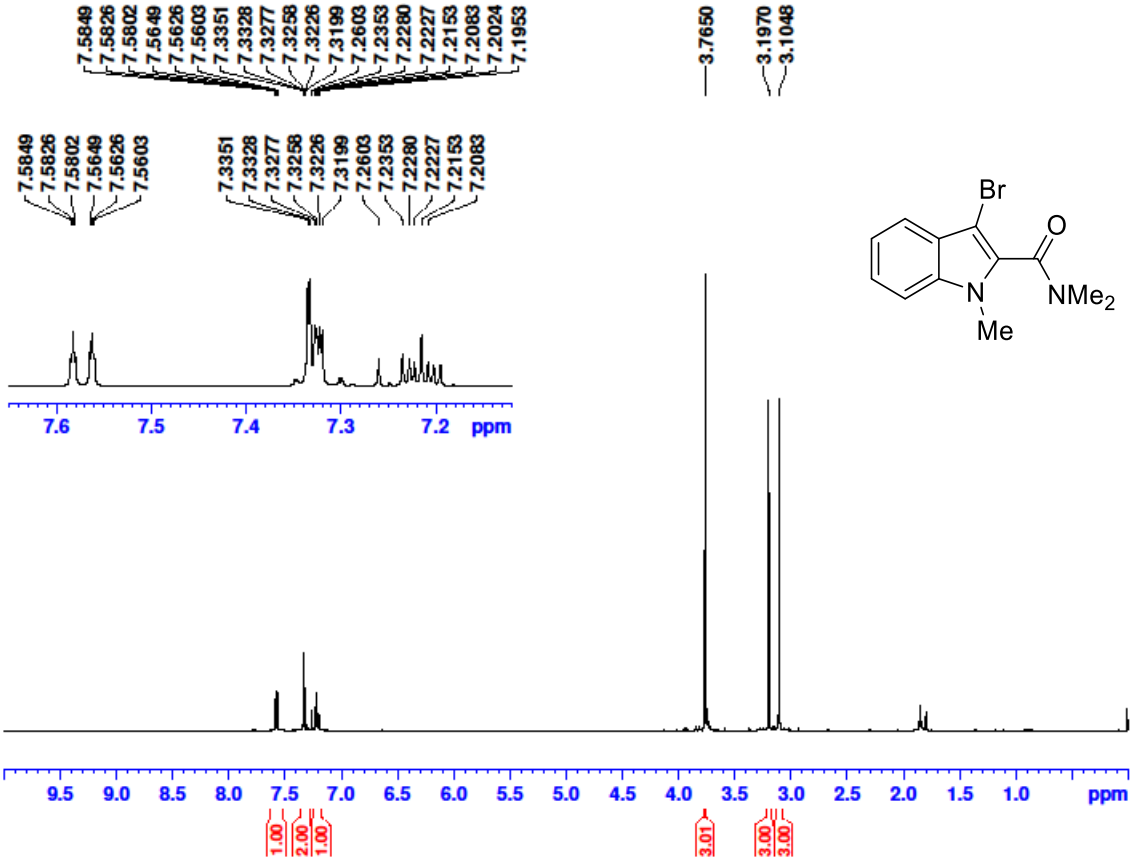
140
120
100
80
60
40
20
0
ppm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7.3226
7.3199
7.2603
7.2353
7.2280
7.2227
7.2153
7.2083
7.2024
7.1953
3.7650
3.1970
3.1048
Br
O
N
NMe2
Me
7.6
7.5
7.4
7.3
7.2
ppm
9.5
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8.5
8.0
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
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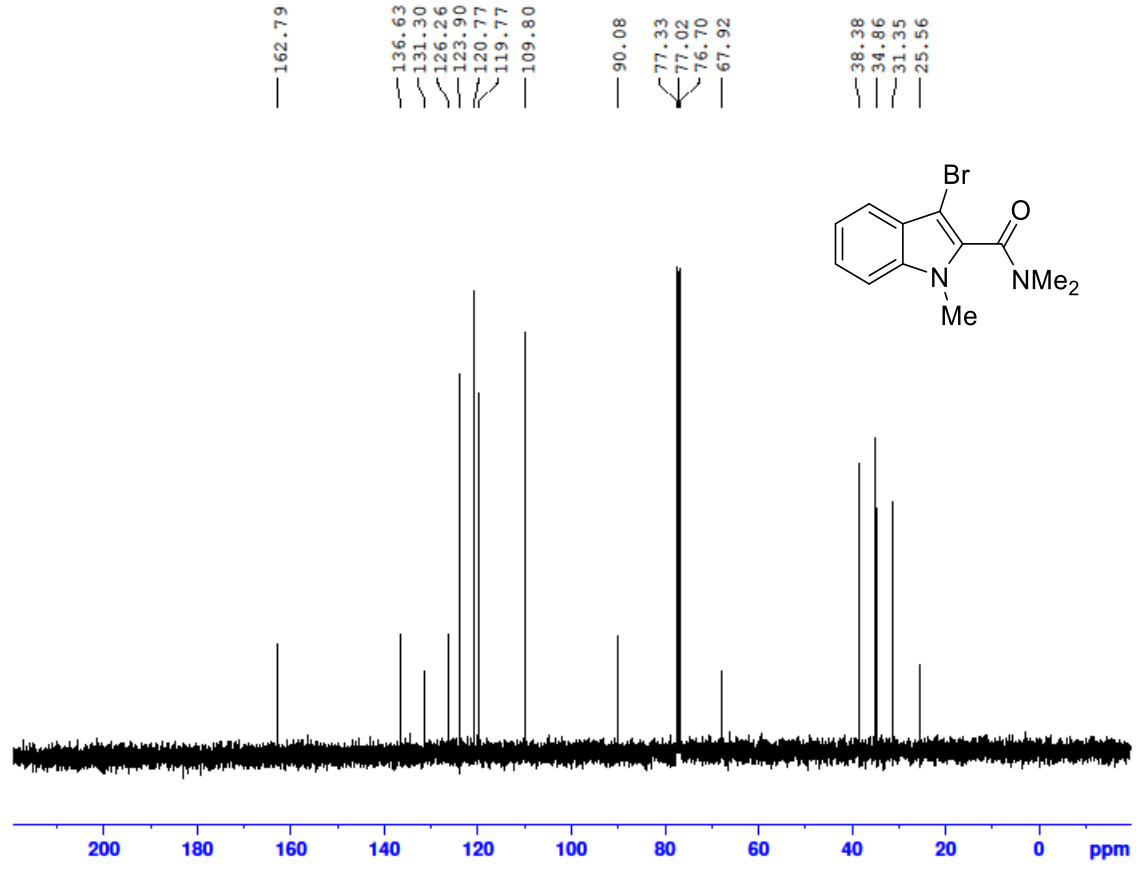
2.00
1.00
3.01
3.00
3.00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120.77
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90.08
77.33
77.02
76.70
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38.38
34.86
31.35
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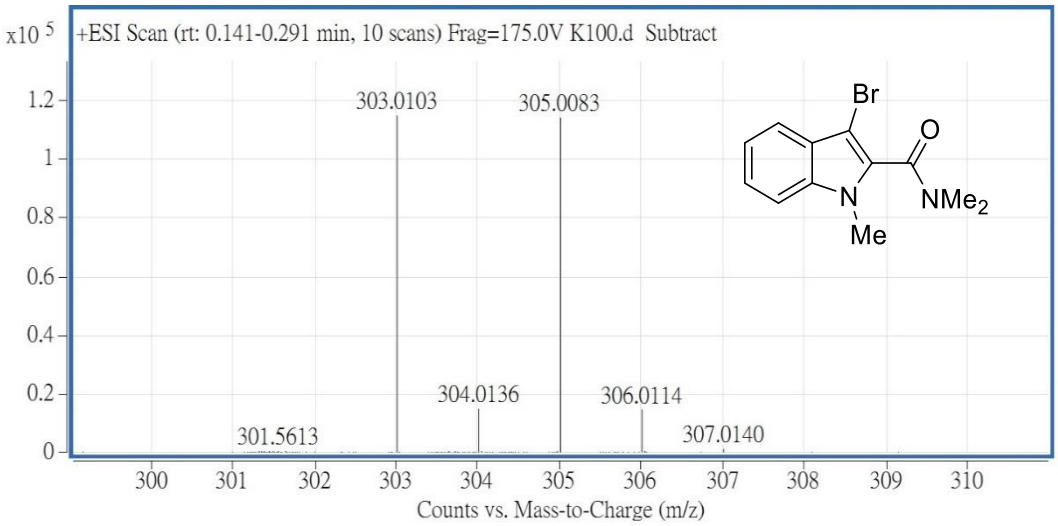
Br
O
N
NMe2
Me
200
180
160
140
120
100
80
60
40
20
0
ppm



Mass	Calc. Mass	mDa	PPM	Formula
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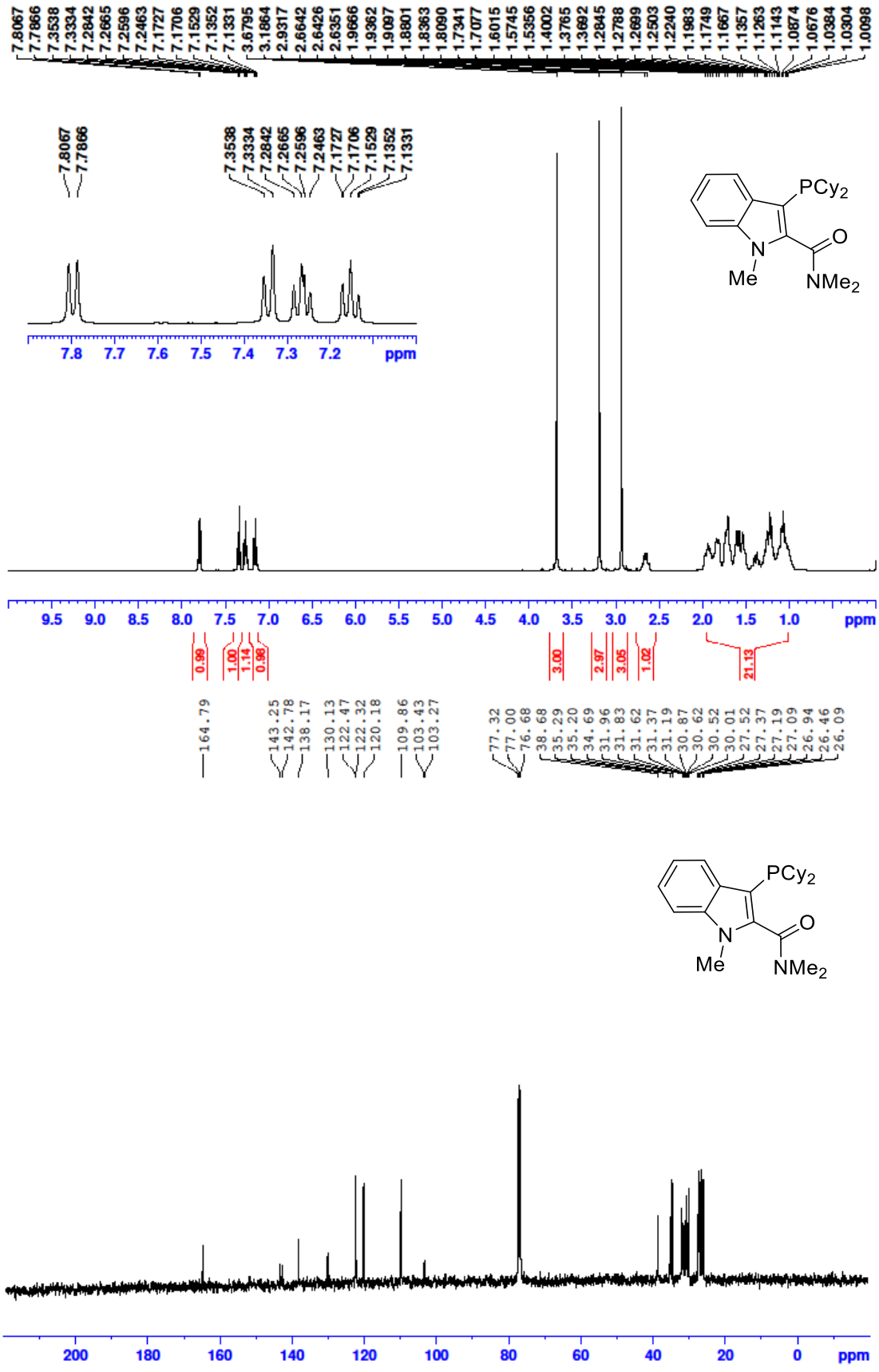
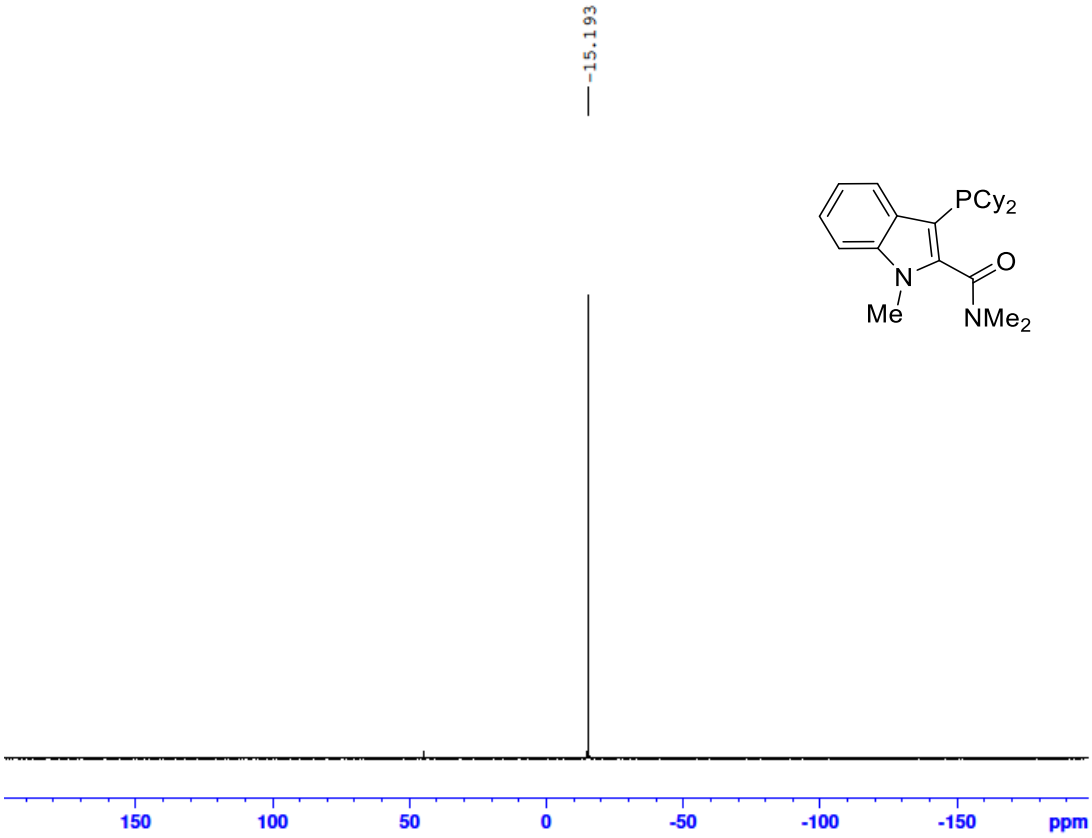
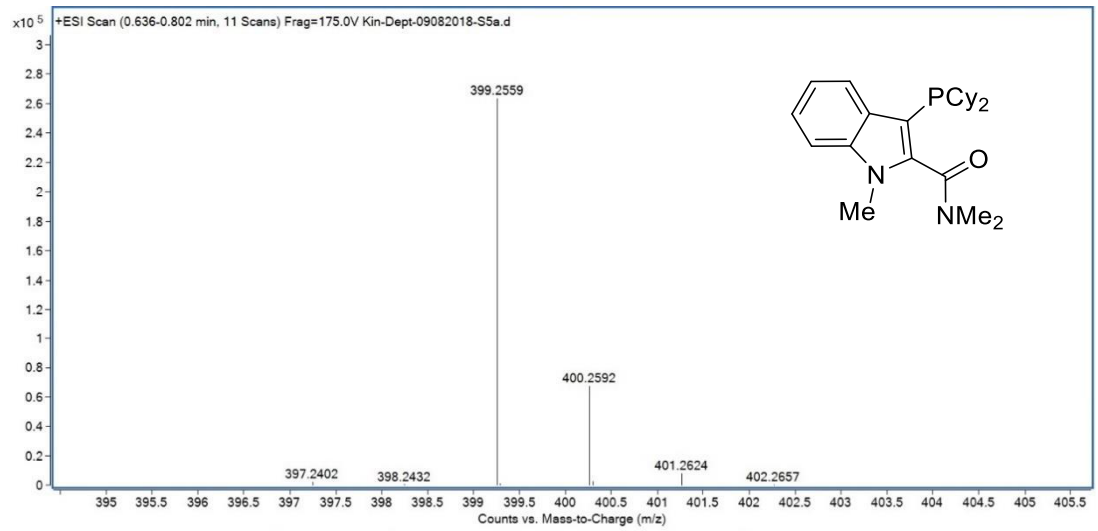

7.8067 7.7866 7.3538 7.3334 7.2842 7.2665 7.2596 7.2463 7.1727 7.1706 7.1529 7.1352 7.1331 3.6795 3.1864 2.9317 2.6642 2.6426 2.6351 1.9666 1.9362 1.9097 1.8801 1.8363 1.8090 1.7341 1.7077 1.6015 1.5745 1.5356 1.4002 1.3765 1.3692 1.2845 1.2788 1.2699 1.2503 1.2240 1.1983 1.1749 1.1667 1.1357 1.1263 1.1143 1.0874 1.0676 1.0384 1.0304 1.0098
PCy2
O
N
Me
NMe2
7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
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 ppm
0.99 1.00 1.14 0.98 3.00 2.97 3.05 1.02 21.13
164.79 143.25 142.78 138.17 130.13 122.47 122.32 120.18 109.86 103.43 103.27
77.32 77.00 76.68 38.68 35.29 35.20 34.69 31.96 31.83 31.62 31.37 31.19 30.87 30.62 30.52 30.01 27.52 27.37 27.19 27.09 26.94 26.46 26.09
PCy2
O
N
Me
NMe2
200 180 160 140 120 100 80 60 40 20 0 ppm





Mass	Calc. Mass	mDa	PPM	Formula
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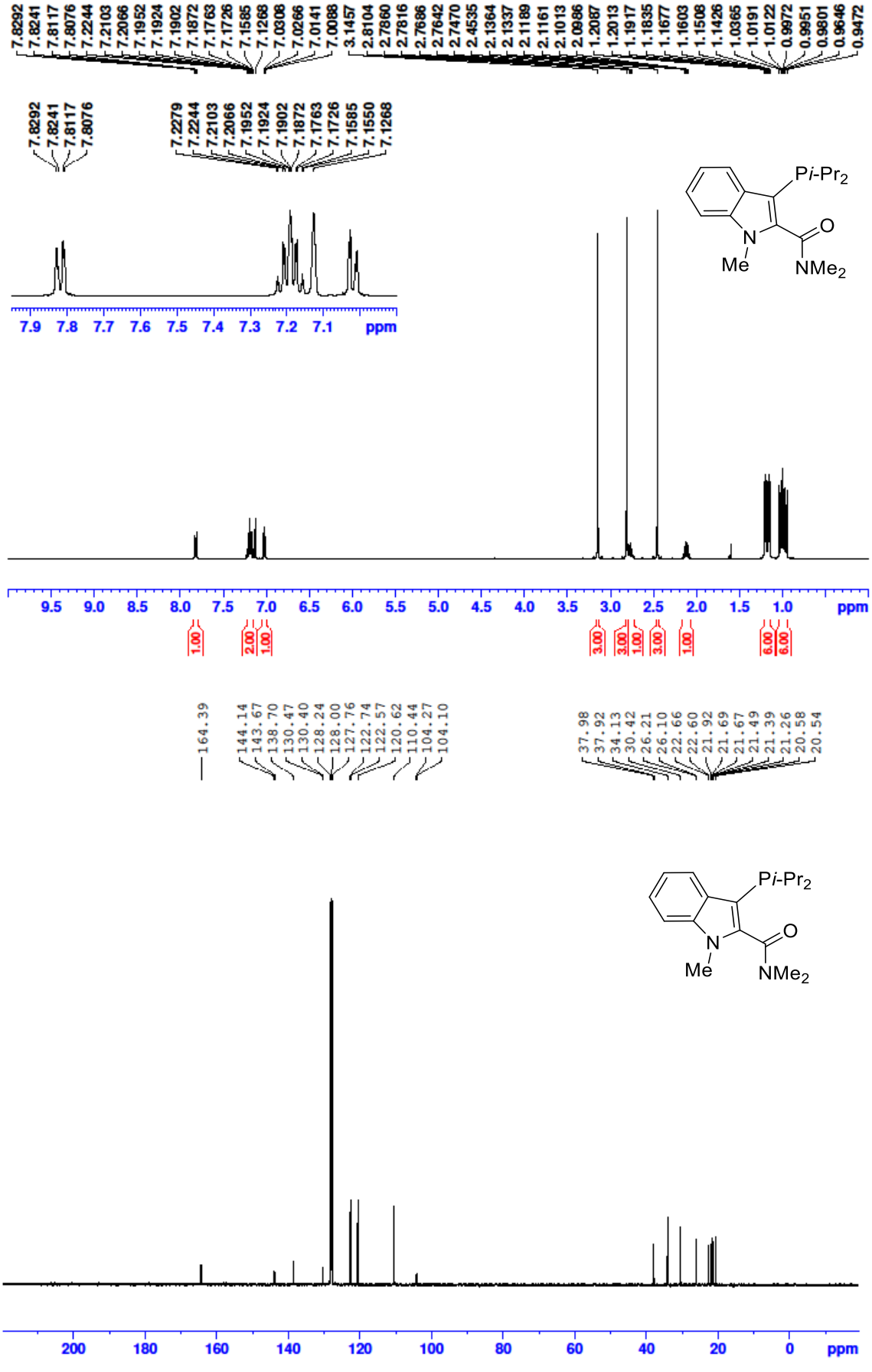
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7.1924
7.1902
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7.1763
7.1726
7.1585
7.1268
7.0308
7.0266
7.0141
7.0088
3.1457
2.8104
2.7860
2.7816
2.7686
2.7642
2.7470
2.4535
2.1364
2.1337
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2.1161
2.1013
2.0986
2.0867
1.2013
1.1917
1.1835
1.1677
1.1603
1.1508
1.1426
1.0365
1.0191
1.0122
0.9972
0.9951
0.9801
0.9646
0.9472
7.2279
7.2244
7.2103
7.2066
7.1952
7.1924
7.1902
7.1872
7.1763
7.1726
7.1585
7.1550
7.1268
P*i*-Pr2
N
Me
O
NMe2
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
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 ppm
1.00
2.00
1.00
3.00
3.00
1.00
3.00
1.00
6.00
6.00
164.39
144.14
143.67
138.70
130.47
130.40
128.24
128.00
127.76
122.74
122.57
120.62
110.44
104.27
104.10
37.98
37.92
34.13
30.42
26.21
26.10
22.66
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20.58
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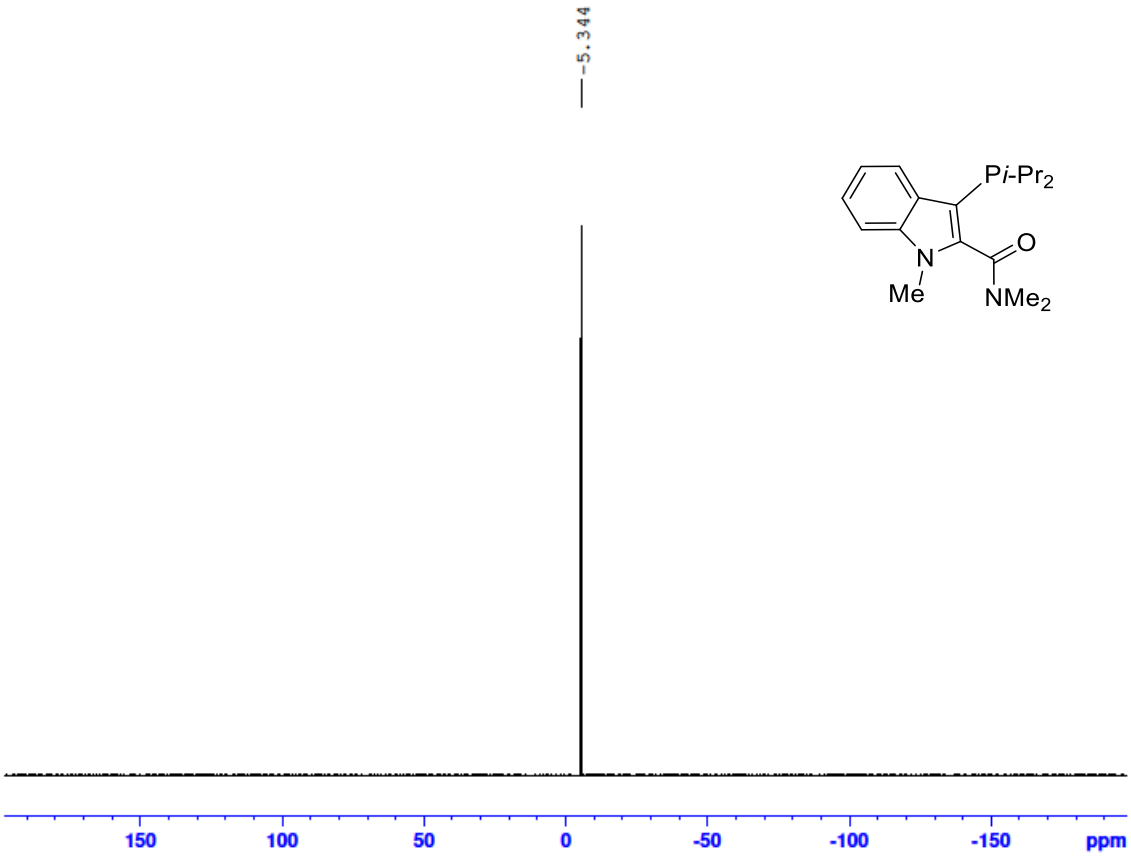

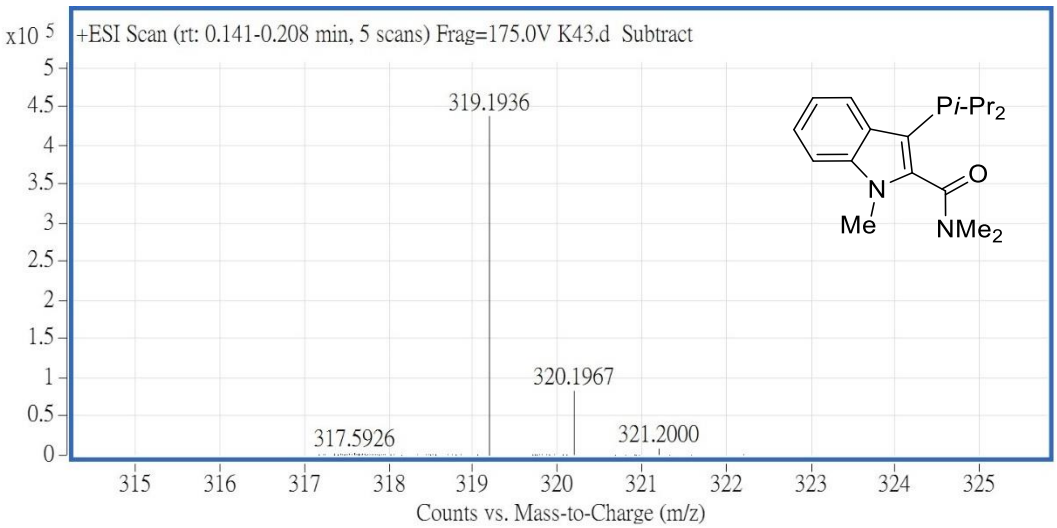

Mass	Calc. Mass	mDa	PPM	Formula
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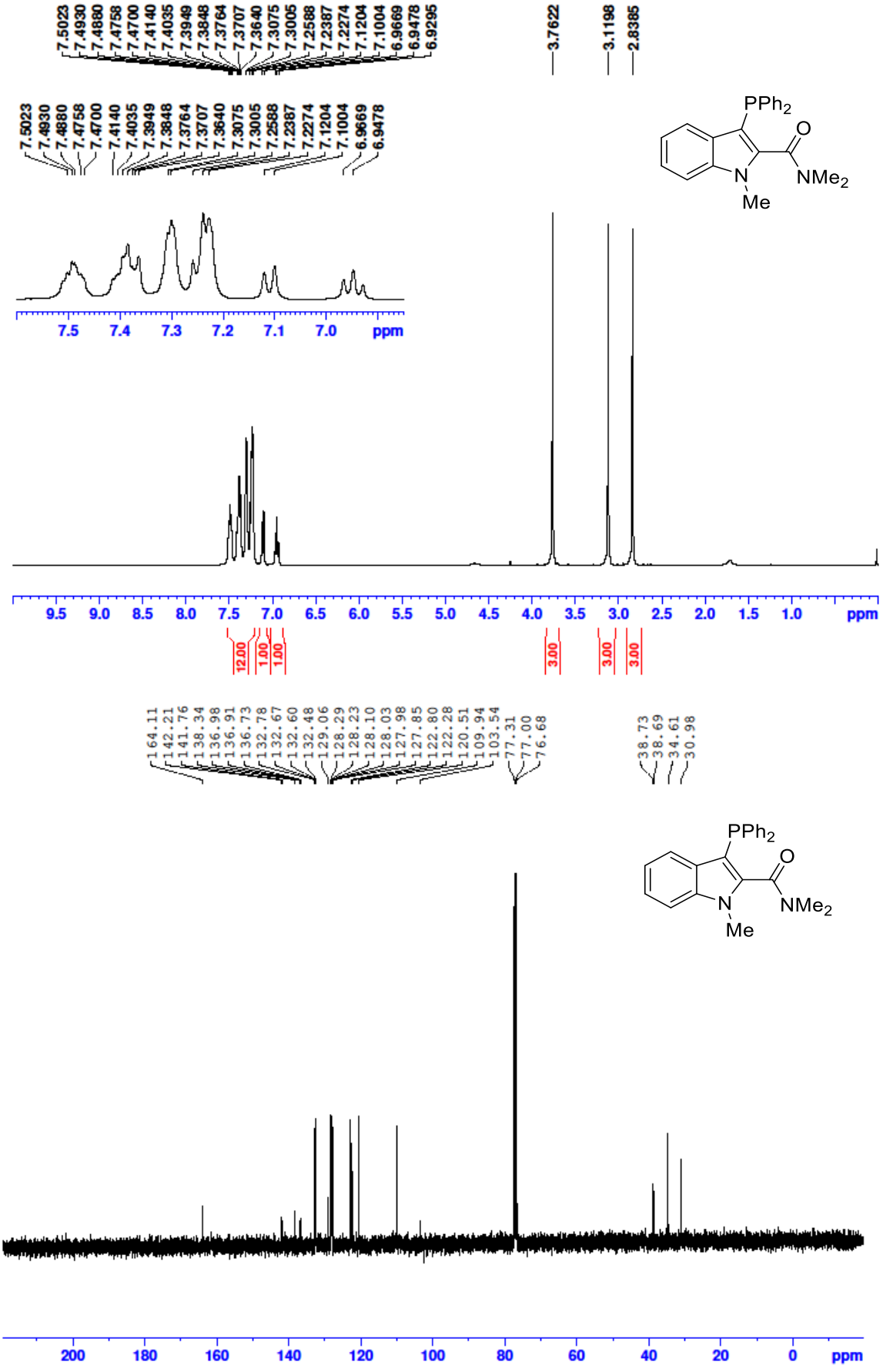
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7.2588
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7.1204
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6.9669
6.9478
6.9295
3.7622
3.1198
2.8385
PPh2
O
N
NMe2
Me
7.5 7.4 7.3 7.2 7.1 7.0 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
12.00
1.00
1.00
3.00
3.00
3.00
164.11
142.21
141.76
138.34
136.98
136.91
136.73
132.78
132.67
132.60
132.48
129.06
128.29
128.23
128.10
128.03
127.98
127.85
122.80
122.28
120.51
109.94
103.54
77.31
77.00
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38.69
34.61
30.98
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O
N
NMe2
Me
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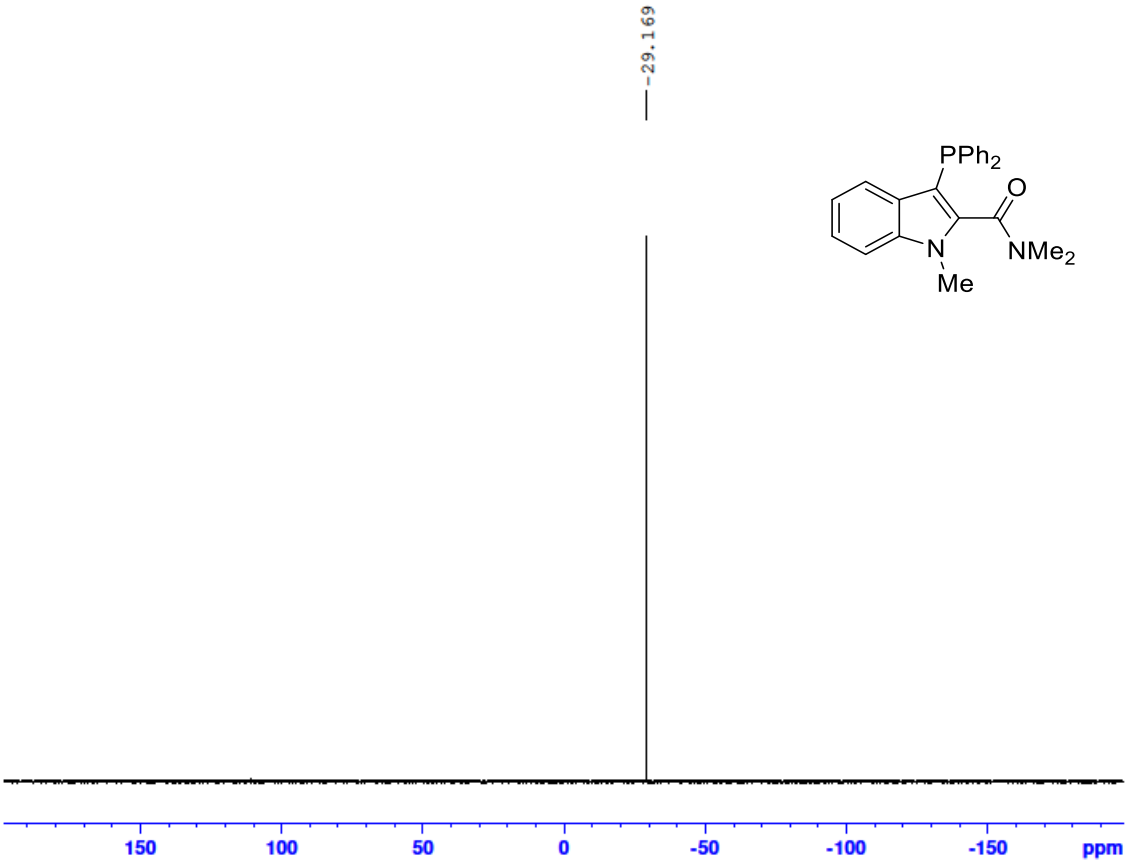

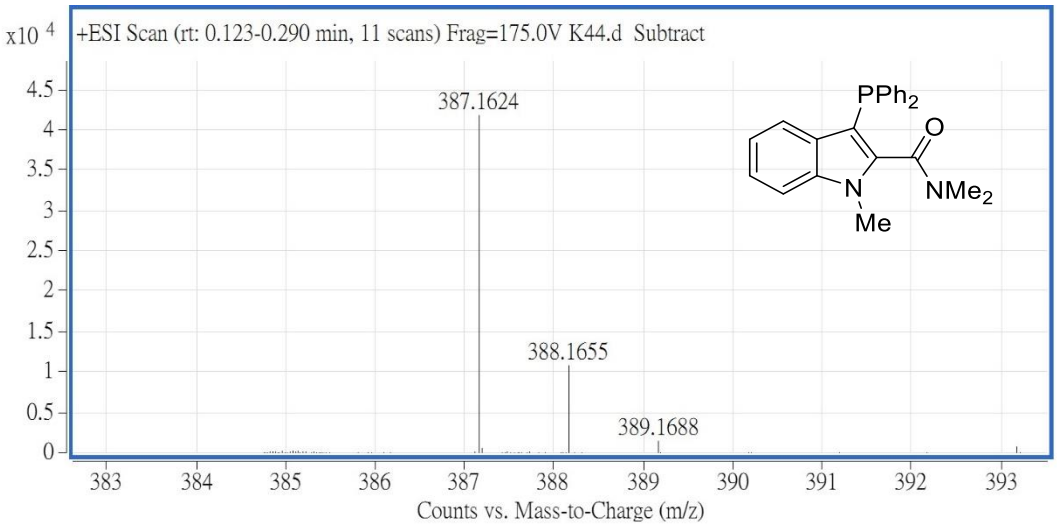

Mass	Calc. Mass	mDa	PPM	Formula
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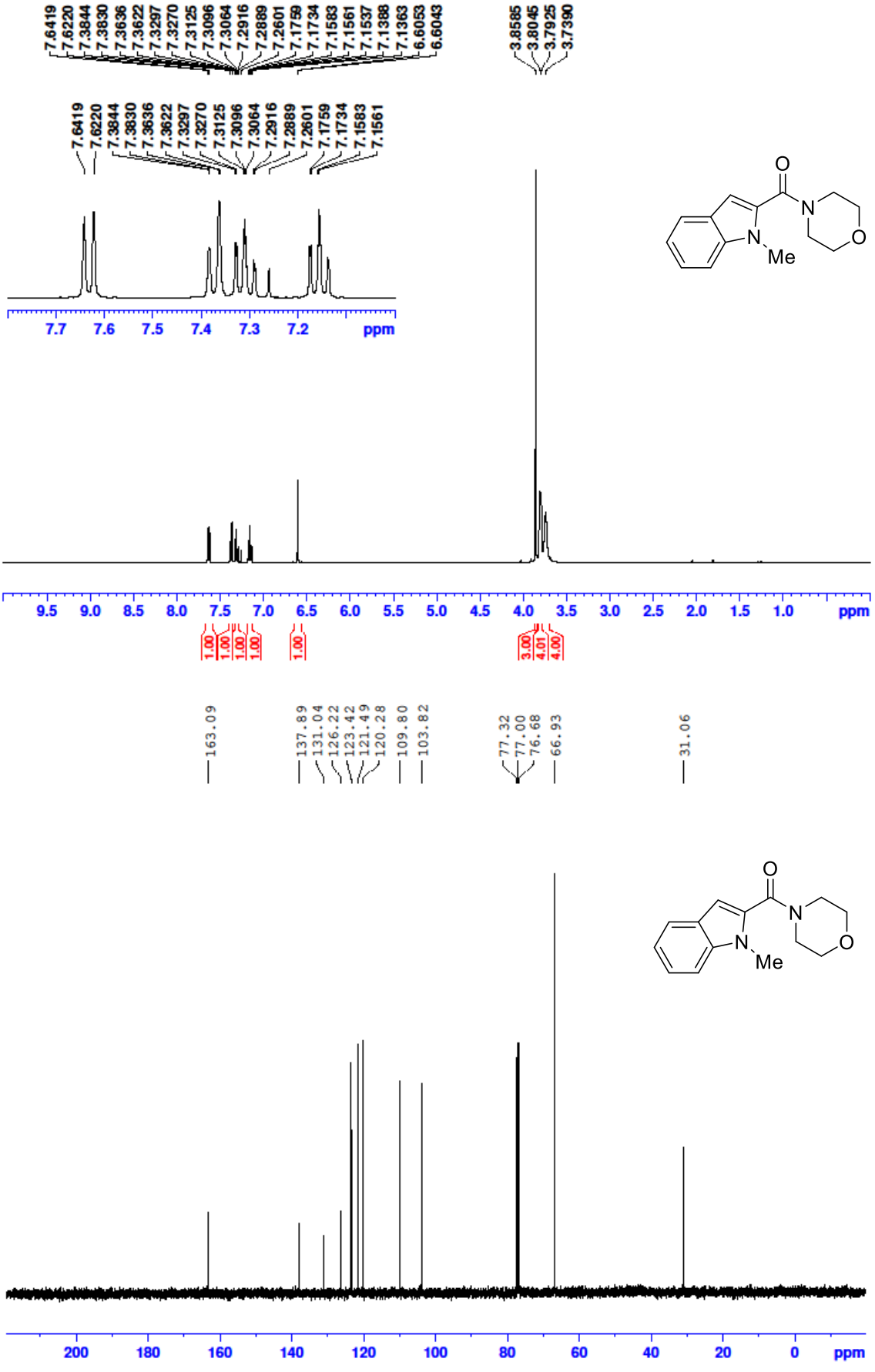
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7.3830
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7.2916
7.2889
7.2601
7.1759
7.1734
7.1583
7.1561
7.1537
7.1388
7.1363
6.6053
6.6043
3.8585
3.8045
3.7925
3.7390
7.7
7.6
7.5
7.4
7.3
7.2
ppm
O
N
N
Me
O
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.00
1.00
1.00
1.00
3.00
4.01
4.00
163.09
137.89
131.04
126.22
123.42
121.49
120.28
109.80
103.82
77.32
77.00
76.68
66.93
31.06
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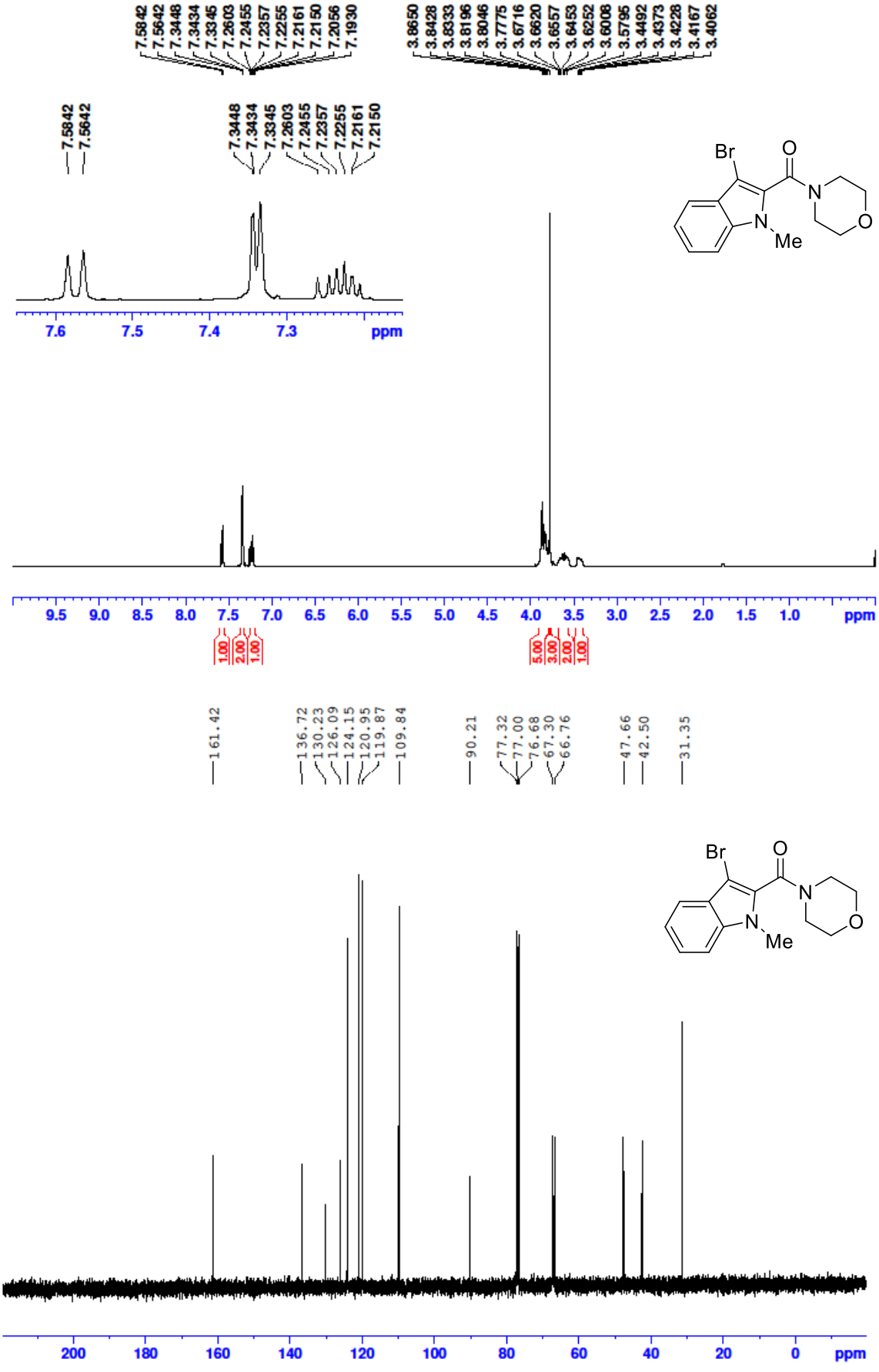
N
N
Me
O
200
180
160
140
120
100
80
60
40
20
0
ppm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7.2255
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7.2150
7.2056
7.1930
3.8650
3.8428
3.8333
3.8196
3.8046
3.7775
3.6716
3.6620
3.6557
3.6453
3.6252
3.6008
3.5795
3.4492
3.4373
3.4228
3.4167
3.4062
Br
O
N
N
Me
O
7.6
7.5
7.4
7.3
ppm
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
ppm
1.00
2.00
1.00
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2.00
1.00
161.42
136.72
130.23
126.09
124.15
120.95
119.87
109.84
90.21
77.32
77.00
76.68
67.30
66.76
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42.50
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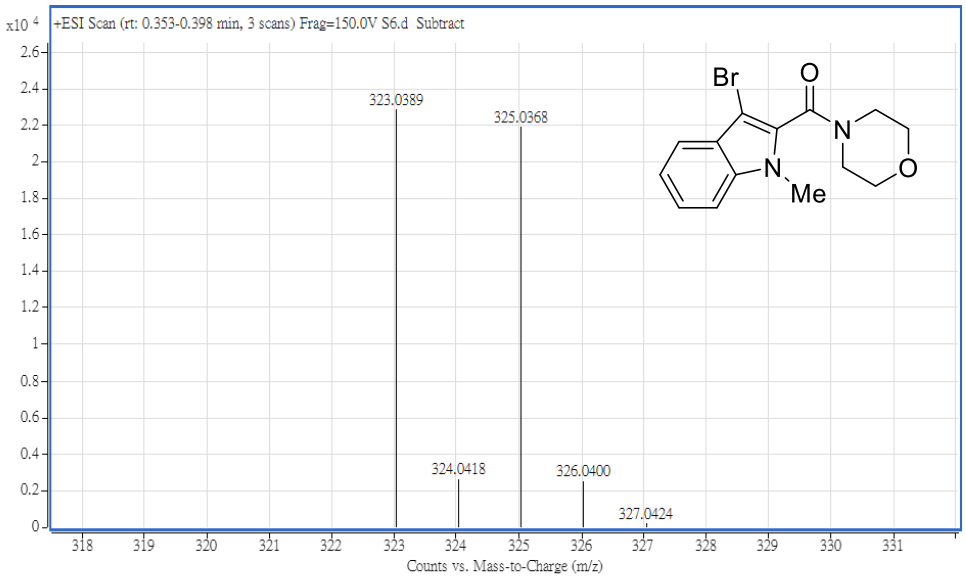
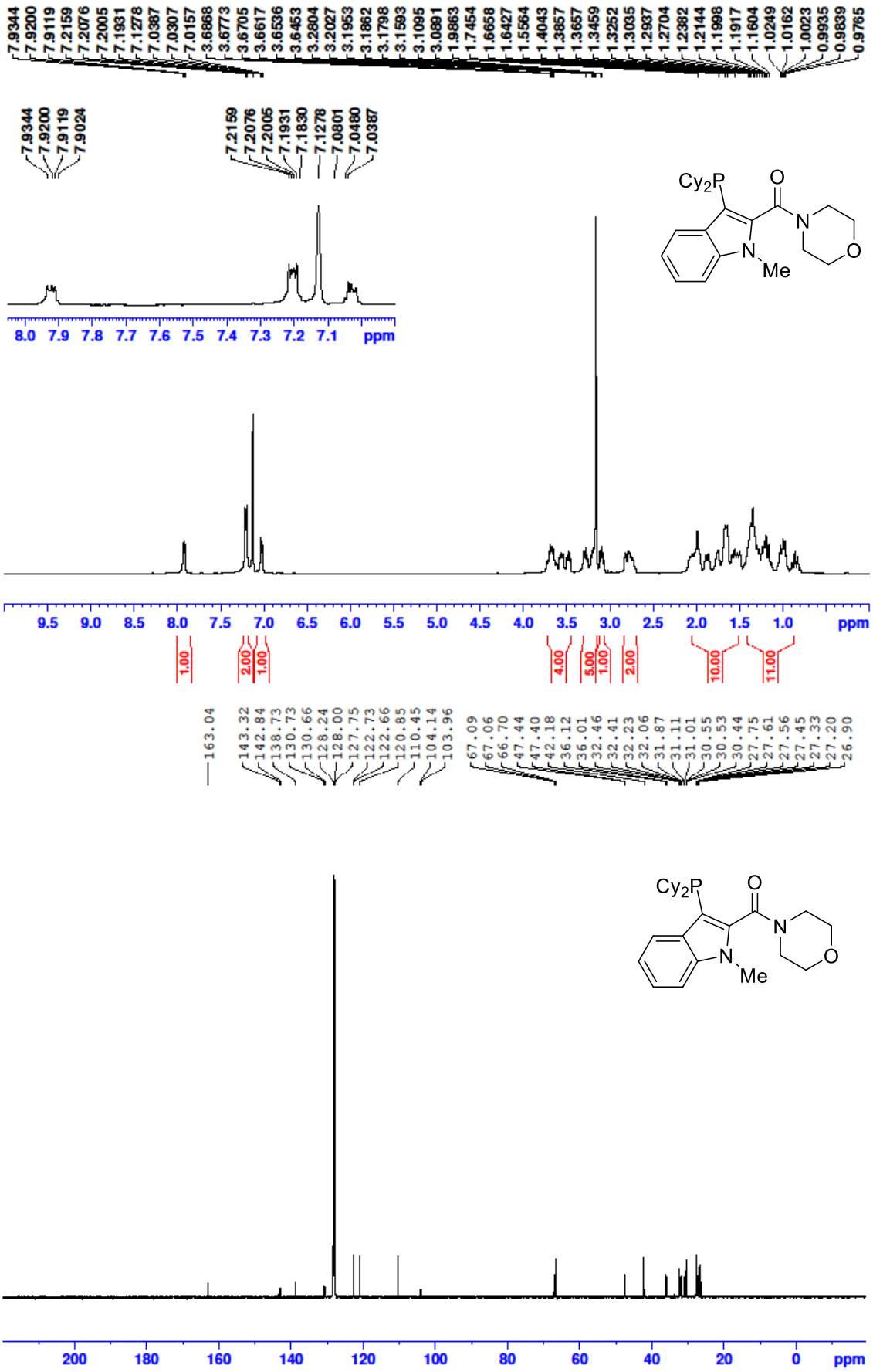
140
120
100
80
60
40
20
0
ppm



Mass	Calc. Mass	mDa	PPM	Formula
323.0389	323.0390	0.07	0.21	C14 H16 Br N2 O2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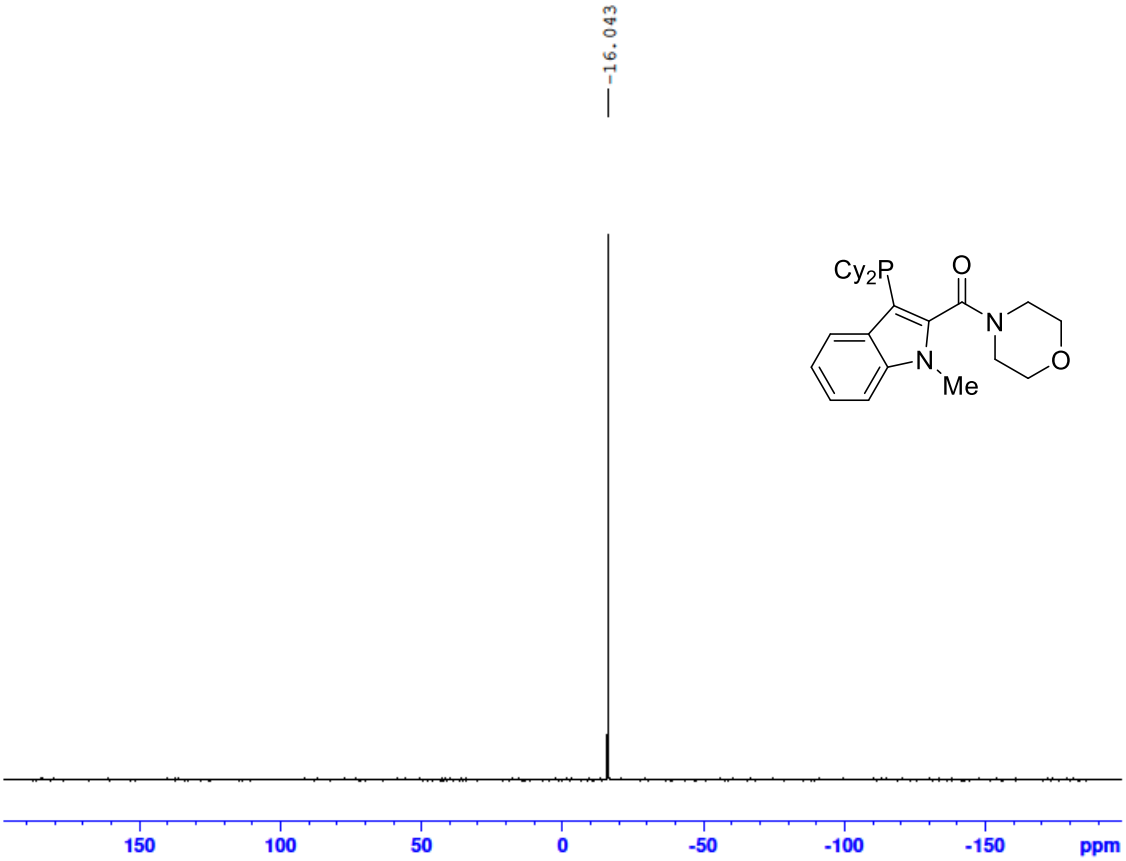
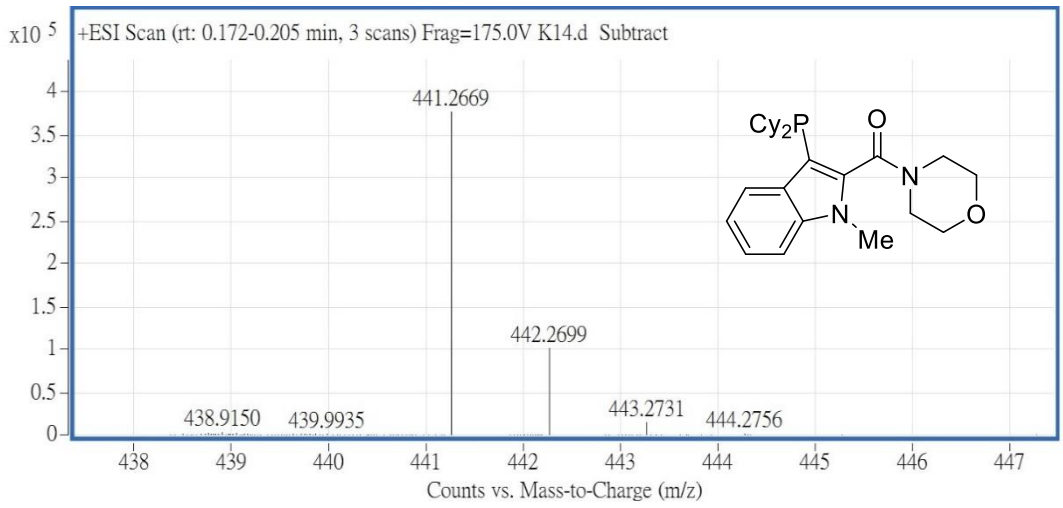
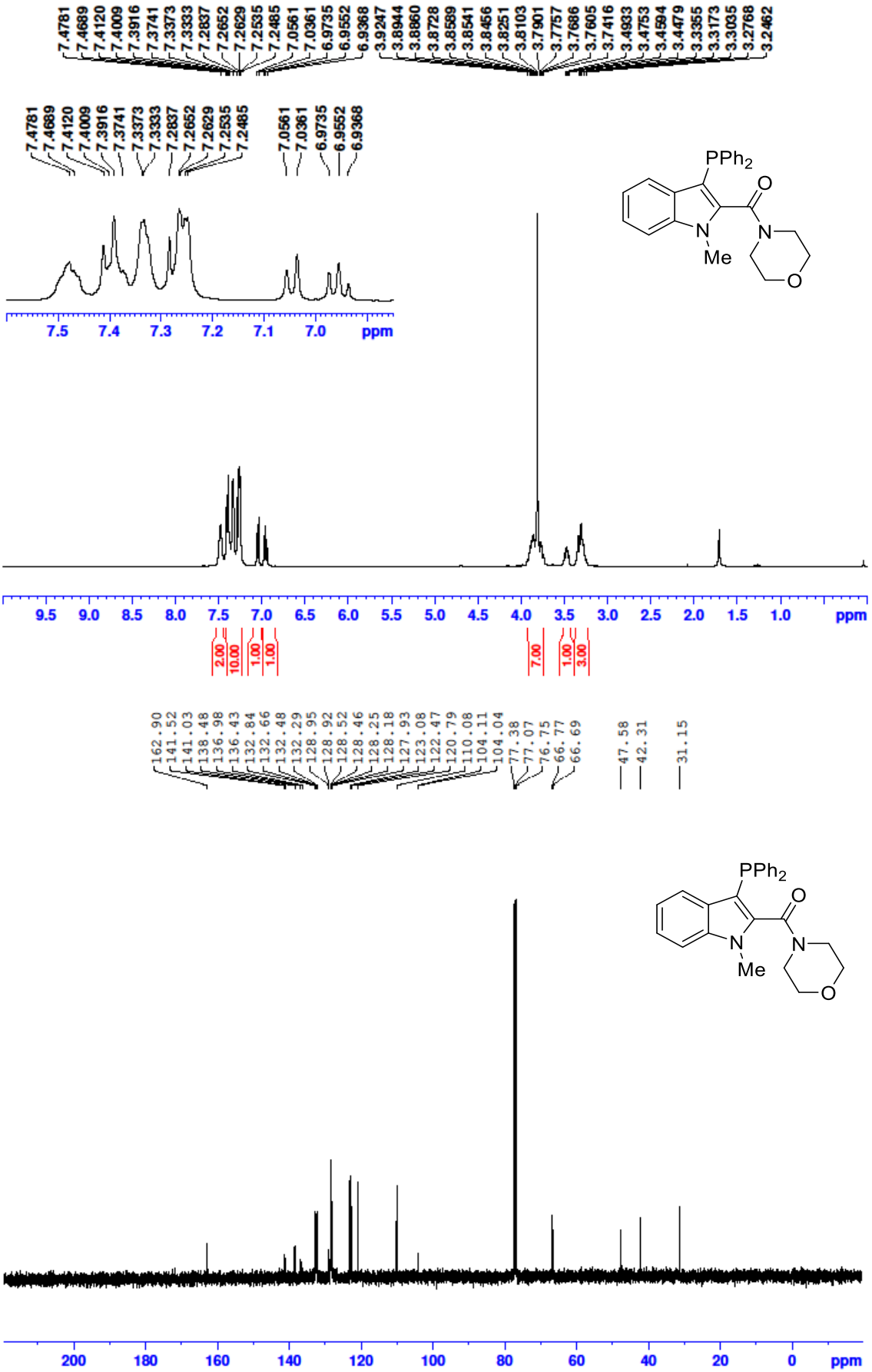
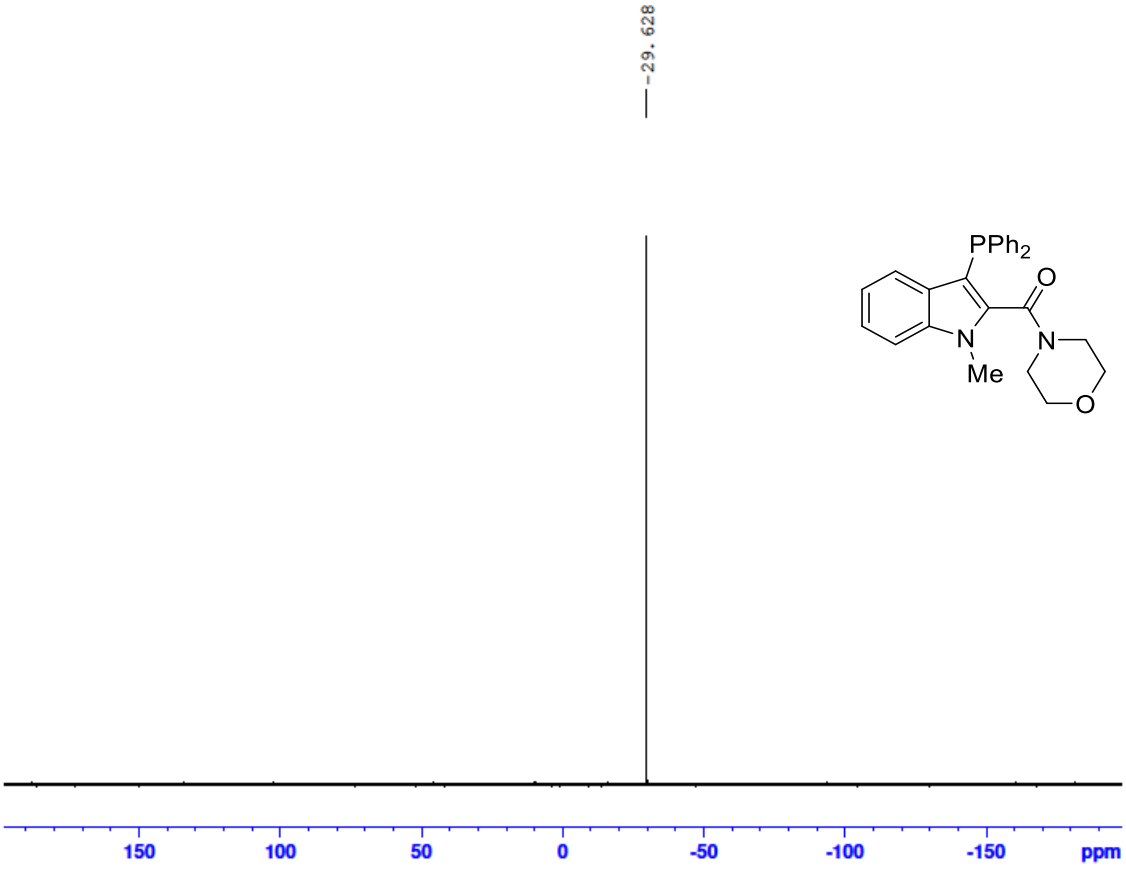
7.9119
7.2159
7.2076
7.2005
7.1931
7.1278
7.0387
7.0307
7.0157
3.6868
3.6773
3.6705
3.6617
3.6536
3.6453
3.2804
3.2027
3.1953
3.1862
3.1798
3.1593
3.1095
3.0891
1.9863
1.7454
1.6658
1.6427
1.5564
1.4043
1.3857
1.3657
1.3459
1.3252
1.3035
1.2937
1.2704
1.2382
1.2144
1.1998
1.1917
1.1604
1.0249
1.0162
1.0023
0.9935
0.9839
0.9765
7.9344
7.9200
7.9119
7.9024
7.2159
7.2076
7.2005
7.1931
7.1830
7.1278
7.0801
7.0480
7.0387
Cy2P
O
N
N
Me
O
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
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 ppm
1.00
2.00
1.00
4.00
5.00
1.00
2.00
10.00
11.00
163.04
143.32
142.84
138.73
130.73
130.66
128.24
128.00
127.75
122.73
122.66
120.85
110.45
104.14
103.96
67.09
67.06
66.70
47.44
47.40
42.18
36.12
36.01
32.46
32.41
32.23
32.06
31.87
31.11
31.01
30.55
30.53
30.44
27.75
27.61
27.56
27.45
27.33
27.20
26.90
Cy2P
O
N
N
Me
O
200 180 160 140 120 100 80 60 40 20 0 ppm

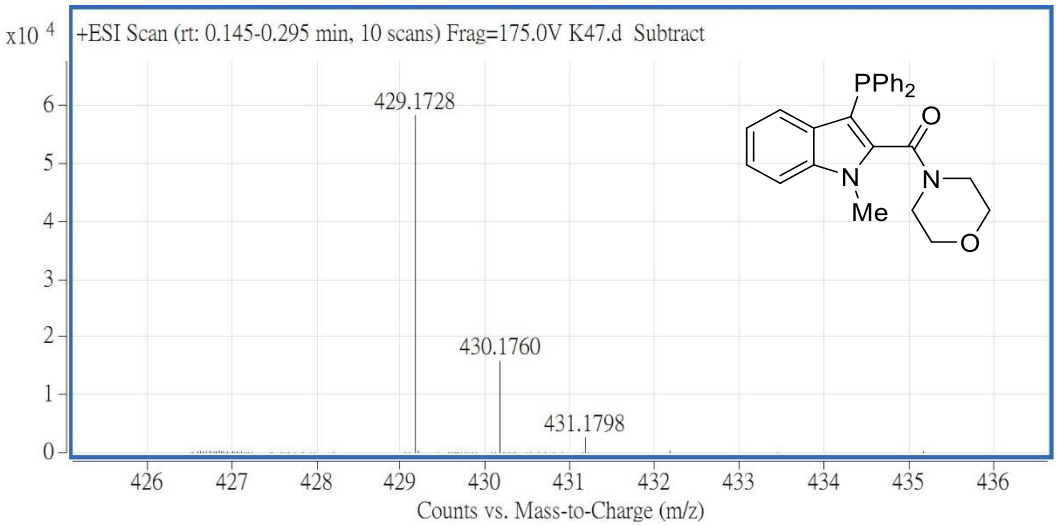




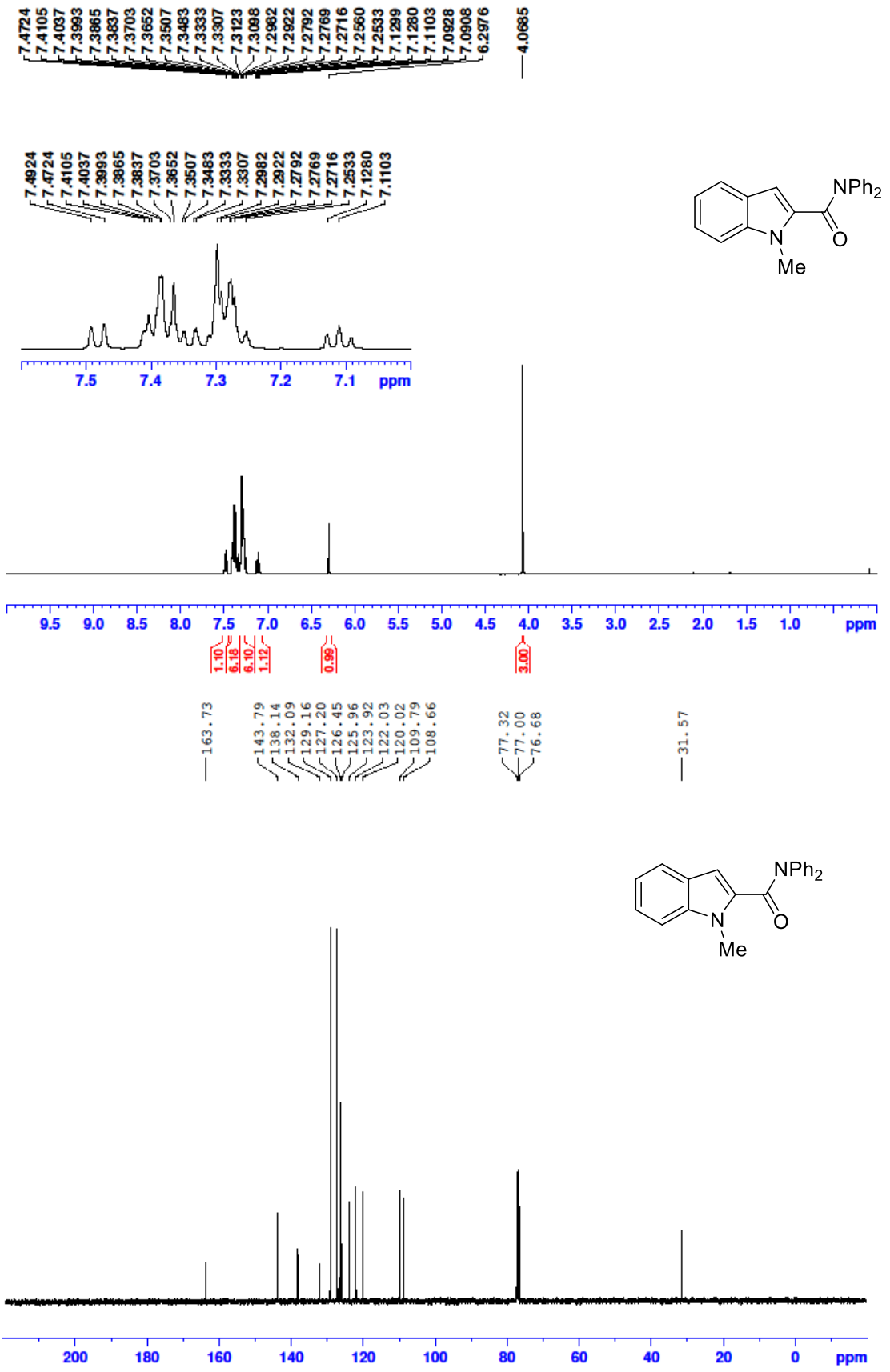
Mass	Calc. Mass	mDa	PPM	Formula
441.2669	441.2665	-0.36	-0.81	C26 H38 N2 O2 P

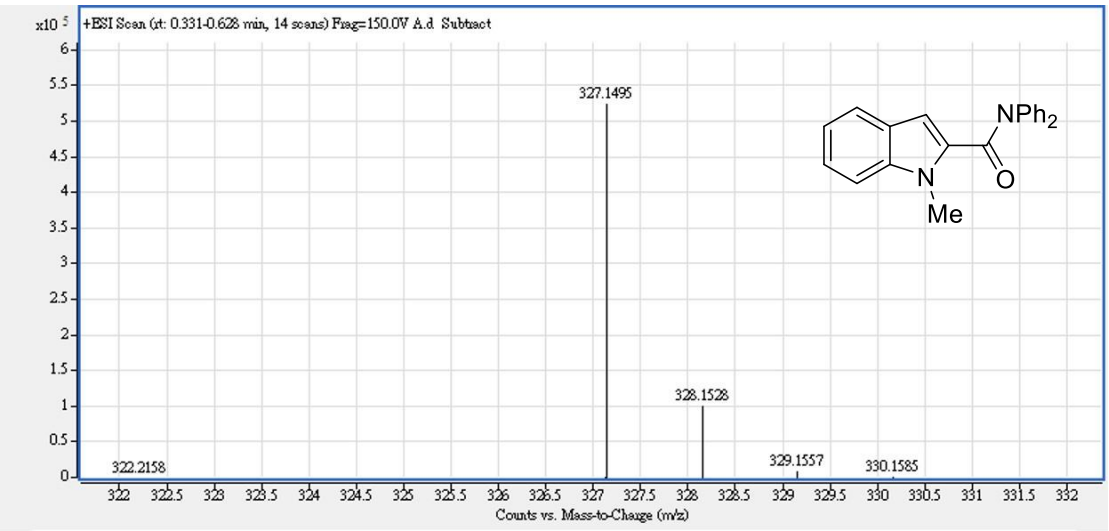

7.4781 7.4689 7.4120 7.4009 7.3916 7.3741 7.3373 7.3333 7.2837 7.2652 7.2629 7.2535 7.2485 7.0561 7.0361 6.9735 6.9552 6.9368 3.9247 3.8944 3.8860 3.8728 3.8589 3.8541 3.8456 3.8251 3.8103 3.7901 3.7757 3.7686 3.7605 3.7416 3.4933 3.4753 3.4594 3.4479 3.3355 3.3173 3.3035 3.2768 3.2462
PPh2
O
N
Me
N
O
7.5 7.4 7.3 7.2 7.1 7.0 ppm
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 ppm
2.00 10.00 1.00 1.00 7.00 1.00 3.00
162.90 141.52 141.03 138.48 136.98 136.43 132.84 132.66 132.48 132.29 128.95 128.92 128.52 128.46 128.25 128.18 127.93 123.08 122.47 120.79 110.08 104.11 104.04 77.38 77.07 76.75 66.77 66.69 47.58 42.31 31.15
PPh2
O
N
Me
N
O
200 180 160 140 120 100 80 60 40 20 0 ppm



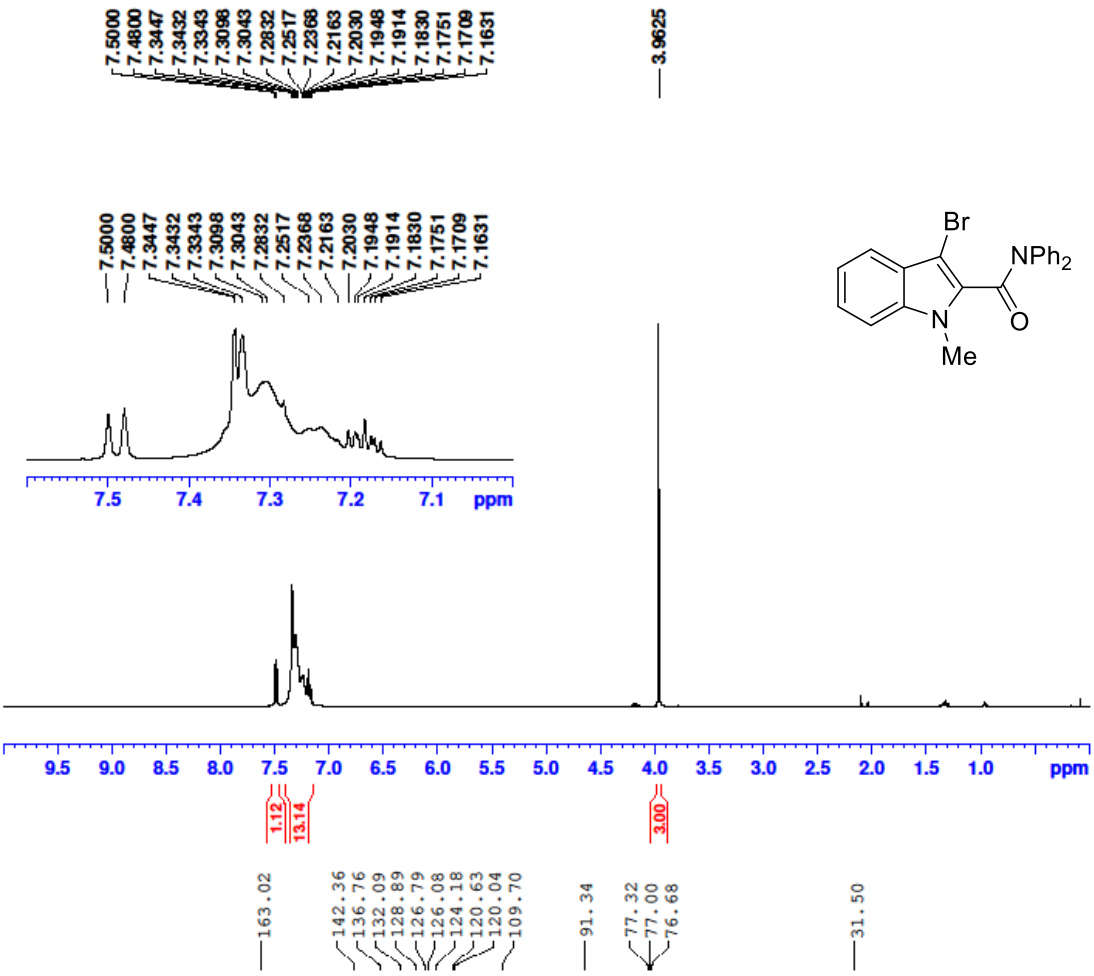


Mass	Calc. Mass	mDa	PPM	Formula
429.1728	429.1726	-0.16	-0.37	C26 H26 N2 O2 P

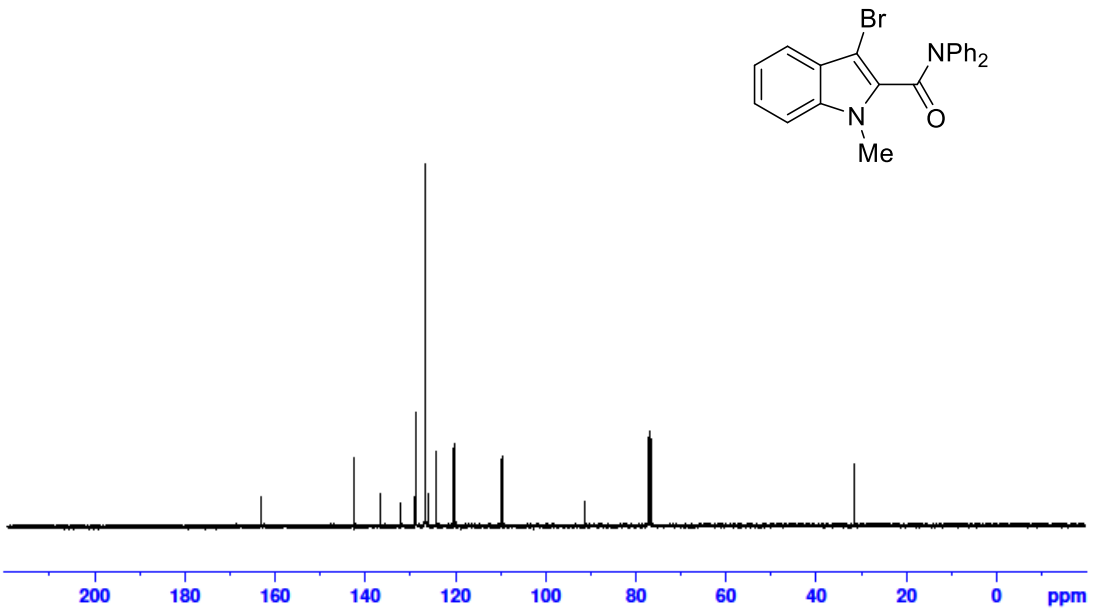

7.4724
7.4105
7.4037
7.3993
7.3865
7.3837
7.3703
7.3652
7.3507
7.3483
7.3333
7.3307
7.3123
7.3098
7.2982
7.2922
7.2792
7.2769
7.2716
7.2560
7.2533
7.1299
7.1280
7.1103
7.0928
7.0908
6.2976
4.0685
NPh2
N
O
Me
7.5
7.4
7.3
7.2
7.1
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
1.10
6.18
6.10
1.12
0.99
3.00
163.73
143.79
138.14
132.09
129.16
127.20
126.45
125.96
123.92
122.03
120.02
109.79
108.66
77.32
77.00
76.68
31.57
200
180
160
140
120
100
80
60
40
20
0

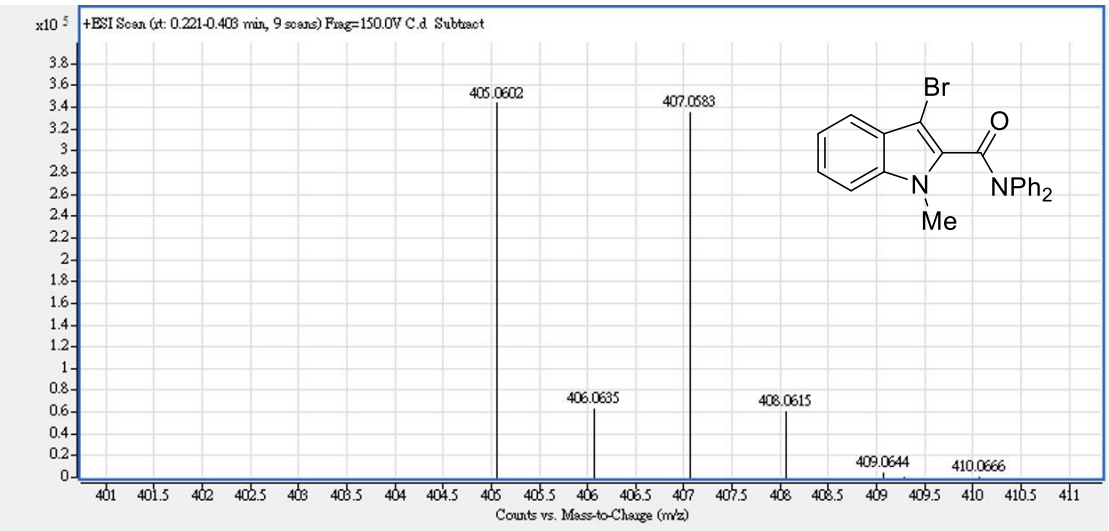


Mass	Calc. Mass	mDa	PPM	Formula
327.1495	327.1492	-0.31	-0.95	C22 H19 N2 O

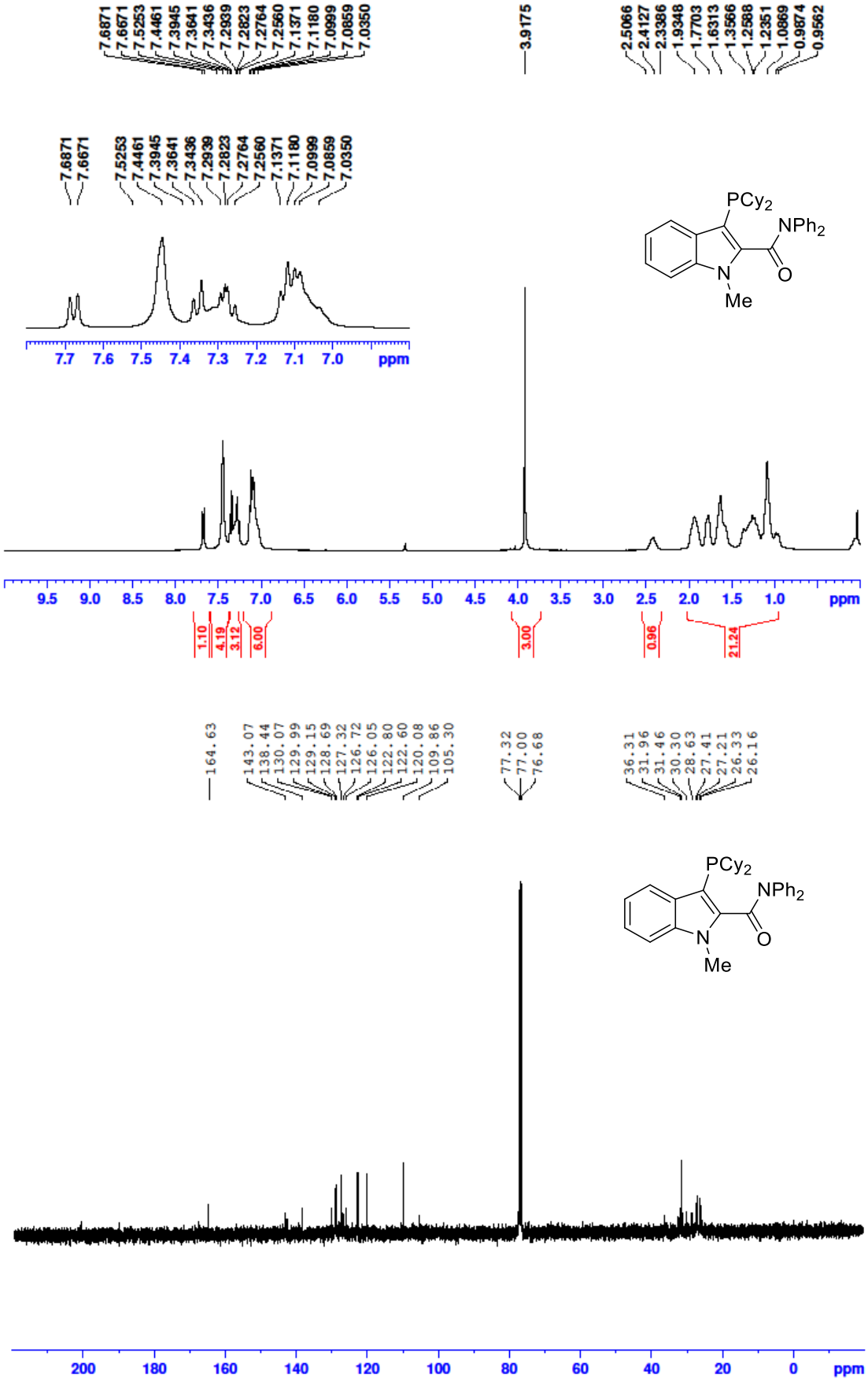

7.5000
7.4800
7.3447
7.3432
7.3343
7.3098
7.3043
7.2832
7.2517
7.2368
7.2163
7.2030
7.1948
7.1914
7.1830
7.1751
7.1709
7.1631
3.9625
Br
NPh2
N
O
Me
7.5
7.4
7.3
7.2
7.1
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.12
13.14
3.00

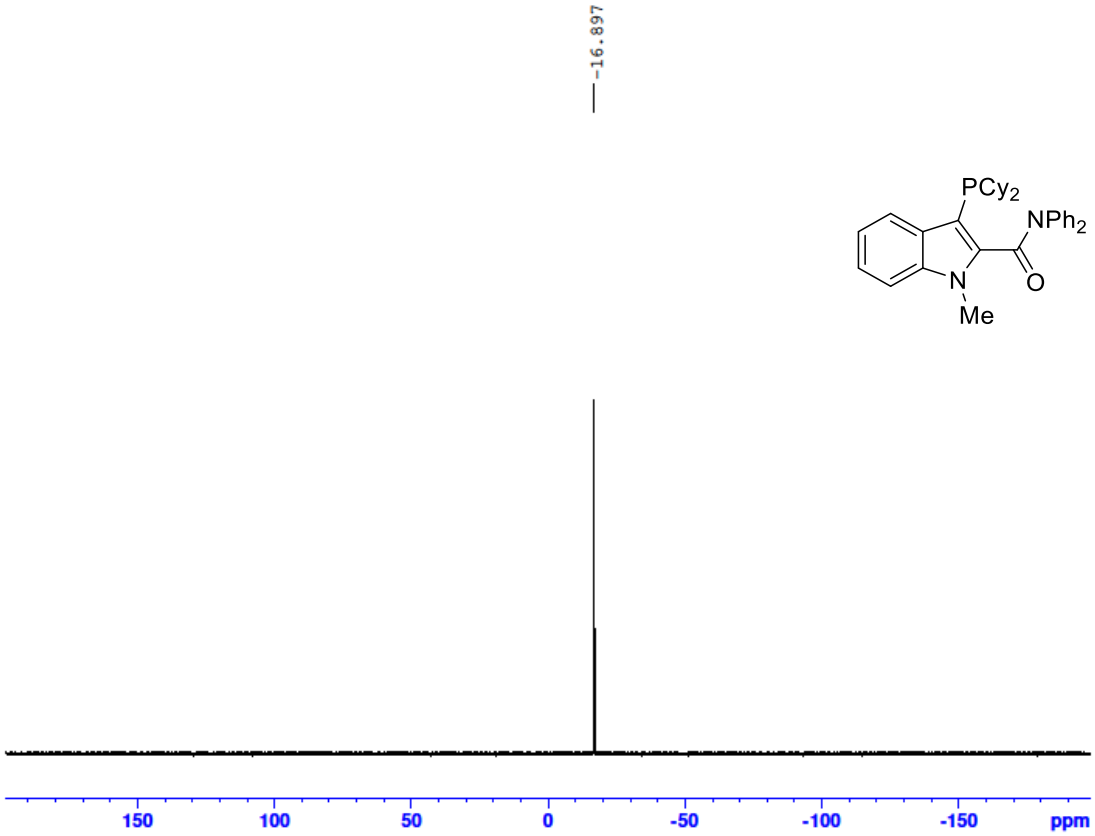
163.02
142.36
136.76
132.09
128.89
126.79
126.08
124.18
120.63
120.04
109.70
91.34
77.32
77.00
76.68
31.50

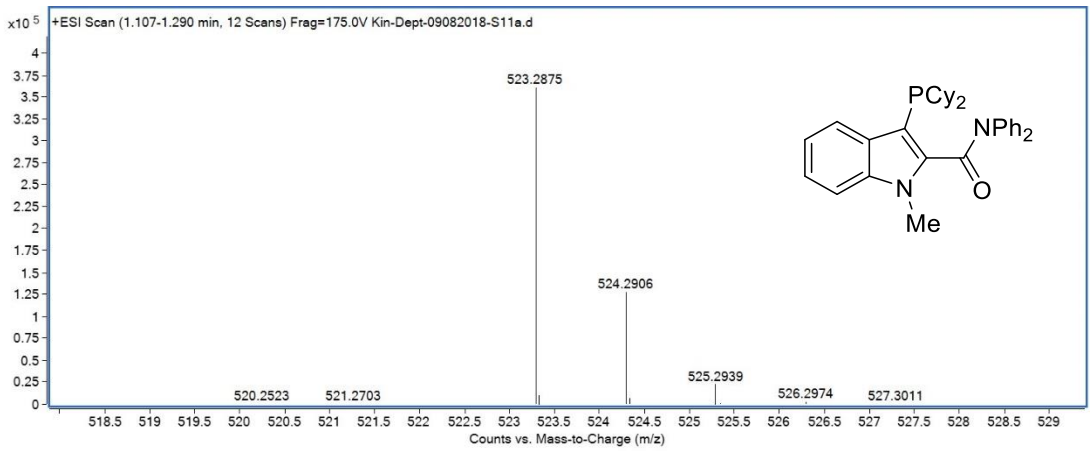

Br
NPh2
N
O
Me
200
180
160
140
120
100
80
60
40
20
0
ppm



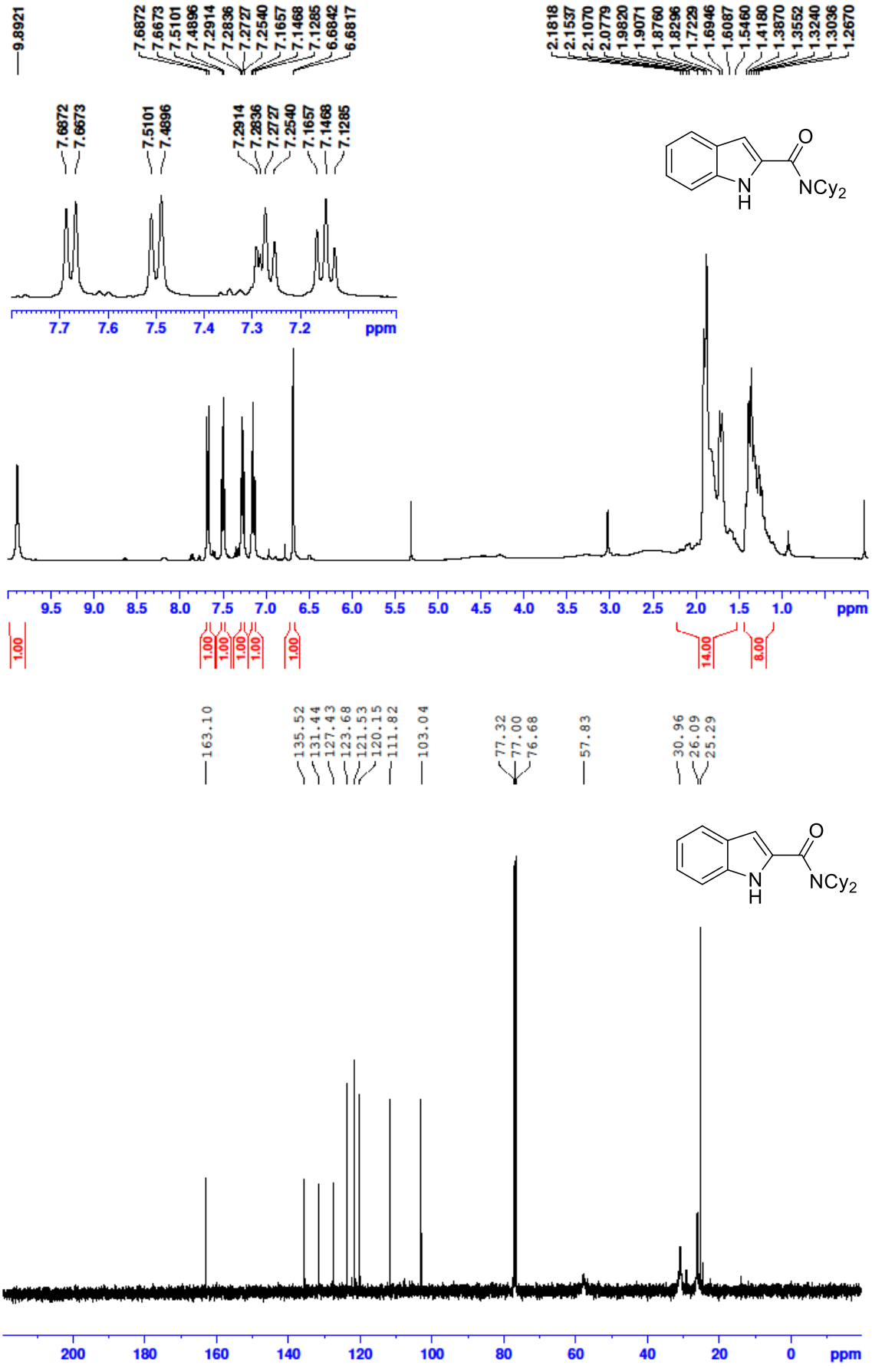
Mass	Calc. Mass	mDa	PPM	Formula
405.0602	405.0597	-0.50	-1.23	C22 H18 Br N2 O

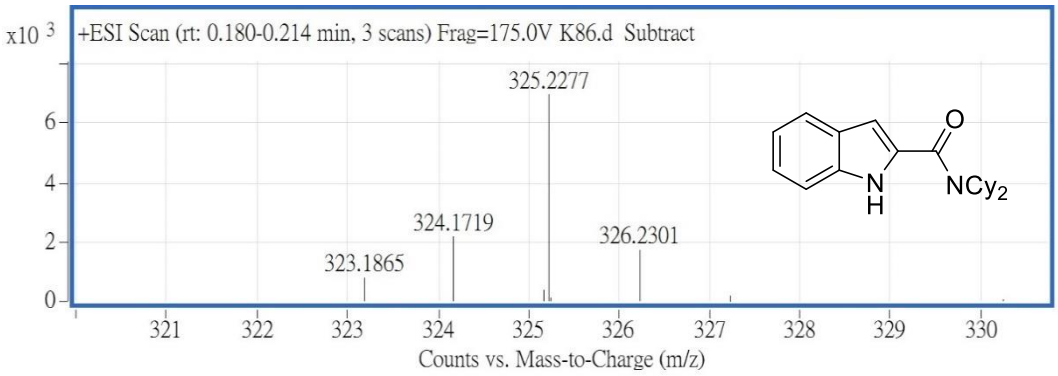

7.6871
7.6671
7.5253
7.4461
7.3945
7.3641
7.3436
7.2939
7.2823
7.2764
7.2560
7.1371
7.1180
7.0999
7.0859
7.0350
3.9175
2.5066
2.4127
2.3386
1.9348
1.7703
1.6313
1.3566
1.2588
1.2351
1.0869
0.9874
0.9562
PCy2
NPh2
N
O
Me
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.10
4.19
3.12
6.00
3.00
0.96
21.24
164.63
143.07
138.44
130.07
129.99
129.15
128.69
127.32
126.72
126.05
122.80
122.60
120.08
109.86
105.30
77.32
77.00
76.68
36.31
31.96
31.46
30.30
28.63
27.41
27.21
26.33
26.16
200 180 160 140 120 100 80 60 40 20 0 ppm



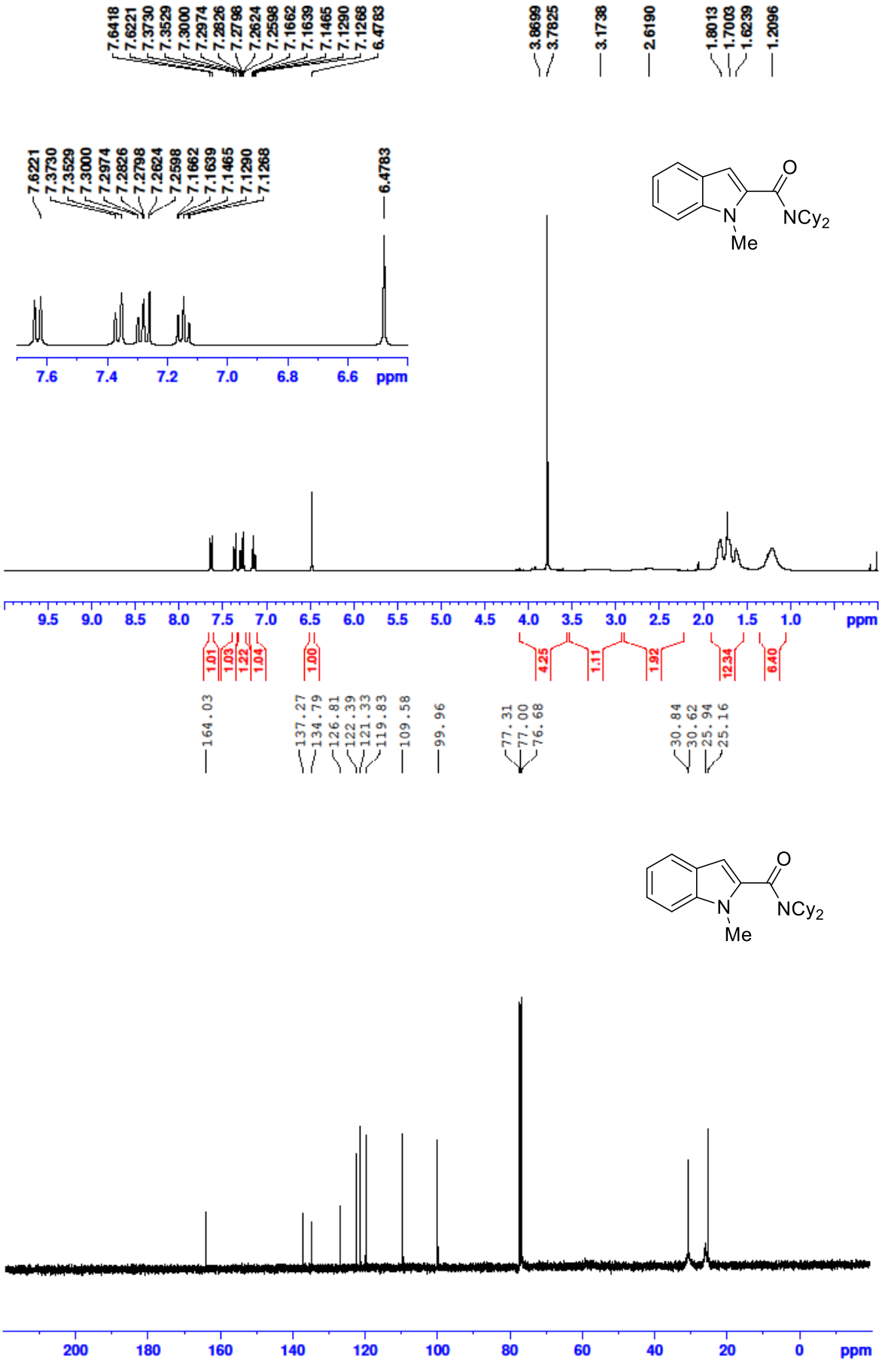


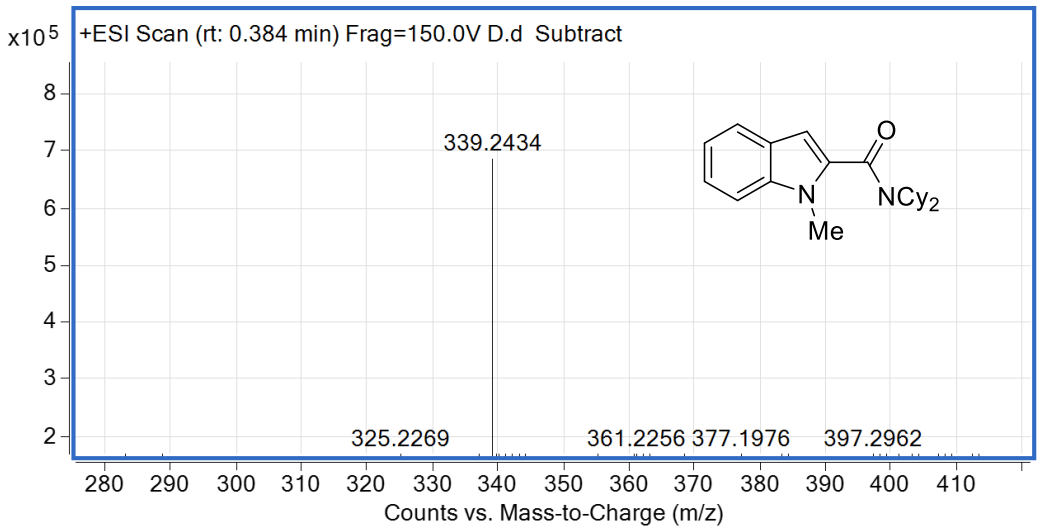
Mass	Calc. Mass	mDa	PPM	Formula
523.2875	523.2873	0.22	0.43	C34 H40 N2 O P


9.8921
7.6872
7.6673
7.5101
7.4896
7.2914
7.2836
7.2727
7.2540
7.1657
7.1468
7.1285
6.6842
6.6817
2.1818
2.1537
2.1070
2.0779
1.9820
1.9071
1.8760
1.8296
1.7229
1.6946
1.6087
1.5460
1.4180
1.3870
1.3552
1.3240
1.3036
1.2670
O
N
H
NCy2
ppm
1.00
14.00
8.00
163.10
135.52
131.44
127.43
123.68
121.53
120.15
111.82
103.04
77.32
77.00
76.68
57.83
30.96
26.09
25.29

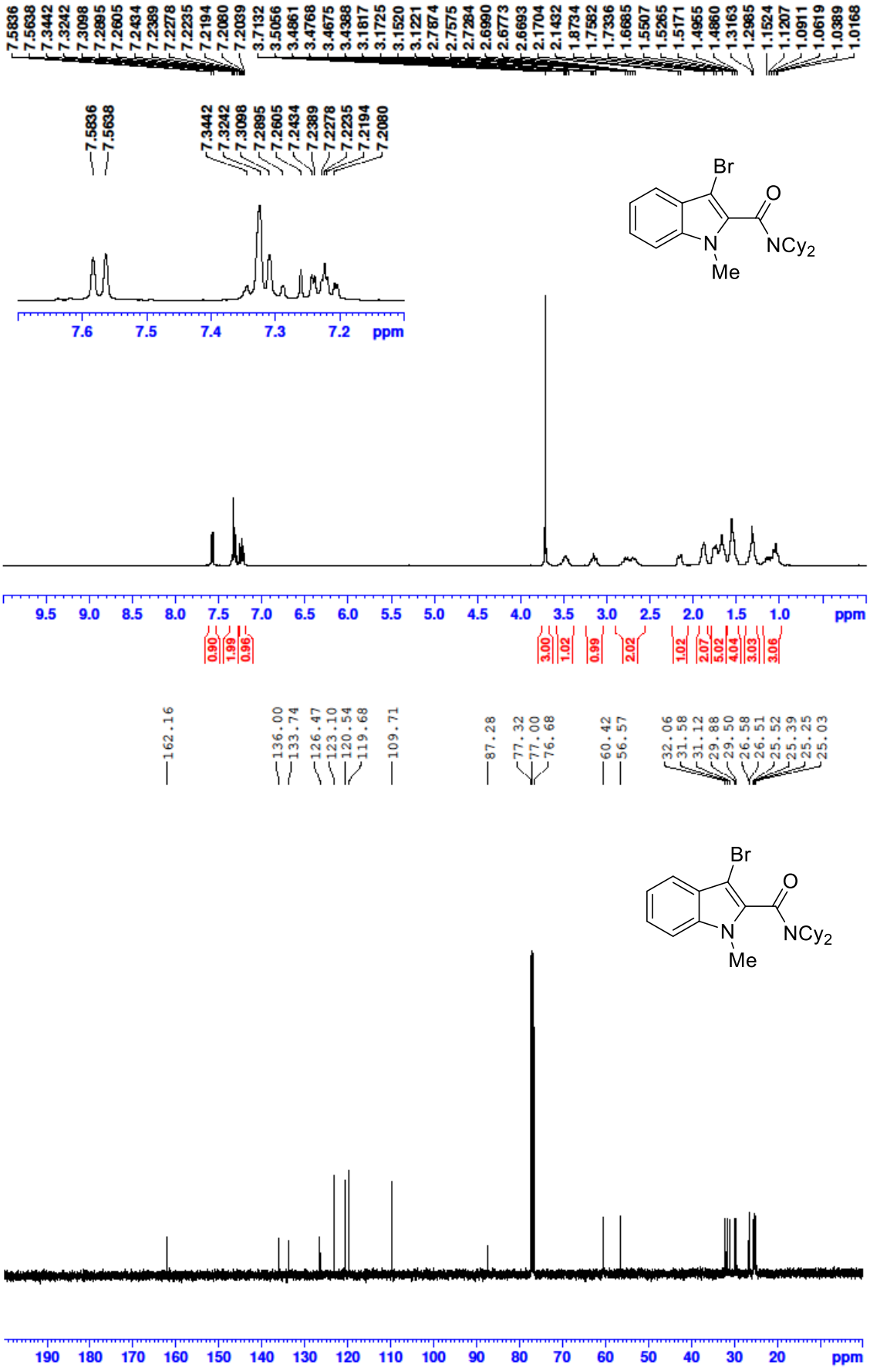


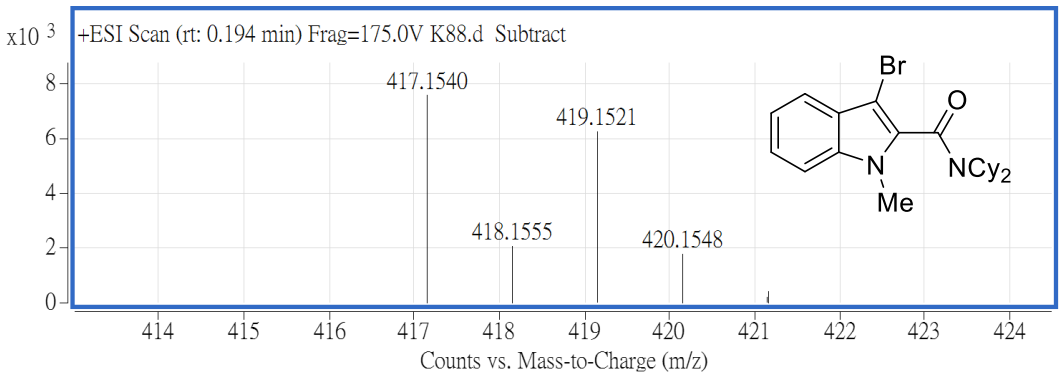
Mass	Calc. Mass	mDa	PPM	Formula
325.2277	325.2274	-0.26	-0.80	C21 H29 N2 O


7.6418
7.6221
7.3730
7.3529
7.3000
7.2974
7.2826
7.2798
7.2624
7.2598
7.1662
7.1639
7.1465
7.1290
7.1268
6.4783
3.8699
3.7825
3.1738
2.6190
1.8013
1.7003
1.6239
1.2096
O
N
Me
NCy2
ppm
1.01
1.03
1.22
1.04
1.00
4.25
1.11
1.92
12.34
6.40
164.03
137.27
134.79
126.81
122.39
121.33
119.83
109.58
99.96
77.31
77.00
76.68
30.84
30.62
25.94
25.16

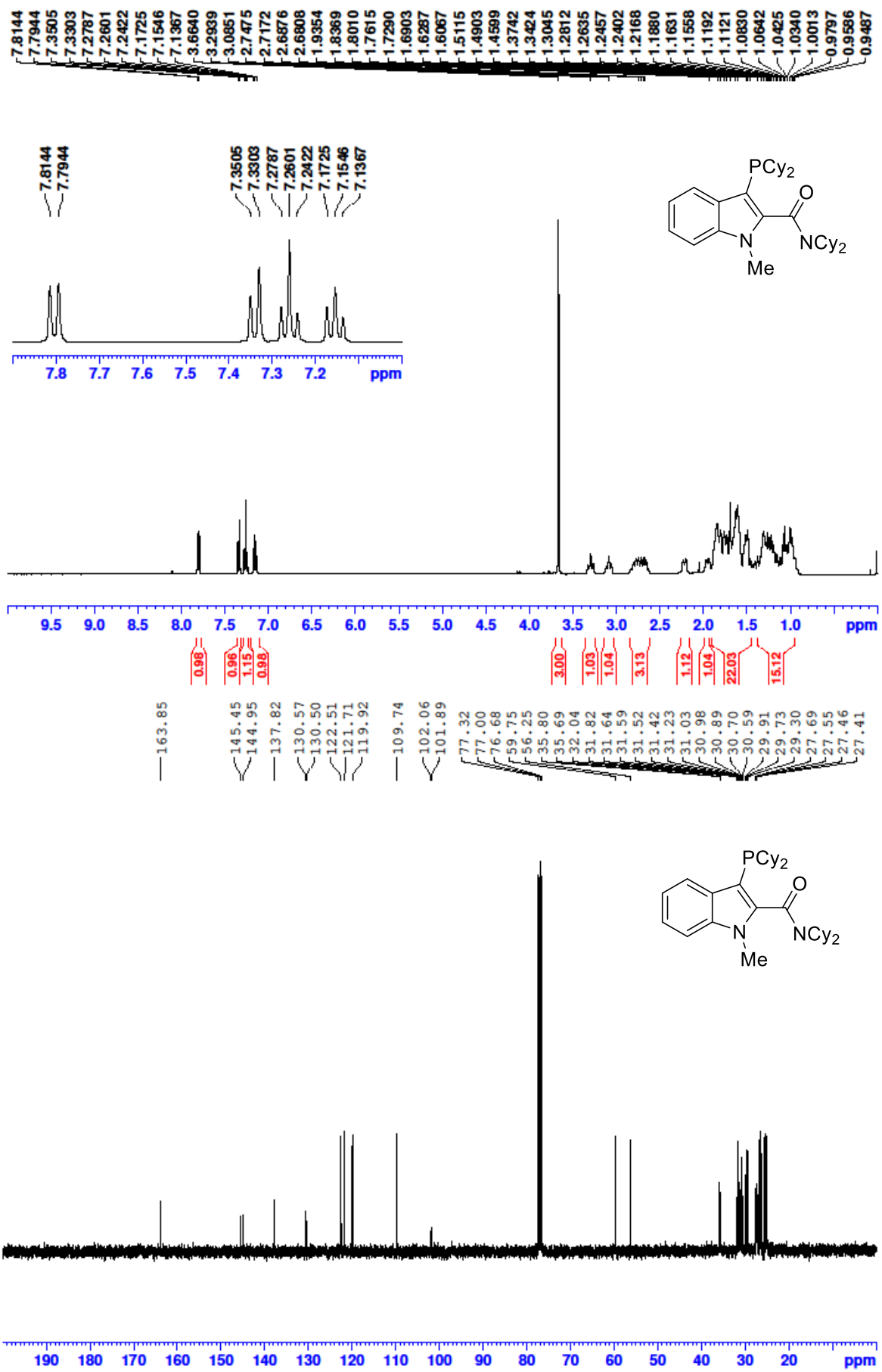


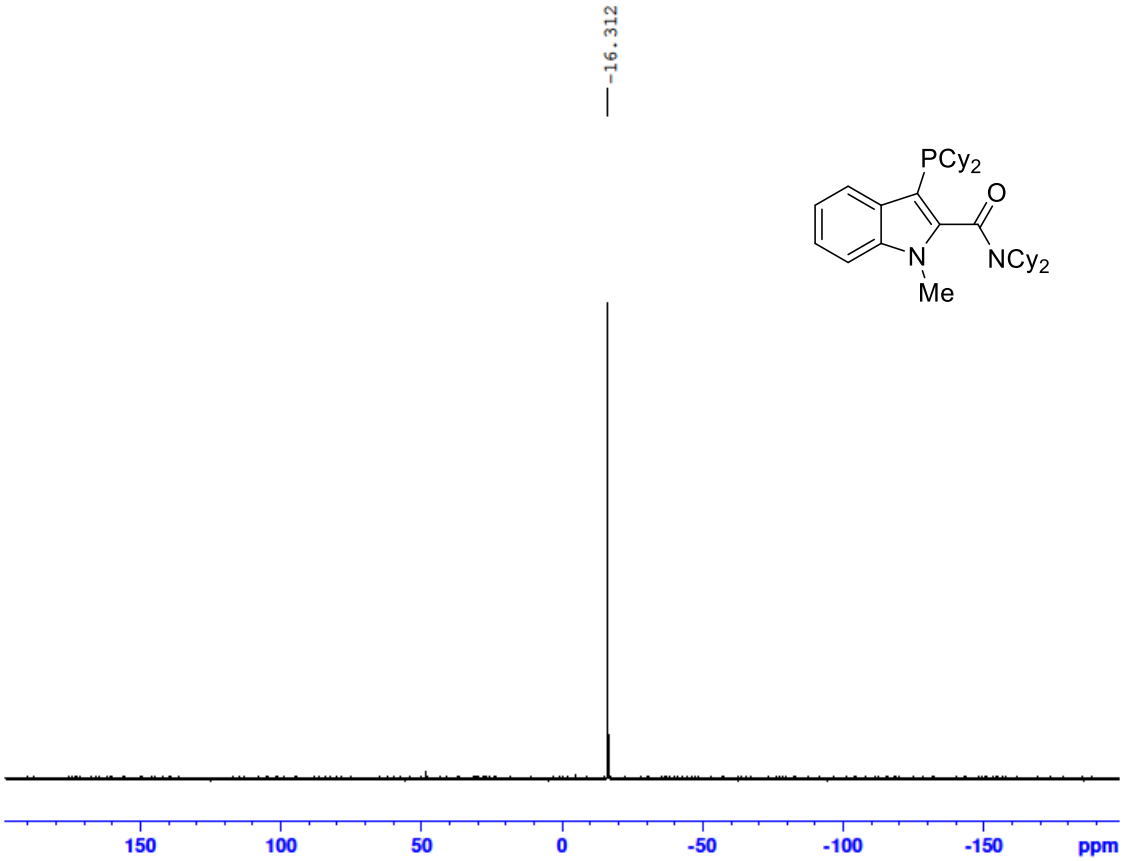
Mass	Calc. Mass	mDa	PPM	Formula
339.2434	339.2431	-0.31	-0.92	$C_{22}H_{31}N_2O$

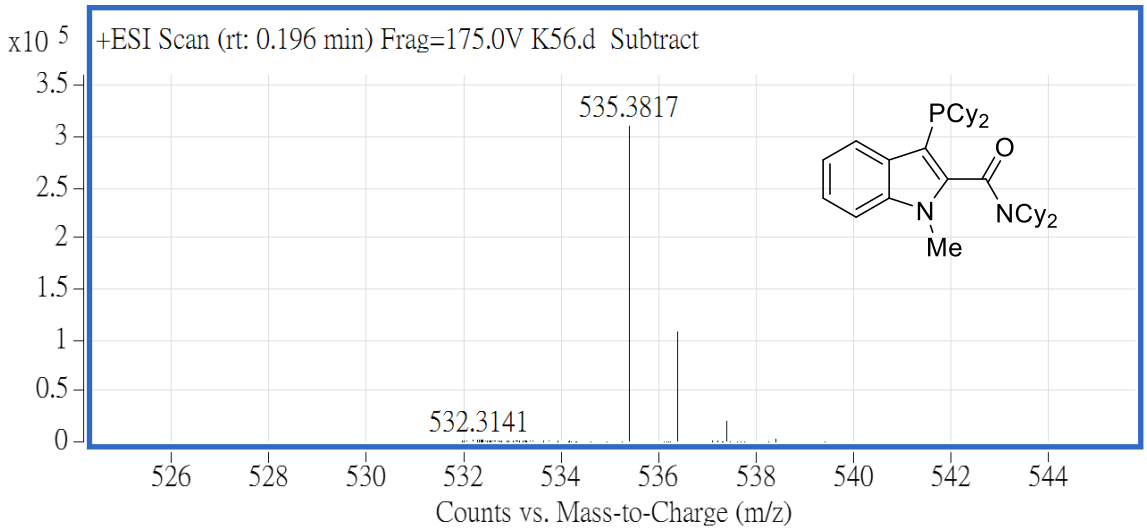

Br
O
NCy2
N
Me
ppm
Br
O
NCy2
N
Me
ppm



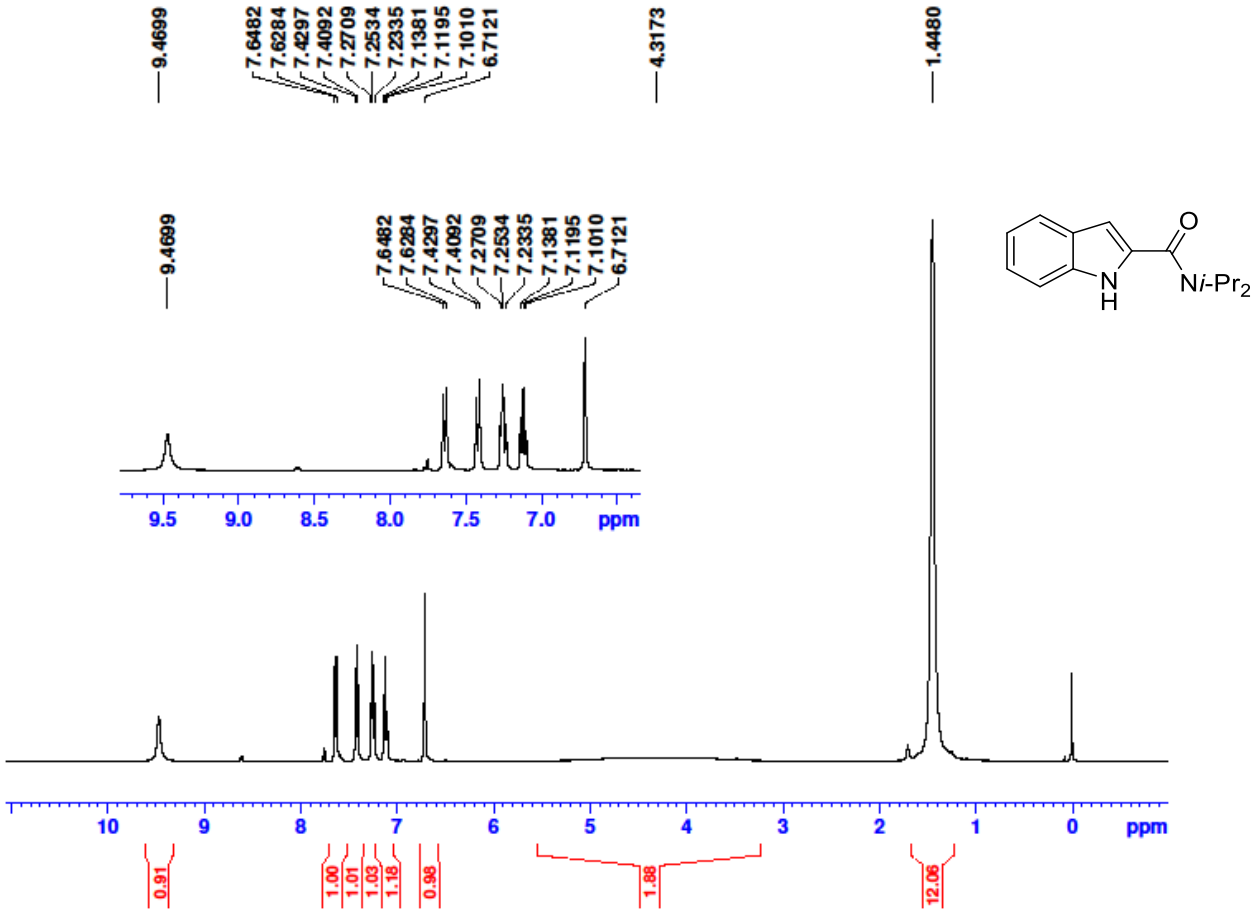
Mass	Calc. Mass	mDa	PPM	Formula
417.1540	417.1536	-0.4	-0.95	C22 H30 Br N2 O

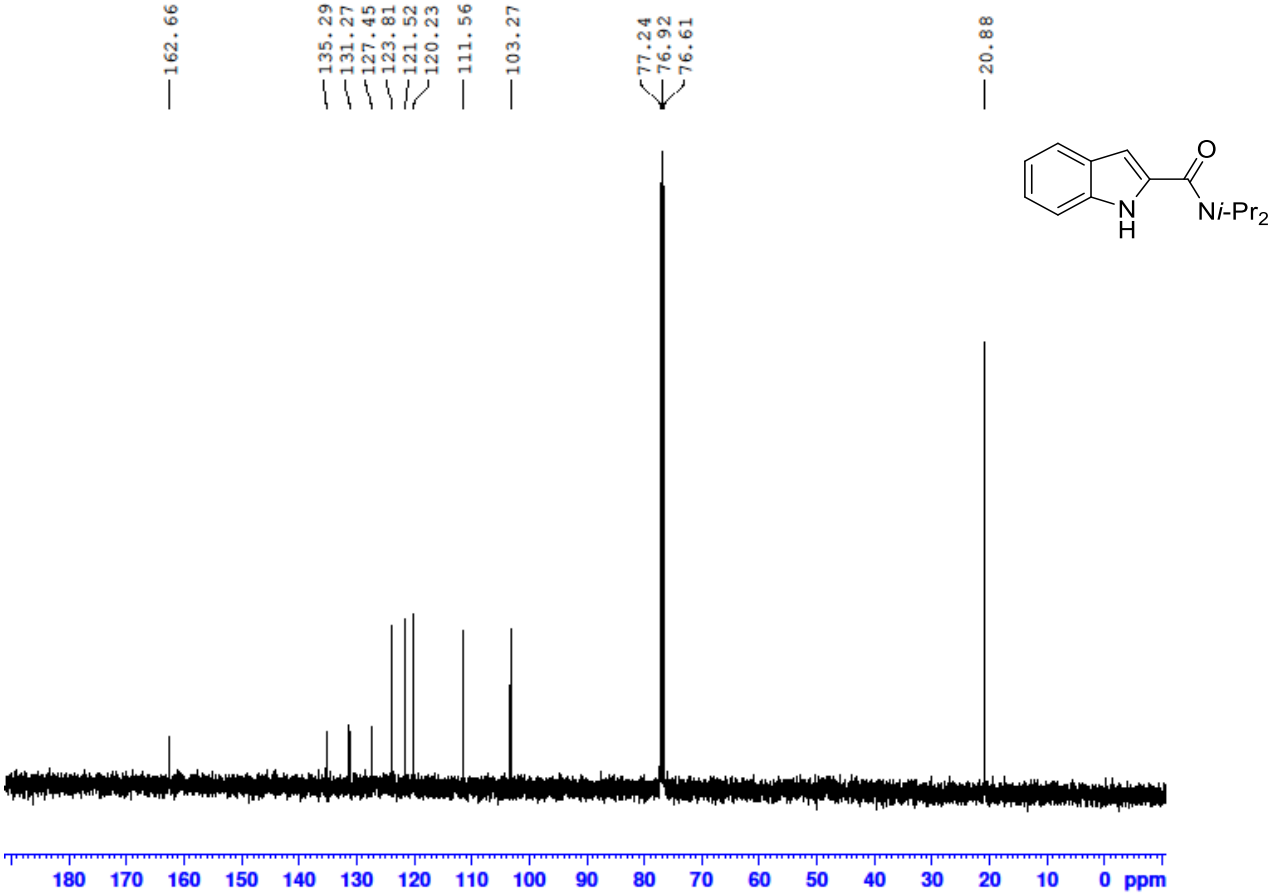

7.8144 7.7944 7.3505 7.3303 7.2787 7.2601 7.2422 7.1725 7.1546 7.1367 3.6640 3.2939 3.0851 2.7475 2.7172 2.6876 2.6808 1.9354 1.8369 1.8010 1.7615 1.7290 1.6903 1.6287 1.6067 1.5115 1.4903 1.4599 1.3742 1.3424 1.3045 1.2812 1.2635 1.2457 1.2402 1.2168 1.1880 1.1631 1.1558 1.1192 1.1121 1.0830 1.0642 1.0425 1.0340 1.0013 0.9797 0.9586 0.9487
PCy2
O
NCy2
N
Me
ppm
0.98 0.96 1.15 0.98 3.00 1.03 1.04 3.13 1.12 1.04 22.03 15.12
163.85 145.45 144.95 137.82 130.57 130.50 122.51 121.71 119.92 109.74 102.06 101.89 77.32 77.00 76.68 59.75 56.25 35.80 35.69 32.04 31.82 31.64 31.59 31.52 31.42 31.23 31.03 30.98 30.89 30.70 30.59 29.91 29.73 29.30 27.69 27.55 27.46 27.41

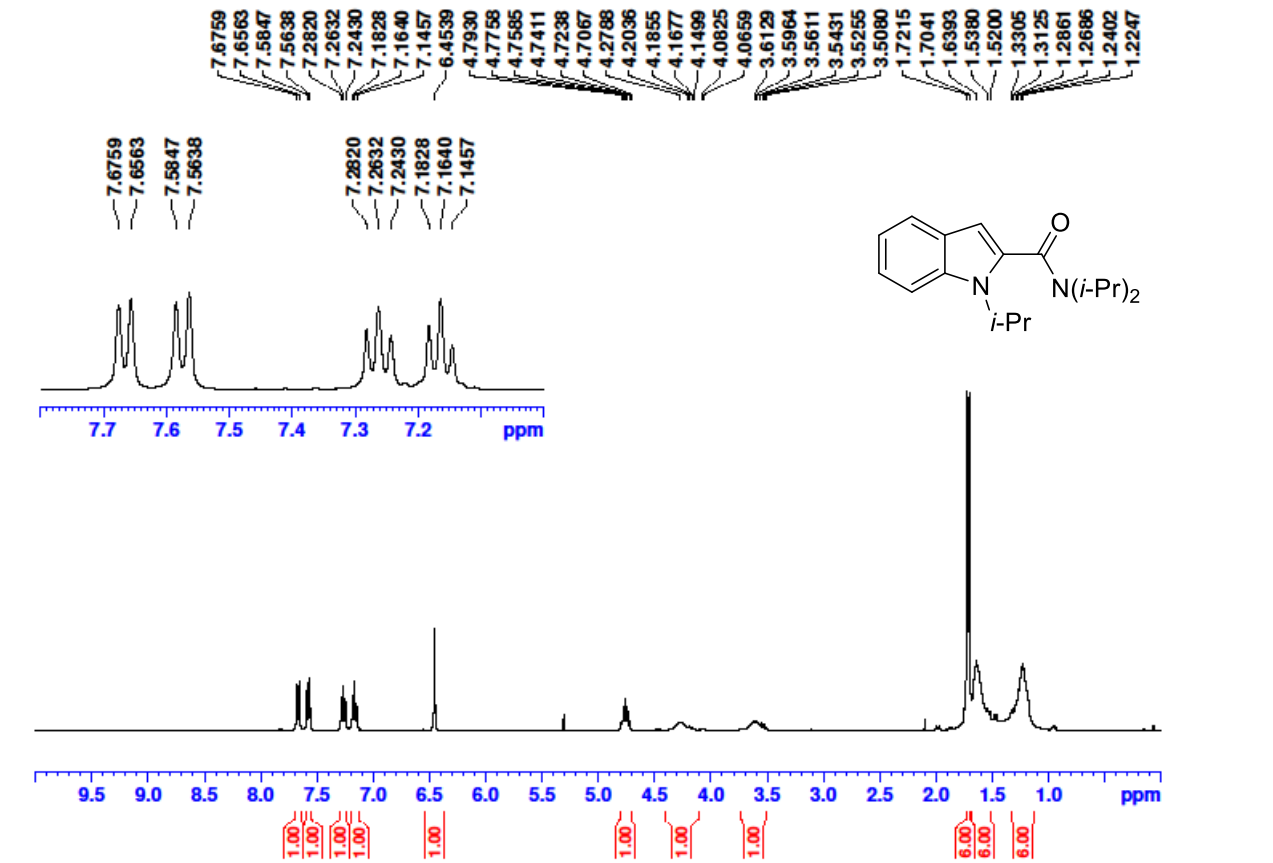


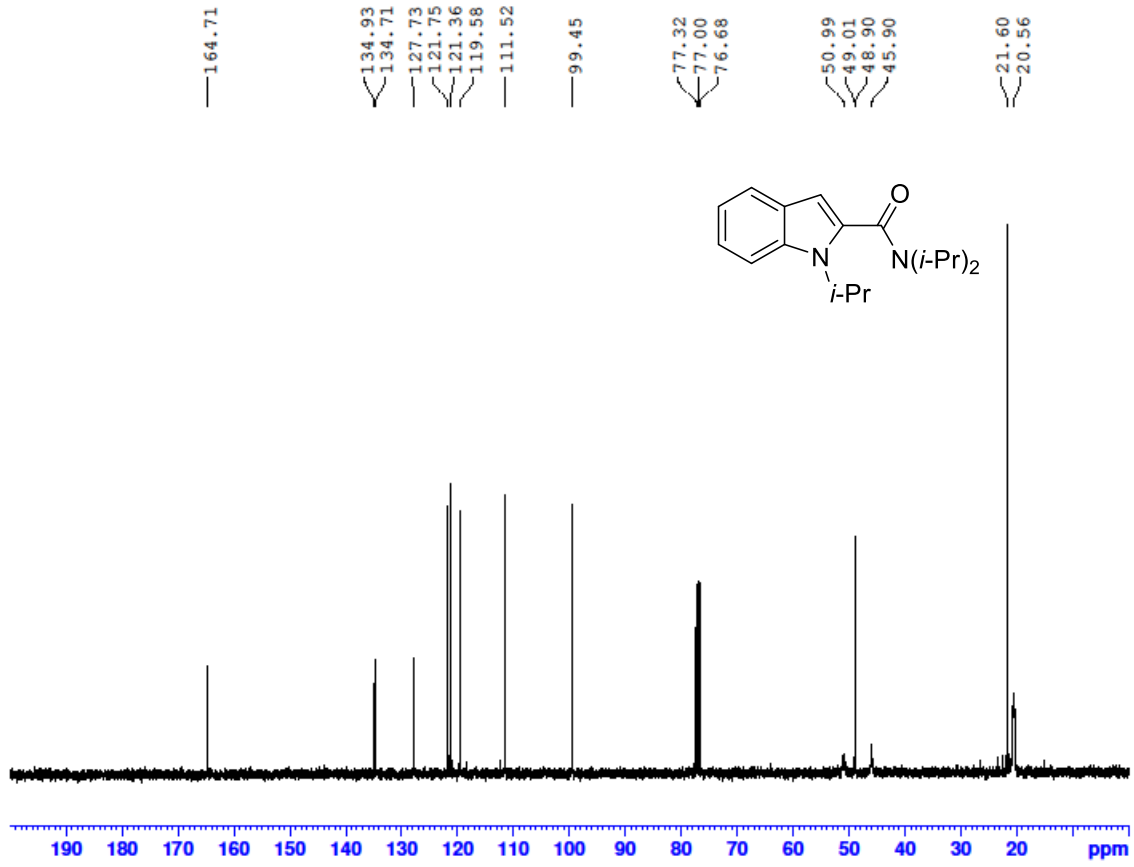


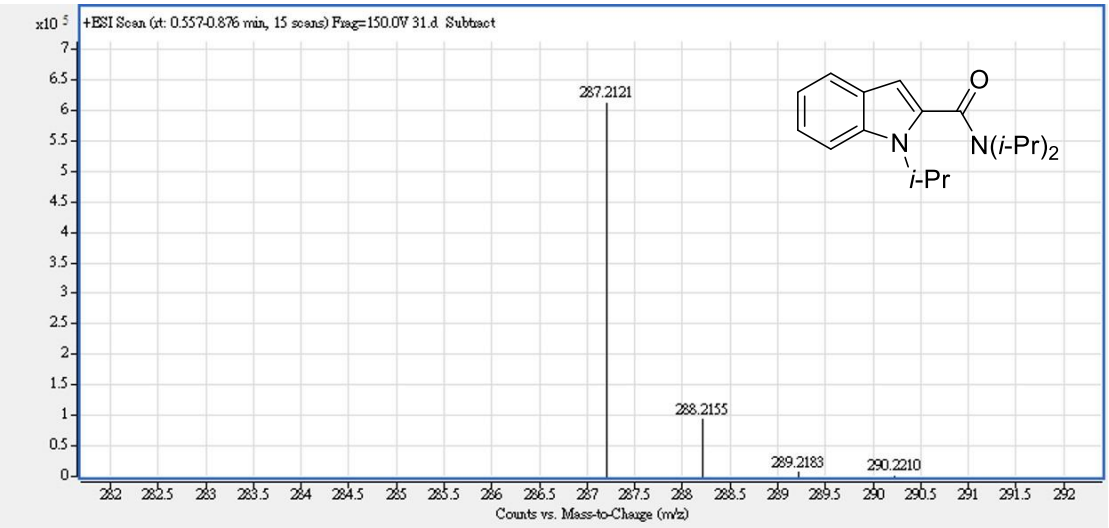
Mass	Calc. Mass	mDa	PPM	Formula
535.3817	535.3812	-0.52	-0.98	C34 H52 N2 O P


9.4699
7.6482
7.6284
7.4297
7.4092
7.2709
7.2534
7.2335
7.1381
7.1195
7.1010
6.7121
4.3173
1.4480
O
N
H
N*i*-Pr$_2$
9.5
9.0
8.5
8.0
7.5
7.0
ppm
10
9
8
7
6
5
4
3
2
1
0
0.91
1.00
1.01
1.03
1.18
0.98
1.86
12.06

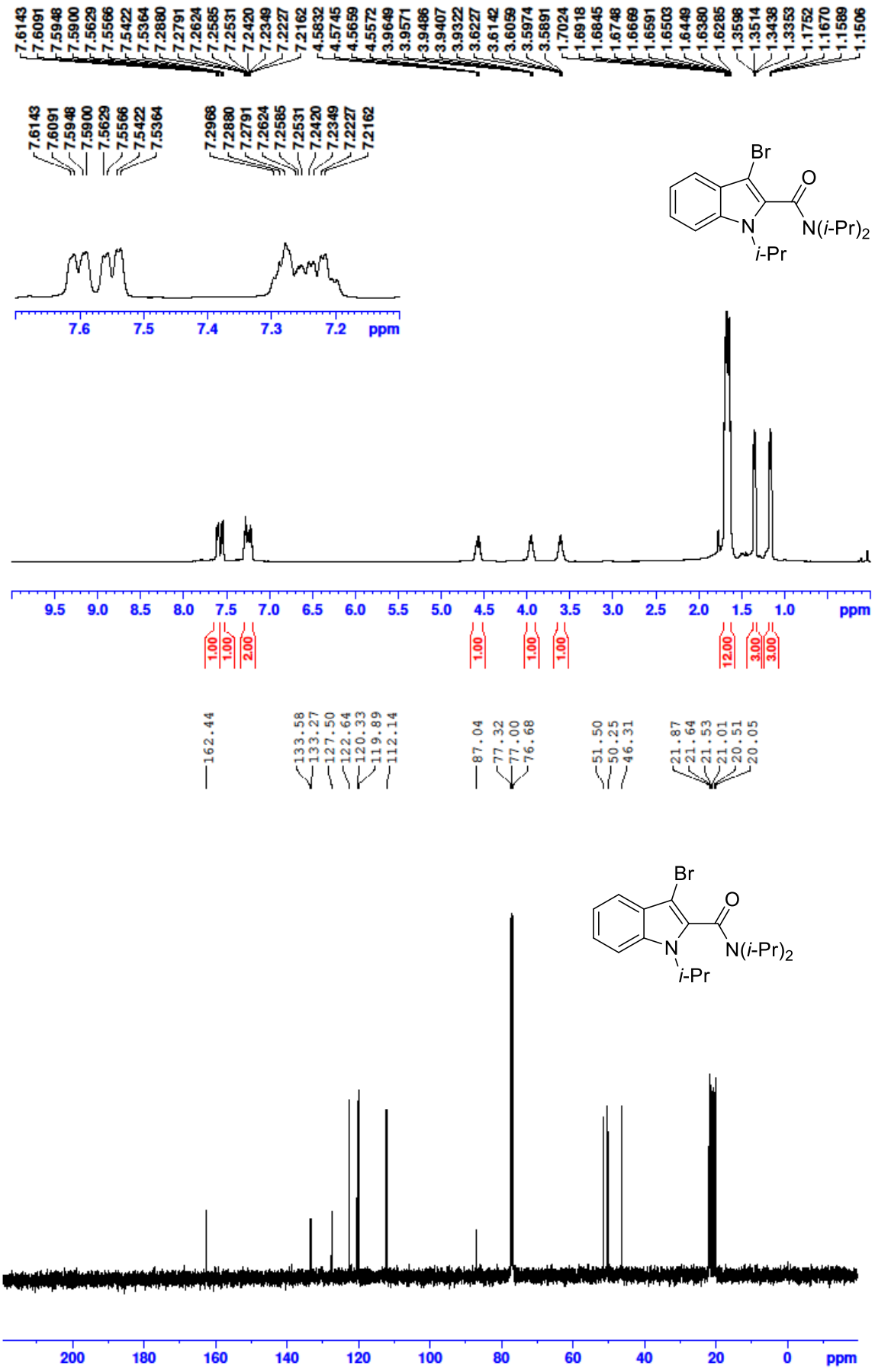

162.66
135.29
131.27
127.45
123.81
121.52
120.23
111.56
103.27
77.24
76.92
76.61
20.88
O
N
H
N*i*-Pr$_2$
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

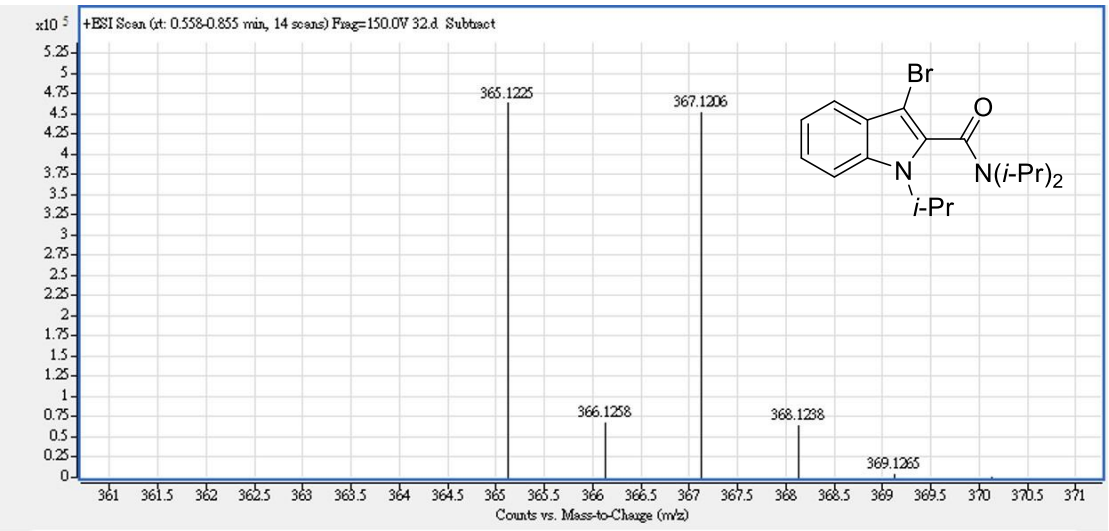

7.6759
7.6563
7.5847
7.5638
7.2820
7.2632
7.2430
7.1828
7.1640
7.1457
6.4539
4.7930
4.7758
4.7585
4.7411
4.7238
4.7067
4.2788
4.2036
4.1855
4.1677
4.1499
4.0825
4.0659
3.6129
3.5964
3.5611
3.5431
3.5255
3.5080
1.7215
1.7041
1.6393
1.5380
1.5200
1.3305
1.3125
1.2861
1.2686
1.2402
1.2247
O
N
N(*i*-Pr)$_2$
i-Pr
7.7 7.6 7.5 7.4 7.3 7.2 ppm
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 ppm
1.00
6.00



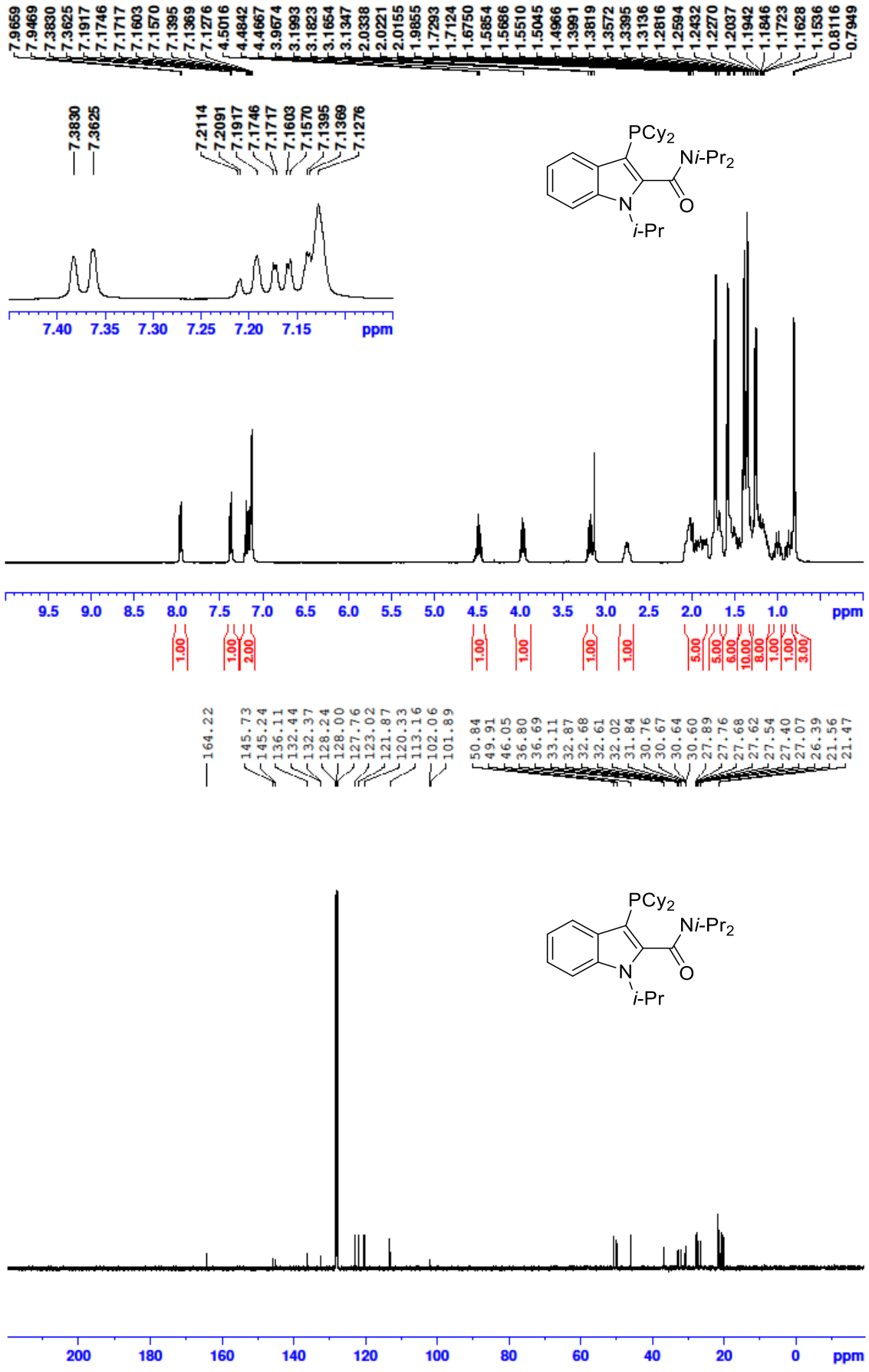


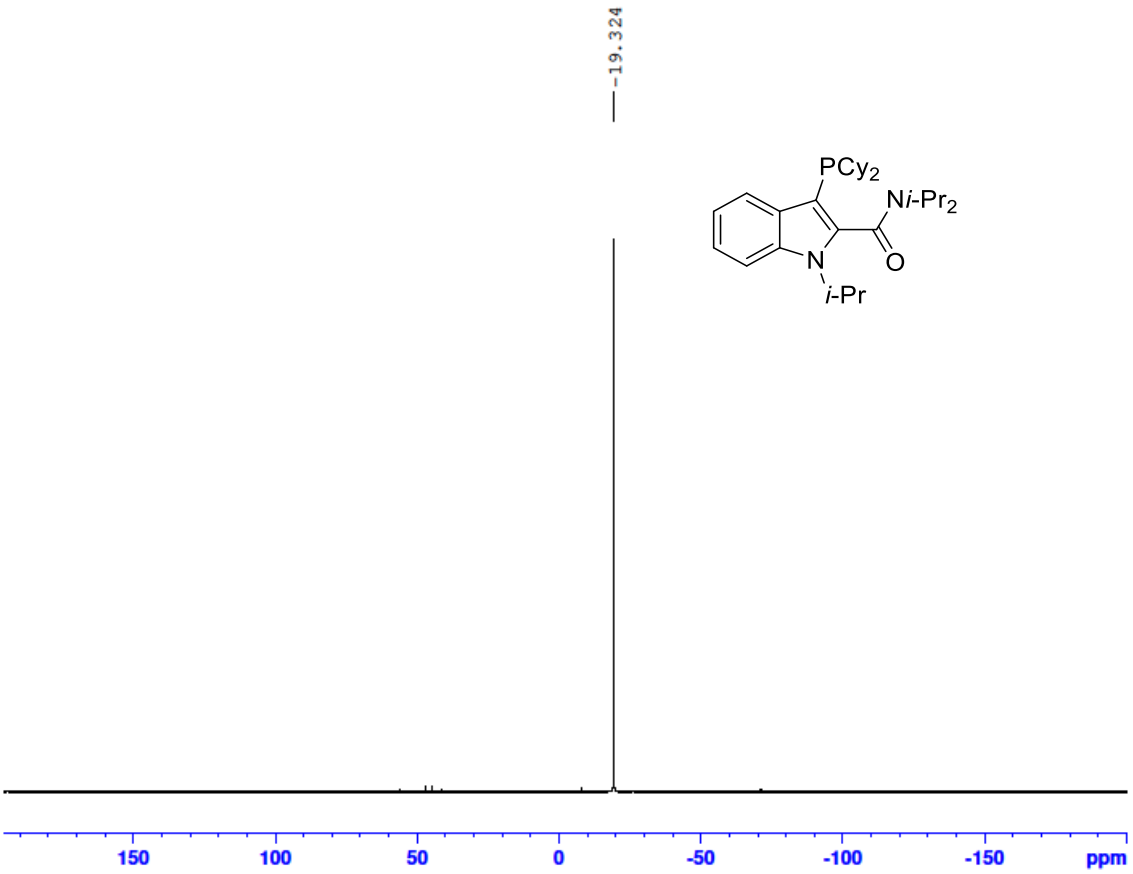
Mass	Calc. Mass	mDa	PPM	Formula
287.2121	287.2118	-0.31	-1.08	C18 H27 N2 O

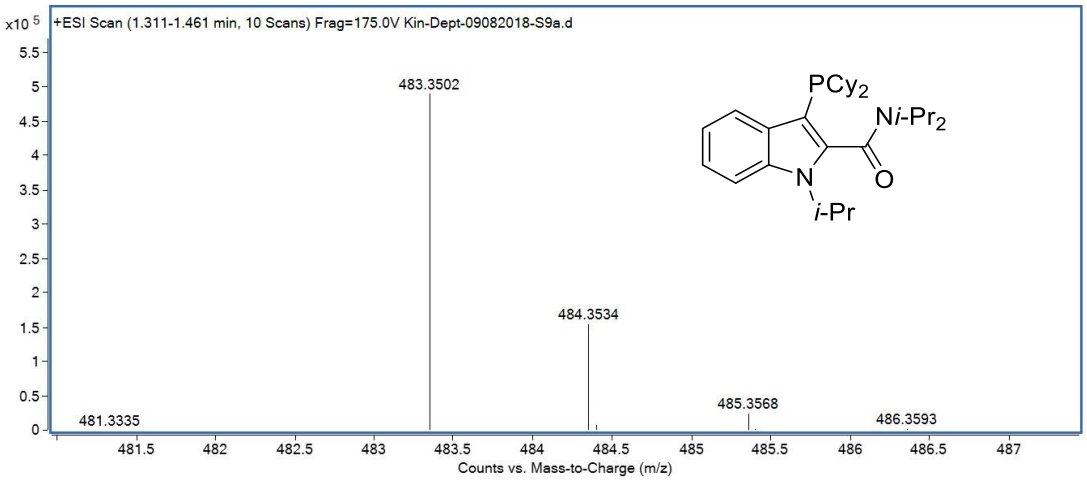

7.6143
7.6091
7.5948
7.5900
7.5629
7.5566
7.5422
7.5364
7.2880
7.2791
7.2624
7.2585
7.2531
7.2420
7.2349
7.2227
7.2162
4.5832
4.5745
4.5659
4.5572
3.9649
3.9571
3.9486
3.9407
3.9322
3.6227
3.6142
3.6059
3.5974
3.5691
1.7024
1.6918
1.6845
1.6748
1.6669
1.6591
1.6503
1.6449
1.6380
1.6285
1.3598
1.3514
1.3438
1.3353
1.1752
1.1670
1.1589
1.1506
Br
O
N
N(i-Pr)2
i-Pr
ppm
1.00
2.00
12.00
3.00
162.44
133.58
133.27
127.50
122.64
120.33
119.89
112.14
87.04
77.32
77.00
76.68
51.50
50.25
46.31
21.87
21.64
21.53
21.01
20.51
20.05



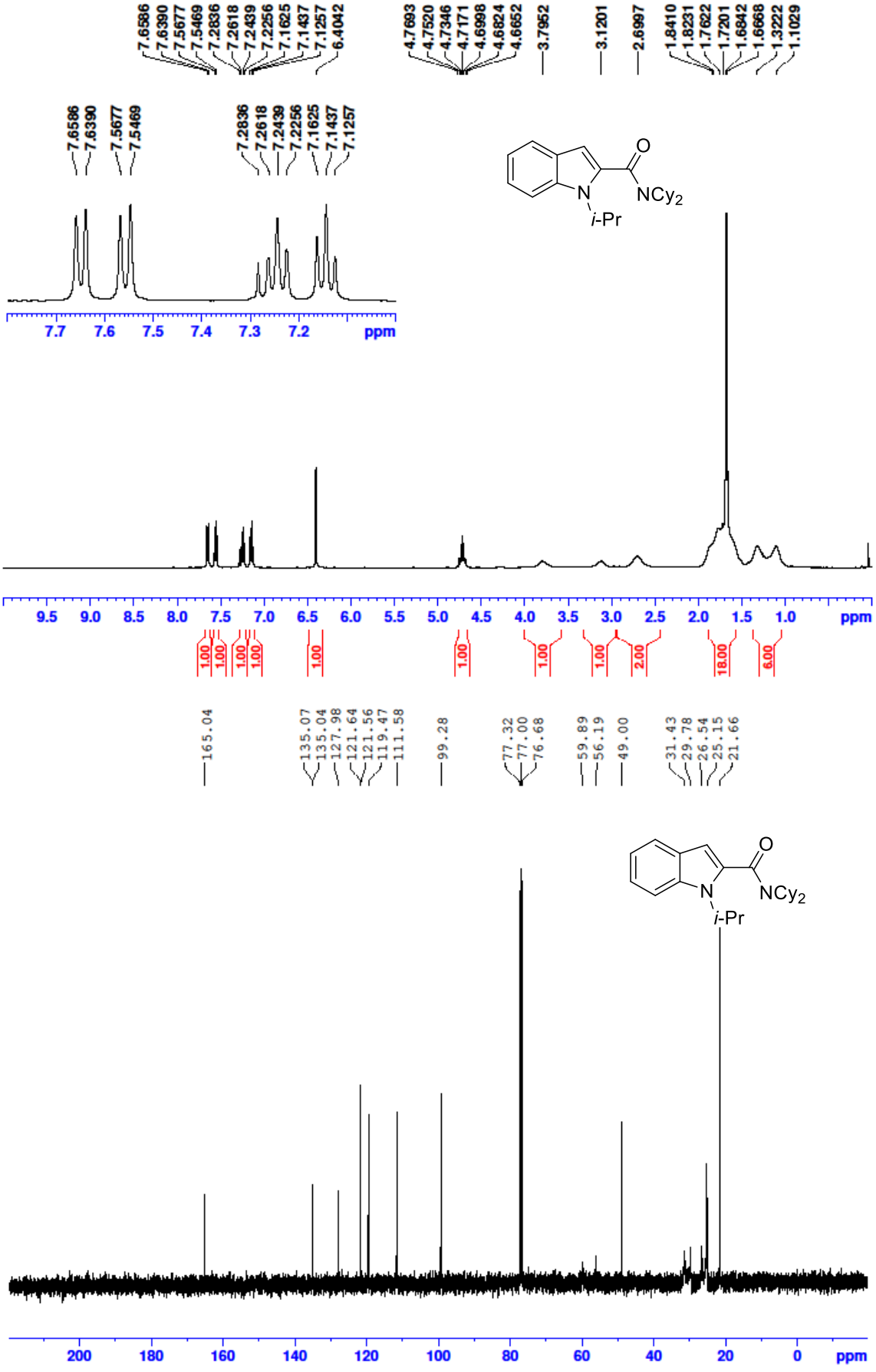
Mass	Calc. Mass	mDa	PPM	Formula
365.1225	365.1223	-0.20	-0.54	C18 H26 Br N2 O

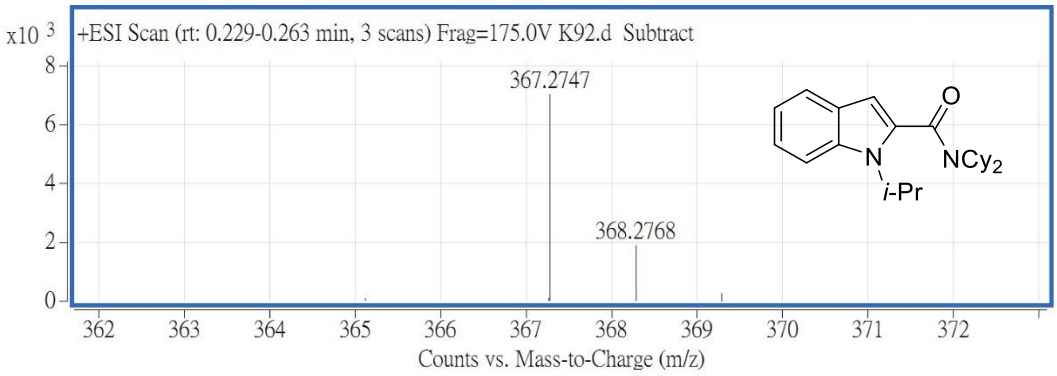

PCy2
Ni-Pr2
N
i-Pr
O
ppm



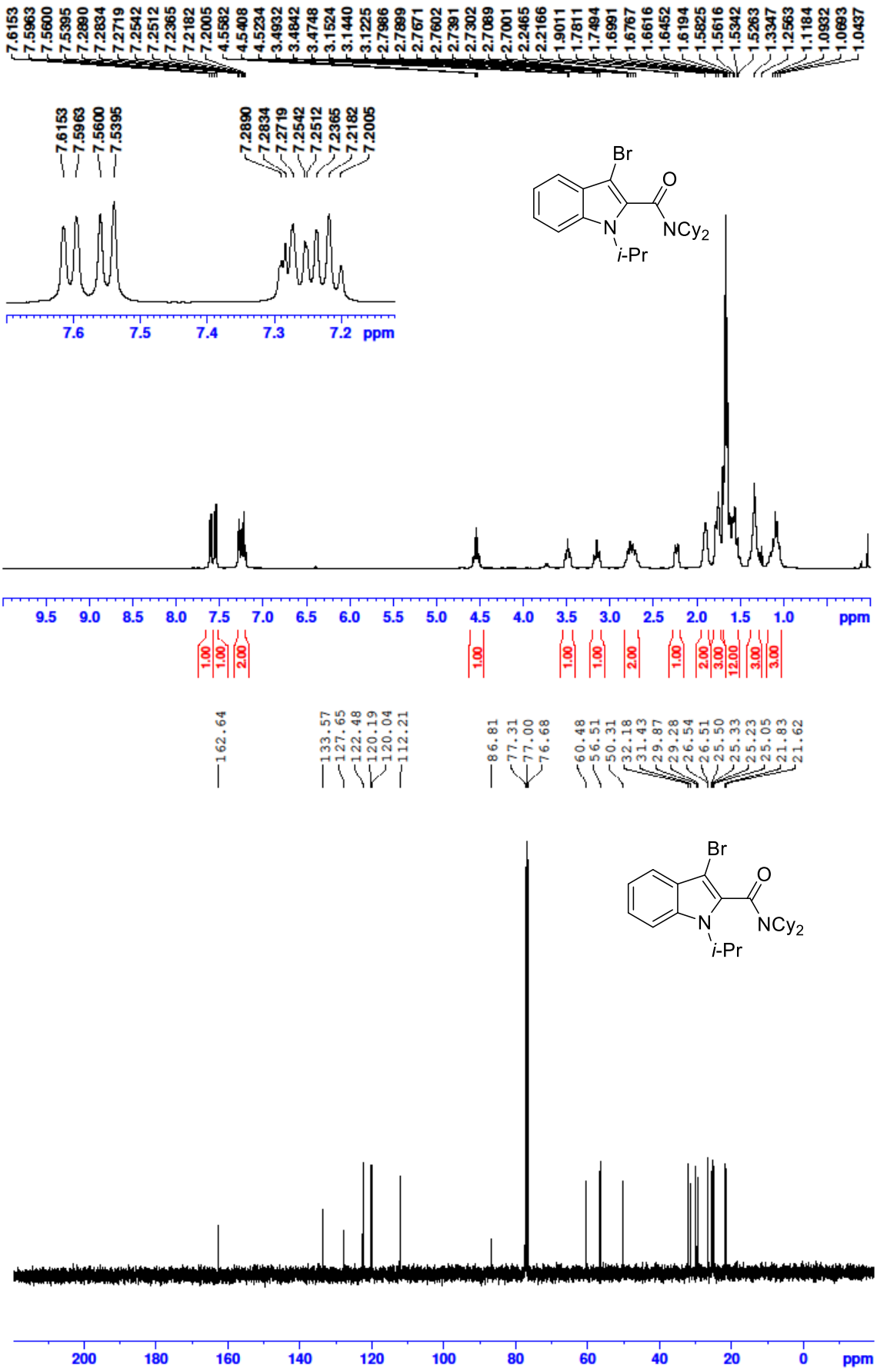


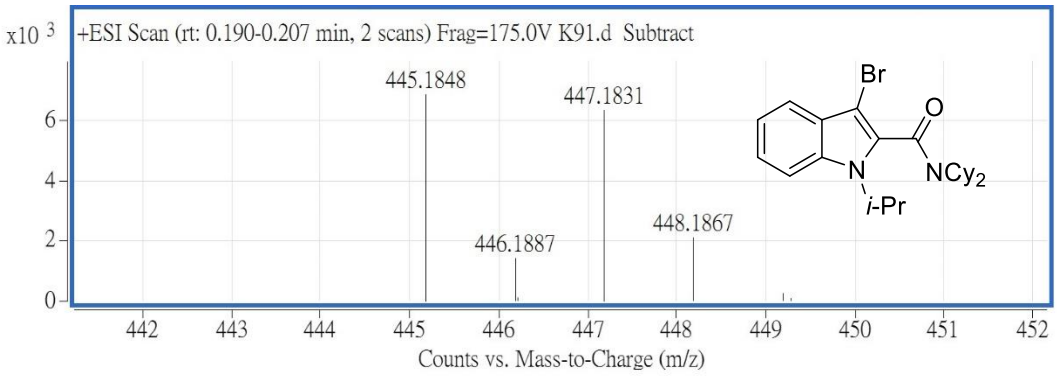
Mass	Calc. Mass	mDa	PPM	Formula
483.3502	483.3499	0.35	0.67	C30 H48 N2 O P


7.6586
7.6390
7.5677
7.5469
7.2836
7.2618
7.2439
7.2256
7.1625
7.1437
7.1257
6.4042
4.7693
4.7520
4.7346
4.7171
4.6998
4.6824
4.6652
3.7952
3.1201
2.6997
1.8410
1.8231
1.7622
1.7201
1.6842
1.6668
1.3222
1.1029
O
N
NCy2
i-Pr
ppm
1.00
2.00
18.00
6.00
165.04
135.07
135.04
127.98
121.64
121.56
119.47
111.58
99.28
77.32
77.00
76.68
59.89
56.19
49.00
31.43
29.78
26.54
25.15
21.66

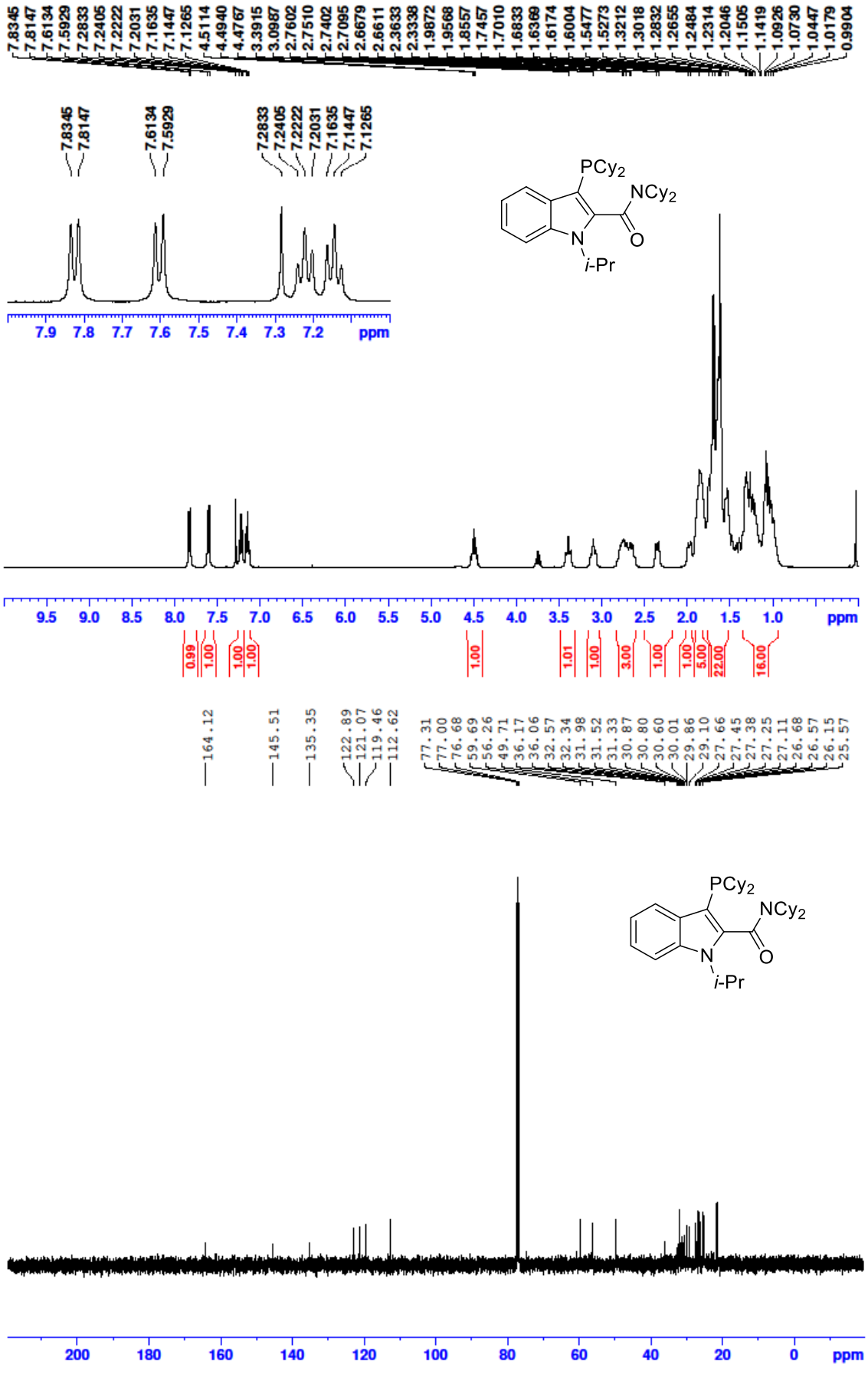


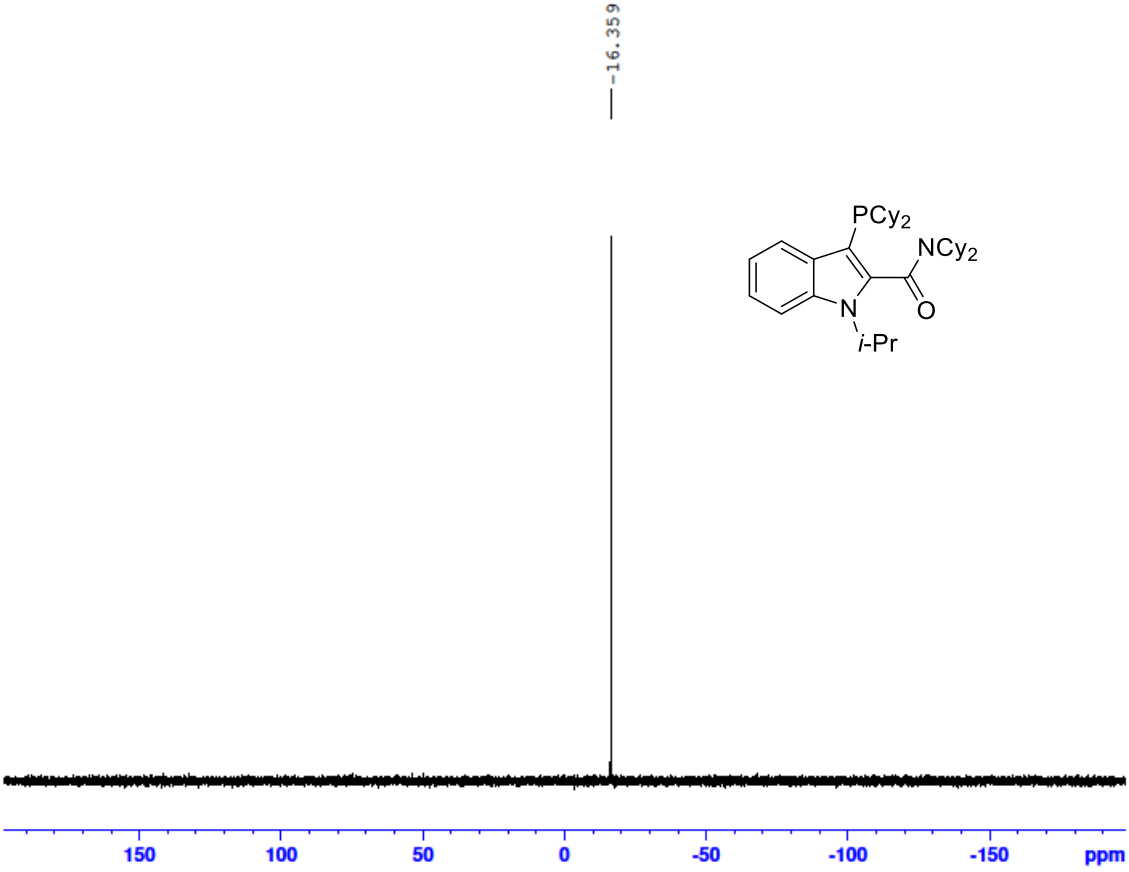
Mass	Calc. Mass	mDa	PPM	Formula
367.2747	367.2744	-0.31	-0.85	C24 H35 N2 O

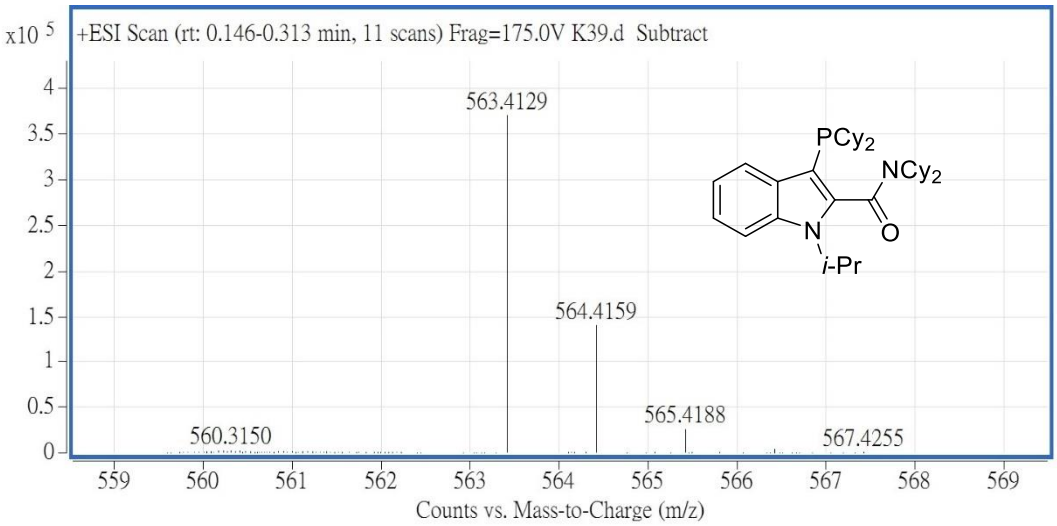

7.6153
7.5963
7.5600
7.5395
7.2890
7.2834
7.2719
7.2542
7.2512
7.2365
7.2182
7.2005
4.5582
4.5408
4.5234
3.4932
3.4842
3.4748
3.1524
3.1440
3.1225
2.7986
2.7899
2.7671
2.7602
2.7391
2.7302
2.7089
2.7001
2.2465
2.2166
1.9011
1.7811
1.7494
1.6991
1.6767
1.6616
1.6452
1.6194
1.5825
1.5616
1.5342
1.5263
1.3347
1.2563
1.1184
1.0932
1.0693
1.0437
Br
O
N
NCy2
i-Pr
7.6
7.5
7.4
7.3
7.2
ppm
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
ppm
1.00
1.00
2.00
1.00
1.00
1.00
2.00
1.00
2.00
3.00
12.00
3.00
3.00
162.64
133.57
127.65
122.48
120.19
120.04
112.21
86.81
77.31
77.00
76.68
60.48
56.51
50.31
32.18
31.43
29.87
29.28
26.54
26.51
25.50
25.33
25.23
25.05
21.83
21.62
Br
O
N
NCy2
i-Pr
200
180
160
140
120
100
80
60
40
20
0
ppm



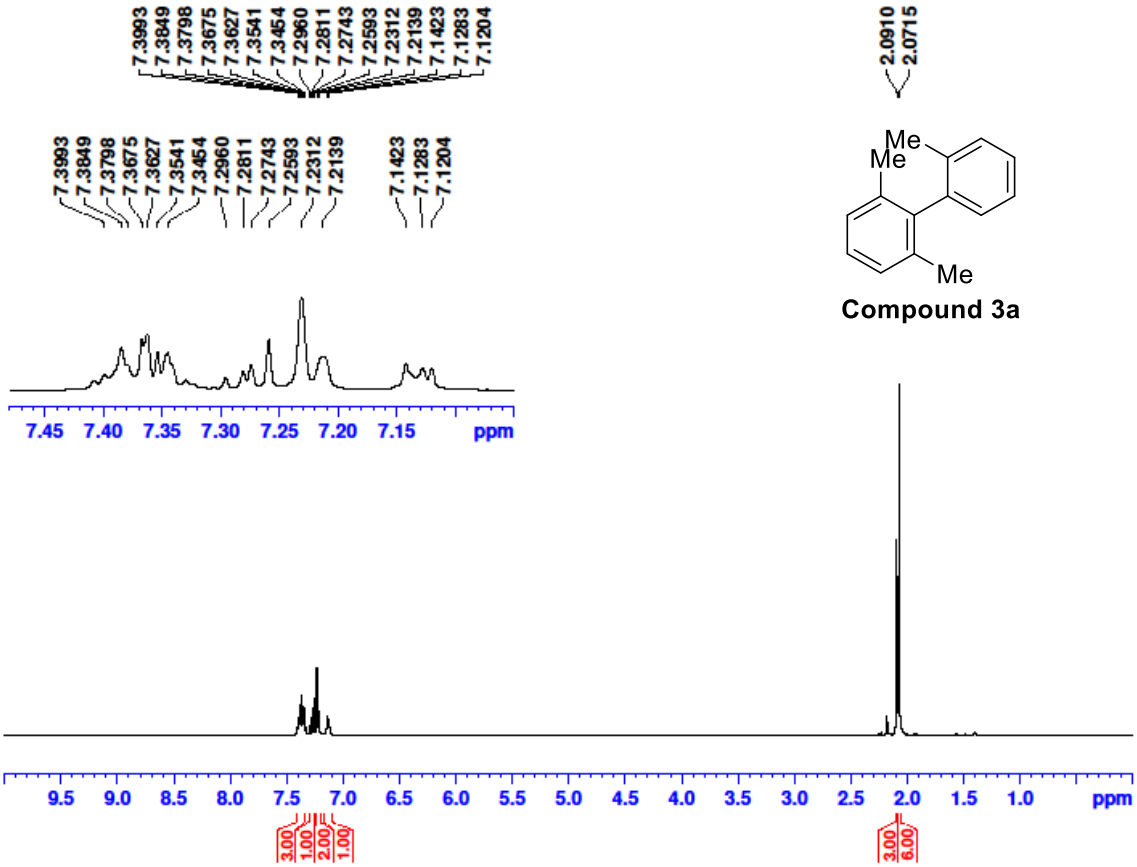
Mass	Calc. Mass	mDa	PPM	Formula
445.1848	445.1849	0.10	0.23	C24 H34 Br N2 O

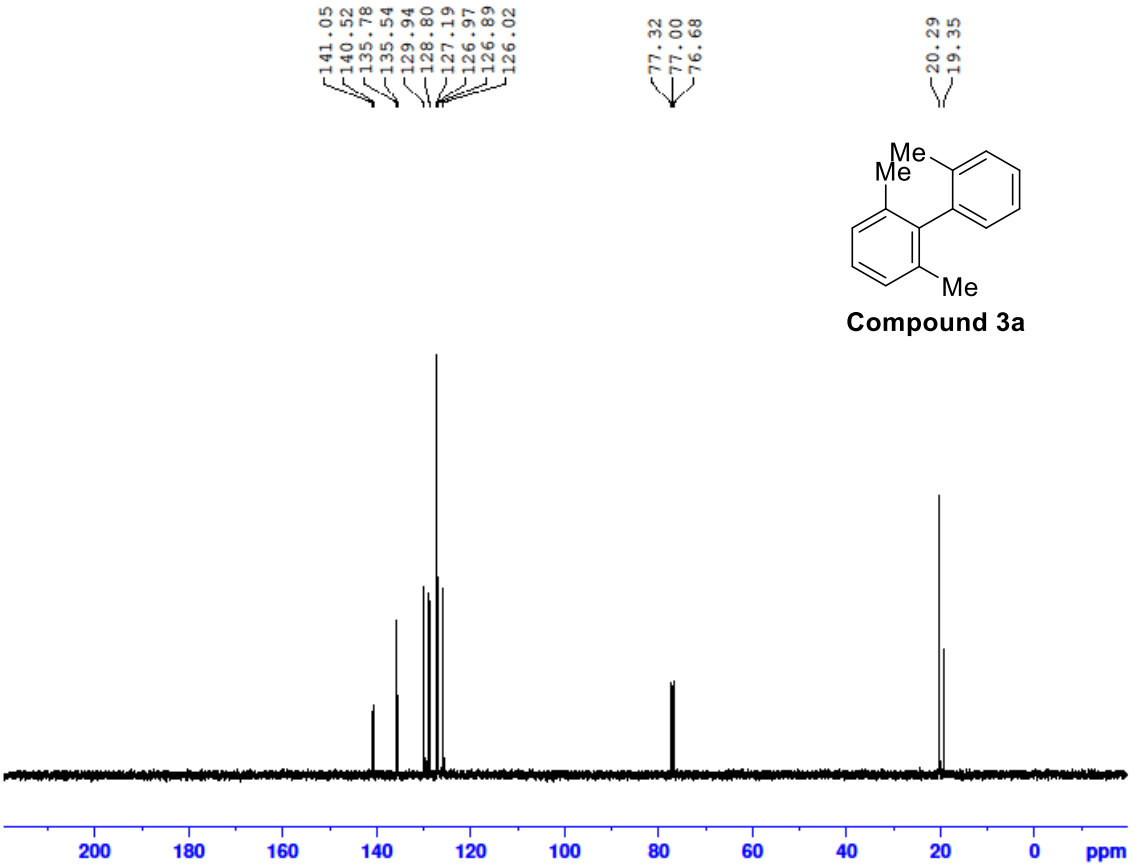

7.8345
7.8147
7.6134
7.5929
7.2833
7.2405
7.2222
7.2031
7.1635
7.1447
7.1265
4.5114
4.4940
4.4767
3.3915
3.0987
2.7602
2.7510
2.7402
2.7095
2.6679
2.6611
2.3633
2.3338
1.9872
1.9568
1.8557
1.7457
1.7010
1.6833
1.6369
1.6174
1.6004
1.5477
1.5273
1.3212
1.3018
1.2832
1.2655
1.2484
1.2314
1.2046
1.1505
1.1419
1.0926
1.0730
1.0447
1.0179
0.9904
PCy2
NCy2
N
O
i-Pr
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
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 ppm
0.99
1.00
1.00
1.00
1.00
1.01
1.00
3.00
1.00
1.00
5.00
22.00
16.00
164.12
145.51
135.35
122.89
121.07
119.46
112.62
77.31
77.00
76.68
59.69
56.26
49.71
36.17
36.06
32.57
32.34
31.98
31.52
31.33
30.87
30.80
30.60
30.01
29.86
29.10
27.66
27.45
27.38
27.25
27.11
26.68
26.57
26.15
25.57
200 180 160 140 120 100 80 60 40 20 0 ppm

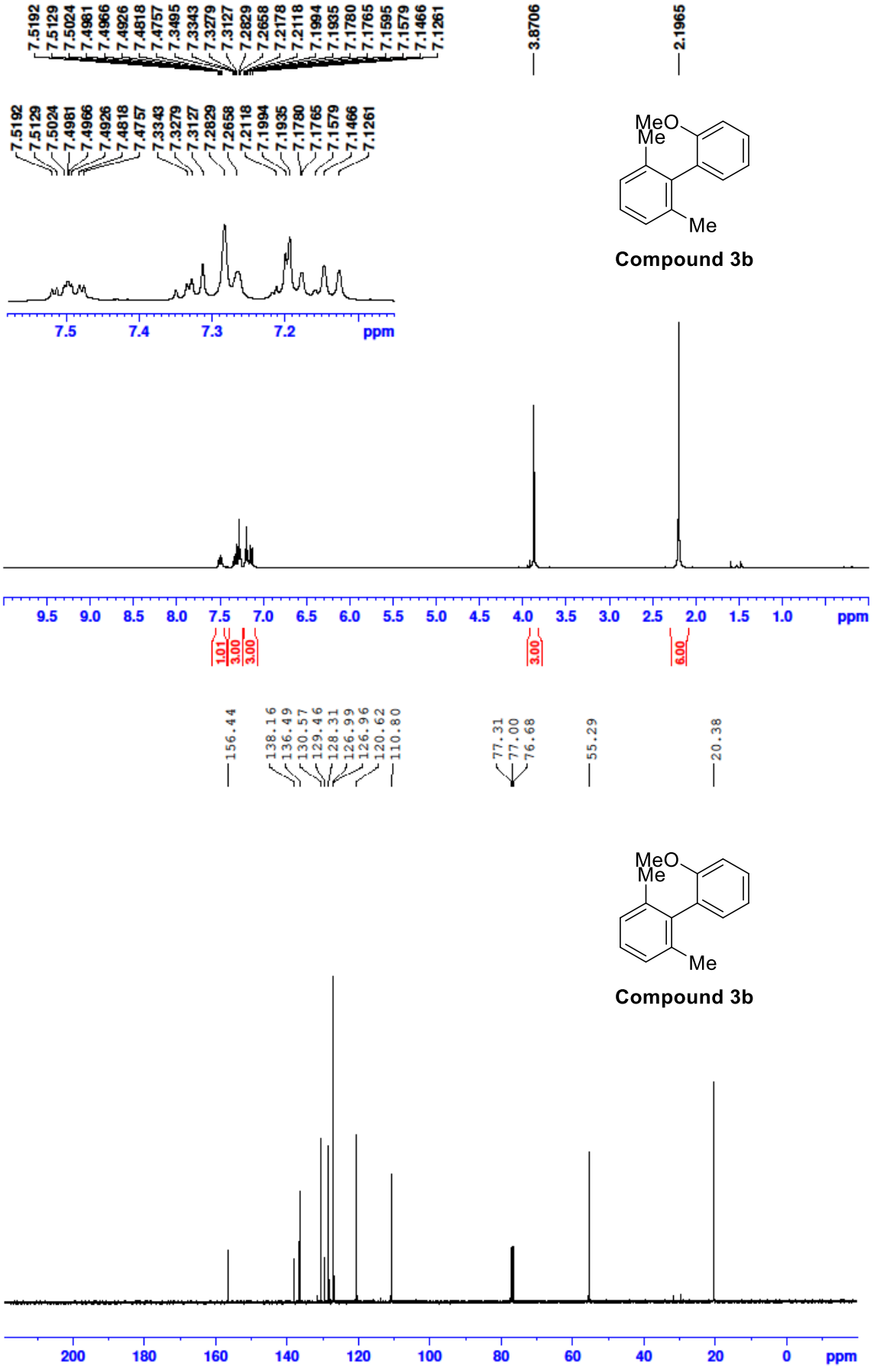


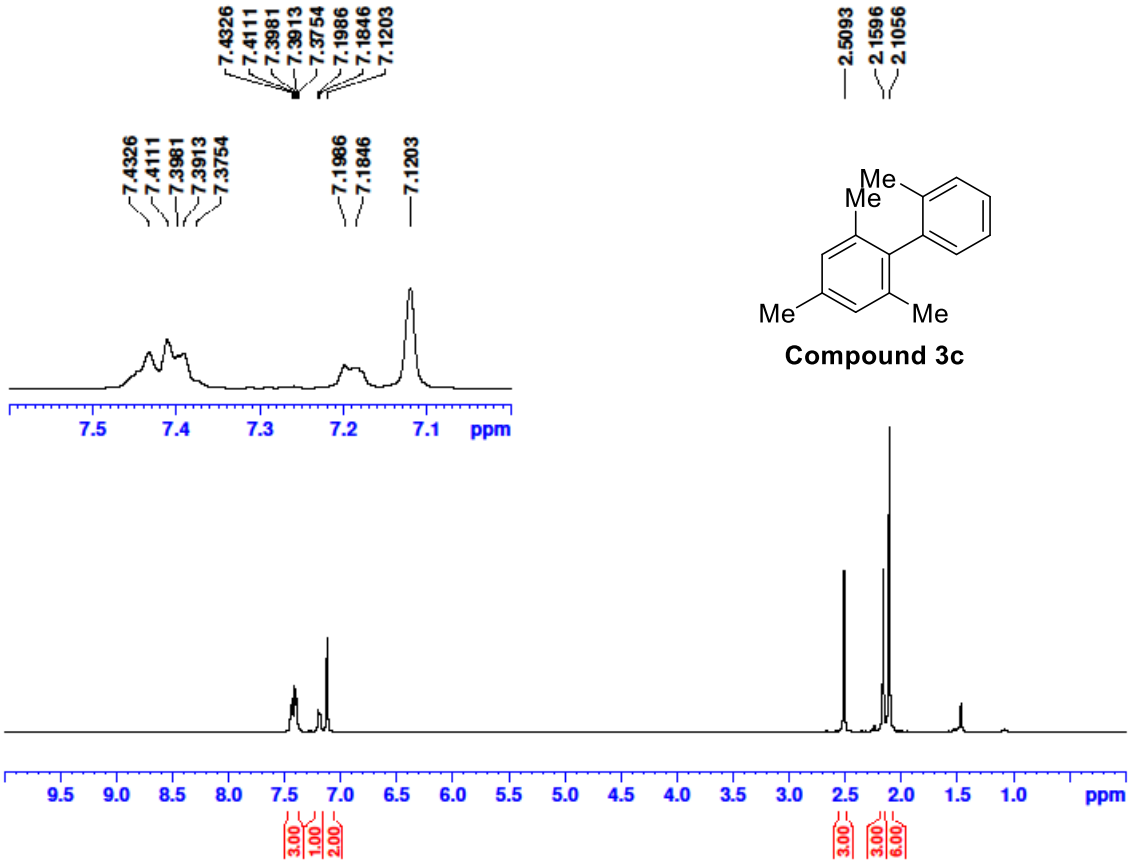


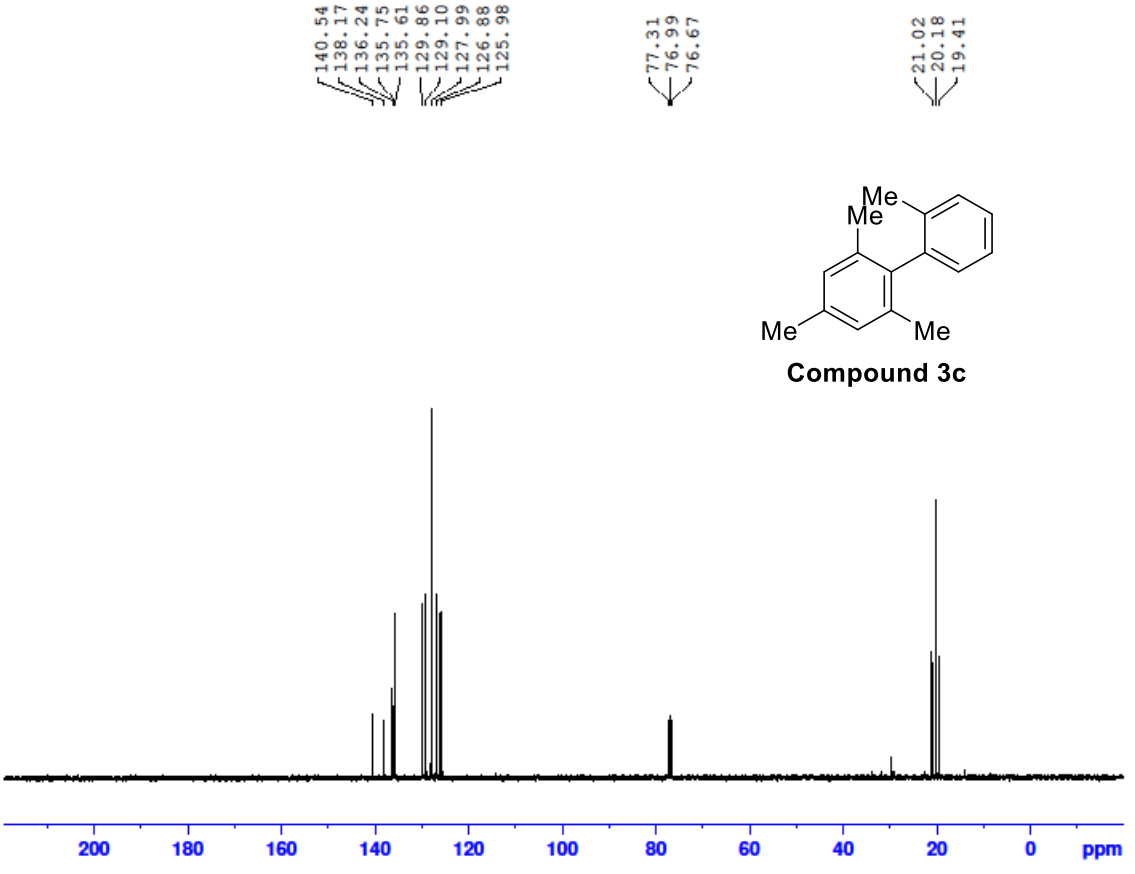
Mass	Calc. Mass	mDa	PPM	Formula
563.4129	563.4125	-0.41	-0.75	C36 H56 N2 O P

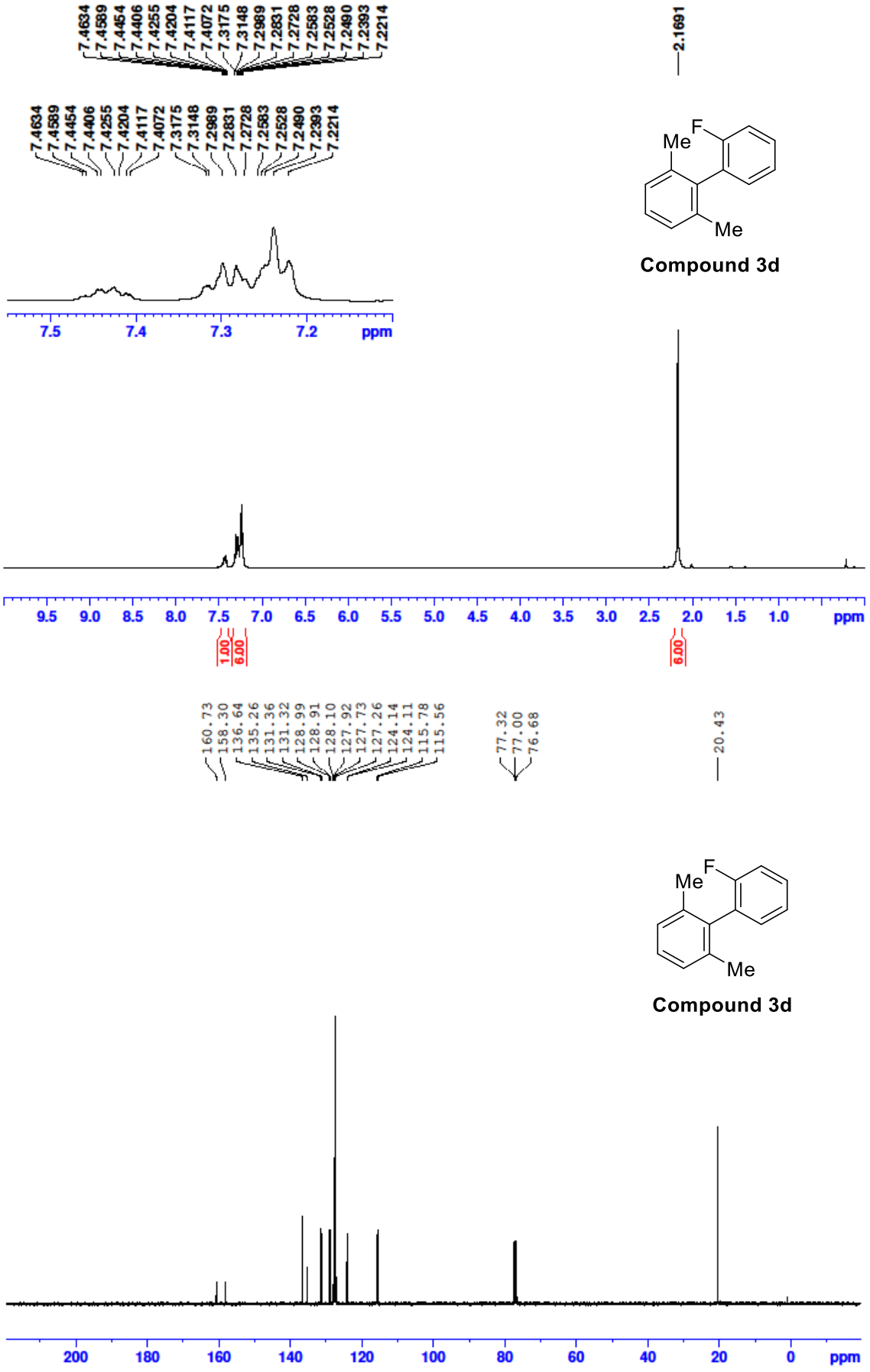

7.3993
7.3849
7.3798
7.3675
7.3627
7.3541
7.3454
7.2960
7.2811
7.2743
7.2593
7.2312
7.2139
7.1423
7.1283
7.1204
2.0910
2.0715
Me
Me
Me
Compound 3a
7.45 7.40 7.35 7.30 7.25 7.20 7.15 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
3.00
1.00
2.00
1.00
3.00
6.00

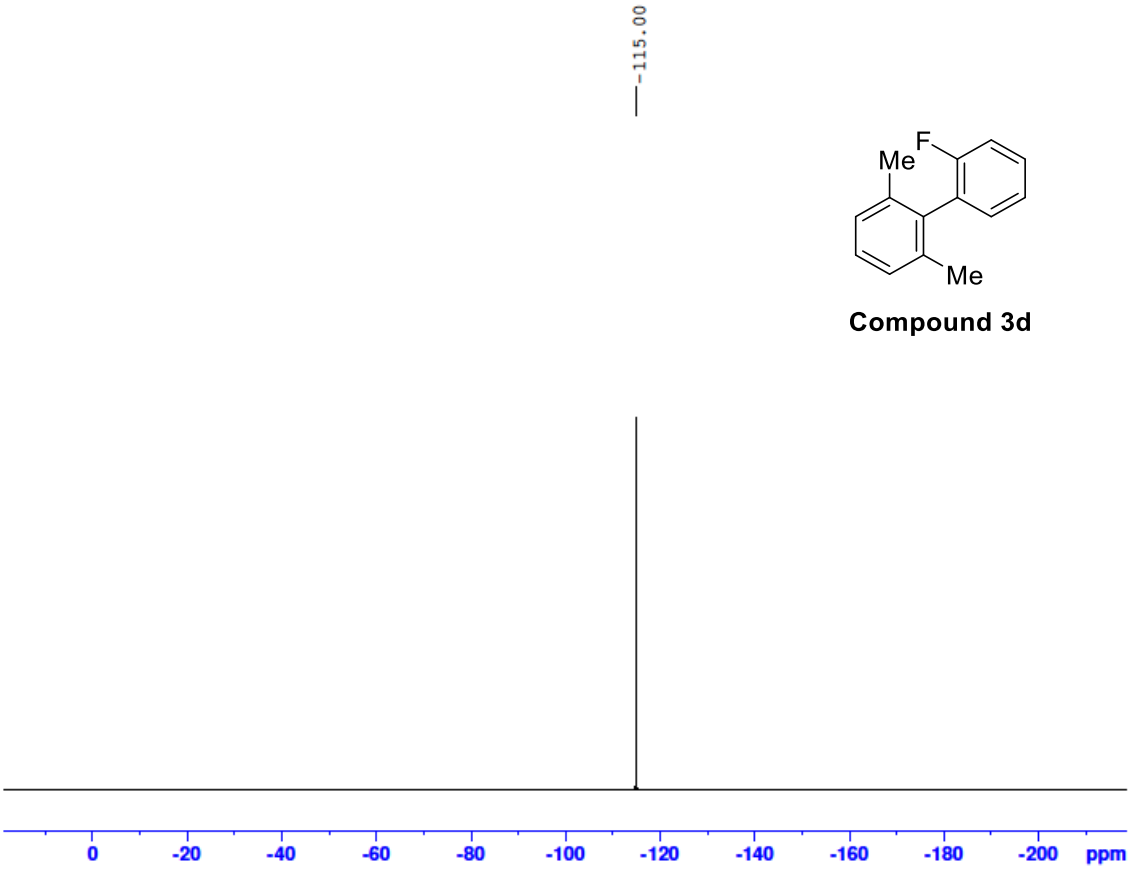

141.05
140.52
135.78
135.54
129.94
128.80
127.19
126.97
126.89
126.02
77.32
77.00
76.68
20.29
19.35
Me
Me
Me
Compound 3a
200 180 160 140 120 100 80 60 40 20 0 ppm


7.5192
7.5129
7.5024
7.4981
7.4966
7.4926
7.4818
7.4757
7.3495
7.3343
7.3279
7.3127
7.2829
7.2658
7.2178
7.2118
7.1994
7.1935
7.1780
7.1765
7.1595
7.1579
7.1466
7.1261
3.8706
2.1965
MeO
Me
Me
Compound 3b
7.5
7.4
7.3
7.2
ppm
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
ppm
1.01
3.00
3.00
3.00
6.00
156.44
138.16
136.49
130.57
129.46
128.31
126.99
126.96
120.62
110.80
77.31
77.00
76.68
55.29
20.38
MeO
Me
Me
Compound 3b
200
180
160
140
120
100
80
60
40
20
0
ppm

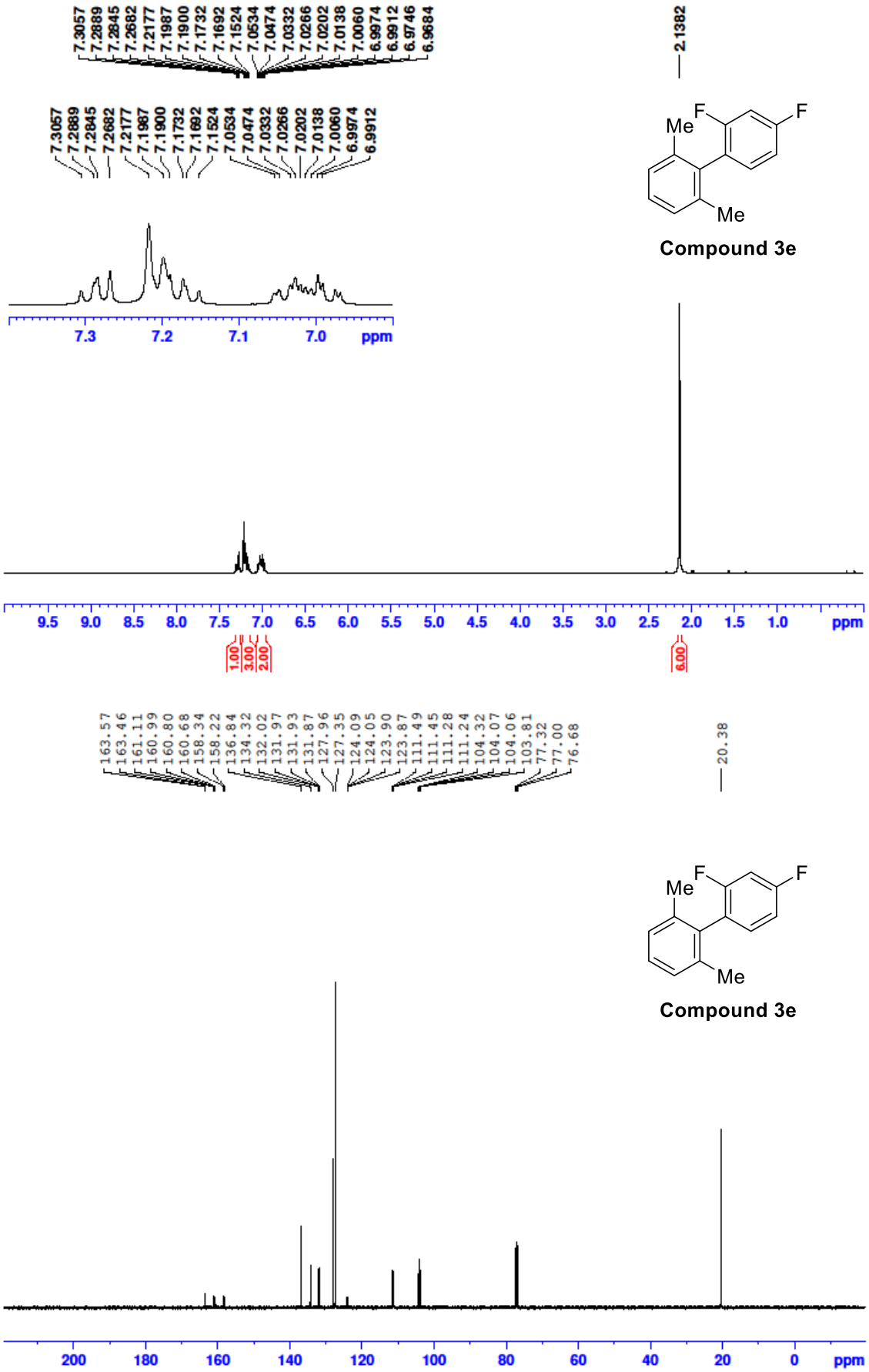

7.4326
7.4111
7.3981
7.3913
7.3754
7.1986
7.1846
7.1203
2.5093
2.1596
2.1056
Me
Me
Me
Me
Compound 3c
7.5
7.4
7.3
7.2
7.1
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
3.00
1.00
2.00
3.00
3.00
6.00

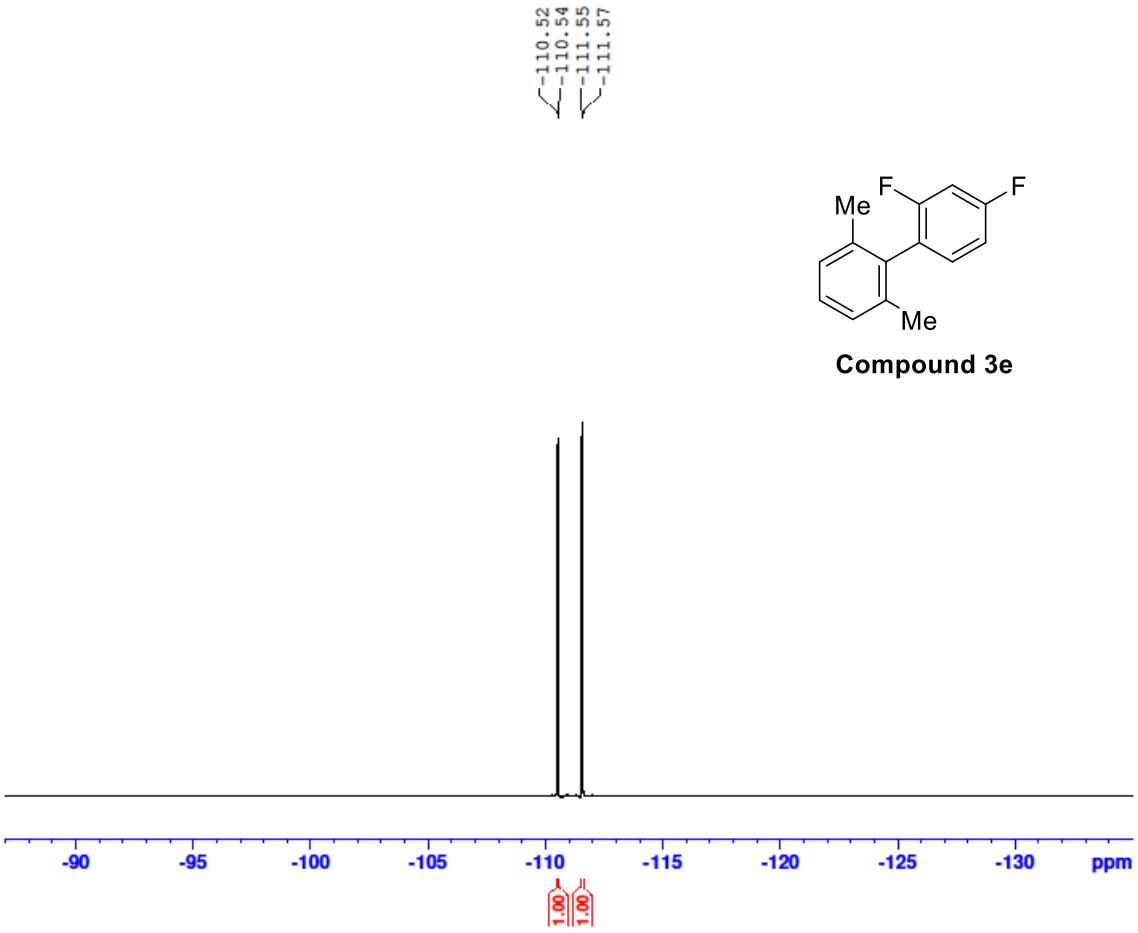

140.54
138.17
136.24
135.75
135.61
129.86
129.10
127.99
126.88
125.98
77.31
76.99
76.67
21.02
20.18
19.41
Me
Me
Me
Me
Compound 3c
200
180
160
140
120
100
80
60
40
20
0
ppm


7.4634
7.4589
7.4454
7.4406
7.4255
7.4204
7.4117
7.4072
7.3175
7.3148
7.2989
7.2831
7.2728
7.2583
7.2528
7.2490
7.2393
7.2214
2.1691
Me
F
Me
Compound 3d
7.5
7.4
7.3
7.2
ppm
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
ppm
1.00
6.00
6.00
160.73
158.30
136.64
135.26
131.36
131.32
128.99
128.91
128.10
127.92
127.73
127.26
124.14
124.11
115.78
115.56
77.32
77.00
76.68
20.43
Me
F
Me
Compound 3d
200
180
160
140
120
100
80
60
40
20
0
ppm

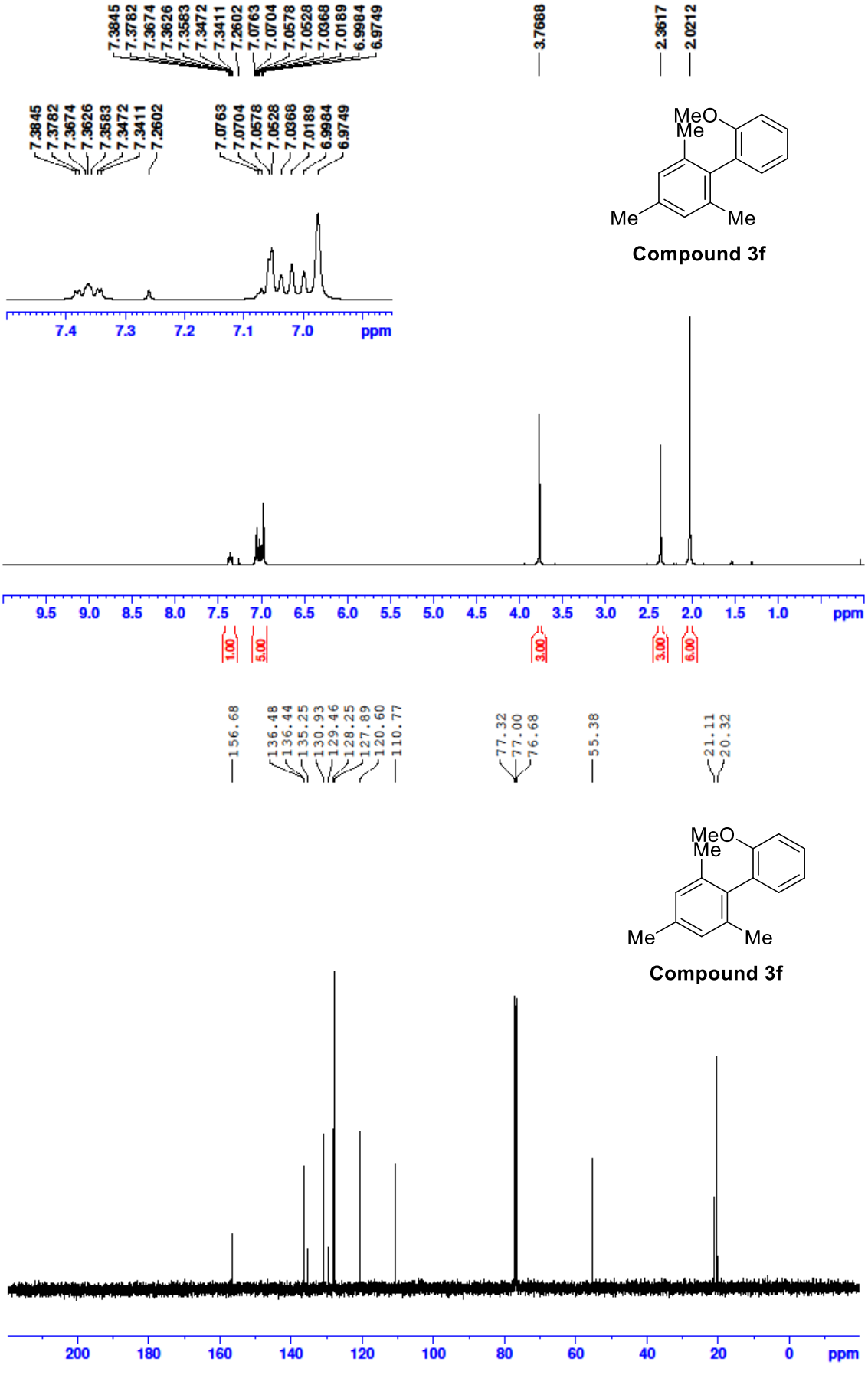


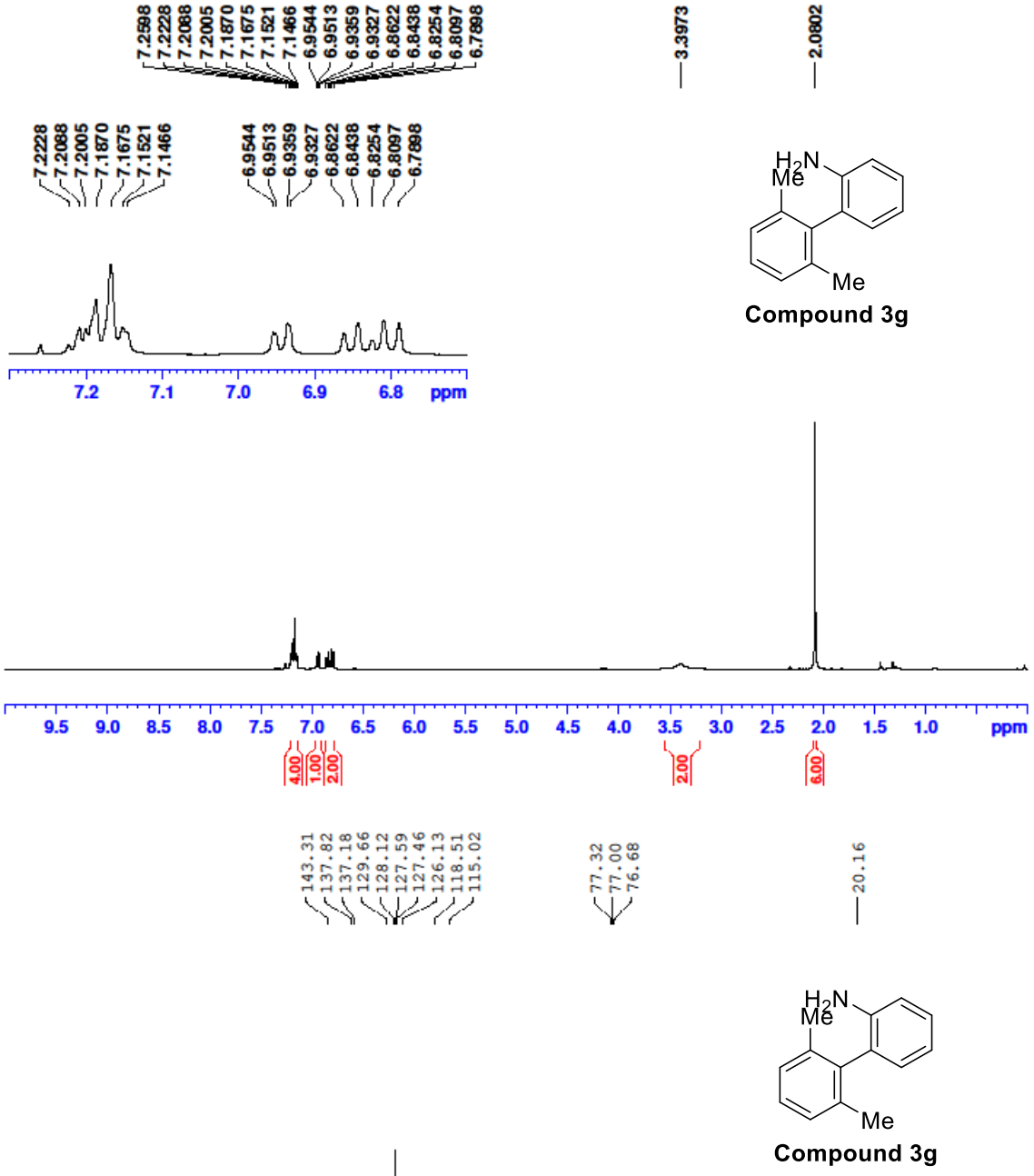
Compound 3d

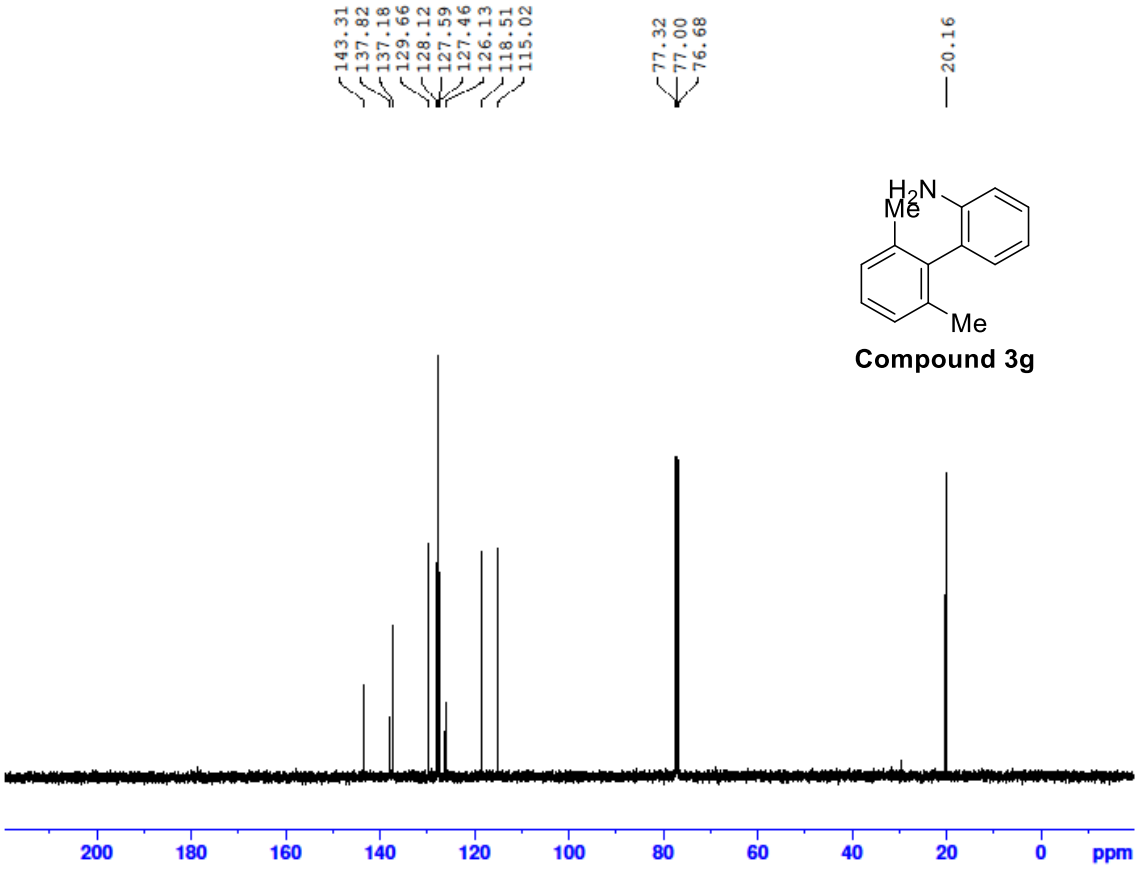

7.3057
7.2889
7.2845
7.2682
7.2177
7.1987
7.1900
7.1732
7.1692
7.1524
7.0534
7.0474
7.0332
7.0266
7.0202
7.0138
7.0060
6.9974
6.9912
6.9746
6.9684
2.1382
Me
F
F
Me
Compound 3e
7.3
7.2
7.1
7.0
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
3.00
2.00
6.00
163.57
163.46
161.11
160.99
160.80
160.68
158.34
158.22
136.84
134.32
132.02
131.97
131.93
131.87
127.96
127.35
124.09
124.05
123.90
123.87
111.49
111.45
111.28
111.24
104.32
104.07
104.06
103.81
77.32
77.00
76.68
20.38
Me
F
F
Me
Compound 3e
200
180
160
140
120
100
80
60
40
20
0
ppm

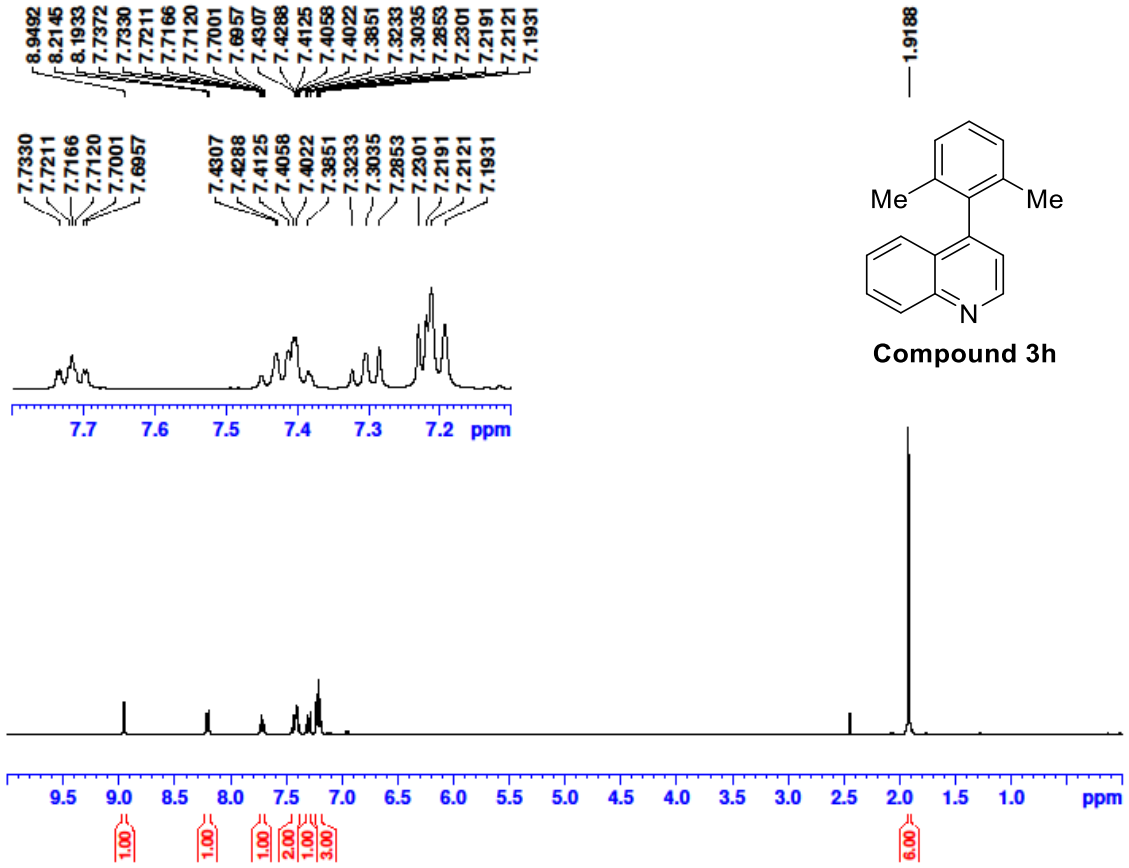

-110.52
-110.54
-111.55
-111.57
F
F
Me
Me
-90
-95
-100
-105
-110
-115
-120
-125
-130
ppm
1.00
1.00

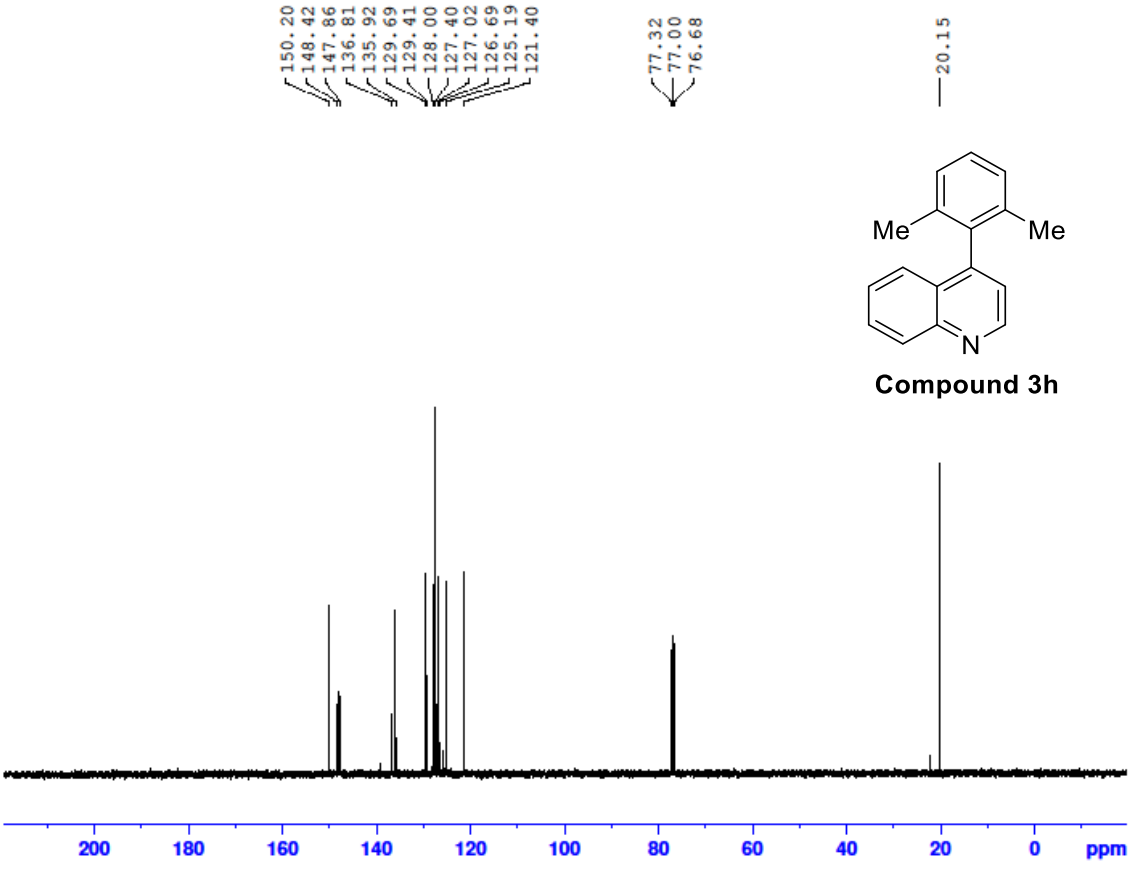
Compound 3e

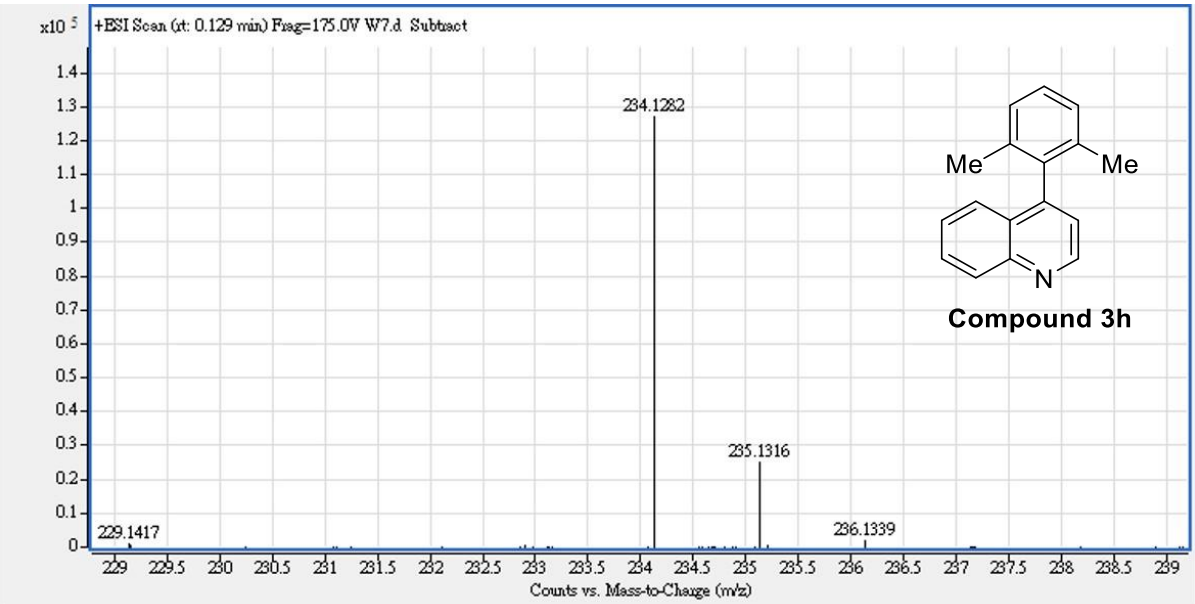

7.3845
7.3782
7.3674
7.3626
7.3583
7.3472
7.3411
7.2602
7.0763
7.0704
7.0578
7.0528
7.0368
7.0189
6.9984
6.9749
3.7688
2.3617
2.0212
MeO
Me
Me
Me
Compound 3f
7.4
7.3
7.2
7.1
7.0
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
5.00
3.00
3.00
6.00
156.68
136.48
136.44
135.25
130.93
129.46
128.25
127.89
120.60
110.77
77.32
77.00
76.68
55.38
21.11
20.32
MeO
Me
Me
Me
Compound 3f
200
180
160
140
120
100
80
60
40
20
0
ppm


7.2598
7.2228
7.2068
7.2005
7.1670
7.1675
7.1521
7.1466
6.9544
6.9513
6.9359
6.9327
6.8622
6.8438
6.8254
6.8097
6.7898
3.3973
2.0802
H2N
Me
Me
Compound 3g
7.2 7.1 7.0 6.9 6.8 ppm
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 ppm
4.00
1.00
2.00
2.00
6.00

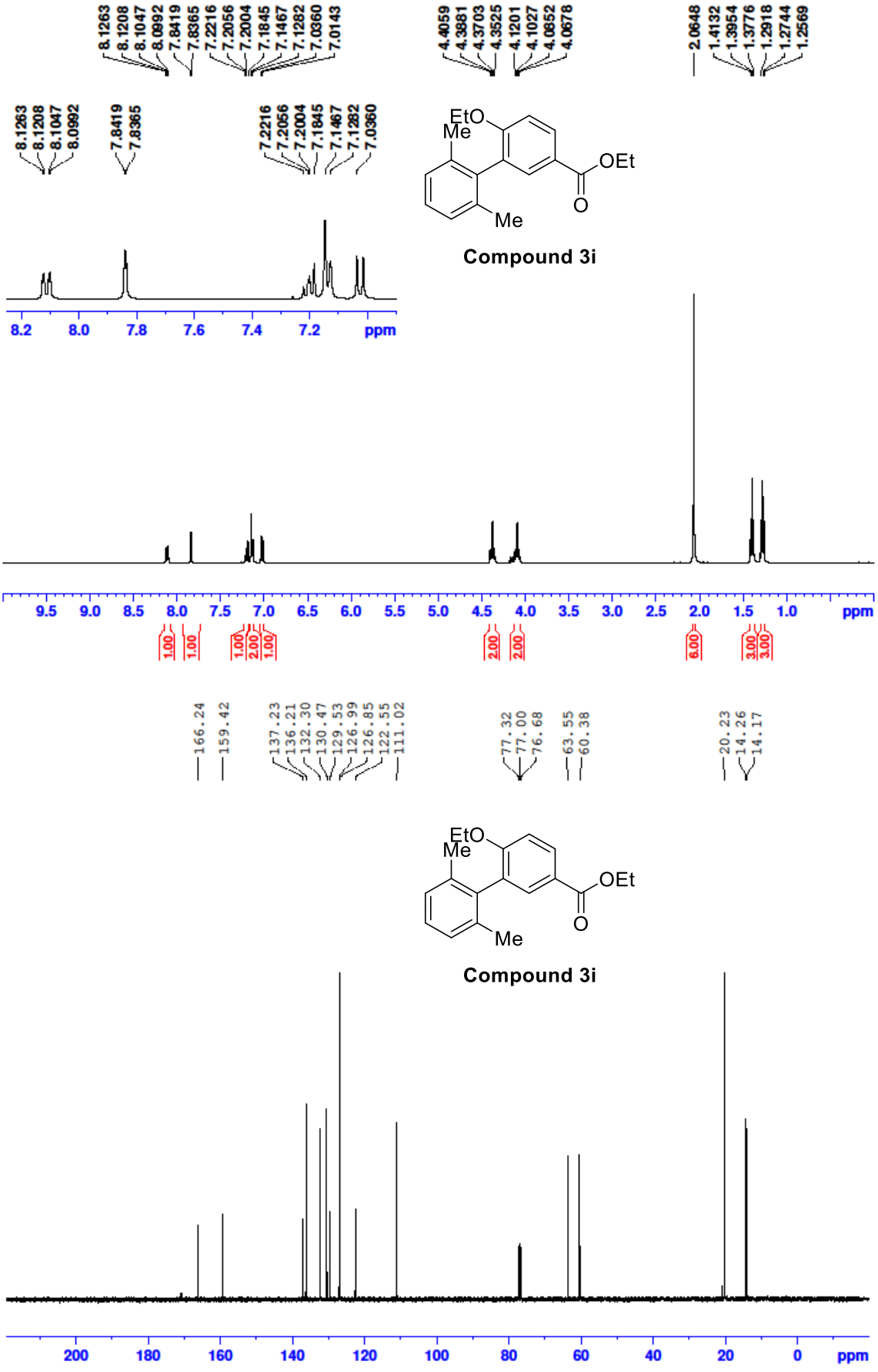

143.31
137.82
137.18
129.66
128.12
127.59
127.46
126.13
118.51
115.02
77.32
77.00
76.68
20.16
H2N
Me
Me
Compound 3g
200 180 160 140 120 100 80 60 40 20 0 ppm

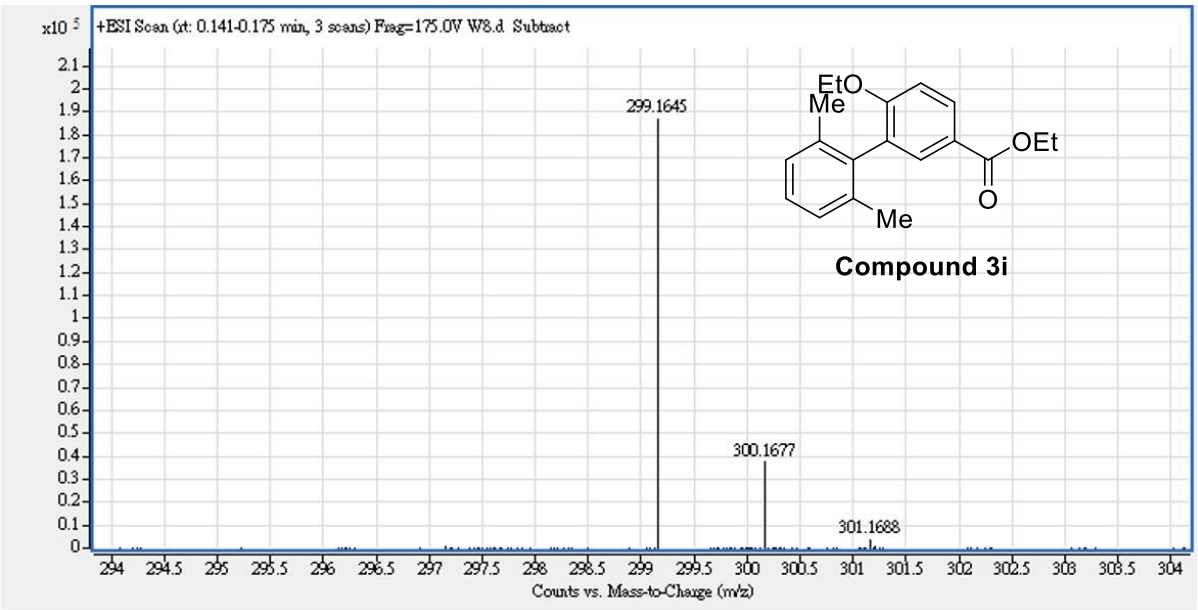

8.9492
8.2145
8.1933
7.7372
7.7330
7.7211
7.7166
7.7120
7.7001
7.6957
7.4307
7.4288
7.4125
7.4058
7.4022
7.3851
7.3233
7.3035
7.2853
7.2301
7.2191
7.2121
7.1931
1.9188
Me
Me
N
Compound 3h
7.7 7.6 7.5 7.4 7.3 7.2 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00 1.00 1.00 2.00 1.00 3.00 6.00


150.20
148.42
147.86
136.81
135.92
129.69
129.41
128.00
127.40
127.02
126.69
125.19
121.40
77.32
77.00
76.68
20.15
Me
Me
N
Compound 3h
200 180 160 140 120 100 80 60 40 20 0 ppm

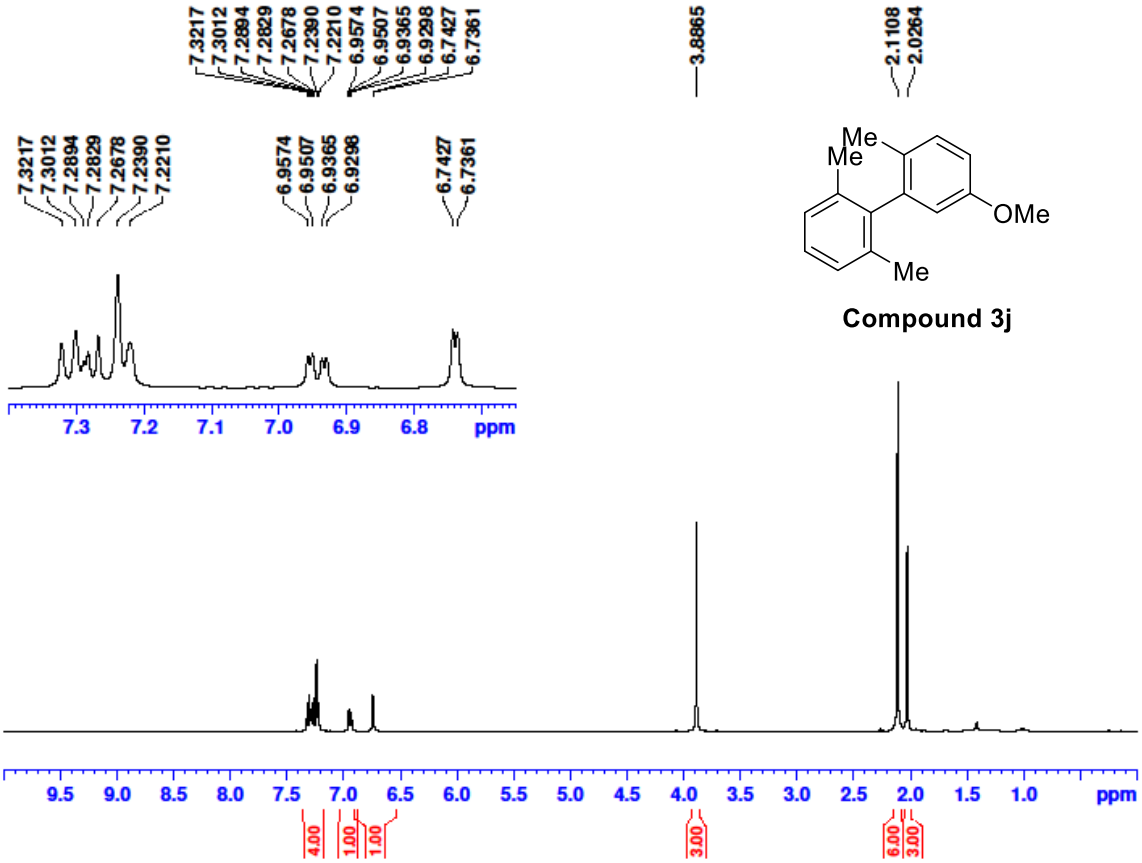


Mass	Calc. Mass	mDa	PPM	Formula
234.1282	234.1277	-0.47	-2.03	C17 H16 N

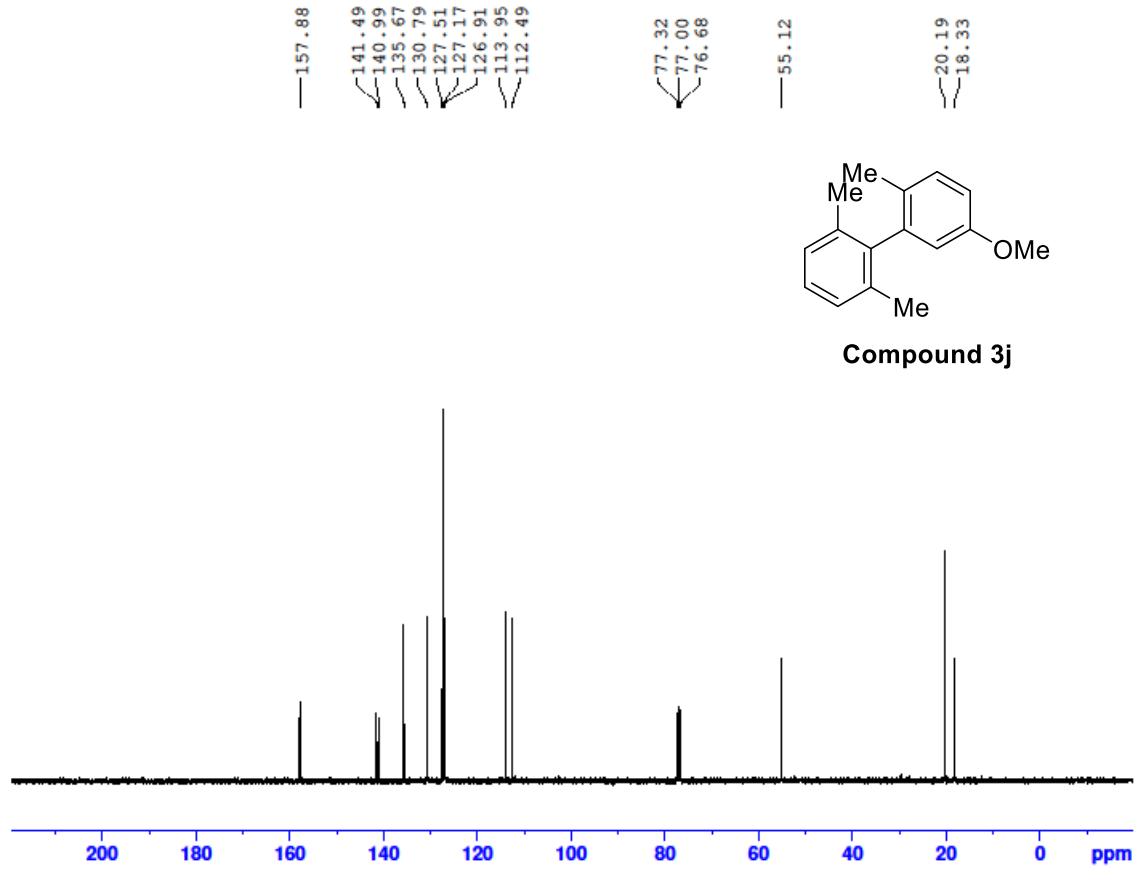

8.1263
8.1208
8.1047
8.0992
7.8419
7.8365
7.2216
7.2056
7.2004
7.1845
7.1467
7.1282
7.0360
7.0143
4.4059
4.3881
4.3703
4.3525
4.1201
4.1027
4.0852
4.0678
2.0648
1.4132
1.3954
1.3776
1.2918
1.2744
1.2569
EtO
Me
OEt
O
Me
Compound 3i
8.2
8.0
7.8
7.6
7.4
7.2
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.00
1.00
2.00
1.00
2.00
2.00
6.00
3.00
3.00
166.24
159.42
137.23
136.21
132.30
130.47
129.53
126.99
126.85
122.55
111.02
77.32
77.00
76.68
63.55
60.38
20.23
14.26
14.17
EtO
Me
OEt
O
Me
Compound 3i
200
180
160
140
120
100
80
60
40
20
0
ppm



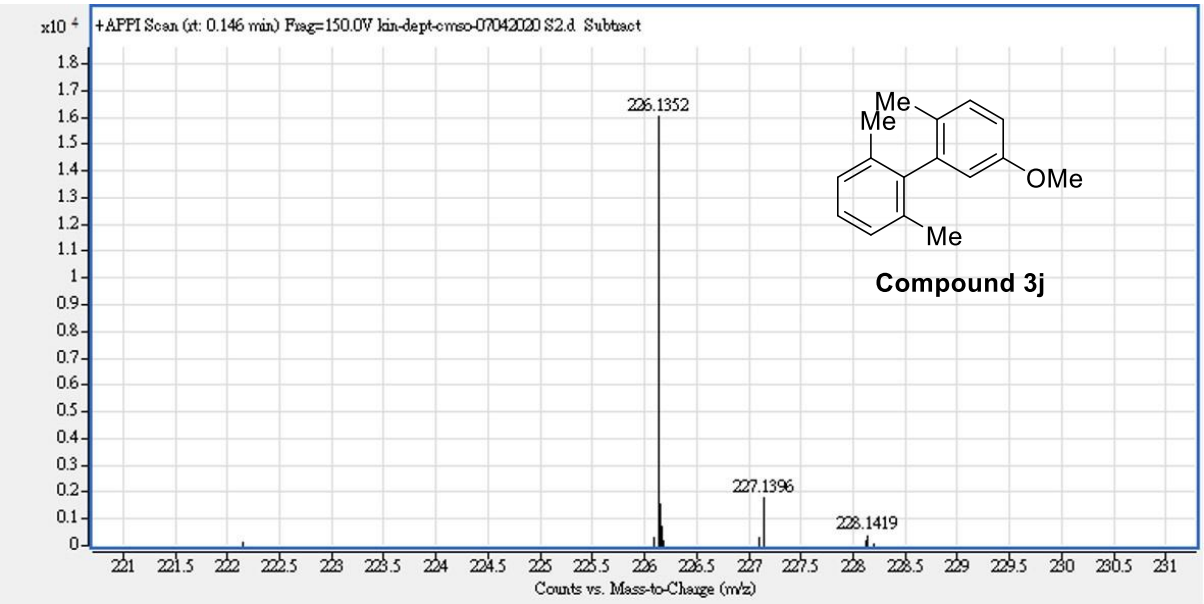
Mass	Calc. Mass	mDa	PPM	Formula
299.1645	299.1642	-0.33	-1.1	C19 H23 O3



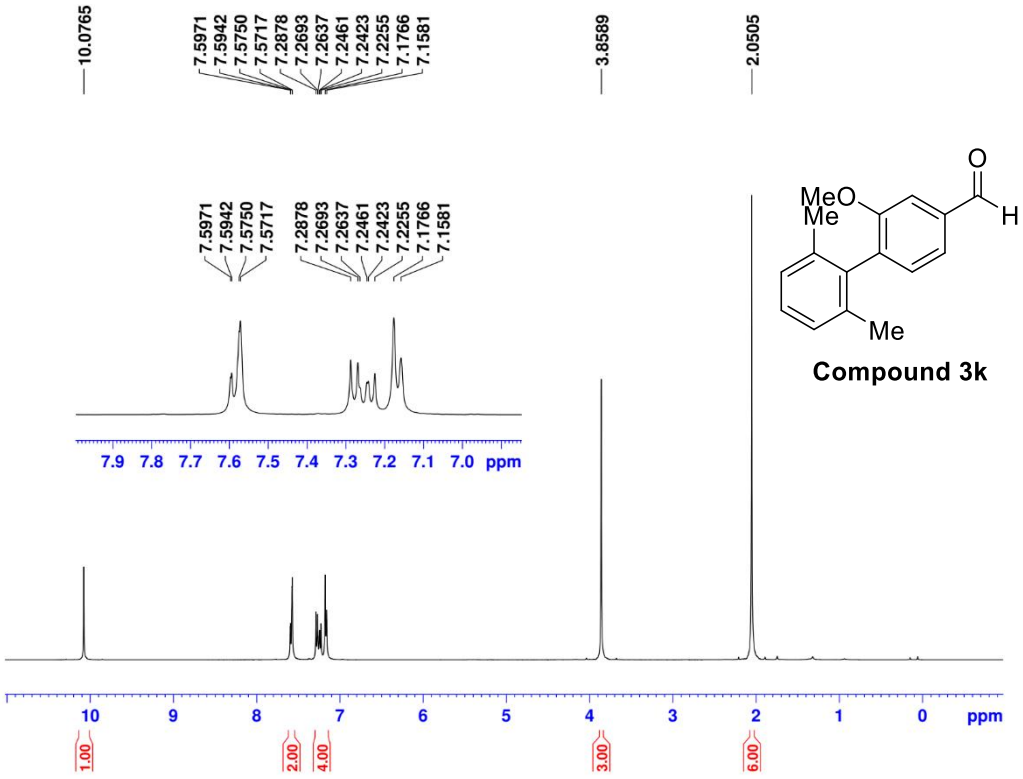
Compound 3j

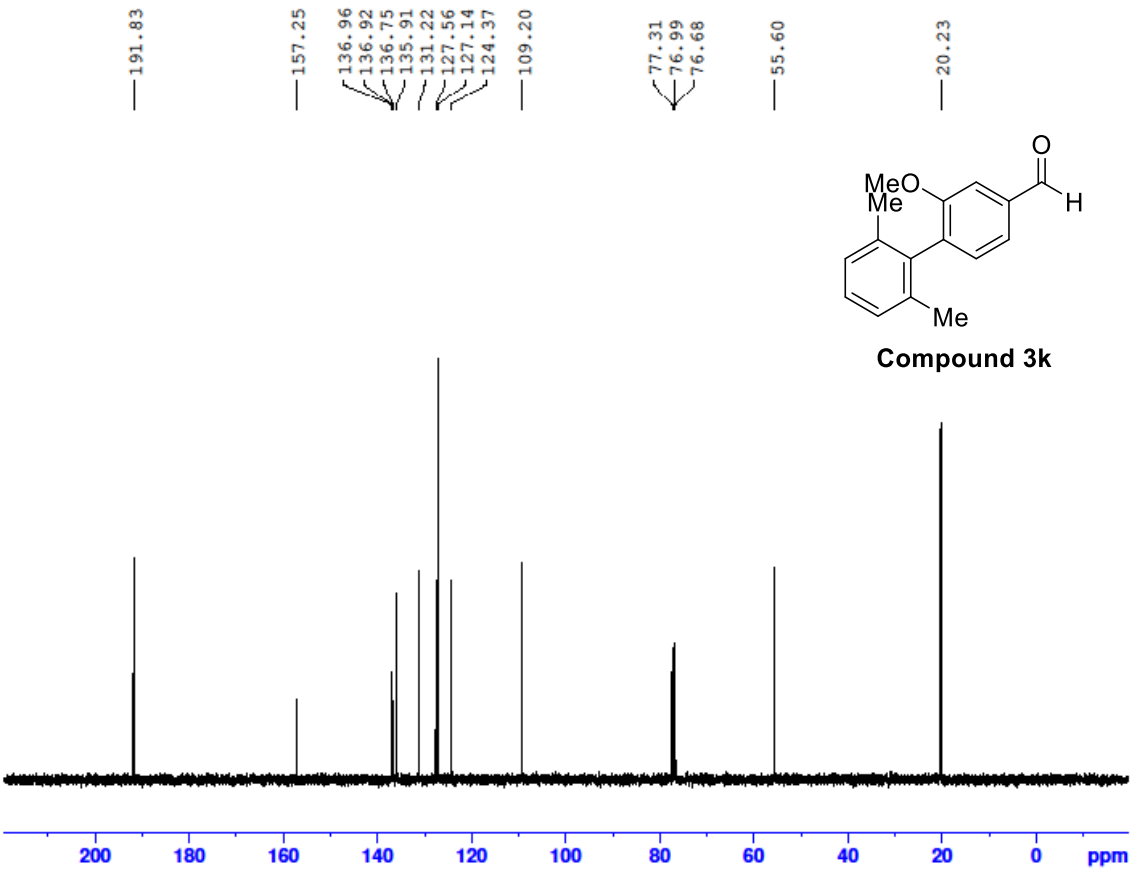


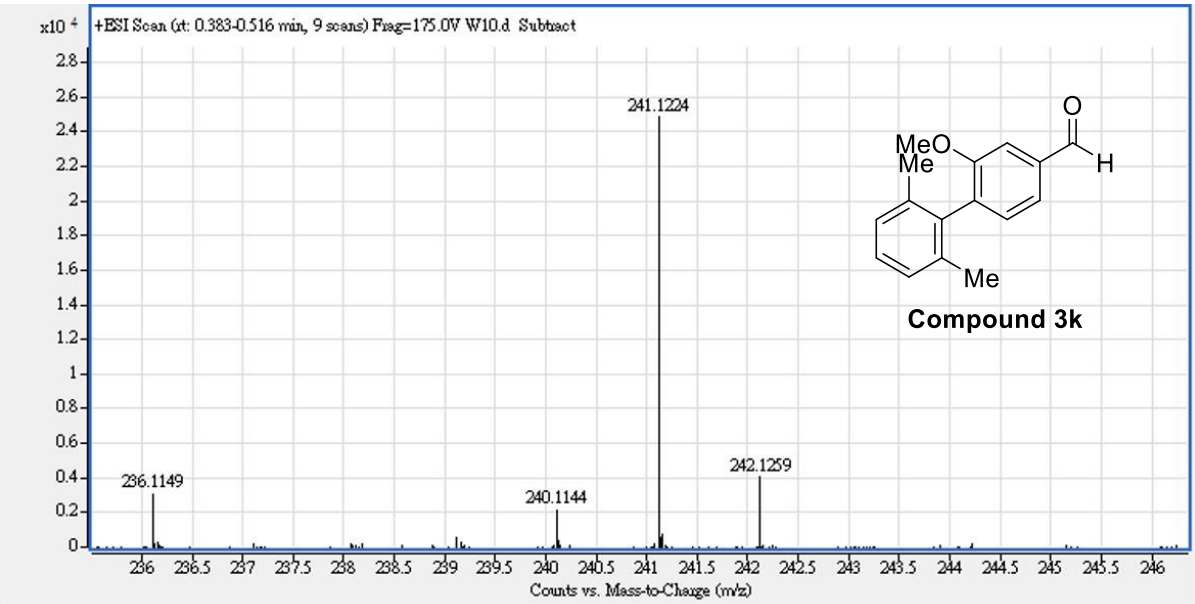
Compound 3j



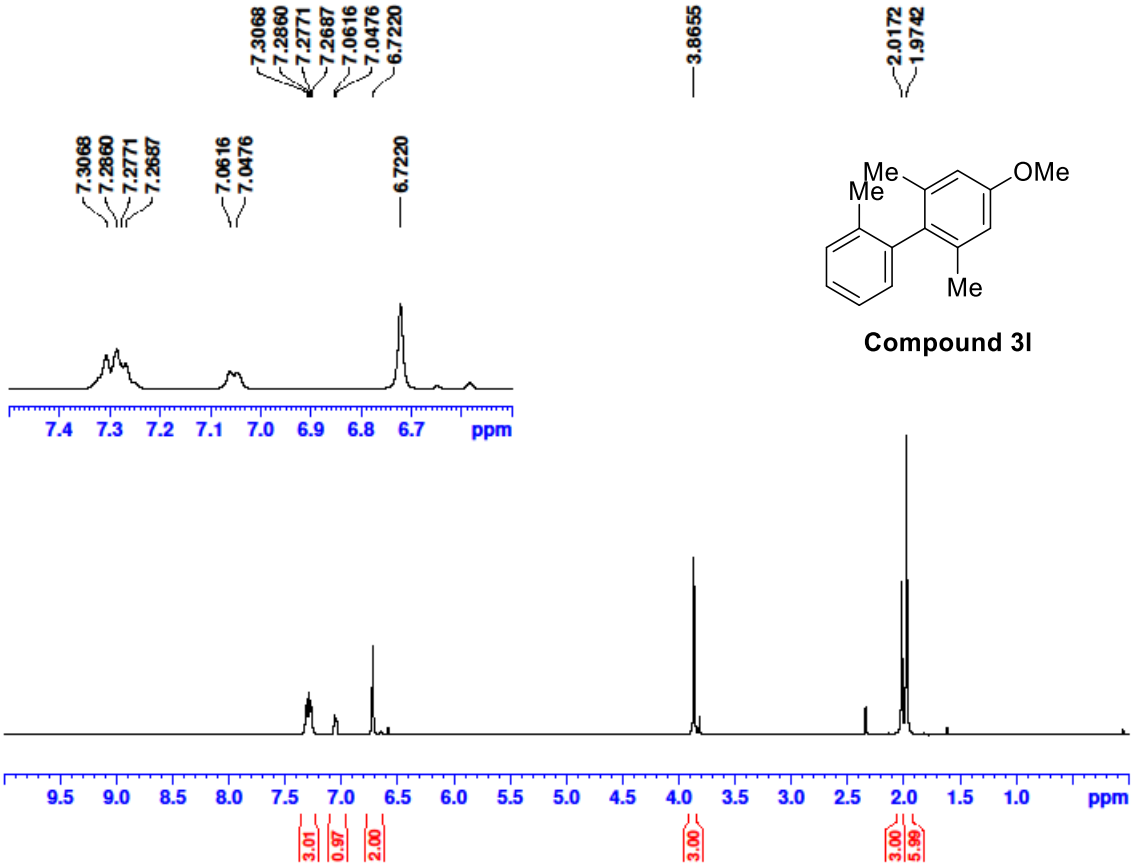
Mass	Calc. Mass	mDa	PPM	Formula
226.1352	226.1352	0.02	0.07	C16 H18 O


10.0765
7.5971
7.5942
7.5750
7.5717
7.2878
7.2693
7.2637
7.2461
7.2423
7.2255
7.1766
7.1581
3.8589
2.0505
MeO
Me
O
H
Me
Compound 3k
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
2.00
4.00
3.00
6.00

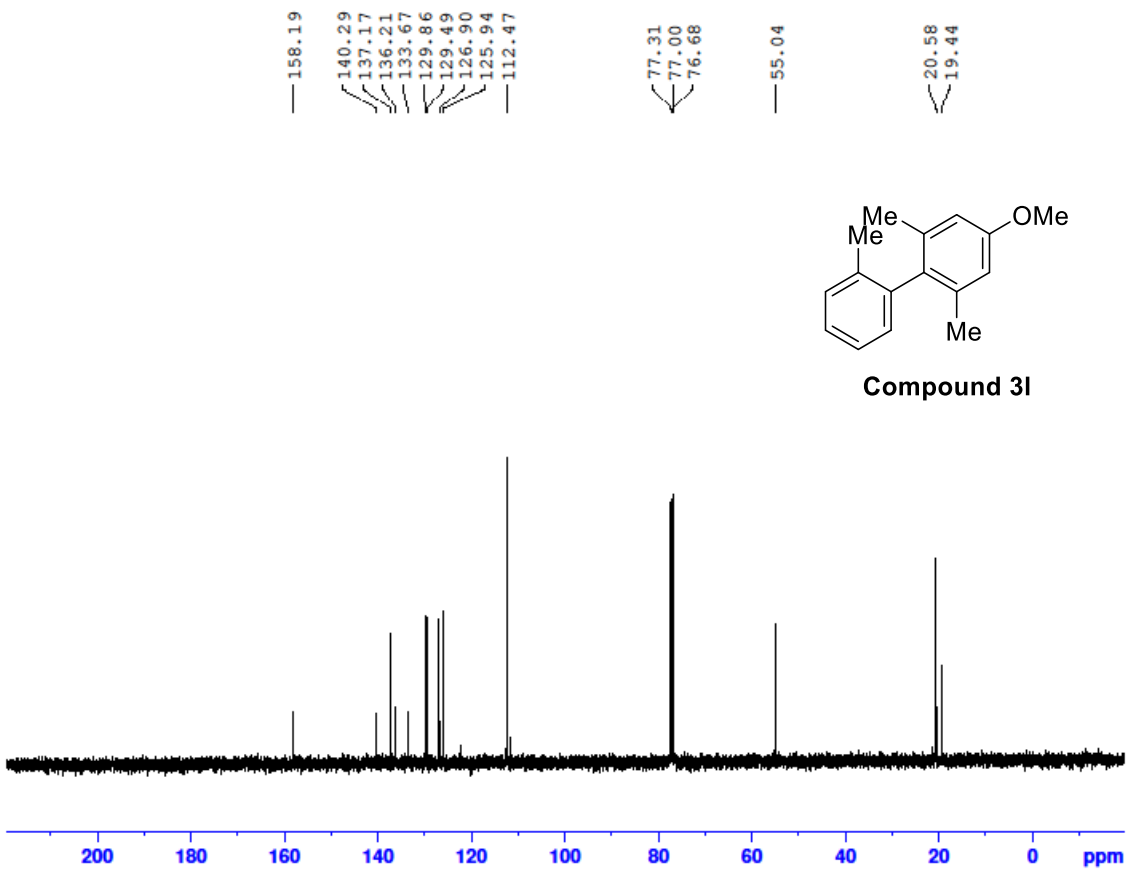

191.83
157.25
136.96
136.92
136.75
135.91
131.22
127.56
127.14
124.37
109.20
77.31
76.99
76.68
55.60
20.23
MeO
Me
O
H
Me
Compound 3k
200 180 160 140 120 100 80 60 40 20 0 ppm



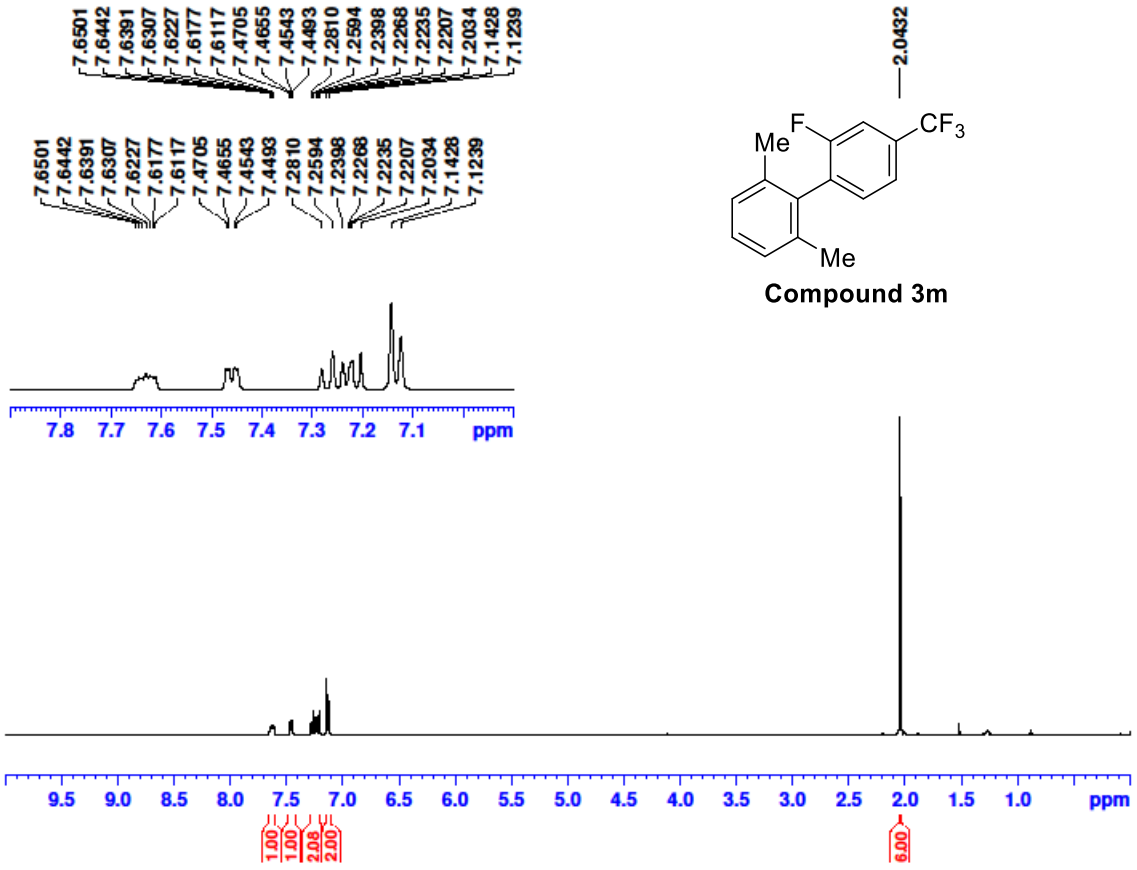
Mass	Calc. Mass	mDa	PPM	Formula
241.1224	241.1223	-0.09	-0.39	C16 H17 O2

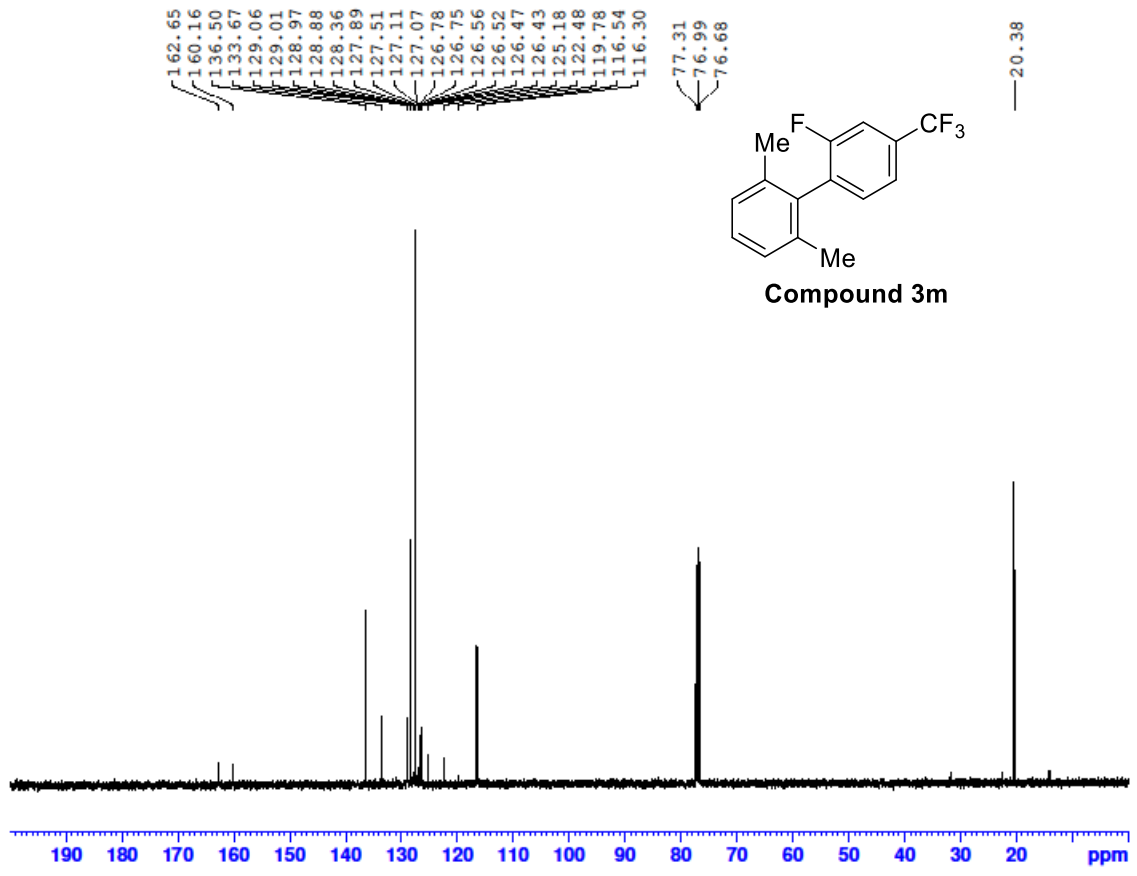


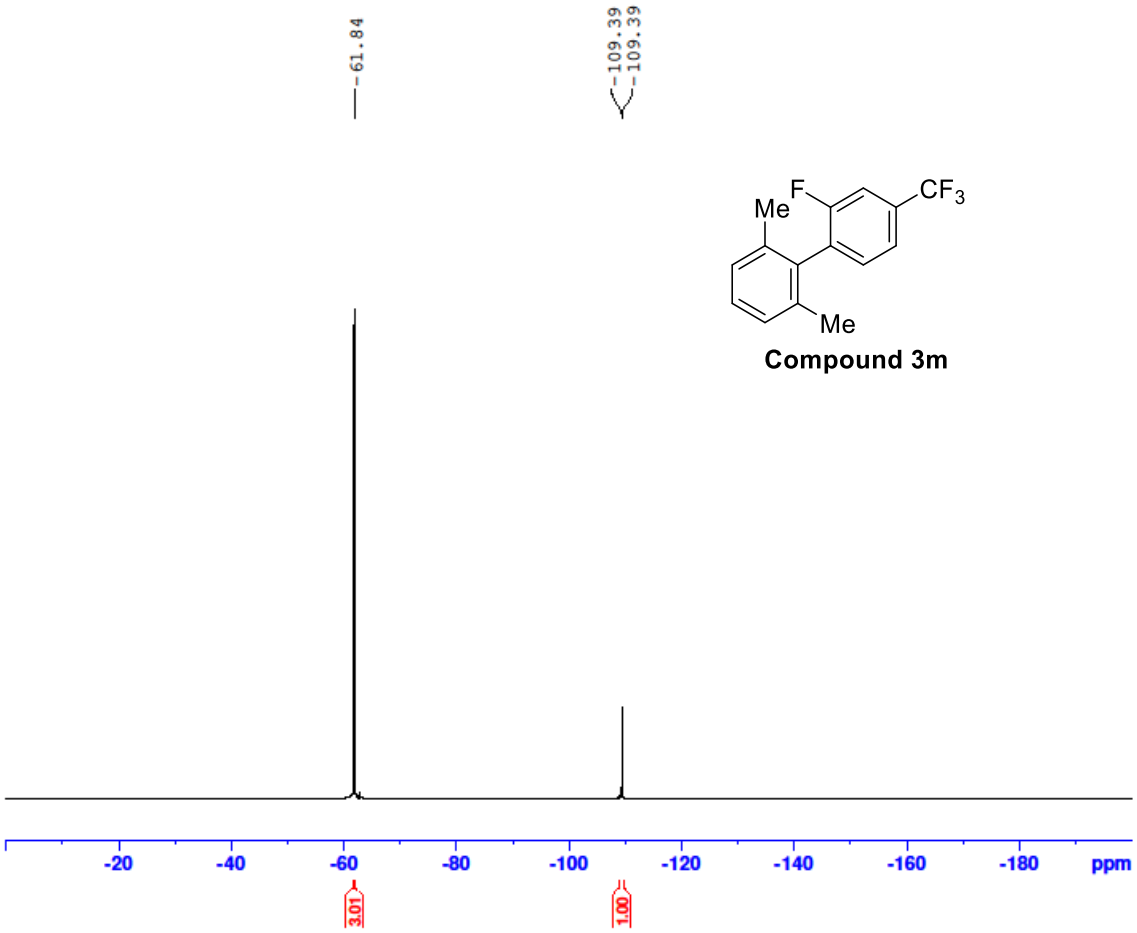
Compound 3l

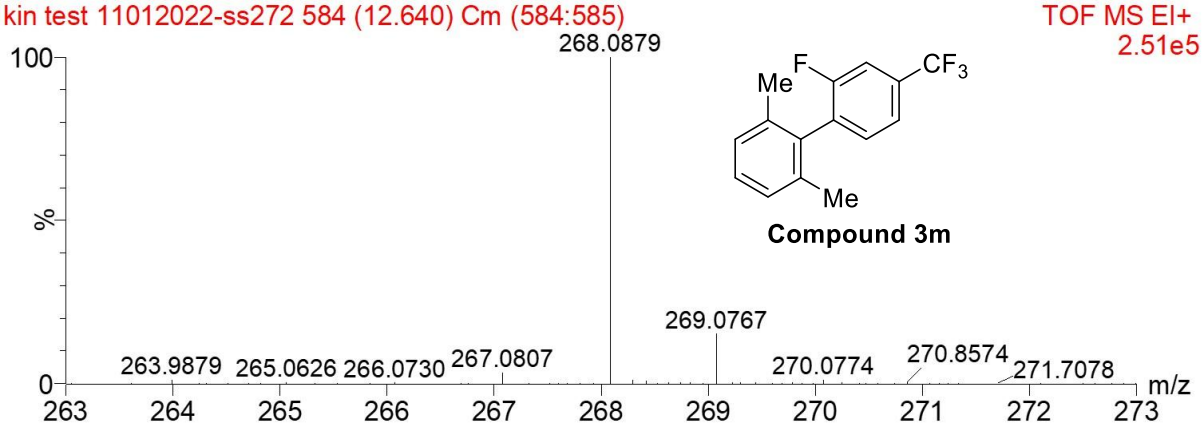


Compound 3l

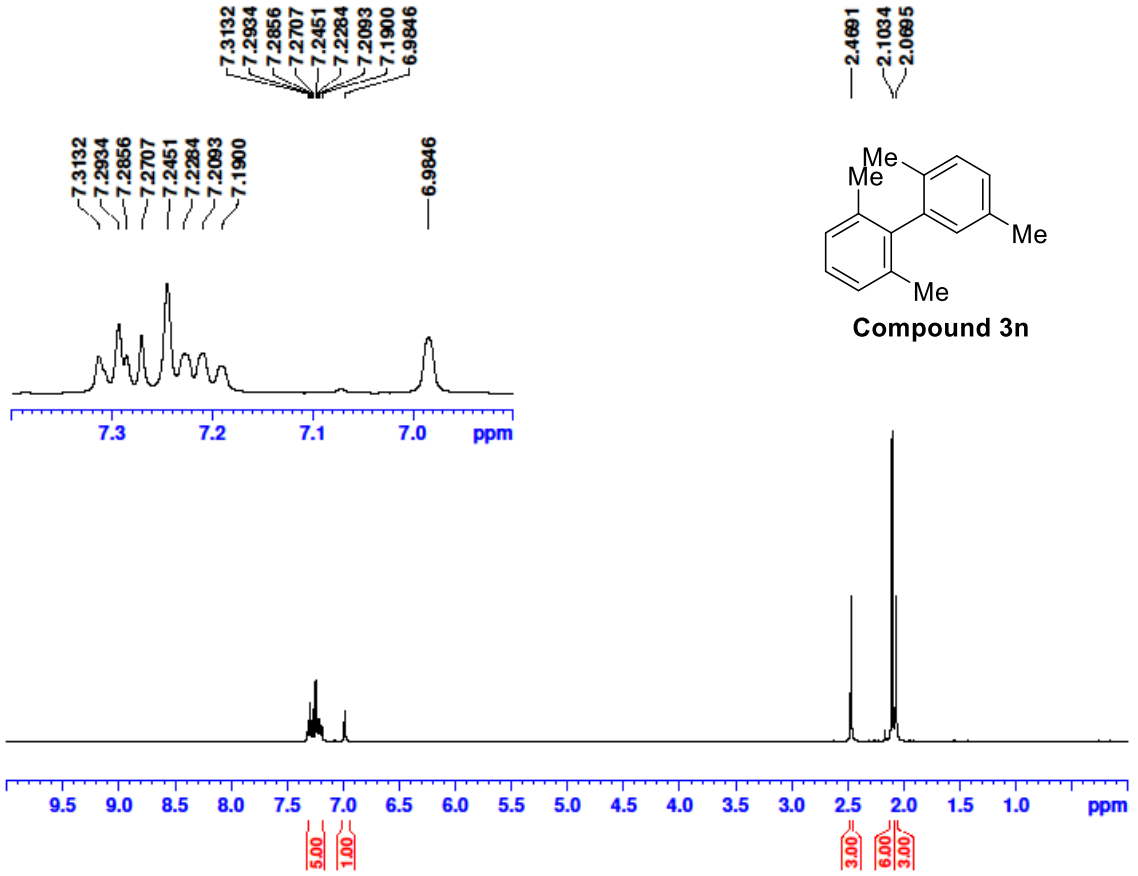

7.6501
7.6442
7.6391
7.6307
7.6227
7.6177
7.6117
7.4705
7.4655
7.4543
7.4493
7.2810
7.2594
7.2398
7.2268
7.2235
7.2207
7.2034
7.1428
7.1239
2.0432
F
CF3
Me
Me
Compound 3m
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.00
2.08
2.00
6.00

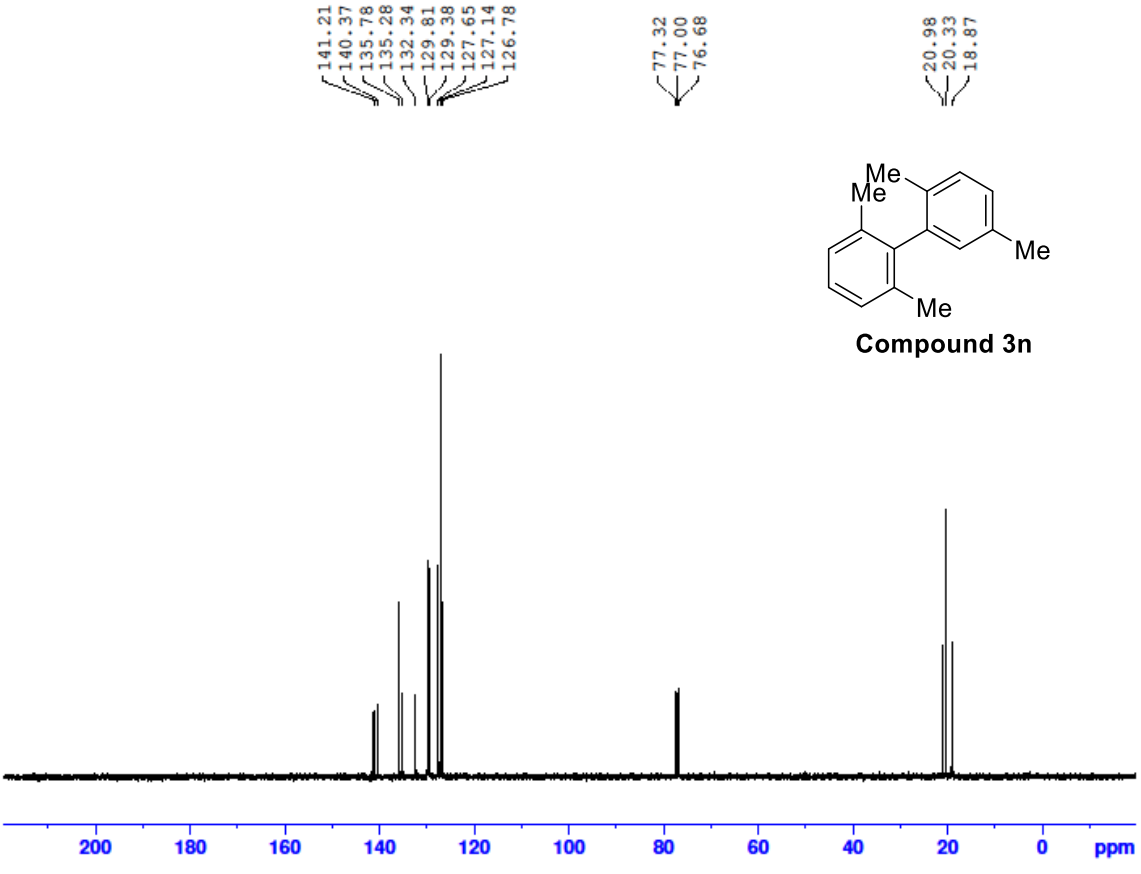

162.65
160.16
136.50
133.67
129.06
129.01
128.97
128.88
128.36
127.89
127.51
127.11
127.07
126.78
126.75
126.56
126.52
126.47
126.43
125.18
122.48
119.78
116.54
116.30
77.31
76.99
76.68
20.38
F
CF3
Me
Me
Compound 3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

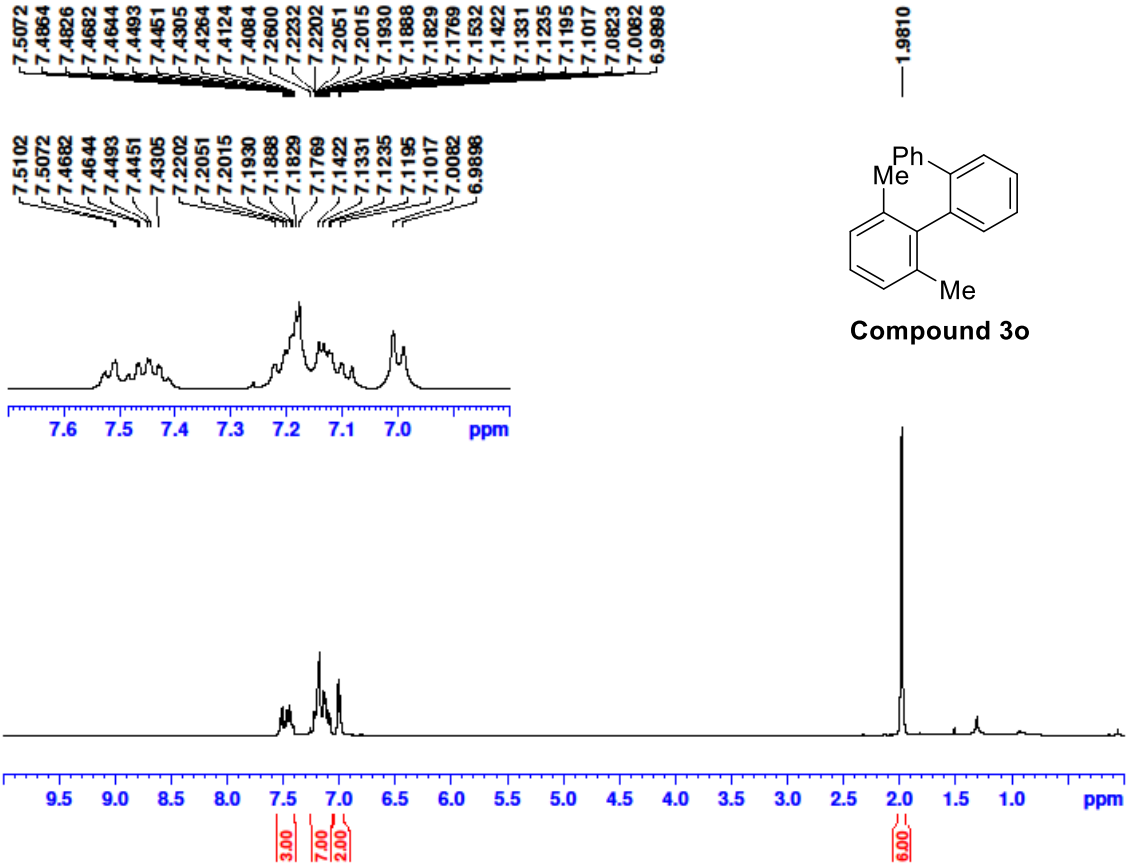


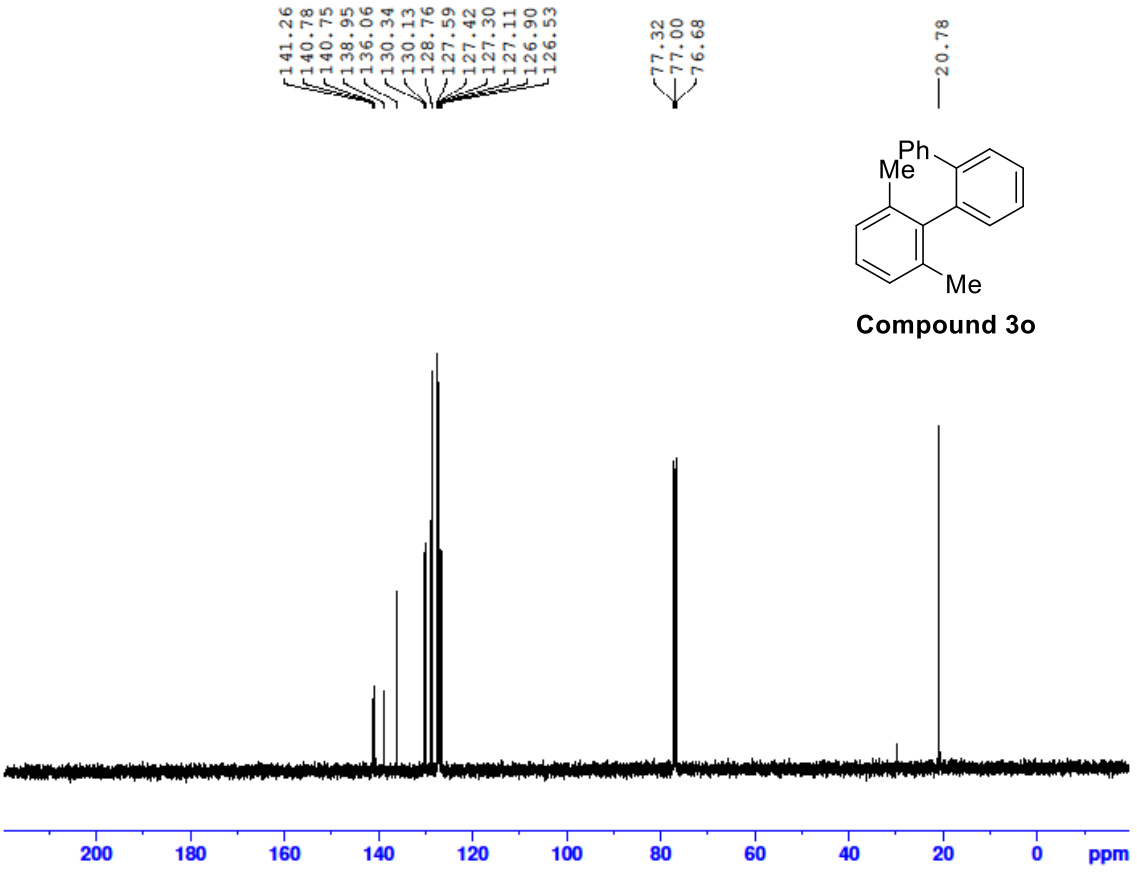


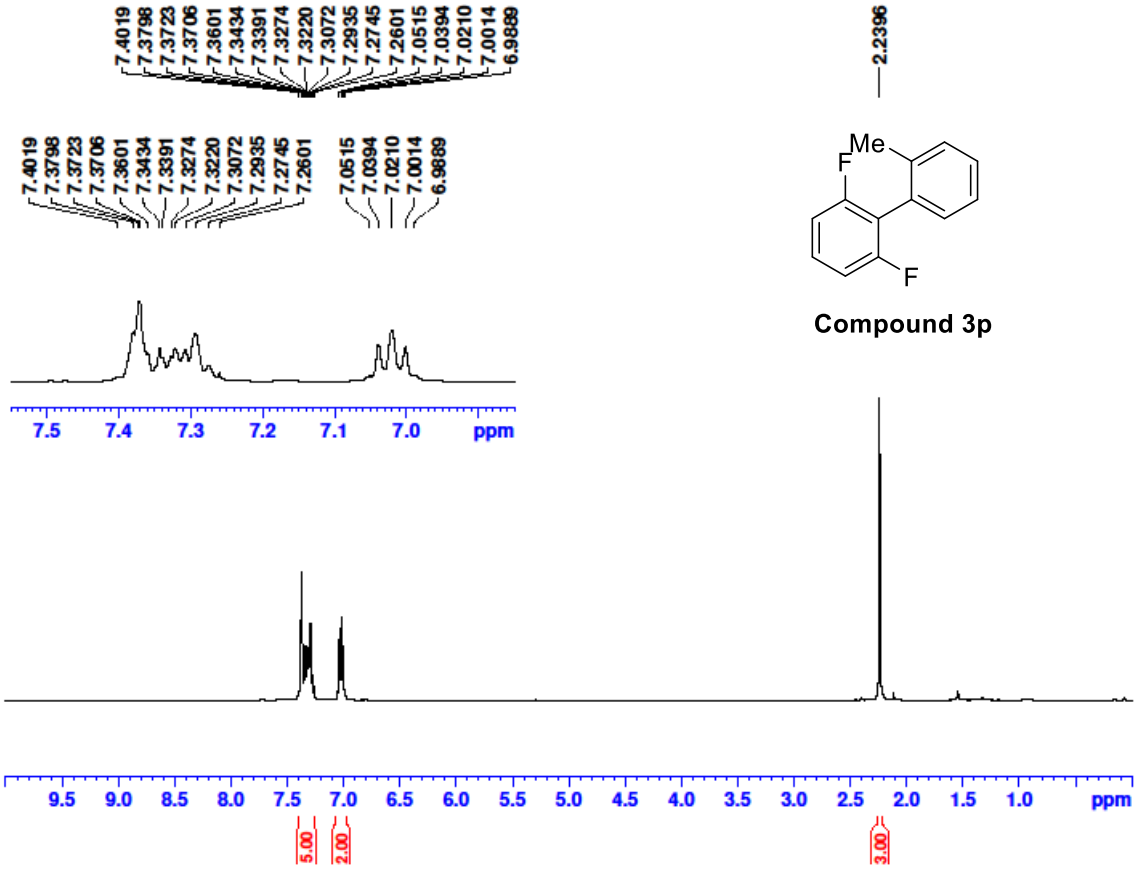
Mass	Calc. Mass	mDa	PPM	Formula
268.0879	268.0870	-0.94	-3.49	C15 H12 F4


7.3132
7.2934
7.2856
7.2707
7.2451
7.2284
7.2093
7.1900
6.9846
2.4691
2.1034
2.0695
Me
Me
Me
Me
Compound 3n
7.3
7.2
7.1
7.0
ppm
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
ppm
5.00
1.00
3.00
6.00
3.00

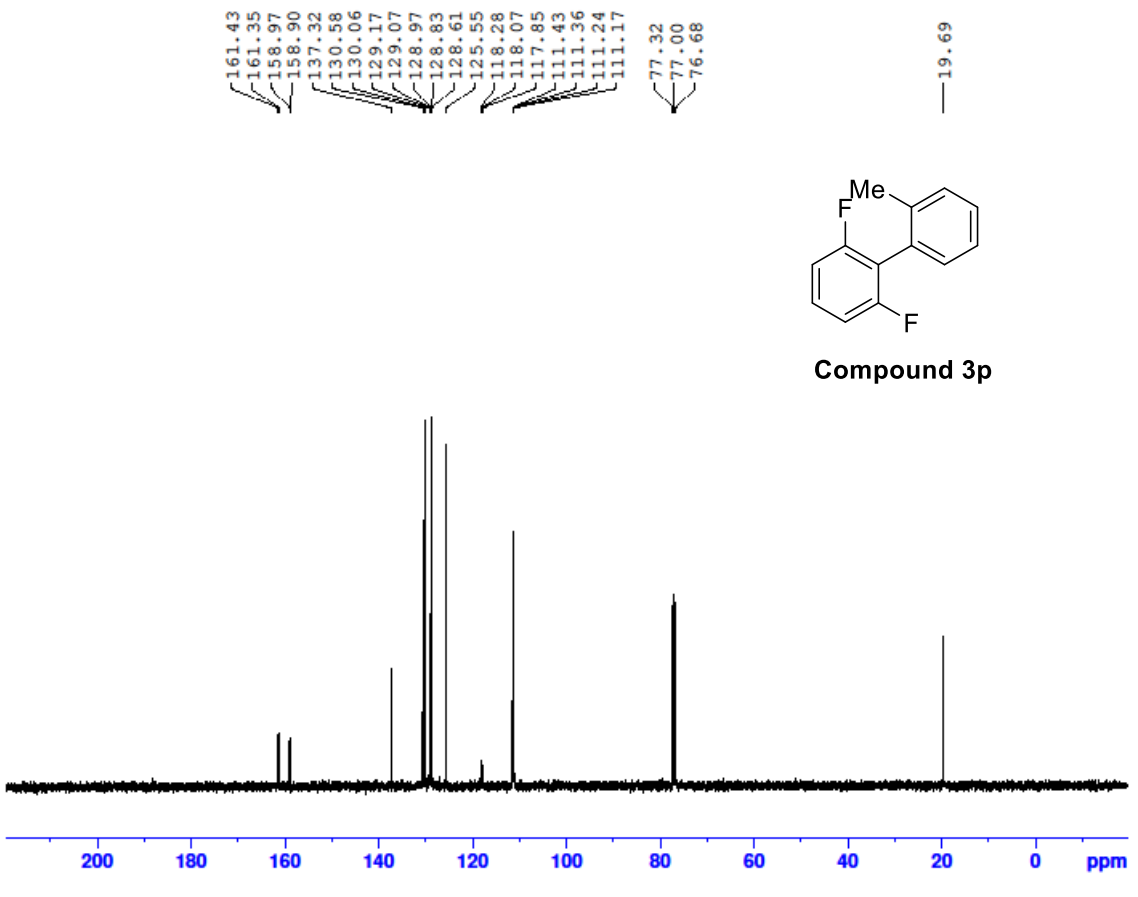

141.21
140.37
135.78
135.28
132.34
129.81
129.38
127.65
127.14
126.78
77.32
77.00
76.68
20.98
20.33
18.87
Me
Me
Me
Me
Compound 3n
200
180
160
140
120
100
80
60
40
20
0
ppm


7.5072
7.4864
7.4826
7.4682
7.4644
7.4493
7.4451
7.4305
7.4264
7.4124
7.4084
7.2600
7.2232
7.2202
7.2051
7.2015
7.1930
7.1888
7.1829
7.1769
7.1532
7.1422
7.1331
7.1235
7.1195
7.1017
7.0823
7.0082
6.9898
1.9810
Ph
Me
Me
Compound 3o
ppm
3.00
7.00
2.00
6.00

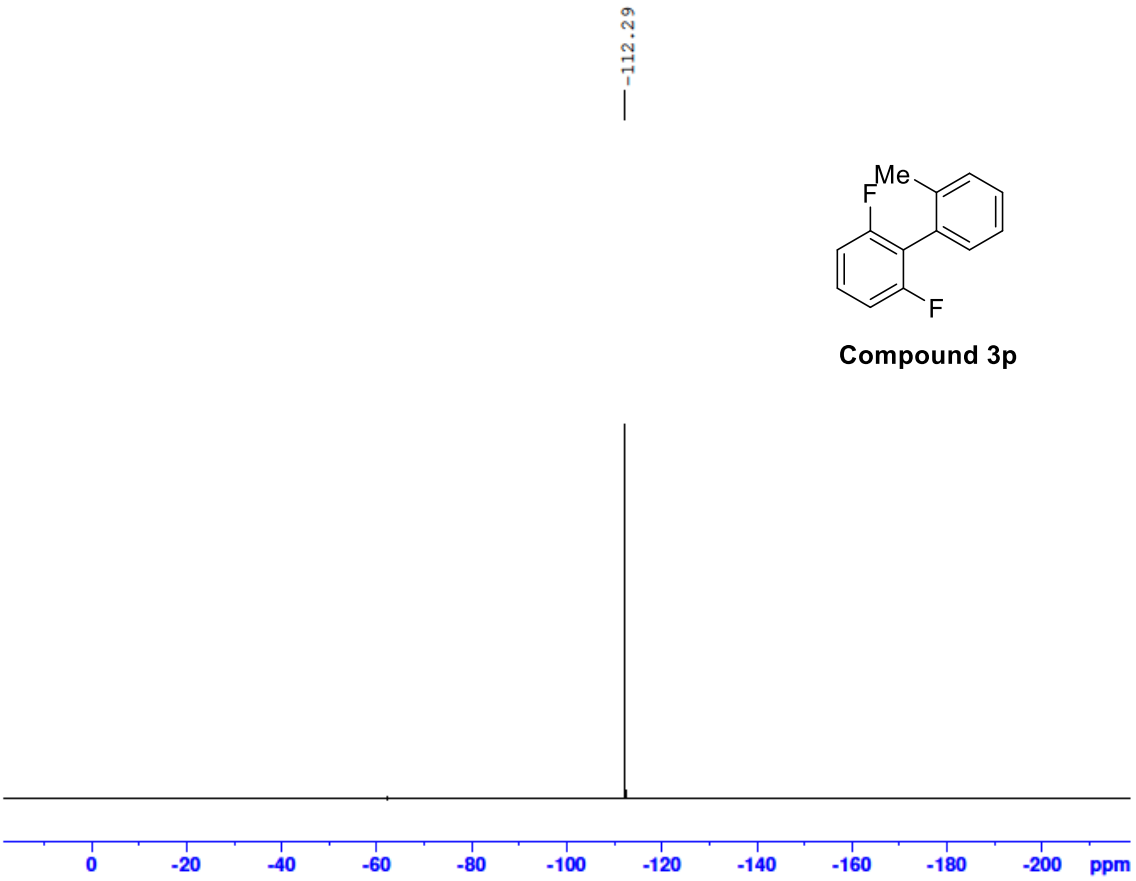

141.26
140.78
140.75
138.95
136.06
130.34
130.13
128.76
127.59
127.42
127.30
127.11
126.90
126.53
77.32
77.00
76.68
20.78
Ph
Me
Me
Compound 3o
ppm



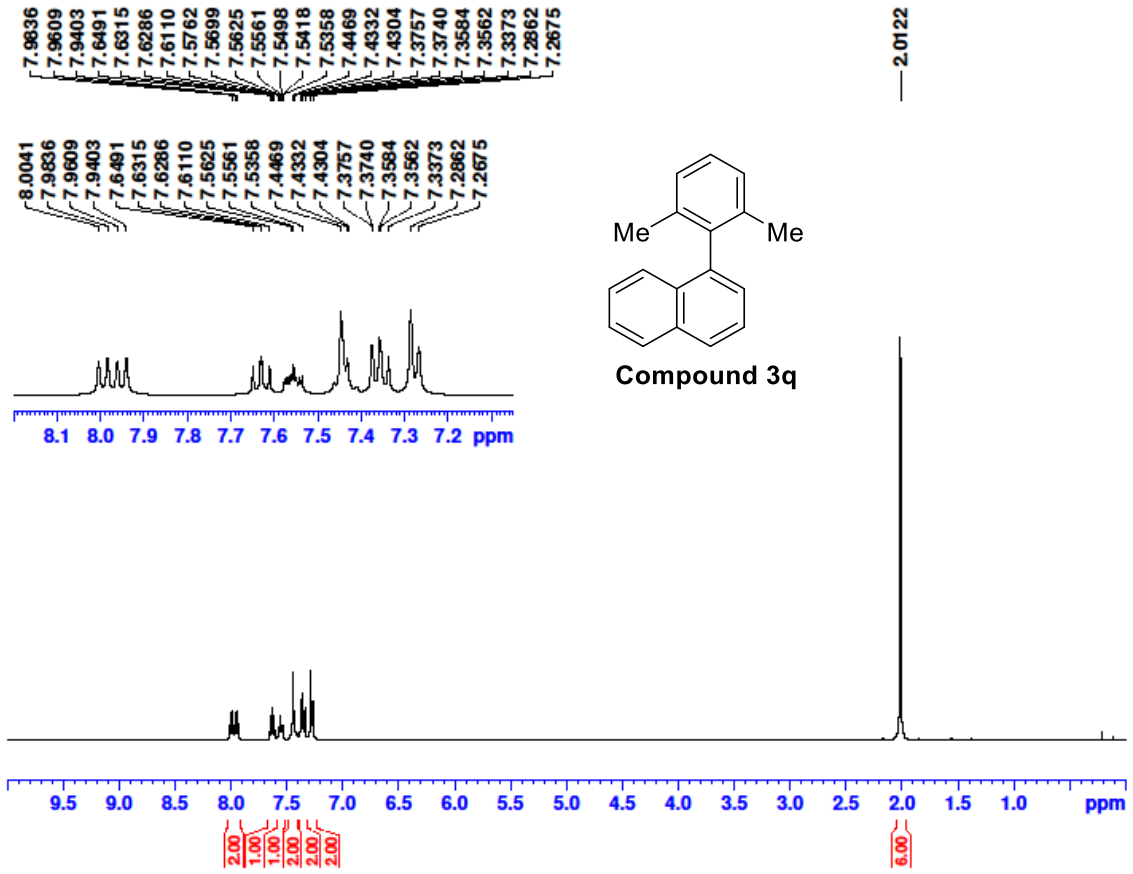
Compound 3p

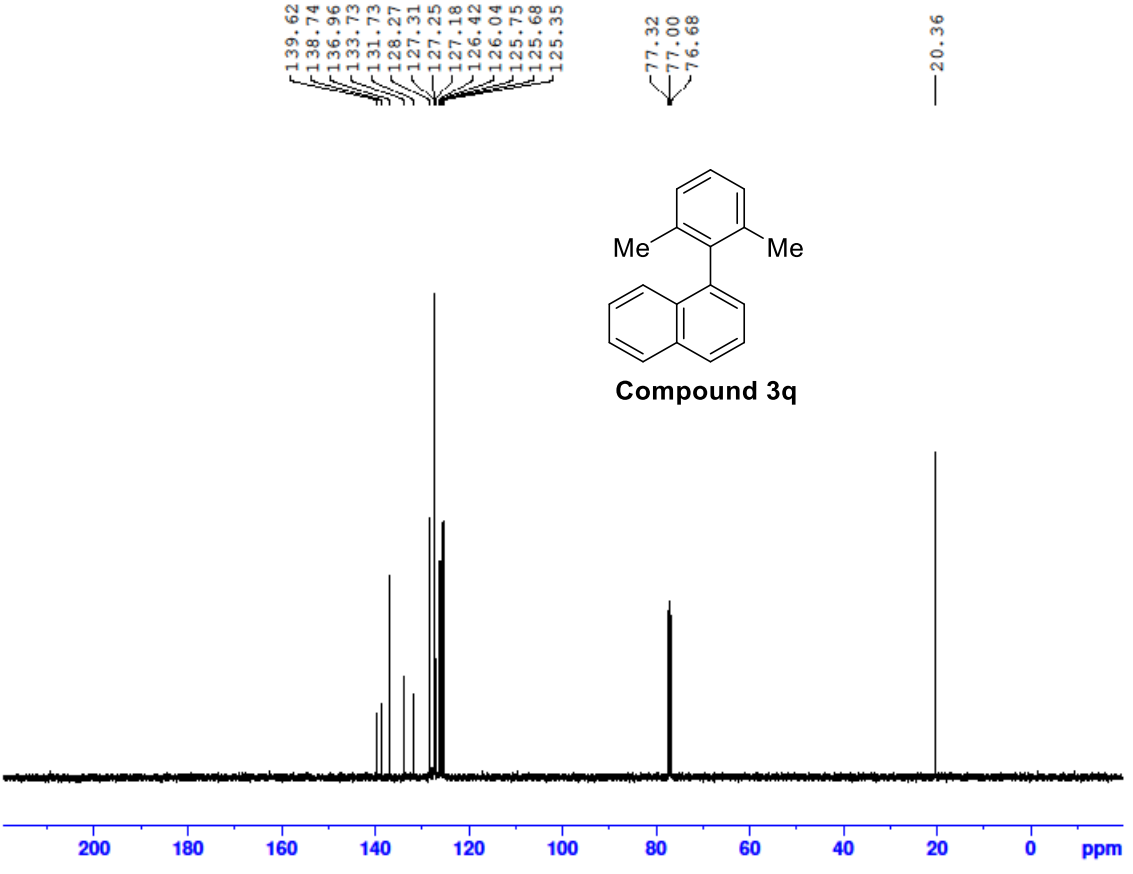


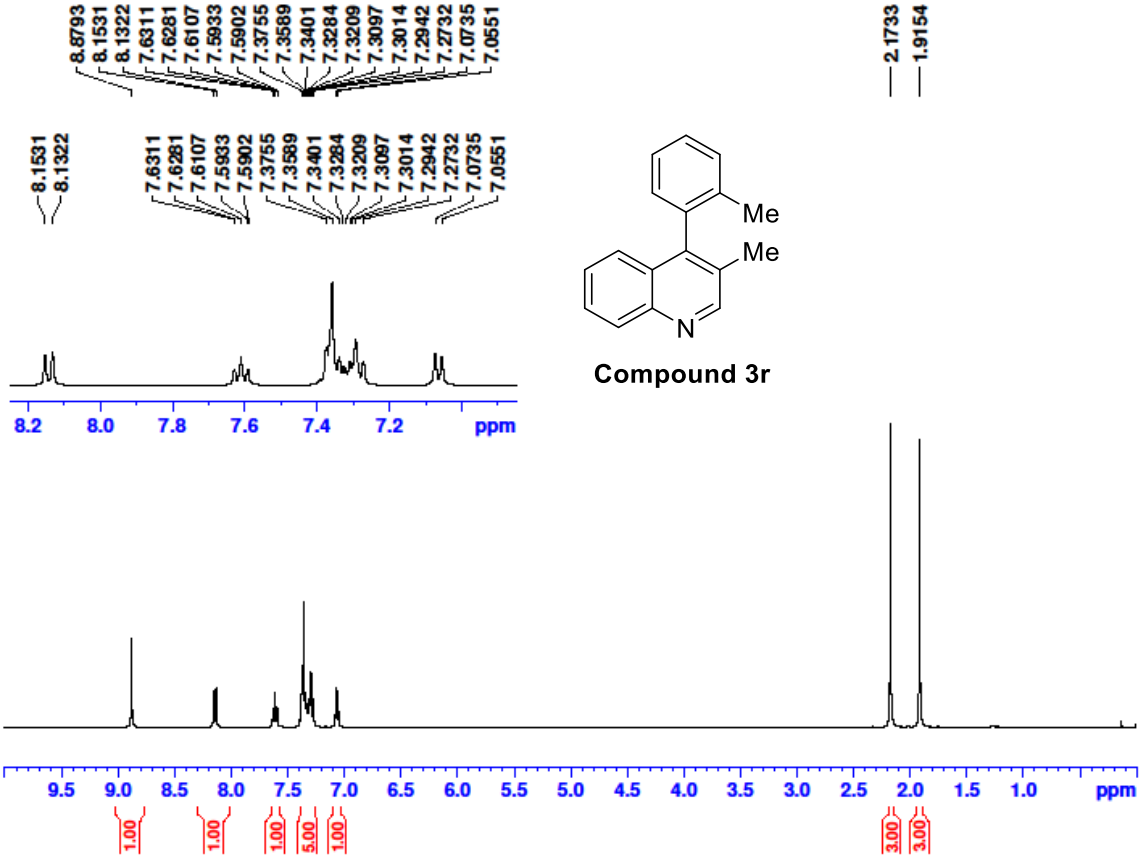
Compound 3p

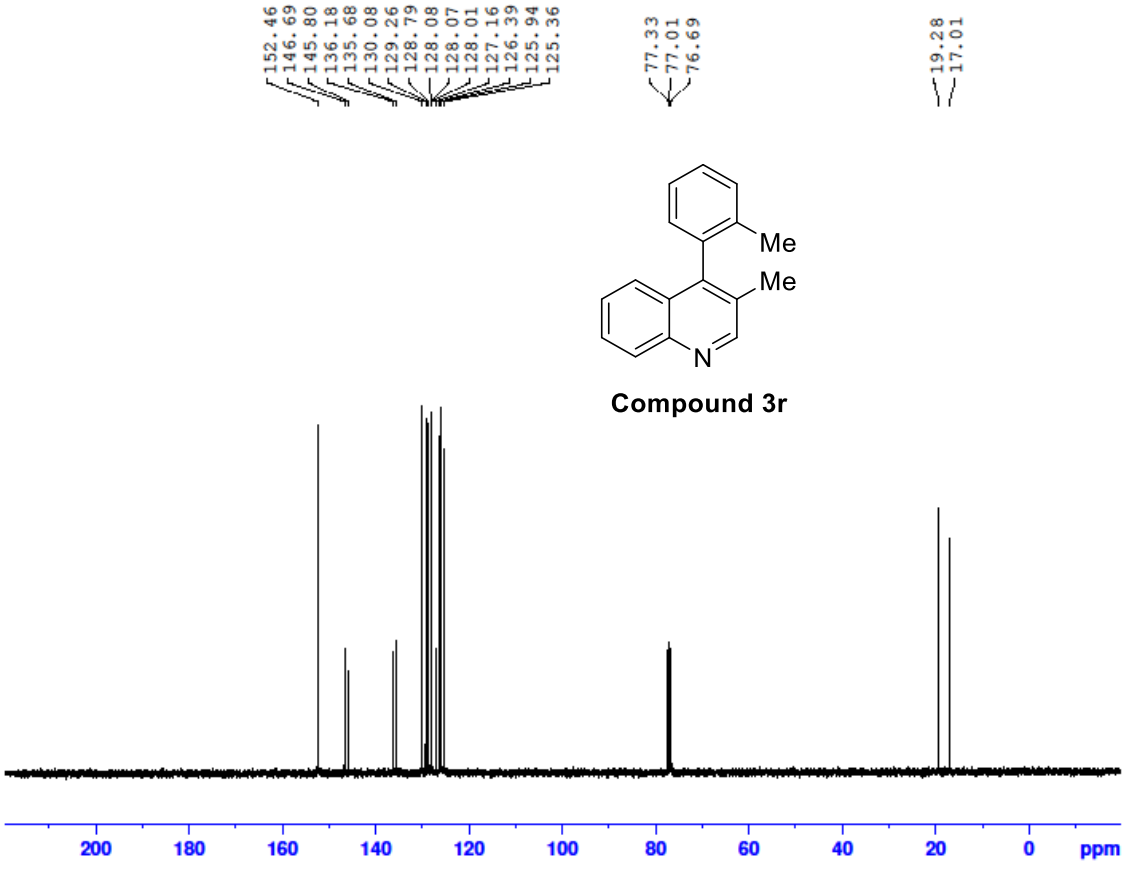


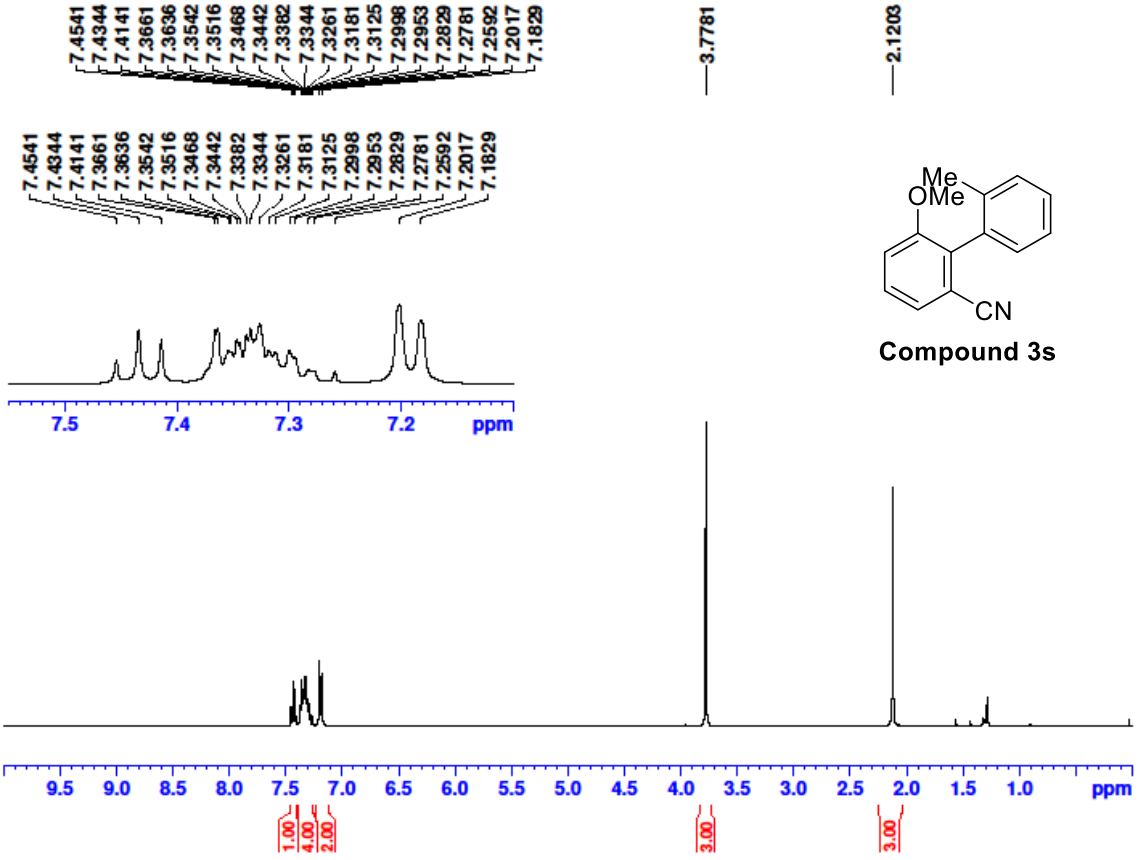
Compound 3p


7.9836
7.9609
7.9403
7.6491
7.6315
7.6286
7.6110
7.5762
7.5699
7.5625
7.5561
7.5498
7.5418
7.5358
7.4469
7.4332
7.4304
7.3757
7.3740
7.3584
7.3562
7.3373
7.2862
7.2675
2.0122
Me
Me
Compound 3q
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
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 ppm
2.00
1.00
1.00
2.00
2.00
2.00
6.00

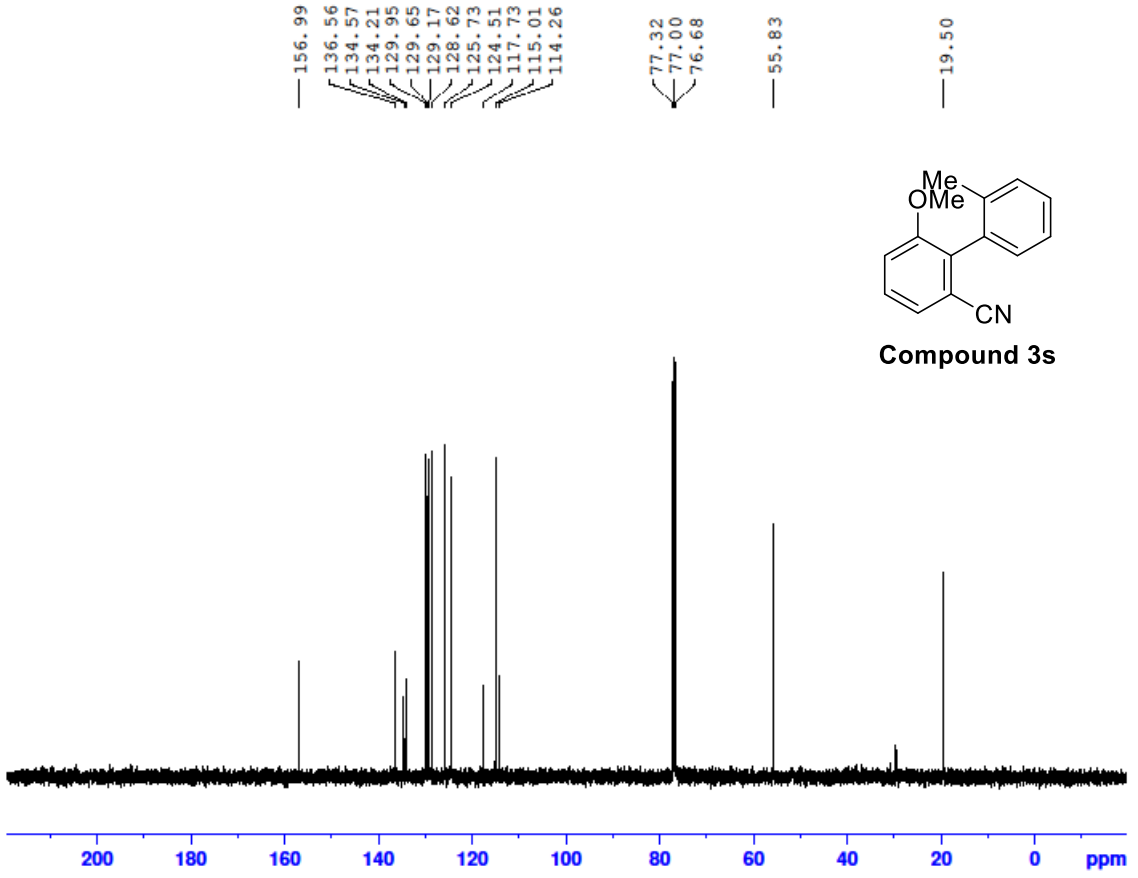

139.62
138.74
136.96
133.73
131.73
128.27
127.31
127.25
127.18
126.42
126.04
125.75
125.68
125.35
77.32
77.00
76.68
20.36
Me
Me
Compound 3q
200 180 160 140 120 100 80 60 40 20 0 ppm


8.8793
8.1531
8.1322
7.6311
7.6281
7.6107
7.5933
7.5902
7.3755
7.3589
7.3401
7.3284
7.3209
7.3097
7.3014
7.2942
7.2732
7.0735
7.0551
2.1733
1.9154
Me
Me
N
Compound 3r
8.2
8.0
7.8
7.6
7.4
7.2
ppm
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
ppm
1.00
1.00
1.00
5.00
1.00
3.00
3.00

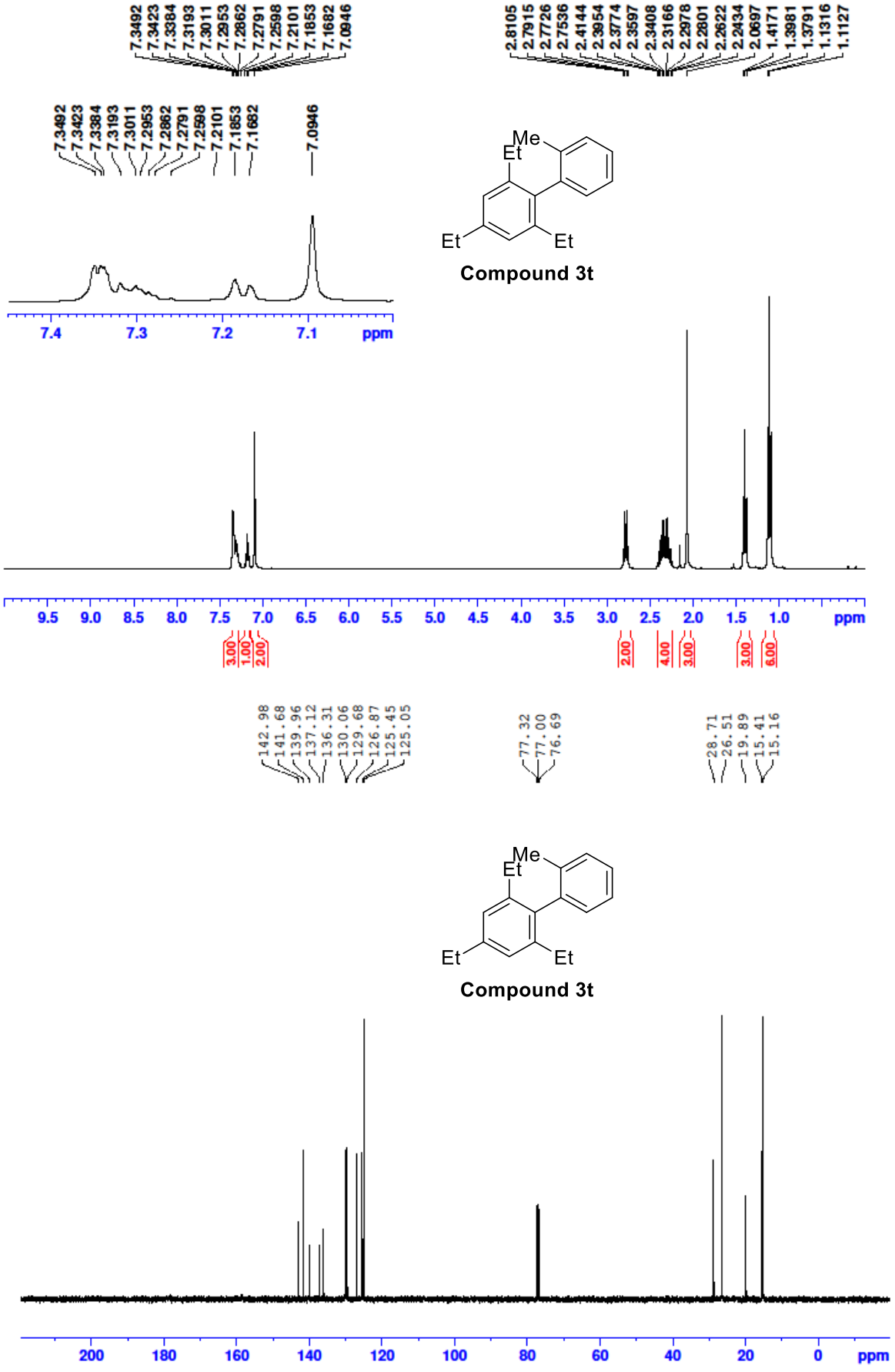

152.46
146.69
145.80
136.18
135.68
130.08
129.26
128.79
128.08
128.07
128.01
127.16
126.39
125.94
125.36
77.33
77.01
76.69
19.28
17.01
Me
Me
N
Compound 3r
200
180
160
140
120
100
80
60
40
20
0
ppm

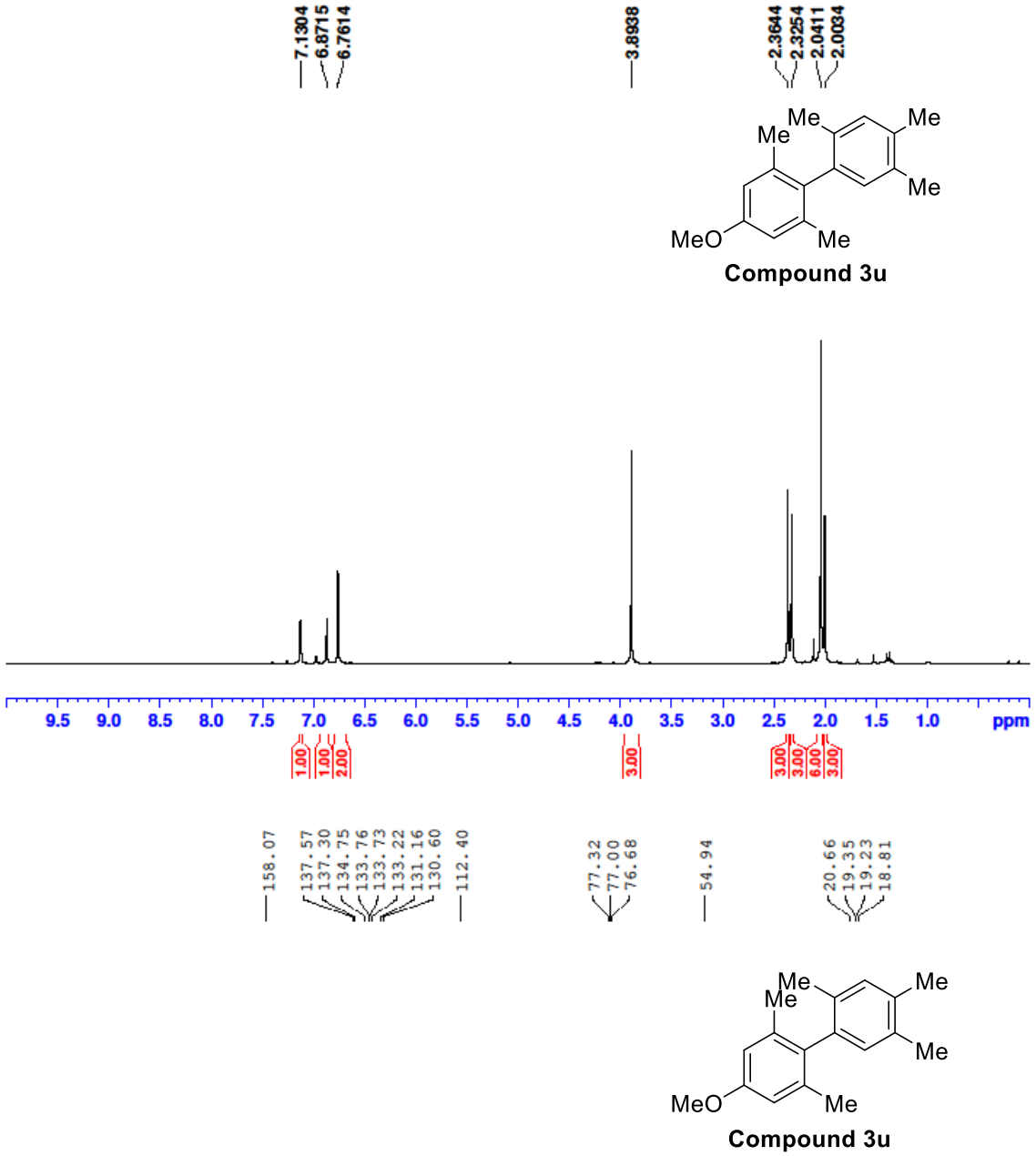


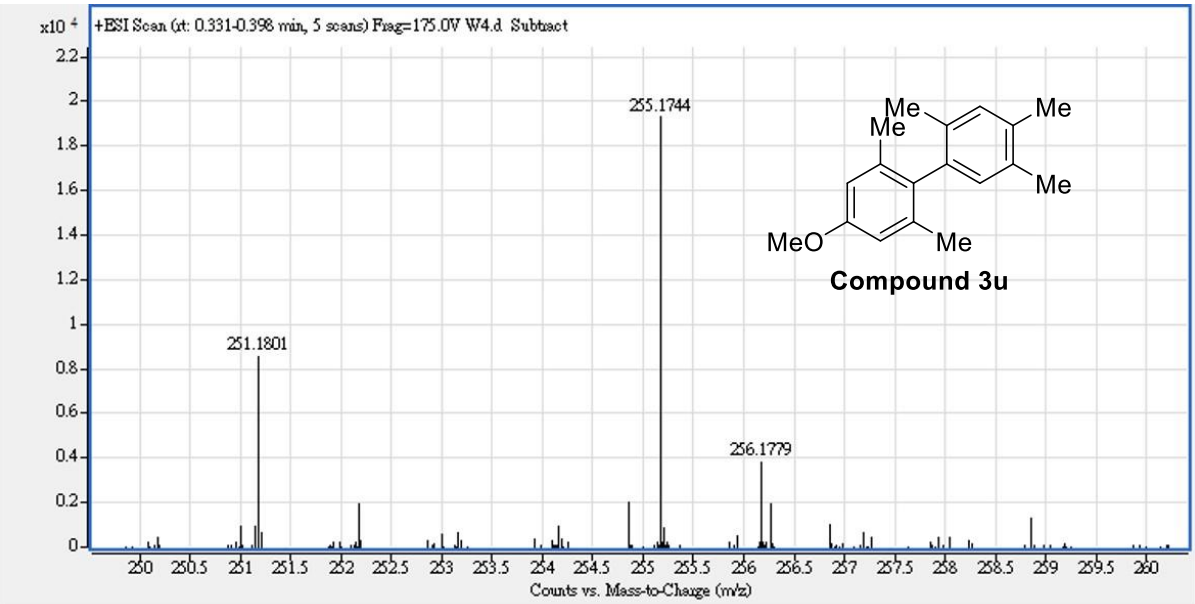
Compound 3s



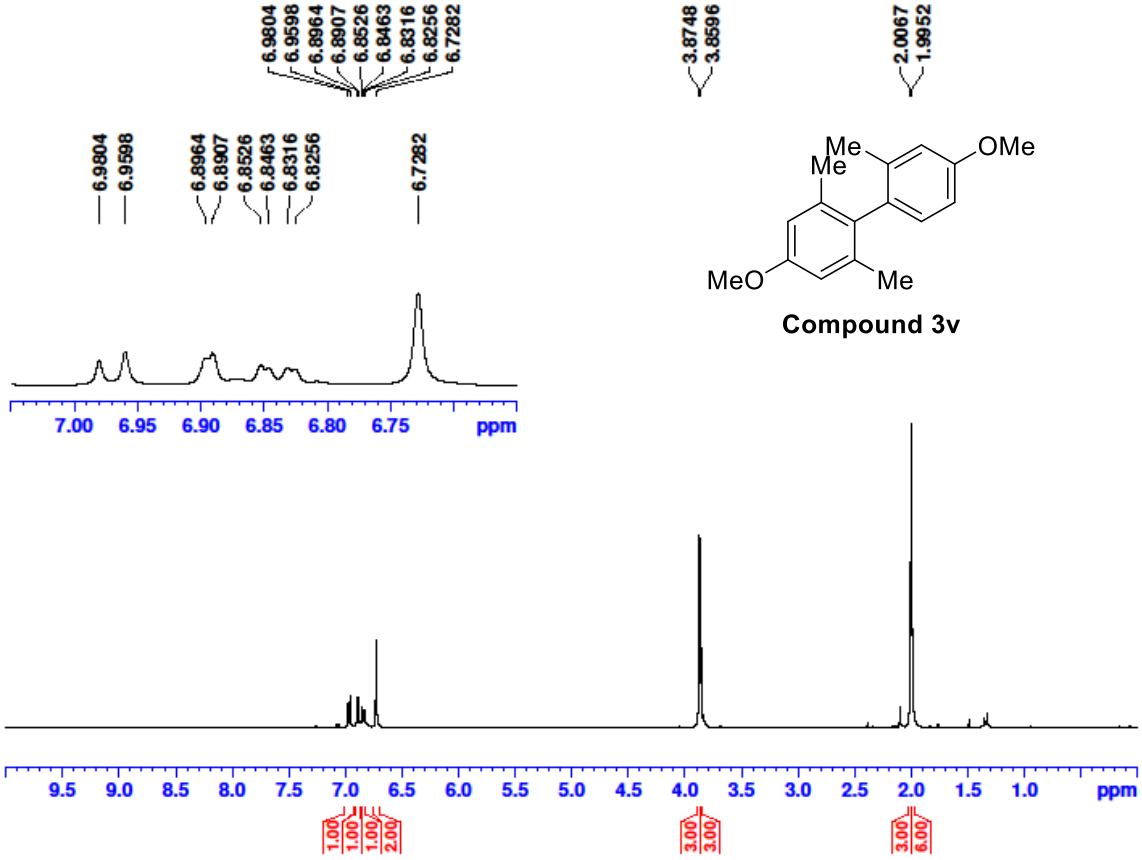
Compound 3s

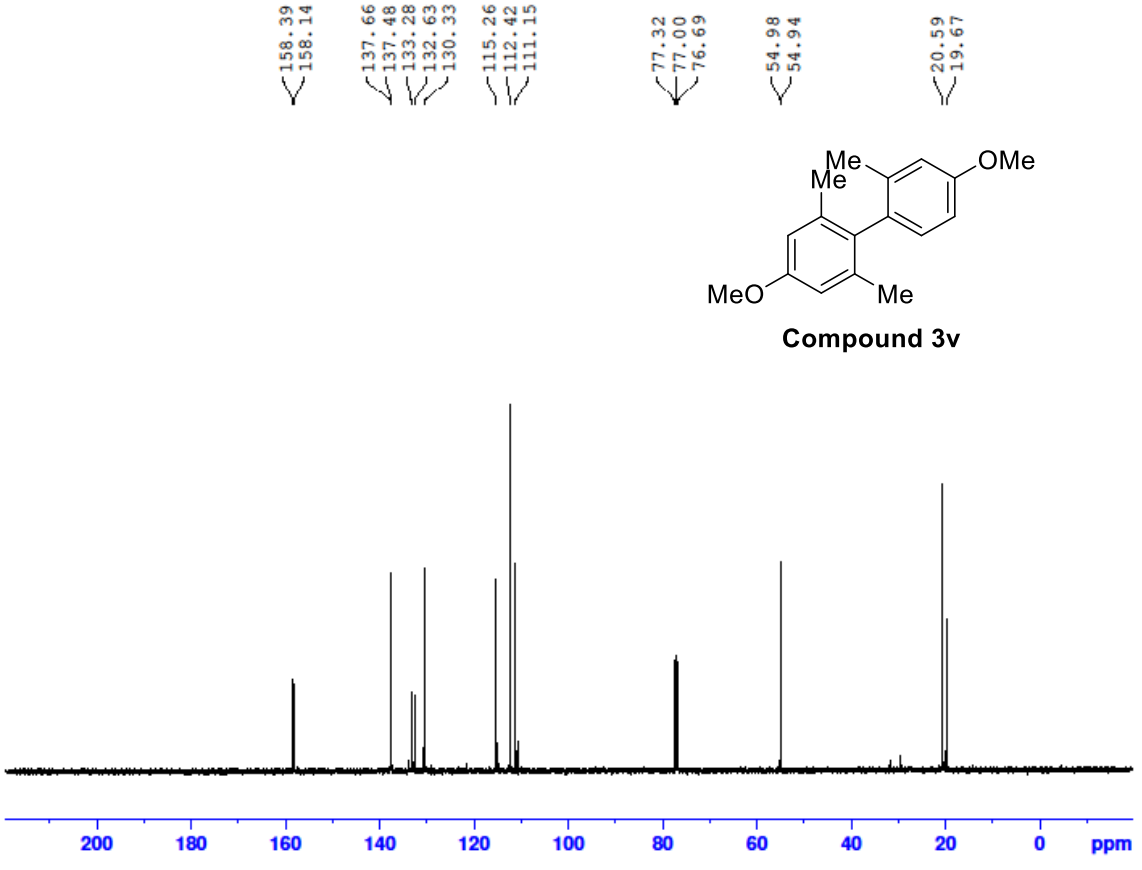

7.3492
7.3423
7.3384
7.3193
7.3011
7.2953
7.2862
7.2791
7.2598
7.2101
7.1853
7.1682
7.0946
2.8105
2.7915
2.7726
2.7536
2.4144
2.3954
2.3774
2.3597
2.3408
2.3166
2.2978
2.2801
2.2622
2.2434
2.0697
1.4171
1.3981
1.3791
1.1316
1.1127
Me
Et
Et
Et
Compound 3t
7.4
7.3
7.2
7.1
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
3.00
1.00
2.00
2.00
4.00
3.00
3.00
6.00
142.98
141.68
139.96
137.12
136.31
130.06
129.68
126.87
125.45
125.05
77.32
77.00
76.69
28.71
26.51
19.89
15.41
15.16
Me
Et
Et
Et
Compound 3t
200
180
160
140
120
100
80
60
40
20
0
ppm

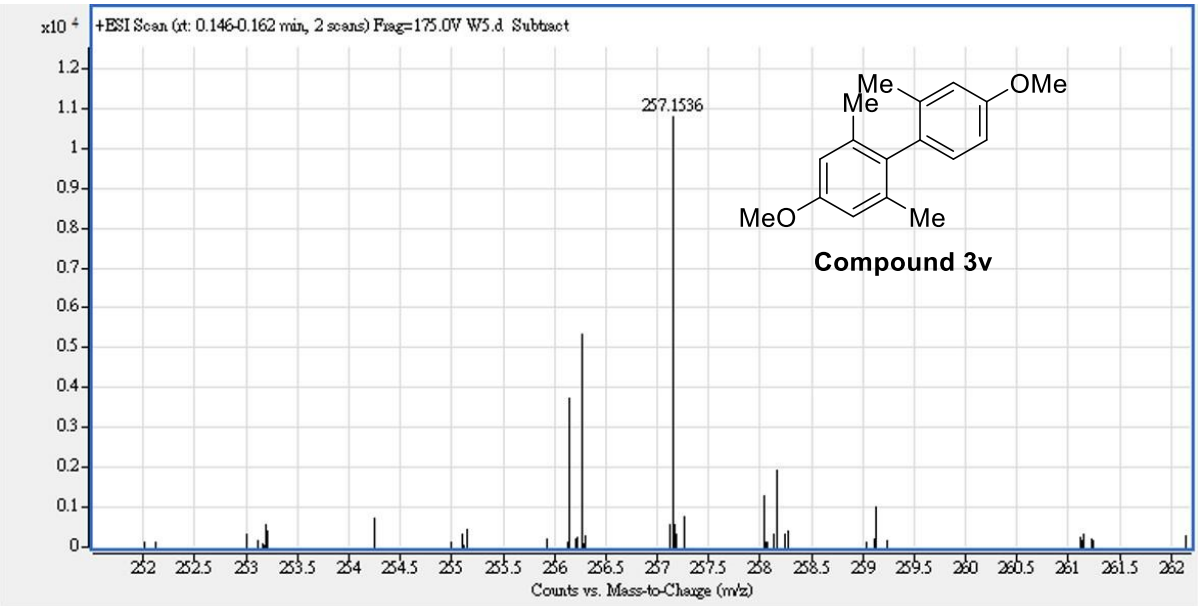

7.1304
6.8715
6.7614
3.8938
2.3644
2.3254
2.0411
2.0034
Me
Me
Me
Me
MeO
Me
Compound 3u
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.00
2.00
3.00
3.00
3.00
6.00
3.00
158.07
137.57
137.30
134.75
133.76
133.73
133.22
131.16
130.60
112.40
77.32
77.00
76.68
54.94
20.66
19.35
19.23
18.81
Me
Me
Me
Me
MeO
Me
Compound 3u
200 180 160 140 120 100 80 60 40 20 0 ppm



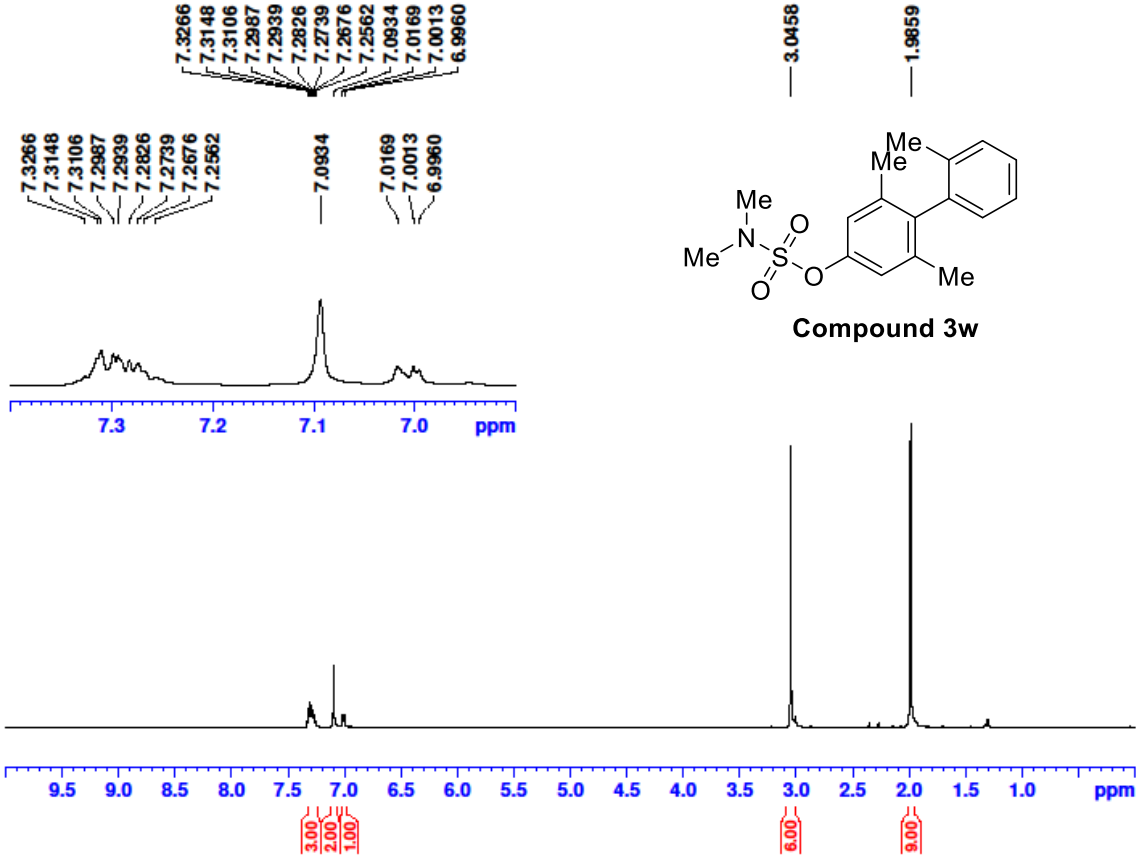
Mass	Calc. Mass	mDa	PPM	Formula
255.1744	255.1743	-0.06	-0.23	C18 H23 O

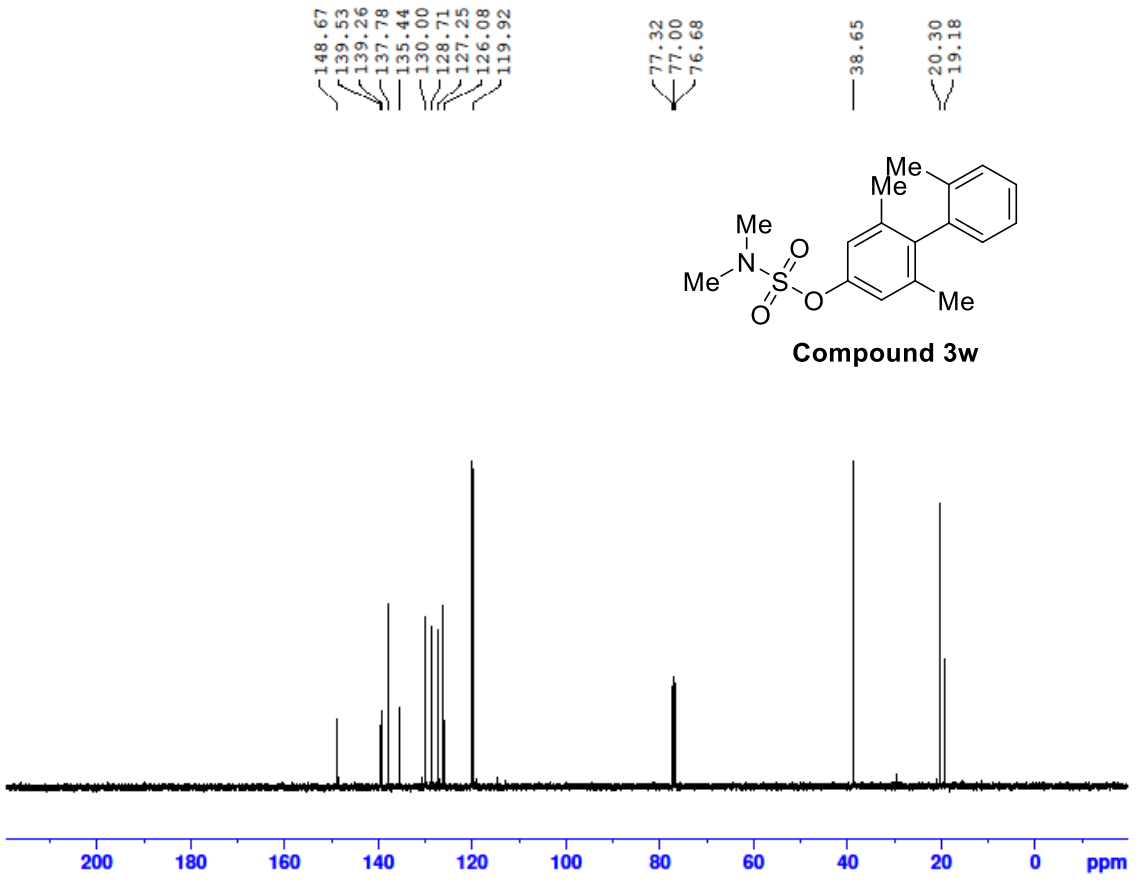

6.9804
6.9598
6.8964
6.8907
6.8526
6.8463
6.8316
6.8256
6.7282
3.8748
3.8596
2.0067
1.9952
Me
Me
OMe
MeO
Me
Compound 3v
7.00 6.95 6.90 6.85 6.80 6.75 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.00
1.00
2.00
3.00
3.00
3.00
6.00

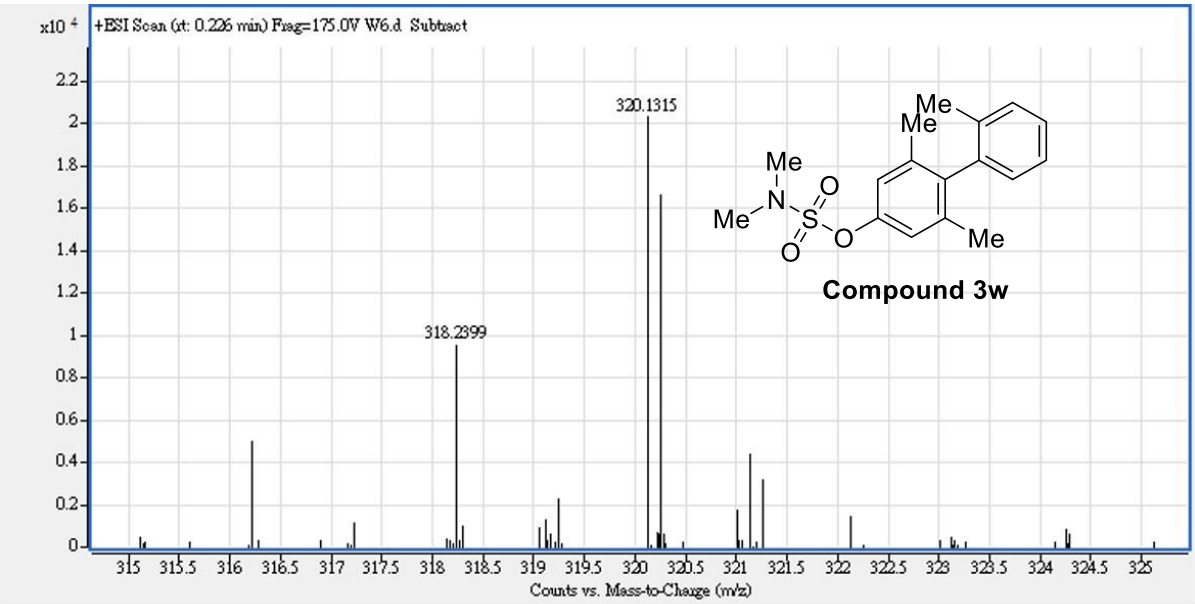

158.39
158.14
137.66
137.48
133.28
132.63
130.33
115.26
112.42
111.15
77.32
77.00
76.69
54.98
54.94
20.59
19.67
Me
Me
OMe
MeO
Me
Compound 3v
200 180 160 140 120 100 80 60 40 20 0 ppm



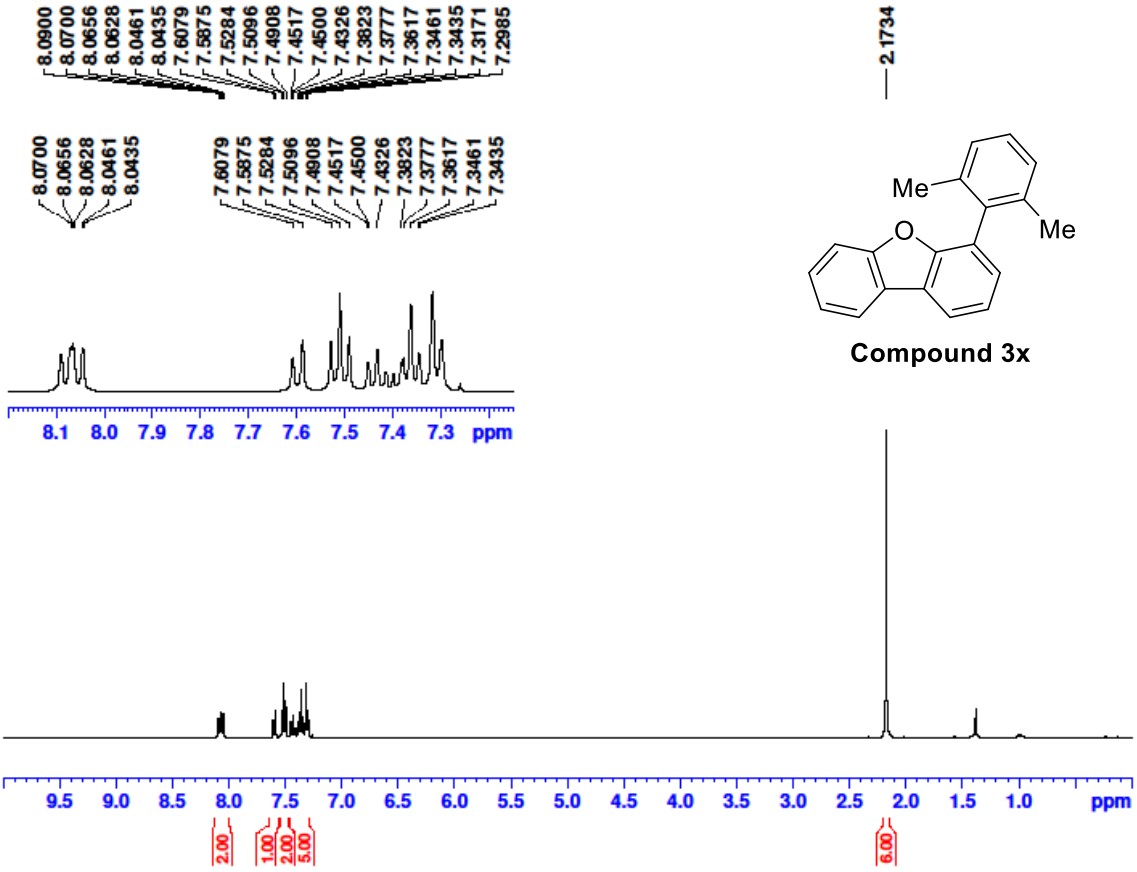
Mass	Calc. Mass	mDa	PPM	Formula
257.1536	257.1536	0.01	0.02	C17 H21 O2

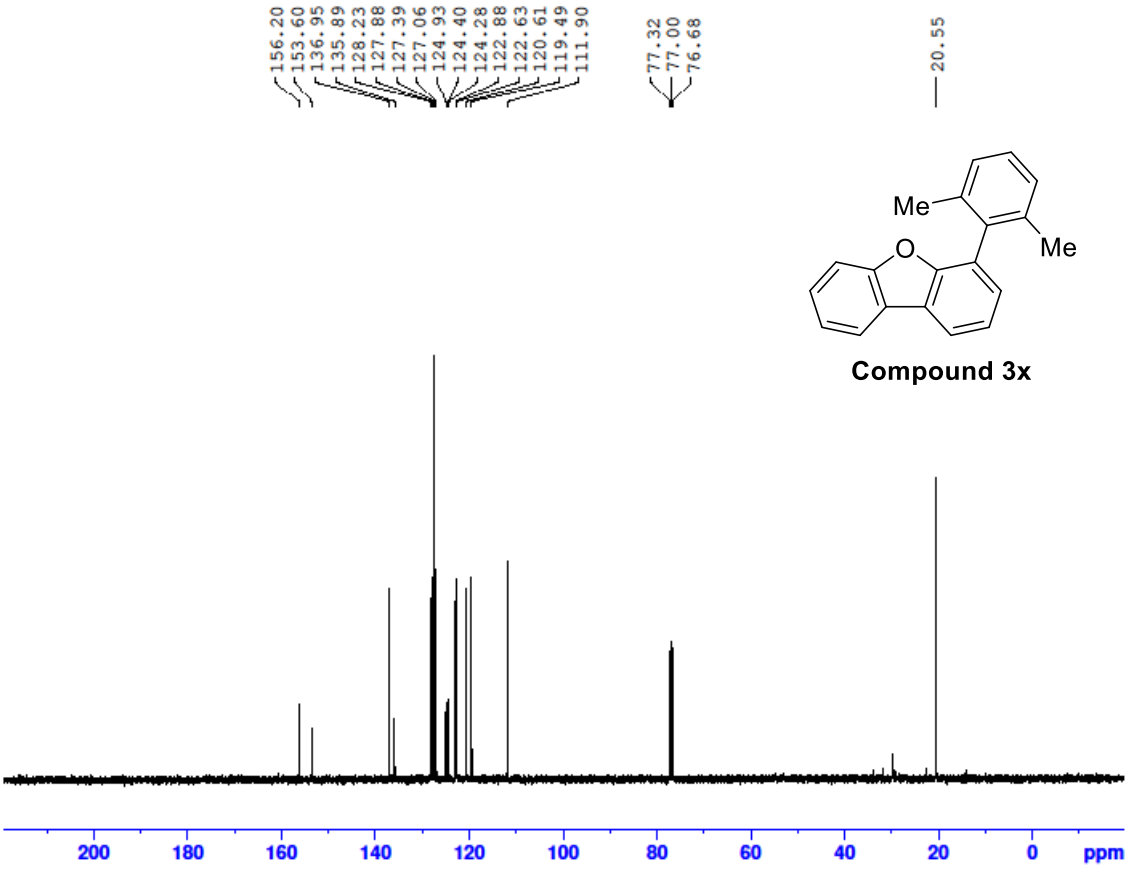

7.3266
7.3148
7.3106
7.2987
7.2939
7.2826
7.2739
7.2676
7.2562
7.0934
7.0169
7.0013
6.9960
3.0458
1.9859
Me
Me
Me
N
S
O
O
O
O
Me
Me
Compound 3w
7.3
7.2
7.1
7.0
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
3.00
2.00
1.00
6.00
9.00

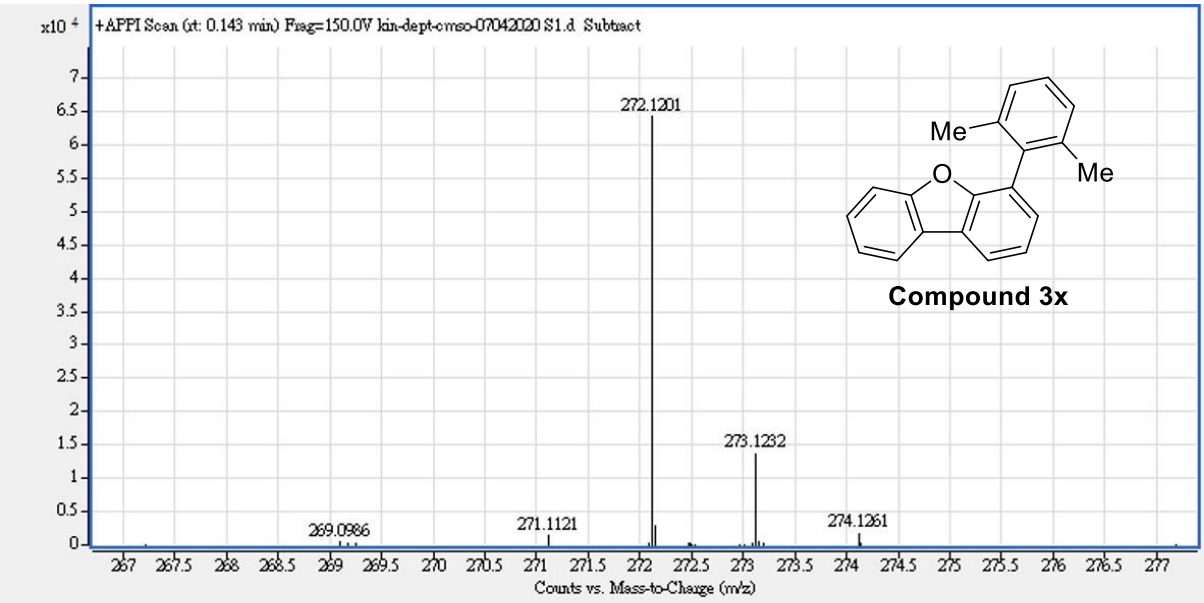

148.67
139.53
139.26
137.78
135.44
130.00
128.71
127.25
126.08
119.92
77.32
77.00
76.68
38.65
20.30
19.18
Me
Me
Me
N
S
O
O
O
O
Me
Me
Compound 3w
200
180
160
140
120
100
80
60
40
20
0
ppm



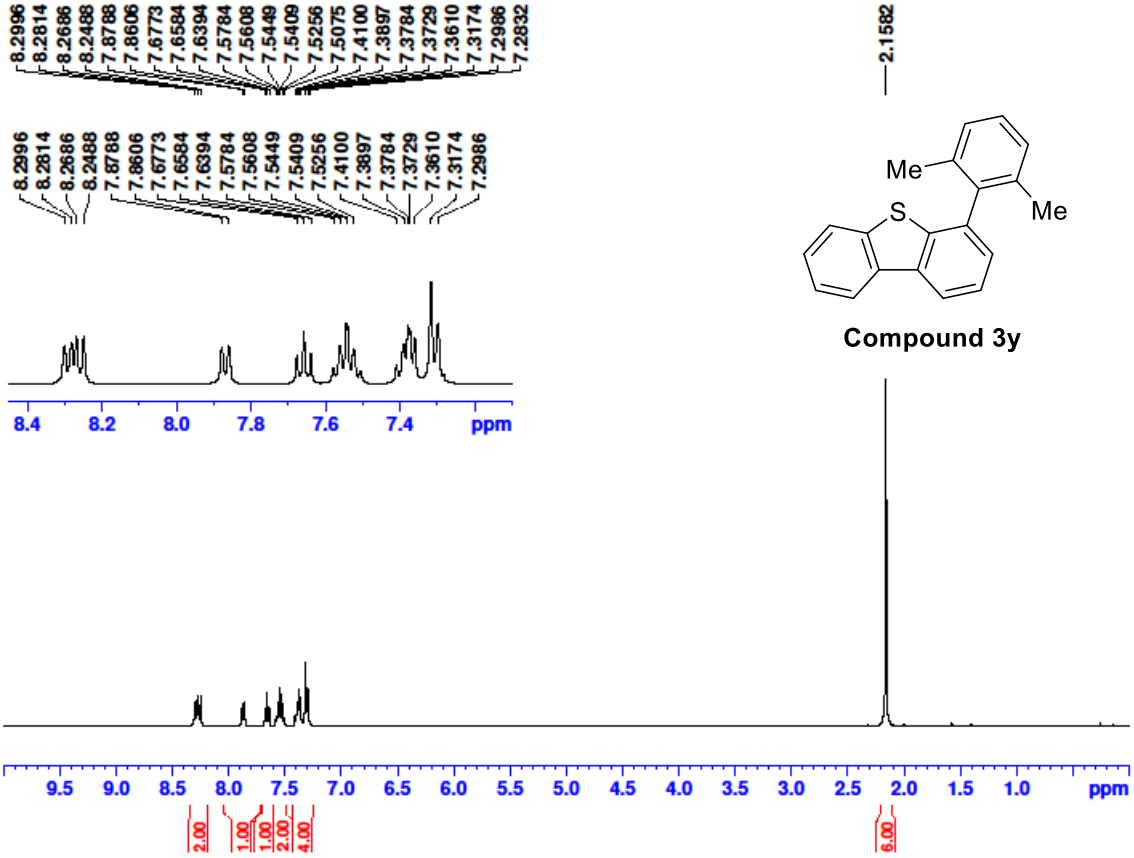
Mass	Calc. Mass	mDa	PPM	Formula
320.1315	320.1315	-0.01	-0.03	C17 H22 N O3 S


8.0900
8.0700
8.0656
8.0628
8.0461
8.0435
7.6079
7.5875
7.5284
7.5096
7.4908
7.4517
7.4500
7.4326
7.3823
7.3777
7.3617
7.3461
7.3435
7.3171
7.2985
2.1734
Me
Me
O
Compound 3x
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 ppm
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 ppm
2.00
1.00
2.00
5.00
6.00

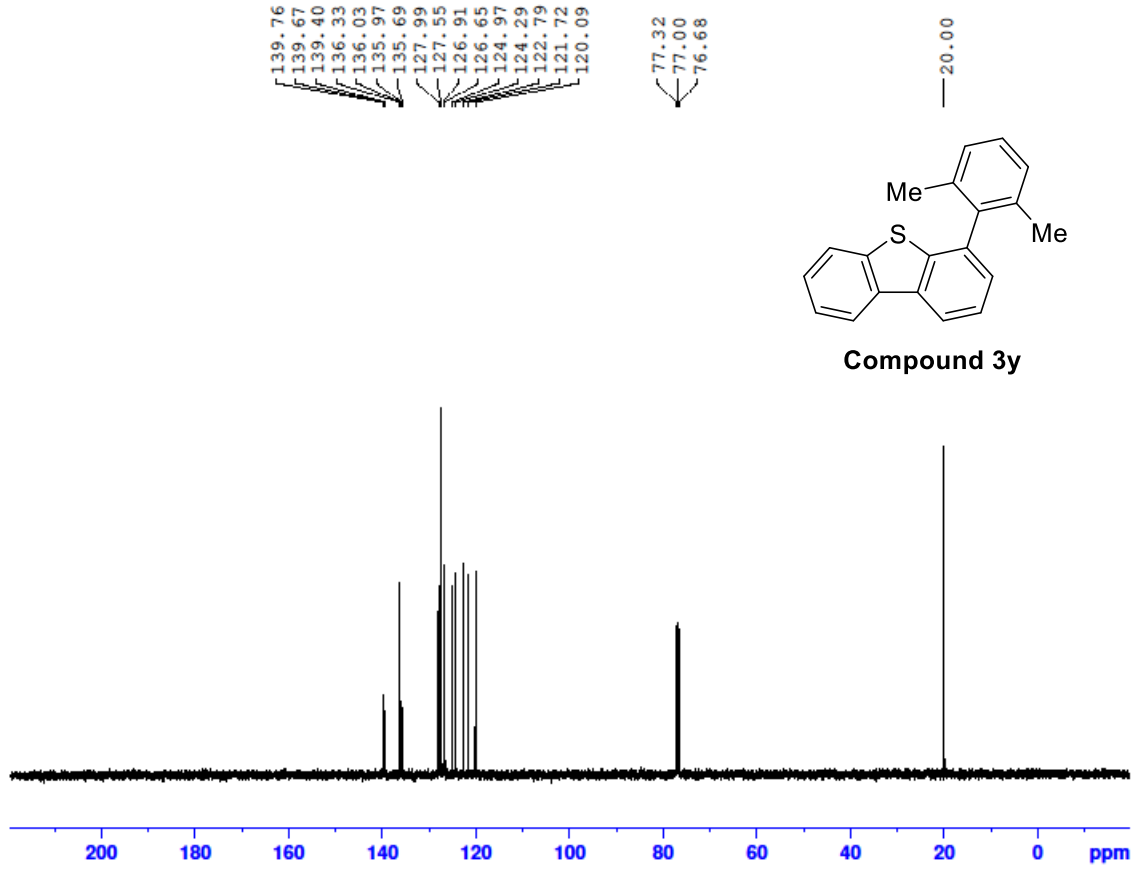

156.20
153.60
136.95
135.89
128.23
127.88
127.39
127.06
124.93
124.40
124.28
122.88
122.63
120.61
119.49
111.90
77.32
77.00
76.68
20.55
Me
Me
O
Compound 3x
200 180 160 140 120 100 80 60 40 20 0 ppm



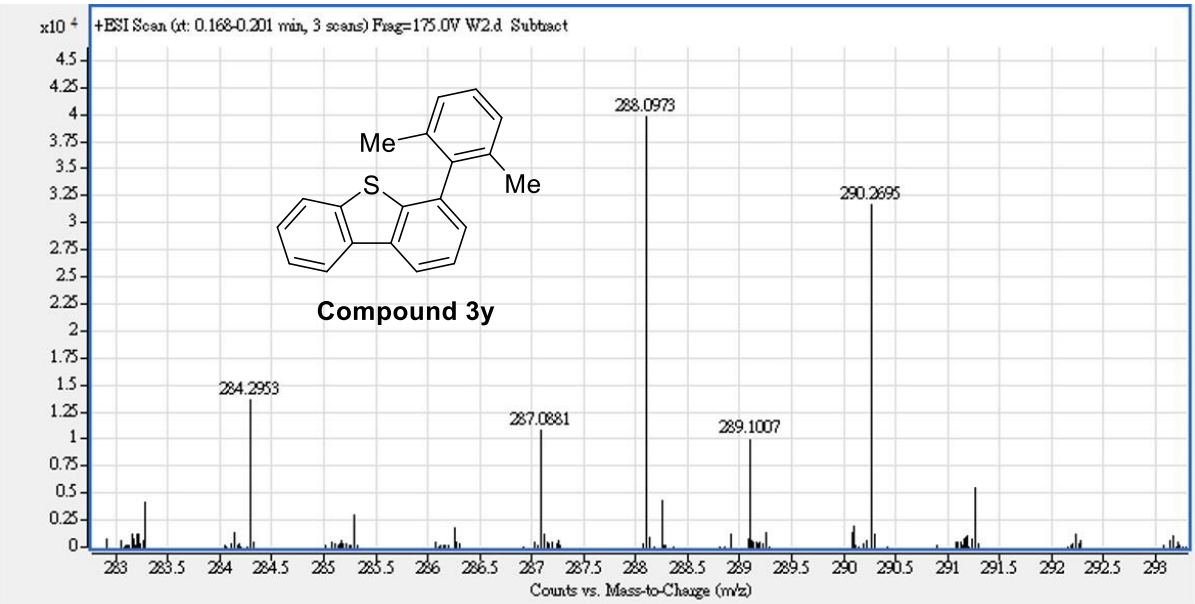
Mass	Calc. Mass	mDa	PPM	Formula
272.1201	272.1196	-0.53	-1.97	C20 H16 O



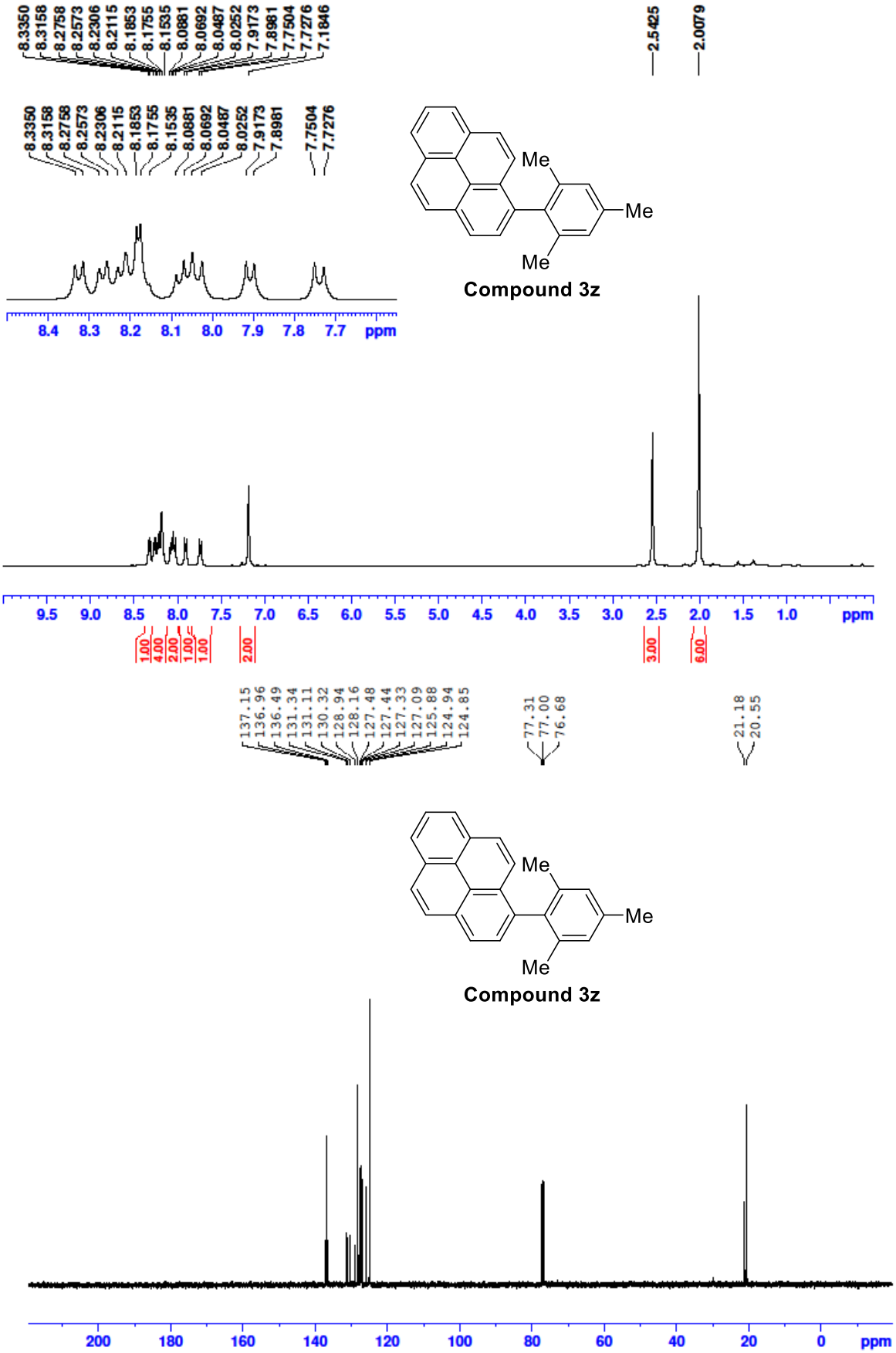
Compound 3y

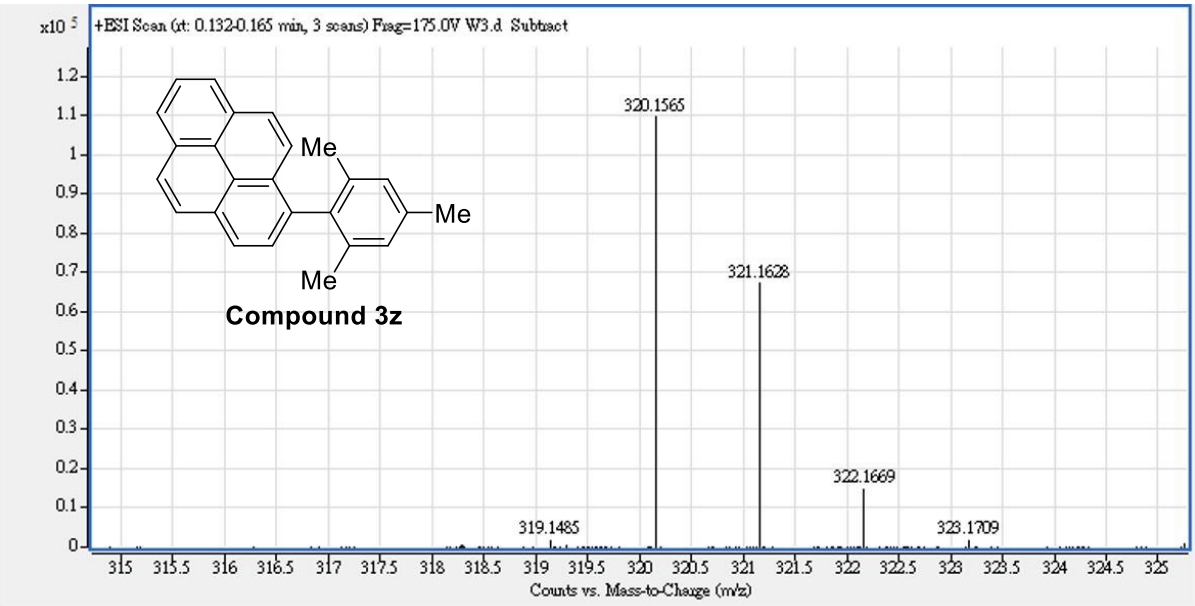


Compound 3y

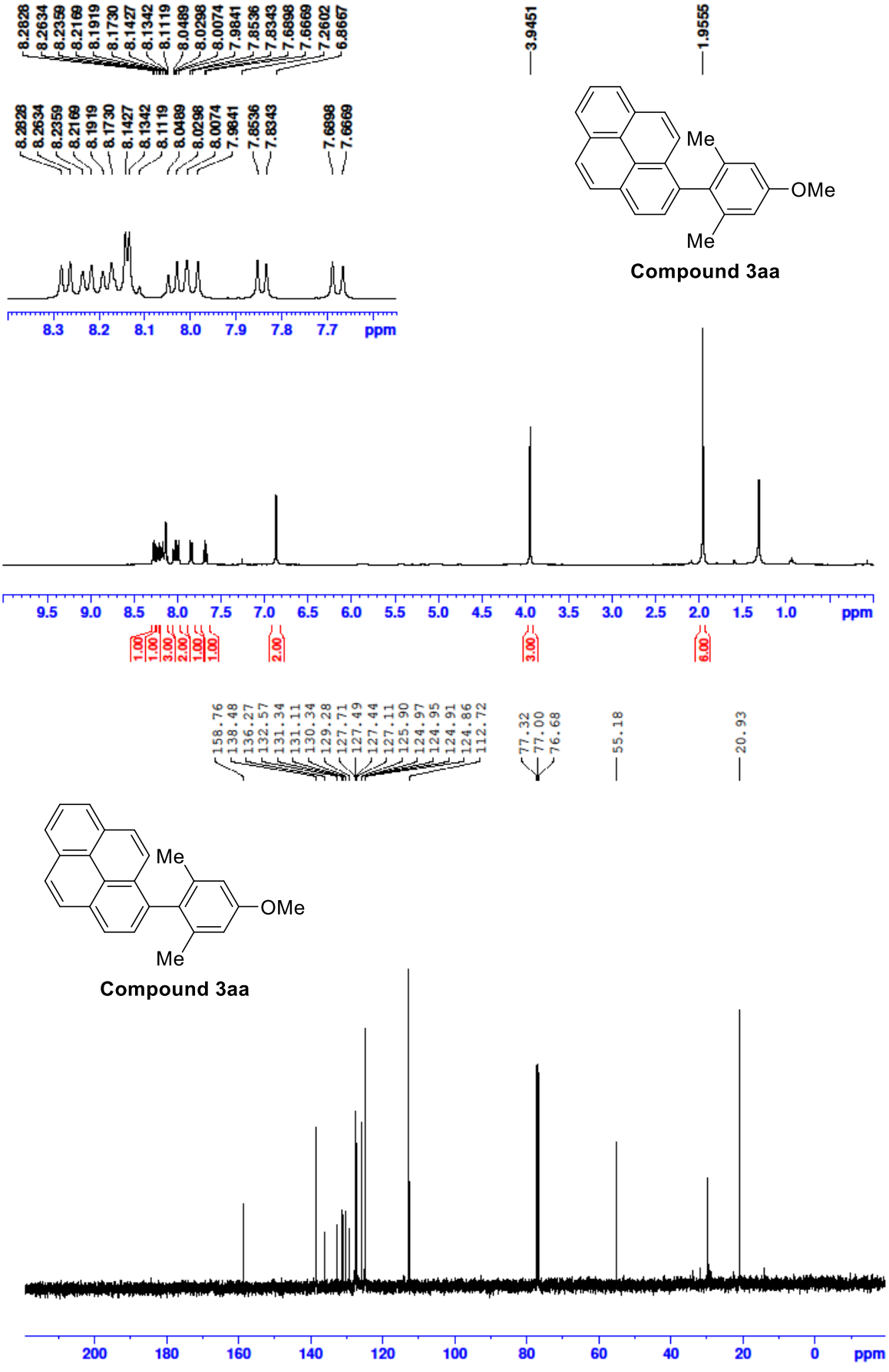


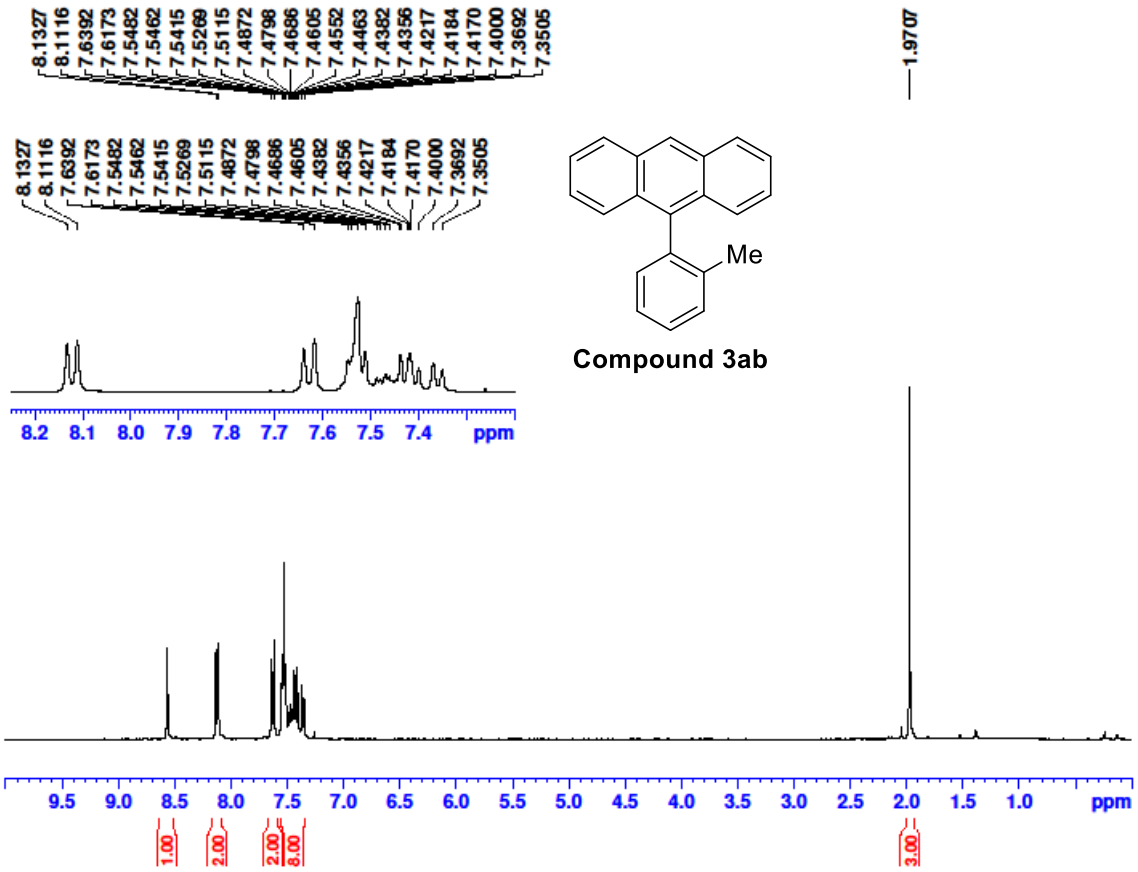
Mass	Calc. Mass	mDa	PPM	Formula
288.0973	288.0973	-0.03	-0.10	C20 H16 S

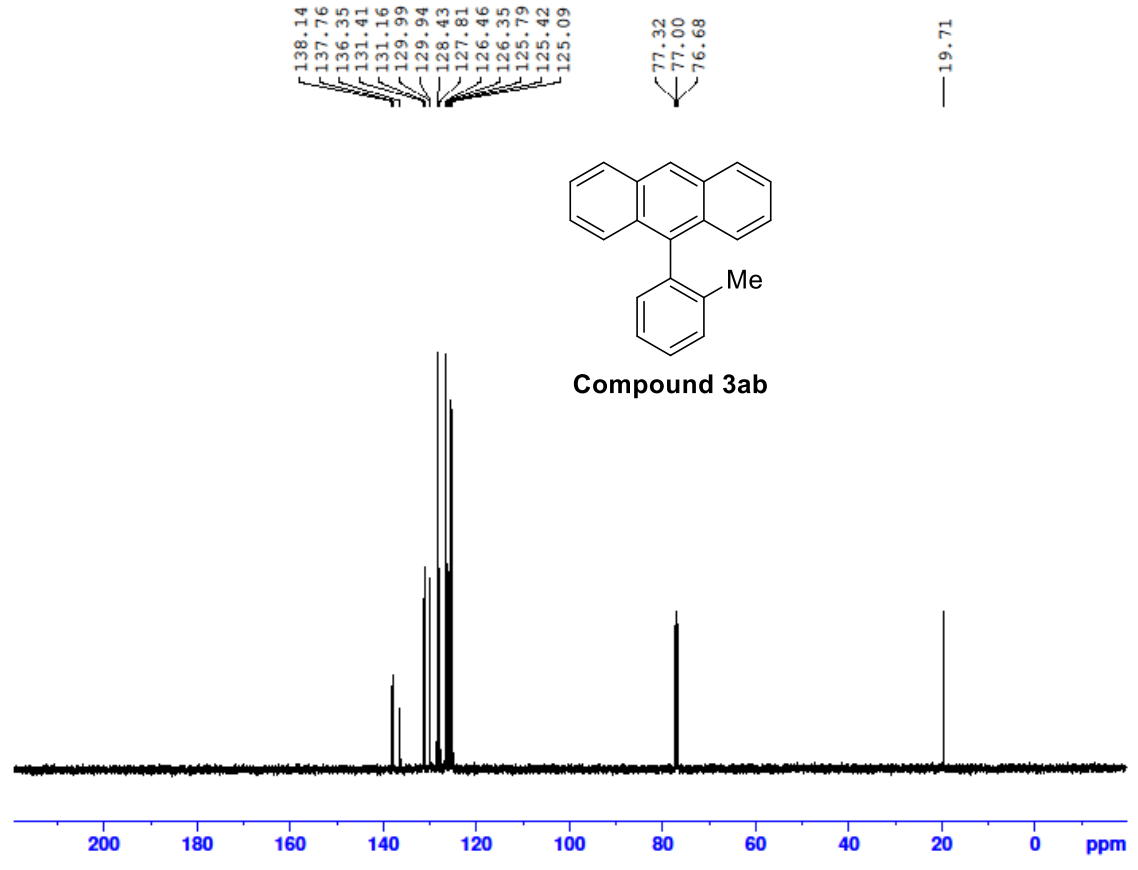

8.3350
8.3158
8.2758
8.2573
8.2306
8.2115
8.1853
8.1755
8.1535
8.0881
8.0692
8.0487
8.0252
7.9173
7.8981
7.7504
7.7276
7.1846
2.5425
2.0079
Me
Me
Me
Compound 3z
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
4.00
2.00
1.00
1.00
2.00
3.00
6.00
137.15
136.96
136.49
131.34
131.11
130.32
128.94
128.16
127.48
127.44
127.33
127.09
125.88
124.94
124.85
77.31
77.00
76.68
21.18
20.55
Me
Me
Me
Compound 3z
200 180 160 140 120 100 80 60 40 20 0 ppm

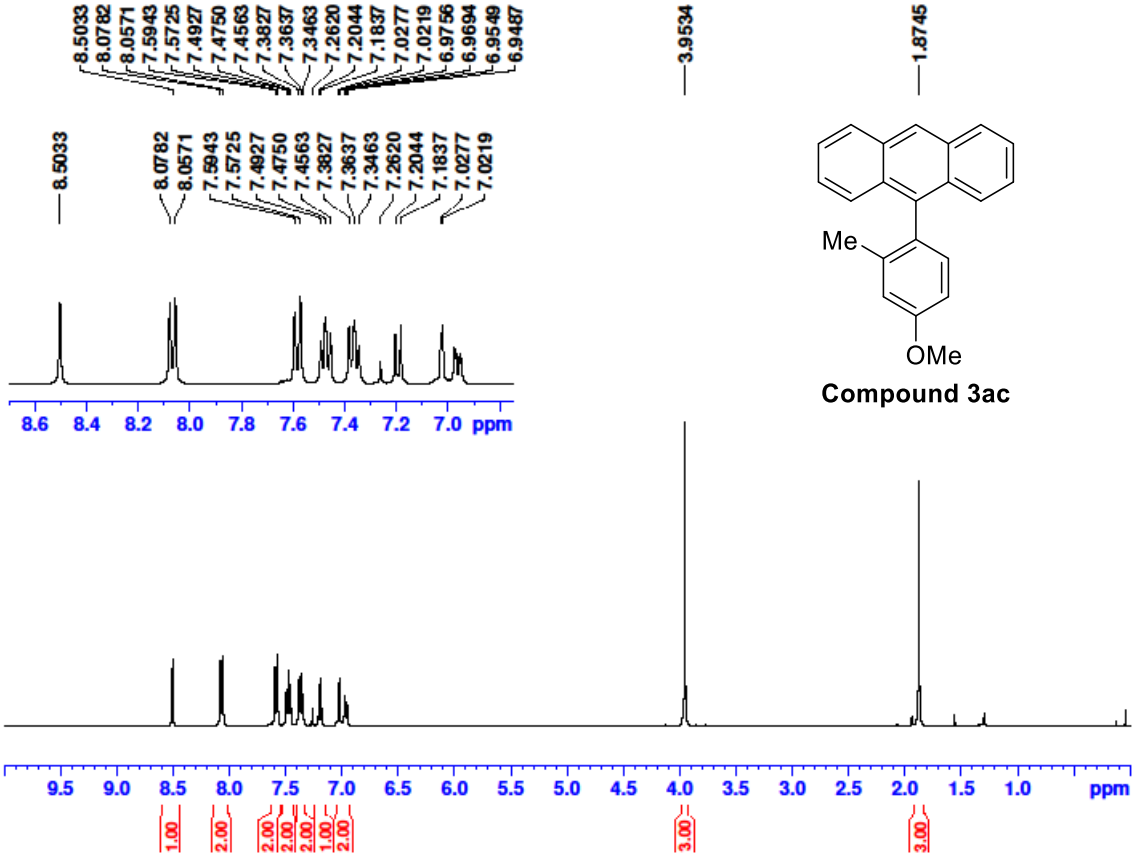


Mass	Calc. Mass	mDa	PPM	Formula
320.1565	320.1565	0.00	0.00	C25 H20

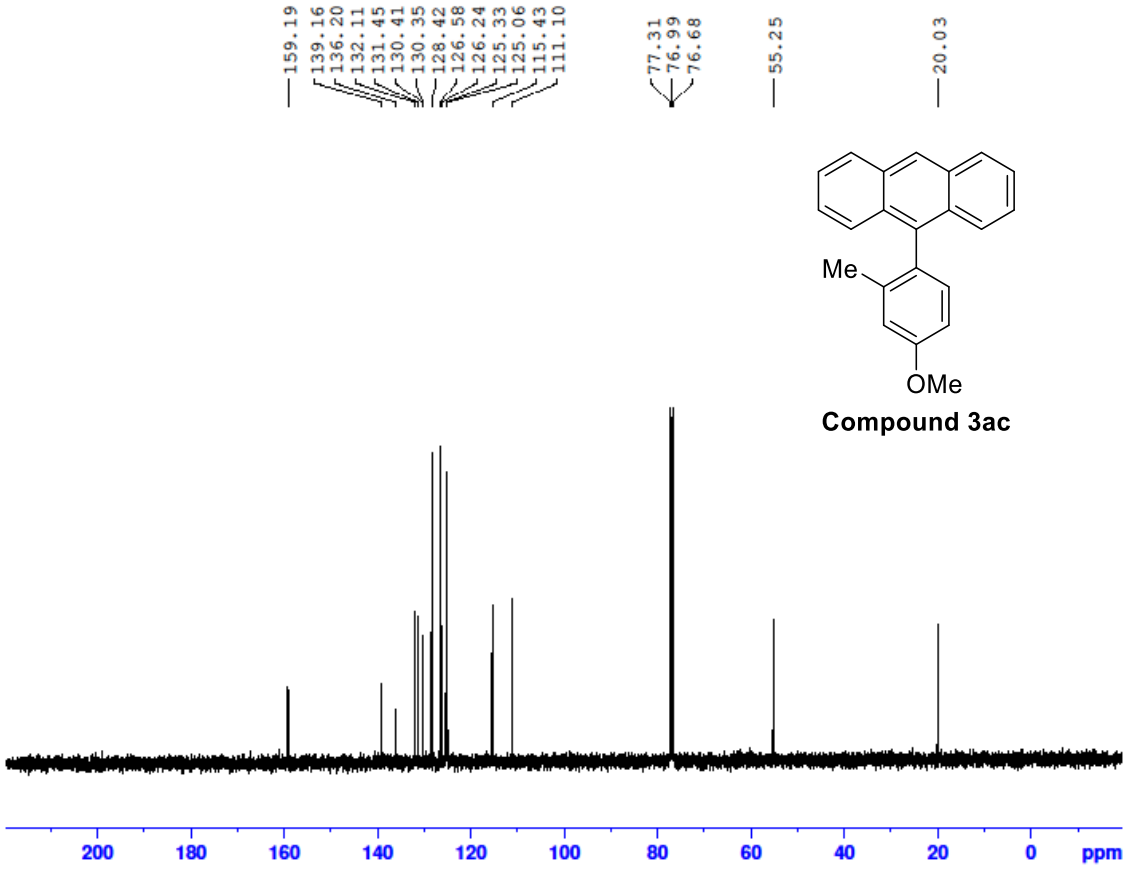

8.2828
8.2634
8.2359
8.2169
8.1919
8.1730
8.1427
8.1342
8.1119
8.0489
8.0298
8.0074
7.9841
7.8536
7.8343
7.6898
7.6669
7.2602
6.8657
3.9451
1.9555
Me
OMe
Me
Compound 3aa
8.3 8.2 8.1 8.0 7.9 7.8 7.7 ppm
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00 1.00 3.00 2.00 1.00 1.00 2.00 3.00 6.00
158.76
138.48
136.27
132.57
131.34
131.11
130.34
129.28
127.71
127.49
127.44
127.11
125.90
124.97
124.95
124.91
124.86
112.72
77.32
77.00
76.68
55.18
20.93
Me
OMe
Me
Compound 3aa
200 180 160 140 120 100 80 60 40 20 0 ppm


8.1327
8.1116
7.6392
7.6173
7.5482
7.5462
7.5415
7.5269
7.5115
7.4872
7.4798
7.4686
7.4605
7.4552
7.4463
7.4382
7.4356
7.4217
7.4184
7.4170
7.4000
7.3692
7.3505
1.9707
Me
Compound 3ab
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
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 ppm
1.00
2.00
2.00
8.00
3.00

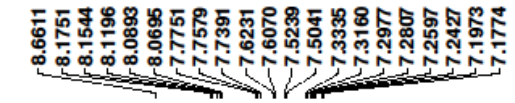

138.14
137.76
136.35
131.41
131.16
129.99
129.94
128.43
127.81
126.46
126.35
125.79
125.42
125.09
77.32
77.00
76.68
19.71
Me
Compound 3ab
200 180 160 140 120 100 80 60 40 20 0 ppm

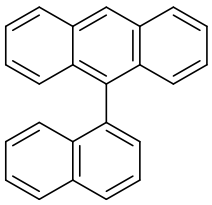


Compound 3ac

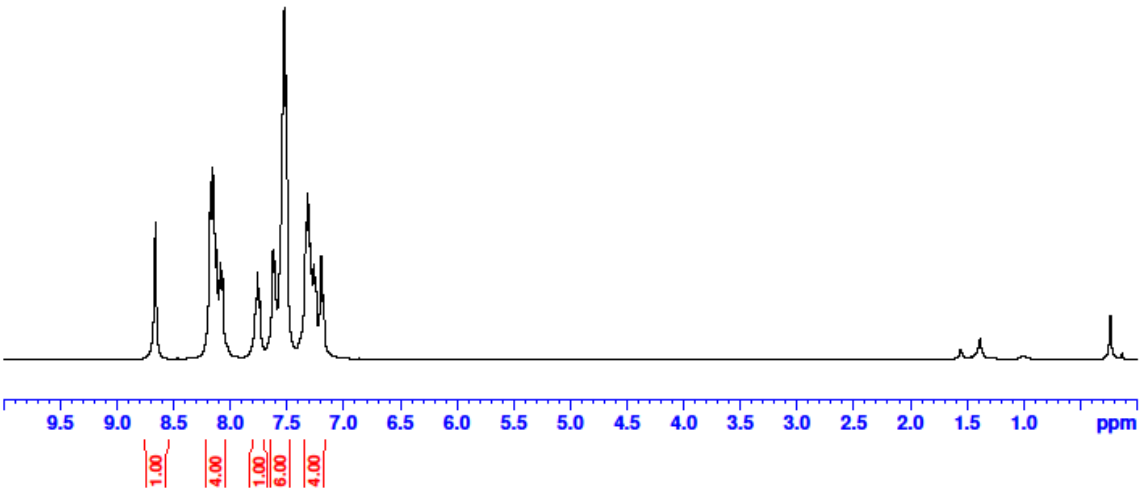


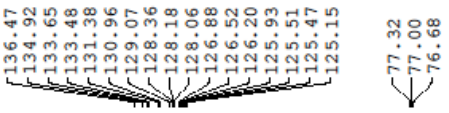
Compound 3ac

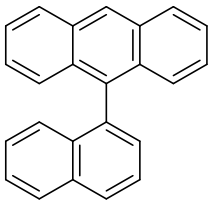




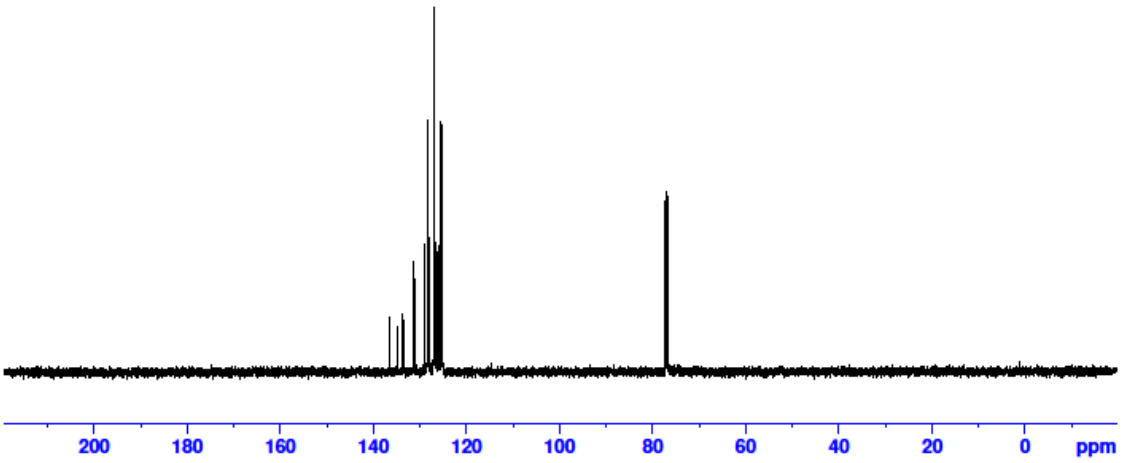
Compound 3ad

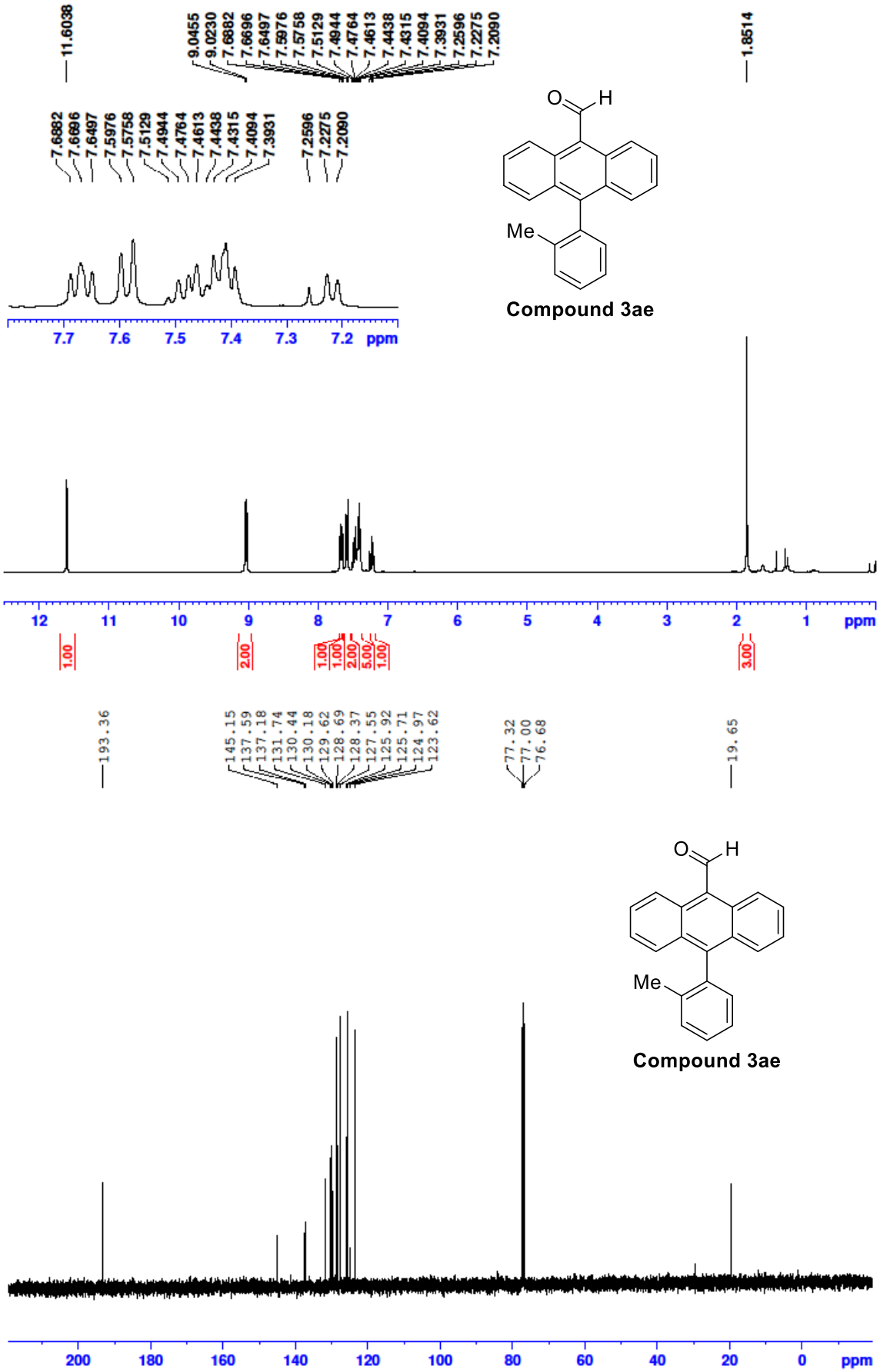


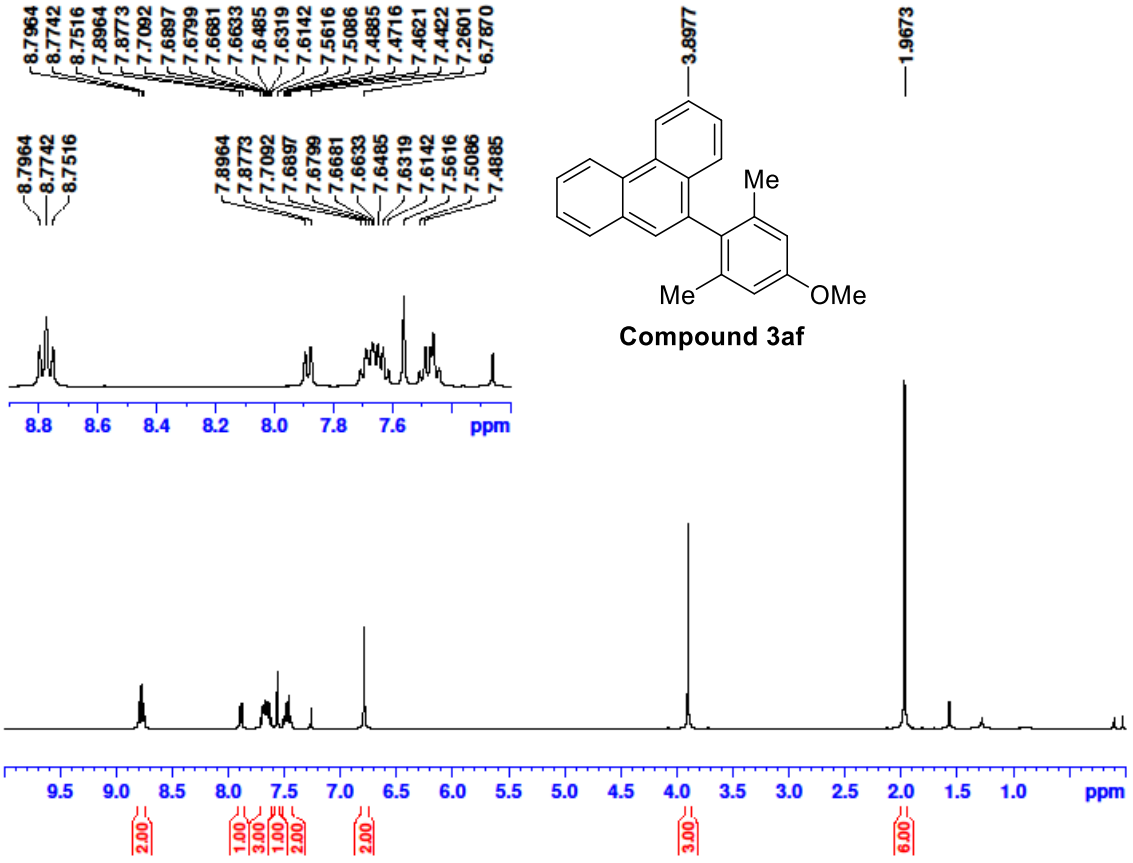




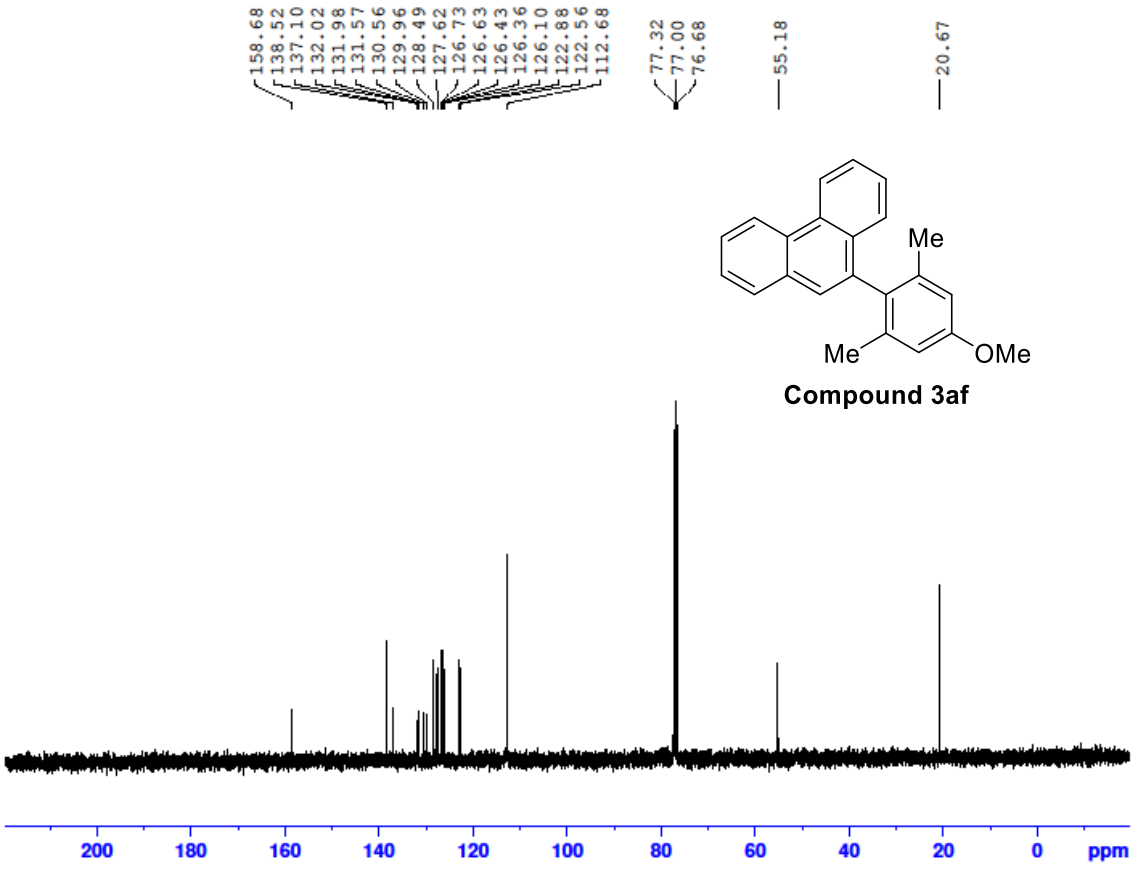
Compound 3ad




11.6038
9.0455
9.0230
7.6882
7.6696
7.6497
7.5976
7.5758
7.5129
7.4944
7.4764
7.4613
7.4438
7.4315
7.4094
7.3931
7.2596
7.2275
7.2090
1.8514
O
H
Me
Compound 3ae
7.7
7.6
7.5
7.4
7.3
7.2
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.00
1.00
1.00
2.00
5.00
1.00
3.00
193.36
145.15
137.59
137.18
131.74
130.44
130.18
129.62
128.69
128.37
127.55
125.92
125.71
124.97
123.62
77.32
77.00
76.68
19.65
O
H
Me
Compound 3ae
200
180
160
140
120
100
80
60
40
20
0
ppm



Compound 3af



Compound 3af

10. References

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