A General Strategy for the Construction of Functionalized Azaindolines via Domino Palladium Catalyzed Heck Cyclization/Suzuki Coupling

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Supporting Information

General Methods

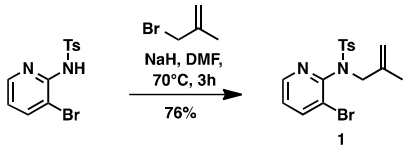
All reactions were carried out under a nitrogen atmosphere. All commercial reagents and anhydrous solvents were used without additional purification. Nuclear magnetic resonance (NMR) spectra were acquired on a Bruker BioSpin GmbG operating at 400 and 100 MHz for ^{1}H and ^{13}C, respectively, and are referenced internally according to residual solvent signals. NMR data were processed using MNova software and recorded as follows: ^{1}H-NMR - chemical shift (δ, ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), coupling constant (Hz), and integration; ^{13}C-NMR – chemical shift (δ, ppm). High-resolution mass spectra (HRMS) were recorded on a Thermo Scientific Orbitrap Q Exact mass spectrometer. Thin-layer chromatography was performed on EMD TLC Silica gel 60 F254 plates and visualized with UV light. Reactions were monitored by a Shimadzu LCMS/UV system with LC-30AD solvent pump, 2020 MS, Sil-30AC autosampler, SPD-M30A UV detector, CTO-20A column oven, using a 2-98% acetonitrile/0.1% formic acid (or 0.001% ammonia) gradient over 2.5 minutes. Flash column chromatography purifications were done on a Teledyne Isco Combiflash Rf utilizing Silicycle HP columns using a mobile phase composed of either heptane/isopropyl acetate or dichloromethane/methanol.

General procedure for the preparation of tosylates

p-Toluenesulfonyl chloride (1.1 equiv) was added to a solution of the substrate (1.0 equiv) in pyridine (1.0 M) and the reaction was heated at 90°C for 3 h. After cooling the rt, the pyridine was removed under reduced pressure. The crude residue was dissolved in dichloromethane and washed with saturated aqueous sodium bicarbonate (3x). The organic layer was dried with sodium sulfate, concentrated, and the crude residue was purified by flash column chromatography to give the desired product in sufficient purity (>80% - contaminated with the bis-tosyl product), which was used directly in the next reaction.

General Procedure 1 – Alkylation of Amino Arenes

Sodium hydride (60% in oil, 1.2 equiv.) was added to a solution of the substrate (1 equiv.) in DMF (0.4 M) at rt. After 30 min, 3-bromo-2-methyl propene (1.2 equiv.) was added and the solution was then heated at 70˚C. Reaction progress was monitored by LCMS (3-16 h). Once complete, the reaction was cooled to rt, and water was carefully added to the solution. The reaction was diluted with isopropyl acetate and additional water. The organic was extracted with isopropyl acetate (3x). The combined organic layers were washed with brine, dried with sodium sulfate, concentrated and the crude residue was purified by flash column chromatography.



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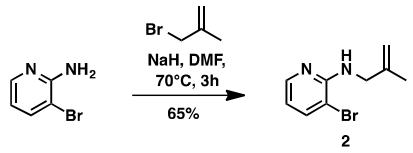
***N*-(3-bromopyridin-2-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide (1)–** Using General Procedure 1, purified by flash column chromatography (silica, 10% → 100% isopropyl acetate – heptane) to give 21.27 g, 55.79 mmol (76%) as a yellowish solid.

Melting point 113-117 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 4.6, 1.7 Hz, 1H), 8.01 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.70 – 7.62 (m, 2H), 7.34 – 7.27 (m, 2H), 7.12 (dd, *J* = 7.9, 4.6 Hz, 1H), 4.70 – 4.65 (m, 1H), 4.65 – 4.60 (m, 1H), 4.03 (d, *J* = 0.9 Hz, 2H), 2.44 (s, 3H), 1.81 (t, *J* = 1.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 147.1, 143.8, 142.6, 139.6, 135.3, 129.4, 128.6, 124.2, 123.7, 115.7, 56.2, 21.6, 20.6.

HRMS (ESI) calcd for $C_{16}H_{18}BrN_2O_2S$ $[M+H]^+$: 381.0272, found: 381.0257.

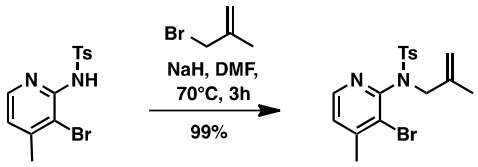


3-bromo-*N*-(2-methylallyl)pyridin-2-amine (2) – Using General Procedure 1, purified by flash column chromatography (silica, 50% → 100% isopropyl acetate – heptane) to give 10.25 g, 45.15 mmol (65%) as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.61 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.45 (dd, *J* = 7.6, 4.9 Hz, 1H), 5.14 (bs, 1H), 4.94 – 4.89 (m, 1H), 4.89 – 4.83 (m, 1H), 4.06 (dd, *J* = 6.0, 1.6 Hz, 2H), 1.84 – 1.78 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 146.8, 142.9, 139.5, 113.4, 110.0, 105.5, 47.0, 20.6.

HRMS (ESI) calcd for $C_9H_{12}BrN_2$ $[M+H]^+$: 227.0184, found: 227.0173



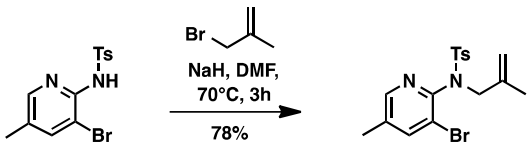
***N*-(3-bromo-4-methylpyridin-2-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide** - Using General Procedure 1, purified by flash column chromatography (silica, 70% isopropyl acetate – heptane) to give 3.94 g, 9.98 mmol (99%) as a light yellow solid.

Melting point 116-117 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 4.7 Hz, 1H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 4.9 Hz, 1H), 4.69 – 4.65 (m, 1H), 4.65 – 4.60 (m, 1H), 4.02 (s, 2H), 2.49 (s, 3H), 2.44 (s, 3H), 1.82 (t, *J* = 1.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 150.7, 146.1, 143.7, 139.7, 135.4, 129.3, 128.7, 126.5, 125.4, 115.7, 56.4, 23.8, 21.6, 20.7.

HRMS (ESI) calcd for $C_{17}H_{20}BrN_2O_2S$ $[M+H]^+$: 395.0429, found: 395.0414



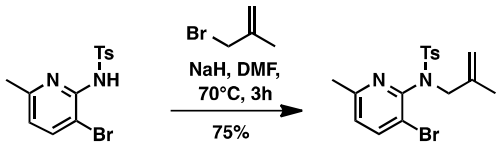
***N*-(3-bromo-5-methylpyridin-2-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide** - Using General Procedure 1, purified by flash column chromatography (silica, 70% isopropyl acetate – heptane) to give 5.11 g, 13.28 mmol (78%) as a yellowish solid.

Melting point 94-97 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 2.2 Hz, 1H), 7.82 (d, *J* = 2.2 Hz, 1H), 7.70 – 7.63 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.69 – 4.65 (m, 1H), 4.65 – 4.61 (m, 1H), 4.01 (s, 2H), 2.44 (s, 3H), 2.33 (s, 3H), 1.81 (t, *J* = 1.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 147.5, 143.7, 142.9, 139.7, 135.4, 134.6, 129.4, 128.6, 123.0, 115.6, 56.1, 21.6, 20.6, 17.6.

HRMS (ESI) calcd for $C_{17}H_{20}BrN_2O_2S$ $[M+H]^+$: 395.0429, found: 395.0410



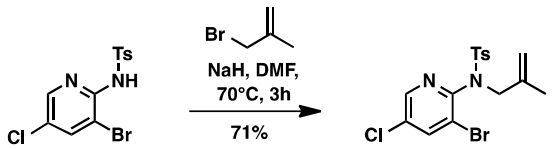
***N*-(3-bromo-6-methylpyridin-2-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide** - Using General Procedure 1, purified by flash column chromatography (silica, 70% isopropyl acetate – heptane) to give 7.50 g, 18.98 mmol (75%) as a white solid.

Melting point 110-114 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 1H), 4.69 – 4.65 (m, 1H), 4.65 – 4.61 (m, 1H), 4.01 (s, 2H), 2.45 (s, 3H), 2.36 (s, 3H), 1.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 150.3, 143.6, 142.5, 139.8, 135.5, 129.11, 128.8, 124.0, 119.9, 115.5, 56.2, 23.4, 21.6, 20.6.

HRMS (ESI) calcd for $C_{17}H_{20}BrN_2O_2S$ $[M+H]^+$: 395.0429, found: 395.0413



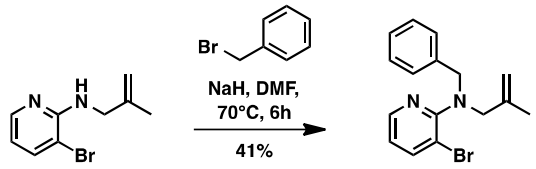
***N*-(3-bromo-5-chloropyridin-2-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide** - Using General Procedure 1, purified by flash column chromatography (silica, 70% isopropyl acetate – heptane) to give 5.52 g, 13.28 mmol (71%) as a yellow solid.

Melting point 100-104 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 2.4 Hz, 1H), 8.01 (d, *J* = 2.4 Hz, 1H), 7.68 – 7.60 (m, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 4.71 – 4.66 (m, 1H), 4.66 – 4.60 (m, 1H), 3.99 (d, *J* = 1.0 Hz, 2H), 2.45 (s, 3H), 1.79 (t, *J* = 1.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.8, 145.9, 144.0, 141.8, 139.3, 135.0, 131.3, 129.5, 128.6, 123.7, 116.0, 56.2, 21.6, 20.5.

HRMS (ESI) calcd for $C_{16}H_{17}BrClN_2O_2S$ $[M+H]^+$: 414.9882, found: 414.9867

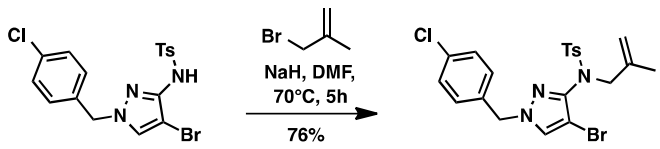


***N*-benzyl-3-bromo-*N*-(2-methylallyl)pyridin-2-amine -** Using General Procedure 1, purified by flash column chromatography (silica, 0% → 20% methanol – dichloromethane) to give 0.255 g, 0.804 mmol (41%) as a clear oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.15 (m, 1H), 7.81 – 7.75 (m, 1H), 7.41 – 7.15 (m, 5H), 6.77 – 6.68 (m, 1H), 4.93 – 4.86 (m, 1H), 4.86 – 4.82 (m, 1H), 4.55 (s, 2H), 3.87 (s, 2H), 1.69 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.32 146.2, 142.5, 142.4, 138.9, 128.2, 128.0, 126.7, 118.2, 112.8, 112.6, 56.1, 53.9, 20.7.

HRMS (ESI) calcd for $C_{16}H_{18}BrN_2$ $[M+H]^+$: 317.0653, found: 317.0641



***N*-(4-bromo-1-(4-chlorobenzyl)-1*H*-pyrazol-3-yl)-4-methyl-*N*-(2-methylallyl) benzenesulfonamide** - Using General Procedure 1, purified by flash column chromatography

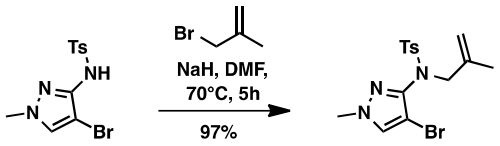
(silica, 50% → 100% isopropyl acetate – heptane) to give 3.49 g, 7.06 mmol (76%) as a yellowish solid.

Melting point 112-115 °C

^{1}H NMR (400 MHz, $CDCl_3$ δ 7.63 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.27 (m, 3H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.05 (d, *J* = 8.3 Hz, 2H), 5.12 (s, 2H), 4.74 (s, 2H), 4.02 (s, 2H), 2.42 (s, 3H), 1.77 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9, 143.6, 139.8, 135.6, 134.3, 134.2, 131.0, 129.4, 129.0, 128.9, 128.2, 115.1, 94.8, 56.8, 56.2, 21.6, 20.0.

HRMS (ESI) calcd for $C_{21}H_{22}BrClN_3O_2S$ $[M+H]^+$: 494.0304, found: 494.0283



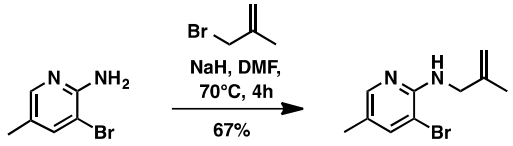
***N*-(4-bromo-1-methyl-1*H*-pyrazol-3-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide -** Using General Procedure 1, purified by flash column chromatography (silica, 50% → 100% isopropyl acetate – heptane) to give 2.03 g, 5.30 mmol (97%) as a white solid.

Melting point 76-79 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.24 (m, 3H), 4.80 – 4.77 (m, 1H), 4.76– 4.73 (m, 1H), 4.02 (s, 2H), 3.80 (s, 3H), 2.43 (s, 3H), 1.53 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 143.6, 139.8, 135.9, 131.5, 129.4, 128.2, 114.9, 93.9, 56.7, 40.1, 21.6, 20.0.

HRMS (ESI) calcd for $C_{15}H_{19}BrN_3O_2S$ $[M+H]^+$: 384.0381, found: 384.0363

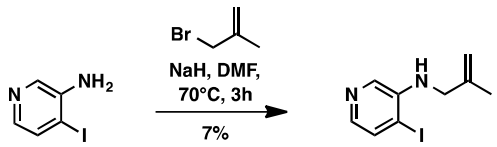


3-bromo-5-methyl-*N*-(2-methylallyl)pyridin-2-amine - Using General Procedure 1, purified by flash column chromatography (silica, 0% → 20% methanol – dichloromethane) to give 0.434 g, 1.80 mmol (67%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 1.8 Hz, 1H), 7.47 (d, *J* = 1.9 Hz, 1H), 4.98 (bs, 1H), 4.92 – 4.88 (m, 1H), 4.87 – 4.81 (m, 1H), 4.06 – 3.99 (m, 2H), 2.16 (s, 3H), 1.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.7, 146.3, 143.1, 140.4, 122.6, 112.2, 109.9, 105.3, 47.1, 20.7, 20.6, 17.0.

HRMS (ESI) calcd for $C_{10}H_{14}BrN_2$ $[M+H]^+$: 241.0340, found: 241.0327

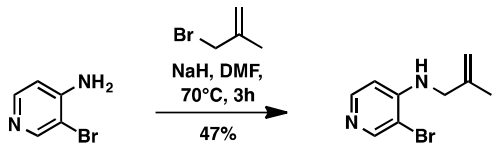


4-iodo-*N*-(2-methylallyl)pyridin-3-amine - Using General Procedure 1, purified by flash column chromatography (silica, 30% → 100% isopropyl acetate – heptane) to give 0.130 g, 0.474 mmol (7%) as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.60 – 7.52 (m, 2H), 4.99 – 4.91 (m, 2H), 4.42 – 4.32 (m, 1H), 3.81 (d, *J* = 5.8 Hz, 2H), 1.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 140.9, 138.9, 133.6, 132.8, 111.7, 94.8, 49.7, 20.3.

HRMS (ESI) calcd for $C_9H_{12}IN_2$ $[M+H]^+$: 275.0045, found: 275.0032

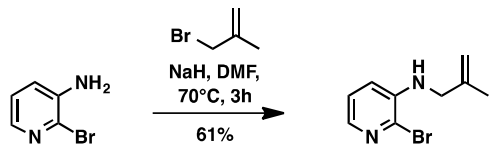


3-bromo-*N*-(2-methylallyl)pyridin-4-amine - Using General Procedure 1, purified by flash column chromatography (silica, 30% → 100% isopropyl acetate – heptane) to give 1.23 g, 5.42 mmol (47%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 8.13 (d, *J* = 5.6 Hz, 1H), 6.44 (d, *J* = 5.7 Hz, 1H), 5.05 (bs, 1H), 4.93 (ddd, *J* = 6.7, 3.3, 1.5 Hz, 2H), 3.79 (d, *J* = 6.3 Hz, 2H), 1.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.7, 149.9, 149.0, 140.4, 111.8, 107.5, 106.3, 48.6, 20.2.

HRMS (ESI) calcd for $C_9H_{12}BrN_2$ $[M+H]^+$: 227.0184, found: 227.0173



2-bromo-*N*-(2-methylallyl)pyridin-3-amine- Using General Procedure 1, purified by flash column chromatography (silica, 30% → 100% isopropyl acetate – heptane) to give 1.61 g, 7.09 mmol (61%) as an orange oil.

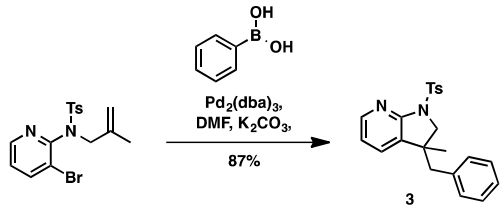
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 4.6, 1.7 Hz, 1H), 7.07 (dd, *J* = 8.0, 4.5 Hz, 1H), 6.78 (dd, *J* = 8.0, 1.7 Hz, 1H), 4.93 (ddt, *J* = 5.7, 2.8, 1.2 Hz, 2H), 4.69 (bs, 1H), 3.74 (dd, *J* = 5.9, 1.8 Hz, 2H), 1.78 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.2, 140.9, 137.2, 130.2, 123.6, 117.5, 111.6, 49.2, 20.2.

HRMS (ESI) calcd for $C_9H_{12}BrN_2$ $[M+H]^+$: 227.0184, found: 227.0176

General Procedure 2 - Tandem Heck-Suzuki Cross Coupling:

Tris(dibenzylideneacetone)dipalladium (5 mol%), potassium carbonate (4 equiv), boronic acid (2 equiv.) were added to a solution of the substrate (1.0 equiv.) in DMF (0.1 M). The solution was degassed with nitrogen for 10 min. The reaction flask was sealed and then heated at 110˚C for 17 hours. After cooling, the reaction was diluted with isopropyl acetate and filtered through a short plug of celite. The filtrate concentrated under reduced pressure. The crude residue was dissolved in isopropyl acetate and washed successfully washed with 3 M aqueous potassium hydroxide then water. The organic layer was dried with sodium sulfate, concentrated and the crude residue was purified by flash column chromatography.



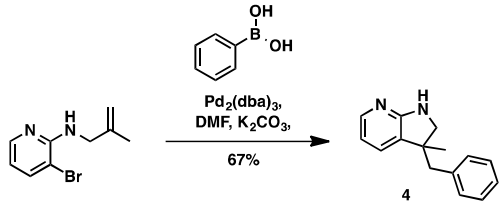
3-benzyl-3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (3) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 80% isopropyl acetate – heptane) to give 0.328 g, 0.867 mmol (87%) as a white soild.

Melting point - Not Determined – turned brown at 250 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 5.1, 1.7 Hz, 1H), 7.99 – 7.86 (m, 2H), 7.27 – 7.20 (m, 5H), 7.02 (dd, *J* = 7.3, 1.7 Hz, 1H), 6.97 – 6.87 (m, 2H), 6.79 (dd, *J* = 7.4, 5.1 Hz, 1H), 4.07 (d, *J* = 9.8 Hz, 1H), 3.52 (d, *J* = 9.8 Hz, 1H), 3.08 – 2.70 (m, 2H), 2.38 (s, 3H), 1.28 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 147.4, 144.0, 136.4, 135.1, 131.9, 131.3, 130.5, 129.4, 128.1, 128.0, 126.8, 117.7, 60.0, 46.2, 42.3, 24.8, 21.6.

HRMS (ESI) calcd for $C_{22}H_{23}N_2O_2S$ $[M+H]^+$: 379.1480, found: 379.1463

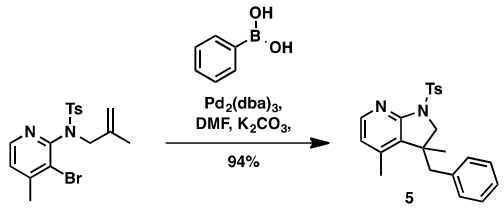


3-benzyl-3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (4) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 100% isopropyl acetate – heptane) to give 0.150 g, 0.669 mmol (67%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 5.3, 1.6 Hz, 1H), 7.30 – 7.18 (m, 3H), 7.06 – 6.97 (m, 2H), 6.91 (dd, *J* = 7.1, 1.6 Hz, 1H), 6.50 (dd, *J* = 7.2, 5.3 Hz, 1H), 4.36 (bs, 1H), 3.54 (dd, *J* = 8.9, 1.1 Hz, 1H), 3.23 (dd, *J* = 8.9, 1.9 Hz, 1H), 2.87 (d, *J* = 1.9 Hz, 2H), 1.31 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.4, 146.4, 137.6, 130.6, 130.5, 129.0, 127.8, 126.4, 113.2, 56.7, 46.0, 44.7, 24.9.

HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1391, found: 225.1380

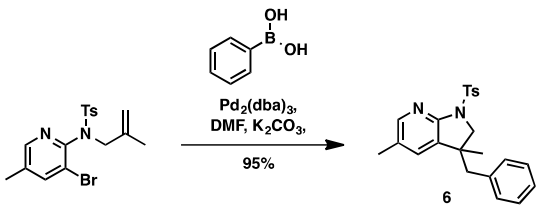


3-benzyl-3,4-dimethyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (5) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 100% isopropyl acetate – heptane) to give 0.370 g, 0.943 mmol (94%) as a white foam.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 5.2 Hz, 1H), 7.94 – 7.85 (m, 2H), 7.25 – 7.15 (m, 5H), 6.94 (dd, *J* = 6.3, 2.9 Hz, 2H), 6.57 (d, *J* = 5.2 Hz, 2H), 4.04 (d, *J* = 9.7 Hz, 1H), 3.34 (d, *J* = 9.7 Hz, 1H), 2.97 – 2.84 (m, 2H), 2.37 (s, 3H), 1.98 (s, 3H), 1.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 147.0, 144.7, 143.8, 136.7, 135.0, 130.3, 129.3, 128.2, 128.1, 128.1, 126.8, 121.1, 59.5, 44.7, 43.6, 23.7, 21.6, 18.2.

HRMS (ESI) calcd for $C_{23}H_{25}N_2O_2S$ $[M+H]^+$: 393.1636 found: 393.1620



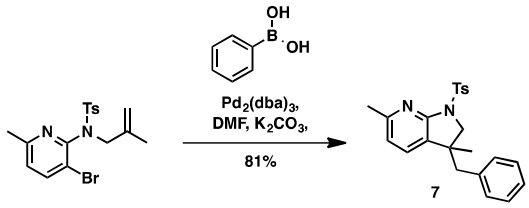
3-benzyl-3,5-dimethyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (6) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 80% isopropyl acetate – heptane) to give 0.374 g, 0.953 mmol (95%) as a white solid.

Melting point 143-146 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.95 (m, 1H), 7.94 – 7.87 (m, 2H), 7.26 –7.19 (m, 5H), 6.97 – 6.89 (m, 2H), 6.83 (d, *J* = 2.1 Hz, 1H), 4.04 (d, *J* = 9.9 Hz, 1H), 3.47 (d, *J* = 9.9 Hz, 1H), 2.91 – 2.72 (m, 2H), 2.37 (s, 3H), 2.18 (s, 3H), 1.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.3, 147.1, 143.9, 136.5, 135.0, 132.9, 131.2, 130.5, 129.3, 128.0, 128.0, 127.1, 126.8, 60.2, 46.1, 42.2, 24.7, 21.6, 18.0.

HRMS (ESI) calcd for $C_{23}H_{25}N_2O_2S$ $[M+H]^+$: 393.1636 found: 393.1618

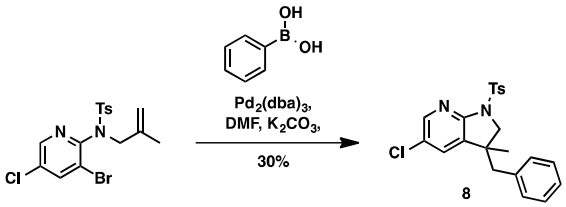


3-benzyl-3,6-dimethyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (7) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 100% isopropyl acetate – heptane) to give 0.318 g, 0.810 mmol (81%) as a light brown solid.
Melting point 98-100 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.92 (m, 2H), 7.27 – 7.18 (m, 5H), 6.97 – 6.89 (m, 2H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 7.4 Hz, 1H), 4.06 (d, *J* = 9.7 Hz, 1H), 3.50 (d, *J* = 9.8 Hz, 1H), 2.81 (d, *J* = 2.8 Hz, 2H), 2.47 (s, 3H), 2.38 (s, 3H), 1.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 154.7, 143.8, 136.6, 135.0, 132.0, 130.5, 129.1, 128.4, 128.0, 127.9, 126.7, 116.9, 60.4, 46.2, 42.1, 24.8, 24.2, 21.6.

HRMS (ESI) calcd for $C_{23}H_{25}N_2O_2S$ $[M+H]^+$: 393.1636 found: 393.1618



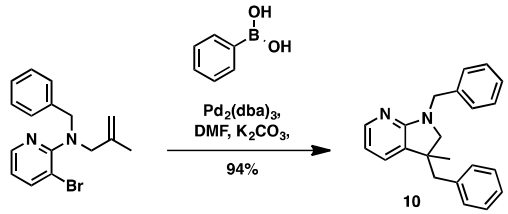
3-benzyl-5-chloro-3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (8) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 40% methanol – dichloromethane) to give 0.123 g, 0.298 mmol (30%) as a white solid.

Melting point 132-134 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 2.4 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.28 – 7.20 (m, 4H), 6.99 – 6.88 (m, 3H), 4.10 (d, *J* = 9.9 Hz, 1H), 3.55 (d, *J* = 10.0 Hz, 1H), 2.85 (d, *J* = 13.4 Hz, 1H), 2.78 (d, *J* = 13.4 Hz, 1H), 2.39 (s, 3H), 1.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.6, 145.7, 144.4, 135.9, 134.7, 133.2, 132.2, 130.4, 129.5, 128.2, 128.0, 127.1, 125.8, 60.5, 46.1, 42.4, 24.7, 21.6.

HRMS (ESI) calcd for $C_{22}H_{22}ClN_2O_2S$ $[M+H]^+$: 413.1090 found: 413.1073

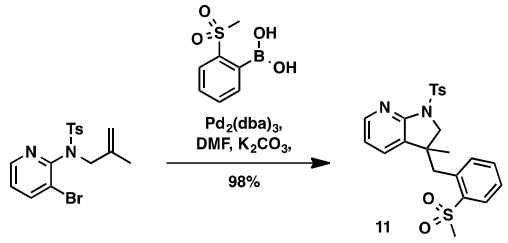


1,3-dibenzyl-3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (10) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.148 g, 0.471 mmol (94%) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.88 (m, 1H), 7.34 – 7.10 (m, 8H), 7.01 – 6.91 (m, 3H), 6.47 (dd, *J* = 7.0, 5.4 Hz, 1H), 4.70 (d, *J* = 15.0 Hz, 1H), 4.35 (d, *J* = 15.0 Hz, 1H), 3.33 (d, *J* = 9.3 Hz, 1H), 2.94 (d, *J* = 9.2 Hz, 1H), 2.85 – 2.73 (m, 2H), 1.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 146.4, 138.1, 137.5, 130.5, 130.0, 129.9, 128.4, 128.0, 127.9, 127.0, 126.4, 112.3, 61.2, 49.1, 46.7, 42.6, 25.4.

HRMS (ESI) calcd for $C_{22}H_{23}N_2$ $[M+H]^+$: 315.1861 found: 315.1846



3-methyl-3-(2-(methylsulfonyl)benzyl)-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (11) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.223 g, 0.488 mmol (98%) as a white solid.

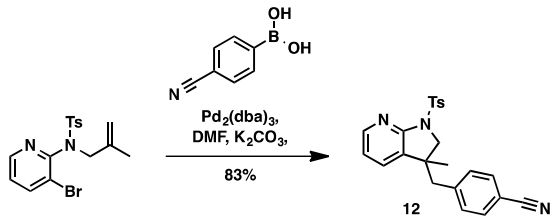
Melting point 185-187 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 5.1, 1.6 Hz, 1H), 8.00 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.85 – 7.78 (m, 2H), 7.40 – 7.23 (m, 3H), 7.16 (d, *J* = 8.1 Hz, 2H), 6.87 (dd, *J* = 7.4, 5.1 Hz, 1H), 6.79

(dd, *J* = 7.6, 1.4 Hz, 1H), 4.05 (d, *J* = 10.3 Hz, 1H), 3.70 (d, *J* = 13.6 Hz, 1H), 3.60 (d, *J* = 10.3 Hz, 1H), 3.17 (d, *J* = 13.7 Hz, 1H), 2.97 (s, 3H), 2.33 (s, 3H), 1.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 147.7, 143.9, 139.8, 136.8, 134.8, 133.2, 132.2, 132.0, 131.6, 129.9, 129.4, 127.9, 127.8, 118.2, 60.0, 45.6, 42.8, 40.9, 26.6, 21.6.

HRMS (ESI) calcd for $C_{23}H_{25}N_2O_4S_2$ $[M+H]^+$: 457.1255 found: 457.1237



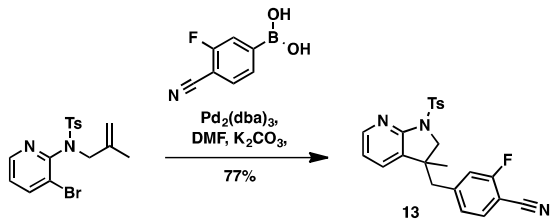
4-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzonitrile (12) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.167 g, 0.414 mmol (83%) as an off-white solid.

Melting point 166-171 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 5.1, 1.6 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 7.06 – 6.93 (m, 3H), 6.82 (dd, *J* = 7.3, 5.1 Hz, 1H), 4.03 (d, *J* = 10.0 Hz, 1H), 3.54 (d, *J* = 9.9 Hz, 1H), 2.89 (d, *J* = 3.8 Hz, 2H), 2.40 (s, 3H), 1.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 147.8, 144.3, 141.9, 134.9, 131.8, 131.8, 131.0, 130.2, 129.4, 128.0, 118.6, 117.8, 110.9, 59.7, 46.5, 42.3, 24.8, 21.6.

HRMS (ESI) calcd for $C_{23}H_{22}N_3O_2S$ $[M+H]^+$: 404.1432 found: 404.1412

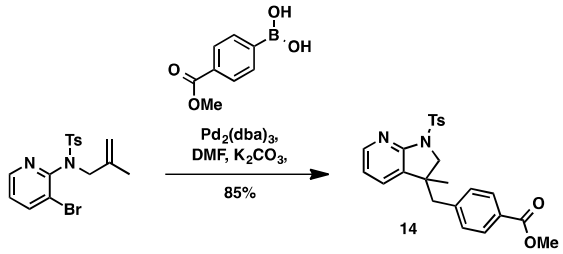


2-fluoro-4-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzonitrile (13) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.162 g, 0.384 mmol (77%) as a light yellow solid.
Melting point 125-131 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 5.1, 1.6 Hz, 1H), 7.94 – 7.87 (m, 2H), 7.41 (dd, *J* = 7.9, 6.7 Hz, 1H), 7.28 – 7.22 (m, 2H), 7.09 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.86 (dd, *J* = 7.4, 5.1 Hz, 1H), 6.85 – 6.70 (m, 2H), 4.01 (d, *J* = 10.0 Hz, 1H), 3.57 (d, *J* = 10.0 Hz, 1H), 2.89 (d, *J* = 3.6 Hz, 2H), 2.41 (s, 3H), 1.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5 (d, *J* = 259.6 Hz), 155.3, 148.0, 145.1 (d, *J* = 7.3 Hz), 144.5, 134.8, 132.9, 131.7, 129.8, 129.4, 127.9, 126.7 (d, *J* = 3.5 Hz), 118.1 (d, *J* = 19.2 Hz), 117.9, 113.7, 99.8 (d, *J* = 15.4 Hz), 59.6, 46.4, 42.3, 24.8, 21.6.

HRMS (ESI) calcd for $C_{23}H_{21}FN_3O_2S$ $[M+H]^+$: 422.1338 found: 422.1321



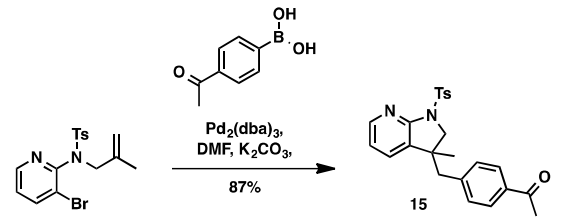
methyl 4-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzoate (14) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.185 g, 0.424 mmol (85%) as a light yellow solid.

Melting point 138-141 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 5.1, 1.7 Hz, 1H), 7.94 – 7.83 (m, 4H), 7.32 – 7.19 (m, 2H), 7.02 – 6.92 (m, 3H), 6.80 (dd, *J* = 7.4, 5.1 Hz, 1H), 4.05 (d, *J* = 9.9 Hz, 1H), 3.91 (s, 3H), 3.54 (d, *J* = 9.8 Hz, 1H), 2.89 (d, *J* = 4.9 Hz, 2H), 2.37 (s, 3H), 1.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8, 155.2, 147.6, 144.1, 141.8, 134.9, 131.9, 130.6, 130.5, 129.4, 129.3, 128.8, 128.0, 117.8, 60.0, 52.1, 46.2, 42.3, 24.9, 21.6.

HRMS (ESI) calcd for $C_{24}H_{25}N_2O_4S$ $[M+H]^+$: 437.1535 found: 437.1517

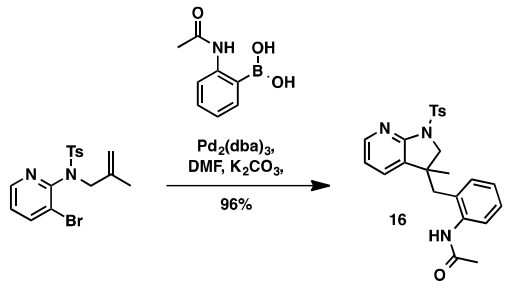


1-(4-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)phenyl)ethan-1-one (15) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.183 g, 0.435 mmol (87%) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 5.1, 1.6 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 2H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.05 – 6.93 (m, 3H), 6.79 (dd, *J* = 7.4, 5.1 Hz, 1H), 4.04 (d, *J* = 9.8 Hz, 1H), 3.50 (d, *J* = 9.9 Hz, 1H), 2.86 (d, *J* = 3.5 Hz, 2H), 2.54 (s, 3H), 2.33 (s, 3H), 1.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.6, 155.2, 147.6, 144.2, 142.0, 135.7, 134.9, 131.9, 130.7, 130.6, 129.4, 128.1, 128.0, 117.8, 60.0, 46.2, 42.3, 26.6, 24.8, 21.6.

HRMS (ESI) calcd for $C_{24}H_{25}N_2O_3S$ $[M+H]^+$: 421.1586 found: 421.1566

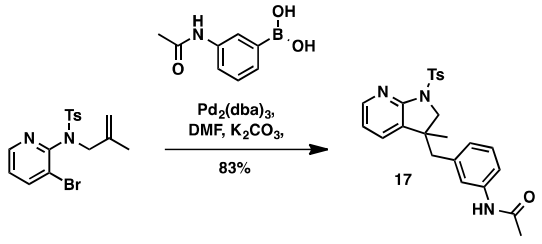


***N*-(2-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)phenyl) acetamide (16)** - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.208 g, 0.478 mmol (96%) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 5.2, 1.7 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 2H), 7.67 (bs, 1H), 7.46 – 7.39 (m, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.18 – 6.99 (m, 3H), 6.80 (dd, *J* = 7.4, 5.1 Hz, 1H), 6.60 (d, *J* = 7.5 Hz, 1H), 4.05 (d, *J* = 9.7 Hz, 1H), 3.45 (d, *J* = 9.9 Hz, 1H), 2.74 (d, *J* = 4.5 Hz, 2H), 2.36 (s, 3H), 2.15 (s, 3H), 1.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 155.1, 147.3, 144.2, 138.0, 137.2, 134.8, 131.9, 131.5, 129.4, 128.6, 128.0, 126.2, 121.8, 118.4, 118.0, 59.9, 46.1, 42.3, 24.8, 24.6, 21.6.

HRMS (ESI) calcd for $C_{24}H_{26}N_3O_3S$ $[M+H]^+$: 436.1695 found: 436.1672



***N*-(3-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)phenyl) acetamide (17)** - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.181 g, 0.416 mmol (83%) as a light yellow solid.

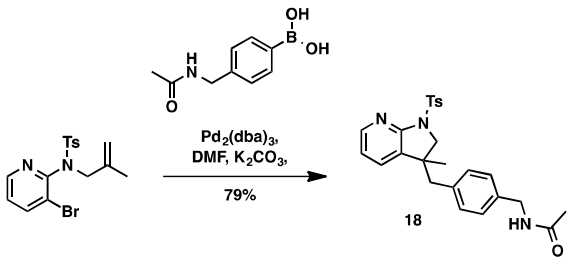
Melting point 189-191 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 5.2, 1.7 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.15 (m, 3H), 7.14 – 7.08 (m, 2H), 6.88 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.79 (dd,

J = 7.3, 5.1 Hz, 1H), 6.52 (bs, 1H), 4.05 (d, *J* = 9.7 Hz, 1H), 3.36 (d, *J* = 9.7 Hz, 1H), 2.90 (d, *J* = 13.9 Hz, 1H), 2.80 (d, *J* = 14.1 Hz, 1H), 2.39 (s, 3H), 1.99 (s, 3H), 1.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1, 155.2, 147.6, 144.4, 136.3, 134.5, 131.9, 131.8, 131.1, 129.7, 129.5, 128.1, 128.0, 125.9, 125.6, 118.4, 60.7, 42.8, 40.7, 23.9, 22.7, 21.6.

HRMS (ESI) calcd for $C_{24}H_{26}N_3O_3S$ $[M+H]^+$: 436.1695 found: 436.1672

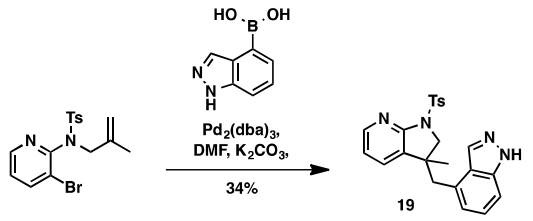


***N*-(4-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzyl)acetamide (18)** - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.178 g, 0.396 mmol (79%) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 5.2, 1.7 Hz, 1H), 7.96 – 7.85 (m, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.15 – 7.05 (m, 3H), 6.87 – 6.76 (m, 3H), 6.20 – 6.08 (m, 1H), 4.44 – 4.27 (m, 2H), 4.05 (d, *J* = 9.9 Hz, 1H), 3.42 (d, *J* = 9.8 Hz, 1H), 2.77 (d, *J* = 1.5 Hz, 2H), 2.35 (s, 3H), 1.98 (s, 3H), 1.25 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 155.2, 147.4, 144.1, 136.9, 135.5, 135.0, 131.8, 131.3, 130.5, 129.4, 127.9, 127.7, 117.9, 59.8, 46.3, 43.4, 42.3, 24.8, 23.2, 21.6.

HRMS (ESI) calcd for $C_{25}H_{28}N_3O_3S$ $[M+H]^+$: 450.1851 found: 450.1830

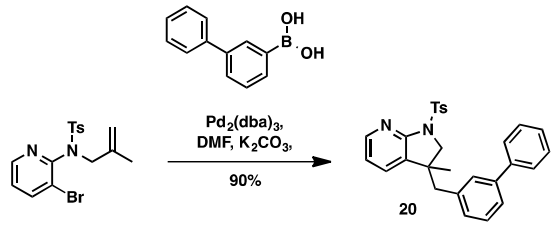


5-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)-1*H*-indazole (19) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 70 mg, 0.167 mmol (34%) as a dark orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.19 (dd, *J* = 5.1, 1.7 Hz, 1H), 7.98 – 7.91 (m, 2H), 7.65 (d, *J* = 1.1 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.21 (m, 3H), 6.90 (dd, *J* = 7.4, 1.6 Hz, 1H), 6.77 – 6.68 (m, 2H), 4.17 (d, *J* = 9.8 Hz, 1H), 3.54 (d, *J* = 9.8 Hz, 1H), 3.29 – 3.09 (m, 2H), 2.38 (s, 3H), 1.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 147.6, 144.1, 134.9, 132.0, 131.2, 129.4, 128.1 (x2), 128.1, 126.6 (x2), 123.6, 123.1, 117.9 (x2), 108.5, 60.7, 43.4, 42.8, 24.7, 21.6.

HRMS (ESI) calcd for $C_{23}H_{23}N_4O_2S$ $[M+H]^+$: 419.1541 found: 419.1521

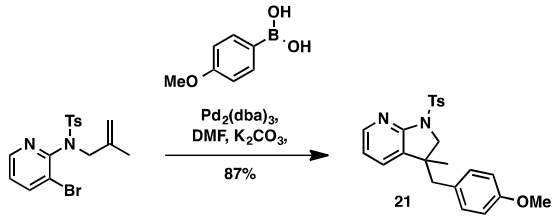


3-([1,1'-biphenyl]-3-ylmethyl)-3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (20) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.204 g, 0.449 mmol (90%) as a light yellow semi-solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 5.1, 1.6 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.25 (m, 7H), 7.17 (d, *J* = 8.2 Hz, 2H), 7.09 – 7.00 (m, 2H), 6.96 – 6.88 (m, 1H), 6.82 (dd, *J* = 7.4, 5.1 Hz, 1H), 4.10 (d, *J* = 9.9 Hz, 1H), 3.57 (d, *J* = 9.9 Hz, 1H), 2.95 – 2.83 (m, 2H), 2.30 (s, 3H), 1.34 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 147.5, 144.0, 141.0, 140.8, 136.9, 135.0, 132.1, 131.2, 129.4, 129.3, 129.3, 128.7, 128.5, 128.0, 127.4, 127.1, 125.7, 117.8, 60.0, 46.3, 42.4, 25.1, 21.5.

HRMS (ESI) calcd for $C_{28}H_{27}N_2O_2S$ $[M+H]^+$: 455.1793 found: 455.1770

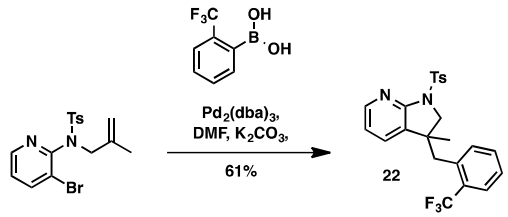


3-(4-methoxybenzyl)-3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (21) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.178 g, 0.436 mmol (87%) as a clear oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 5.2, 1.7 Hz, 1H), 7.96 – 7.85 (m, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.03 (dd, *J* = 7.4, 1.7 Hz, 1H), 6.89 – 6.76 (m, 3H), 6.78 – 6.70 (m, 2H), 4.05 (d, *J* = 9.8 Hz, 1H), 3.77 (s, 3H), 3.51 (d, *J* = 9.8 Hz, 1H), 2.83 – 2.68 (m, 2H), 2.37 (s, 3H), 1.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 155.3, 147.3, 144.0, 135.1, 131.9, 131.4, 129.4, 129.3, 128.5, 128.0, 117.7, 113.5, 59.9, 55.2, 45.4, 42.4, 24.9, 21.6.

HRMS (ESI) calcd for $C_{23}H_{25}N_2O_3S$ $[M+H]^+$: 409.1586 found: 409.1568



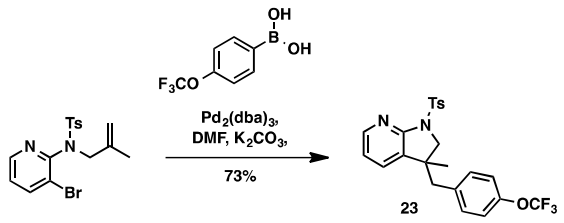
3-methyl-1-tosyl-3-(2-(trifluoromethyl)benzyl)-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (22) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.136 g, 0.305 mmol (61%) as a white solid.

Melting point 136-138 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 5.0, 1.7 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.61 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.32 – 7.15 (m, 5H), 6.90 – 6.77 (m, 2H), 3.89 (d, *J* = 10.1 Hz, 1H), 3.67 (d, *J* = 10.0 Hz, 1H), 3.26 – 3.17 (m, 1H), 3.08 (d, *J* = 14.7 Hz, 1H), 2.36 (s, 3H), 1.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 147.7, 144.0, 135.6, 134.9, 131.6, 131.6, 131.4, 131.3, 129.3, 127.9, 126.9, 126.4 (q, *J* = 5.68 Hz), 125.7, 122.9, 118.0, 60.1, 42.5, 40.8, 27.0, 21.5.

HRMS (ESI) calcd for $C_{23}H_{22}F_3N_2O_2S$ $[M+H]^+$: 447.1354 found: 447.1328

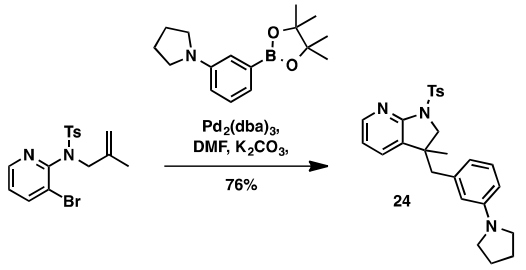


3-methyl-1-tosyl-3-(4-(trifluoromethoxy)benzyl)-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (23) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.168 g, 0.363 mmol (73%) as a clear oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 5.2, 1.6 Hz, 1H), 7.96 – 7.88 (m, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.07 – 6.99 (m, 3H), 6.96 – 6.87 (m, 2H), 6.81 (dd, *J* = 7.4, 5.1 Hz, 1H), 4.03 (d, *J* = 9.9 Hz, 1H), 3.52 (d, *J* = 9.9 Hz, 1H), 2.90 – 2.76 (m, 2H), 2.37 (s, 3H), 1.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 148.2, 147.6, 144.2, 135.1, 134.9, 131.8, 131.7, 130.8, 129.4, 128.0, 120.5, 120.4 (d, *J* = 257.9 Hz), 117.8, 59.8, 45.4, 42.2, 24.7, 21.5.

HRMS (ESI) calcd for $C_{23}H_{22}F_3N_2O_3S$ $[M+H]^+$: 463.1303 found: 463.1281

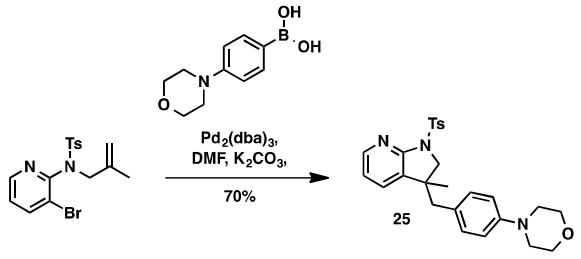


3-methyl-3-(3-(pyrrolidin-1-yl)benzyl)-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (24) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.170 g, 0.380 mmol (76%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 5.1, 1.7 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.15 – 7.03 (m, 2H), 6.80 (dd, *J* = 7.4, 5.1 Hz, 1H), 6.44 (bs, 1H), 6.28 (d, *J* = 7.4 Hz, 1H), 6.07 (bs, 1H), 4.13 (d, *J* = 9.8 Hz, 1H), 3.50 (d, *J* = 9.8 Hz, 1H), 3.20 –3.10 (m, 4H), 2.84 – 2.68 (m, 2H), 2.37 (s, 3H), 2.04 – 1.92 (m, 4H), 1.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 147.3, 147.1, 143.9, 137.3, 135.1, 132.0, 131.9, 129.4, 129.3, 128.8, 128.1, 128.0, 118.2, 117.7, 60.0, 46.6, 42.3, 27.7, 25.4, 25.0, 21.6.

HRMS (ESI) calcd for $C_{26}H_{30}N_3O_2S$ $[M+H]^+$: 448.2058 found: 448.2038



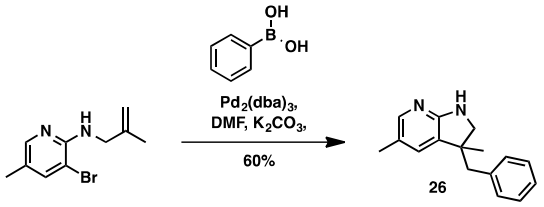
4-(4-((3-methyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)phenyl) morpholine (25) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 0.162 g, 0.349 mmol (70%) as a light brown solid.

Melting point 182-185 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.11 (m, 1H), 7.96 – 7.88 (m, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.03 (dd, *J* = 7.4, 1.7 Hz, 1H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.83 – 6.75 (m, 3H), 4.07 (d, *J* = 9.9 Hz, 1H), 3.93 – 3.79 (m, 4H), 3.49 (d, *J* = 9.8 Hz, 1H), 3.23 – 3.03 (m, 4H), 1.25 (s, 3H), 2.83 – 2.63 (m, 2H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 150.1, 147.3, 144.0, 135.1, 131.9, 131.6, 131.3, 129.4, 128.0, 127.8, 117.7, 115.2, 66.9, 60.1, 49.3, 45.4, 42.5, 24.7, 21.6.

HRMS (ESI) calcd for $C_{26}H_{30}N_3O_3S$ $[M+H]^+$: 464.2008, found: 464.1984

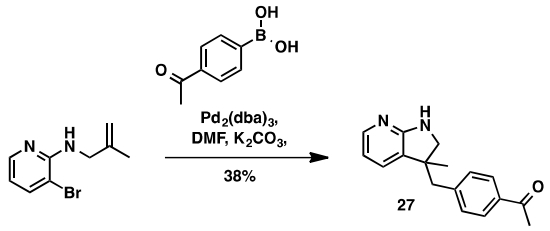


3-benzyl-3,5-dimethyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (26) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 72 mg, 0.302 mmol (60%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.30 – 7.15 (m, 3H), 7.06 – 6.98 (m, 2H), 6.77 (d, *J* = 2.2 Hz, 1H), 4.51 (bs, 1H), 3.53 (d, *J* = 8.9 Hz, 1H), 3.21 (d, *J* = 8.9 Hz, 1H), 2.85 (s, 2H), 2.14 (s, 3H), 1.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5, 145.0, 137.6, 132.1, 130.6, 129.5, 127.8, 126.4, 122.1, 56.9, 45.9, 44.6, 24.7, 17.9.

HRMS (ESI) calcd for $C_{16}H_{19}N_2$ $[M+H]^+$: 239.1548 found: 239.1534

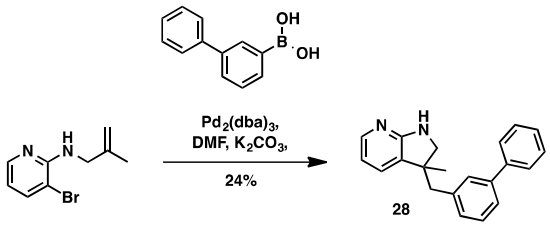


1-(4-((3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)phenyl)ethan-1-one (27) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 51 mg, 0.192 mmol (38%) as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.78 (m, 3H), 7.12 – 7.02 (m, 2H), 6.89 (dd, *J* = 7.2, 1.4 Hz, 1H), 6.51 (dd, *J* = 7.2, 5.3 Hz, 1H), 4.61 (bs, 1H), 3.53 (d, *J* = 9.0 Hz, 1H), 3.28 (d, *J* = 9.0 Hz, 1H), 3.01 – 2.85 (m, 2H), 2.58 (s, 3H), 1.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 163.0, 146.0 (x2), 143.2, 135.6, 130.8, 130.7, 127.9, 113.2, 56.9, 46.0, 44.7, 26.6, 24.9.

HRMS (ESI) calcd for $C_{17}H_{19}N_2O$ $[M+H]^+$: 267.1492 found: 267.1484

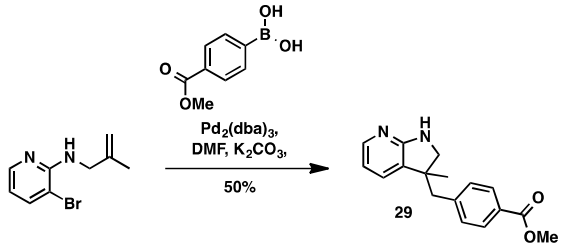


3-([1,1'-biphenyl]-3-ylmethyl)-3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (28) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 36 mg, 0.120 mmol (24%) as a light yellow semi-solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 5.3, 1.6 Hz, 1H), 7.55 – 7.28 (m, 7H), 7.28 – 7.17 (m, 1H), 7.02 (dt, *J* = 7.7, 1.4 Hz, 1H), 6.94 (dd, *J* = 7.1, 1.6 Hz, 1H), 6.52 (dd, *J* = 7.1, 5.3 Hz, 1H), 4.41 (bs, 1H), 3.57 (d, *J* = 9.0 Hz, 1H), 3.27 (dd, *J* = 8.9, 1.7 Hz, 1H), 2.99 – 2.87 (m, 2H), 1.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.4, 146.4, 141.1, 140.8, 138.0, 130.6, 129.5, 129.5, 128.9, 128.7, 128.2, 127.2, 127.1, 125.3, 113.2, 56.8, 46.1, 44.7, 24.9.

HRMS (ESI) calcd for $C_{21}H_{21}N_2$ $[M+H]^+$: 301.1704 found: 301.1689

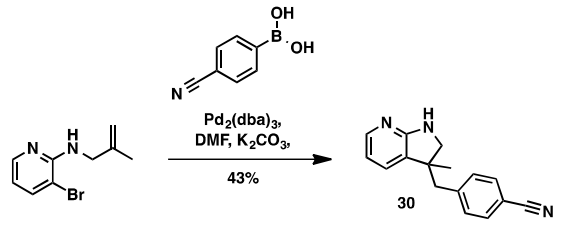


methyl 4-((3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzoate (29) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 70 mg, 0.248 mmol (50%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.88 (m, 2H), 7.87 – 7.80 (m, 1H), 7.10 – 7.03 (m, 2H), 6.87 (dd, *J* = 7.2, 1.5 Hz, 1H), 6.50 (dd, *J* = 7.2, 5.3 Hz, 1H), 4.65 (bs, 1H), 3.91 (s, 3H), 3.53 (d, *J* = 9.0 Hz, 1H), 3.28 (d, *J* = 9.0 Hz, 1H), 2.99 – 2.85 (m, 2H), 1.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0, 163.0, 145.8, 142.9, 130.8, 130.6, 129.1, 128.8, 128.5, 113.1, 56.9, 52.0, 46.0, 44.7, 24.8.

HRMS (ESI) calcd for $C_{17}H_{19}N_2O_2$ $[M+H]^+$: 283.1446 found: 283.1432

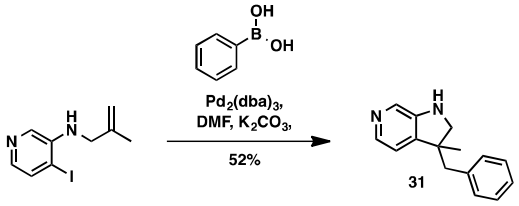


4-((3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzonitrile (30) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 54 mg, 0.217 mmol (43%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 5.5, 1.5 Hz, 1H), 7.61 – 7.44 (m, 2H), 7.11 – 7.02 (m, 2H), 6.87 (dd, *J* = 7.1, 1.5 Hz, 1H), 6.51 (dd, *J* = 7.1, 5.5 Hz, 1H), 4.79 (bs, 1H), 3.52 (d, *J* = 9.2 Hz, 1H), 3.33 (d, *J* = 9.2 Hz, 1H), 2.98 – 2.84 (m, 2H), 1.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 144.8, 142.9, 131.7, 131.2, 131.0, 128.9, 118.8, 113.0, 110.6, 57.0, 46.2, 44.6, 24.8.

HRMS (ESI) calcd for $C_{16}H_{16}N_3$ $[M+H]^+$: 250.1344 found: 250.1331

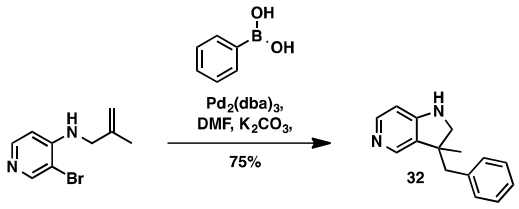


3-benzyl-3-methyl-2,3-dihydro-1*H*-pyrrolo[2,3-*c*]pyridine (31) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 27.5 mg, 0.123 mmol (52%) as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.88 (m, 2H), 7.26 – 7.20 (m, 2H), 7.06 – 6.96 (m, 2H), 6.80 – 6.74 (m, 1H), 3.69 (bs, 1H), 3.55 (d, *J* = 9.1 Hz, 1H), 3.21 (d, *J* = 9.1 Hz, 1H), 2.86 (s, 2H), 1.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.3, 145.0, 140.3, 137.5, 131.6, 130.5, 127.9, 126.5, 118.4, 58.8, 46.4, 45.4, 24.3.

HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1391, found: 225.1381

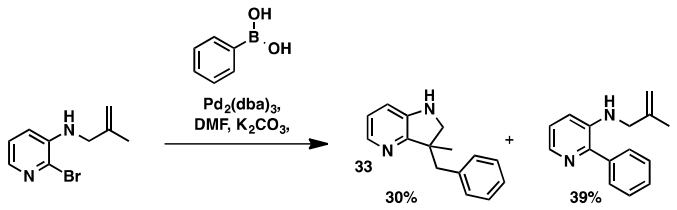


3-benzyl-3-methyl-2,3-dihydro-1*H*-pyrrolo[3,2-*c*]pyridine (32) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 35% methanol – dichloromethane) to give 84.6 mg, 0.377 mmol (75%) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 5.3 Hz, 1H), 7.89 (s, 1H), 7.32 – 7.17 (m, 3H), 7.06 – 6.98 (m, 2H), 6.43 (d, *J* = 5.4 Hz, 1H), 4.14 (bs, 1H), 3.59 (d, *J* = 9.1 Hz, 1H), 3.24 (d, *J* = 9.1 Hz, 1H), 2.88 (s, 2H), 1.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 149.0, 143.9, 137.6, 131.6, 130.5, 127.9, 126.4, 104.0, 58.8, 46.4, 44.8, 25.3.

HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1391, found: 225.1382



3-benzyl-3-methyl-2,3-dihydro-1*H*-pyrrolo[3,2-*b*]pyridine (33) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 20% methanol – dichloromethane) to give 33.6 mg, 0.150 mmol (30%) of the desired product as a dark orange solid and 43.9 mg, 0.196 mmol (39%) as an orange oil.

Desired Product

Melting point 114-116 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.25 – 7.13 (m, 2H), 7.11 – 7.00 (m, 2H), 6.90 (dd, *J* = 7.8, 5.0 Hz, 1H), 6.76 (dd, *J* = 7.8, 1.3 Hz, 1H), 3.63 (d, *J* = 9.2 Hz, 1H), 3.17 (d, *J* = 9.3 Hz, 1H), 3.07 (d, *J* = 13.3 Hz, 1H), 2.91 (d, *J* = 13.4 Hz, 1H), 1.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 144.2, 139.3, 138.4, 130.3, 127.9, 126.2, 122.0, 115.1, 56.5, 46.2, 44.8, 24.5.

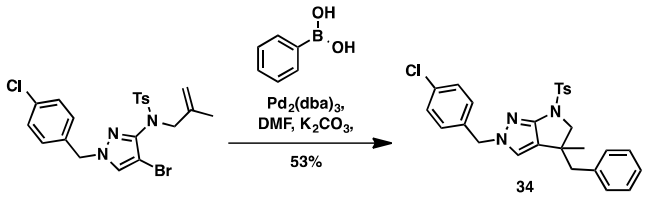
HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1391, found: 225.1379

Undesired Product

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.48 (dd, *J* = 8.2, 6.7 Hz, 2H), 7.43 – 7.35 (m, 1H), 7.09 (dd, *J* = 8.3, 4.7 Hz, 1H), 6.90 (dd, *J* = 8.3, 1.4 Hz, 1H), 4.93 – 4.84 (m, 2H), 4.40 (bt, *J* = 5.9 Hz, 1H), 3.64 (d, *J* = 5.6 Hz, 2H), 1.74 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 141.7, 141.5, 138.6, 137.9, 128.9, 128.7, 128.3, 123.0, 117.4, 111.1, 49.5, 20.3.

HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1391, found: 225.1380



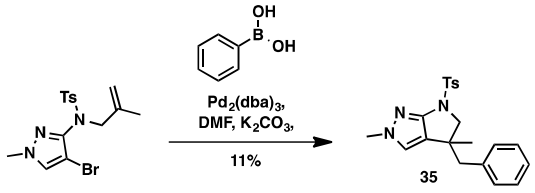
4-benzyl-2-(4-chlorobenzyl)-4-methyl-6-tosyl-2,4,5,6-tetrahydropyrrolo[2,3-*c*]pyrazole (34) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 100% isopropyl acetate – heptane) to give 0.131 g, 0.266 mmol (53%) as a light yellow solid.

Melting point 151-154 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.69 (m, 2H), 7.35 – 7.24 (m, 2H), 7.24 – 7.16 (m, 5H), 7.16 – 7.04 (m, 2H), 6.90 – 6.80 (m, 2H), 6.52 (s, 1H), 5.22 – 5.05 (m, 2H), 4.00 (d, *J* = 10.3 Hz, 1H), 3.74 (d, *J* = 10.3 Hz, 1H), 2.68 (d, *J* = 13.1 Hz, 1H), 2.51 (d, *J* = 13.1 Hz, 1H), 2.39 (s, 3H), 1.09 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.7, 144.0, 137.3, 135.8, 133.7, 133.3, 130.3, 129.3, 128.8, 128.0, 127.8, 126.5, 124.6, 119.8, 68.5, 55.5, 46.6, 41.6, 26.3, 21.6.

HRMS (ESI) calcd for $C_{27}H_{27}ClN_3O_2S$ $[M+H]^+$: 492.1512 found: 492.1490



4-benzyl-2,4-dimethyl-6-tosyl-2,4,5,6-tetrahydropyrrolo[2,3-*c*]pyrazole (35) - Using General Procedure 2, purified by flash column chromatography (silica, 0% → 100% isopropyl acetate – heptane) to give 21 mg, 55.1 μmol (11%) was recovered as a light yellow solid.

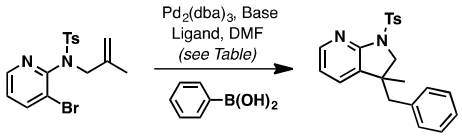
Melting point – Not Determined - turned brown at 170 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 6.6 Hz, 2H), 7.32 – 7.16 (m, 5H), 6.99 – 6.91 (m, 2H), 6.50 (s, 1H), 3.99 (d, *J* = 10.3 Hz, 1H), 3.78 (s, 3H), 3.74 (d, *J* = 10.3 Hz, 1H), 2.67 (d, *J* = 13.0 Hz, 1H), 2.53 (d, *J* = 13.1 Hz, 1H), 2.38 (s, 3H), 1.07 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 144.0, 137.5, 133.7, 130.3, 129.5, 127.9, 127.9, 126.6, 125.1, 119.0, 68.5, 46.8, 41.6, 39.5, 26.3, 21.6.

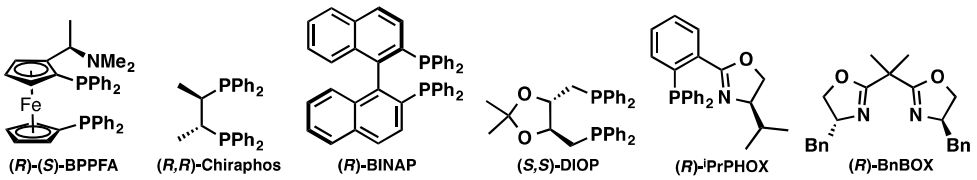
HRMS (ESI) calcd for $C_{21}H_{24}N_3O_2S$ $[M+H]^+$: 382.1589 found: 382.1571

Chiral Ligand Screen

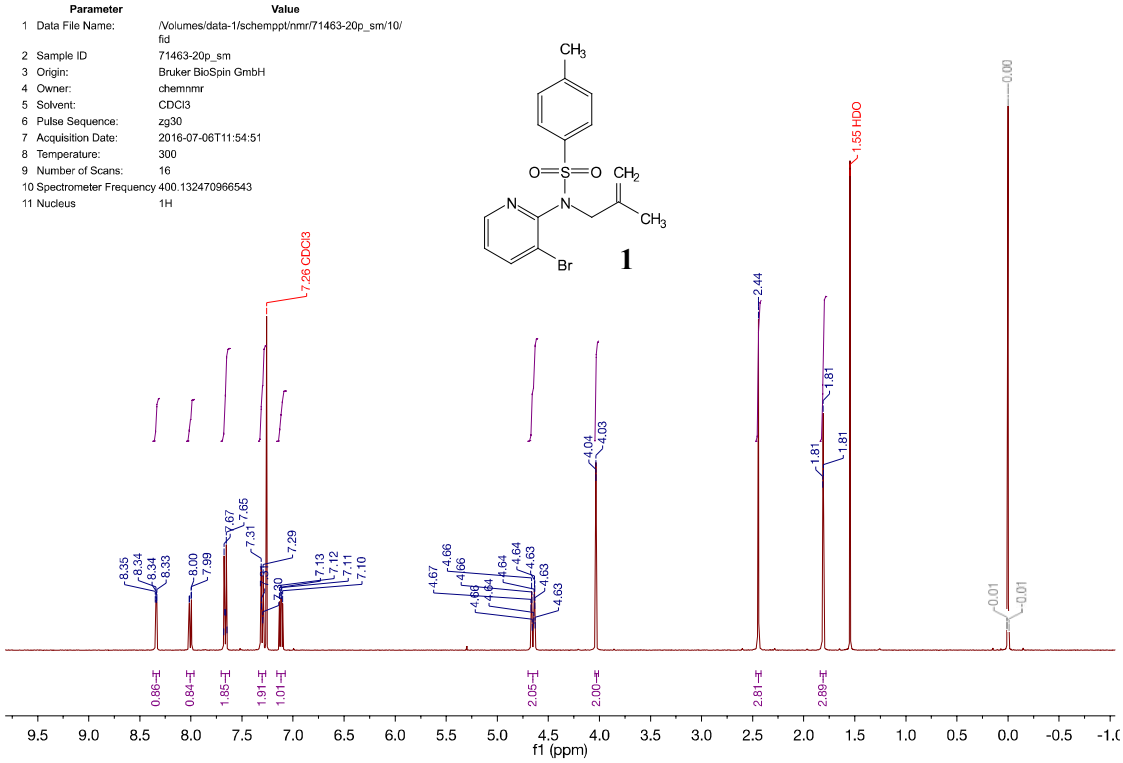


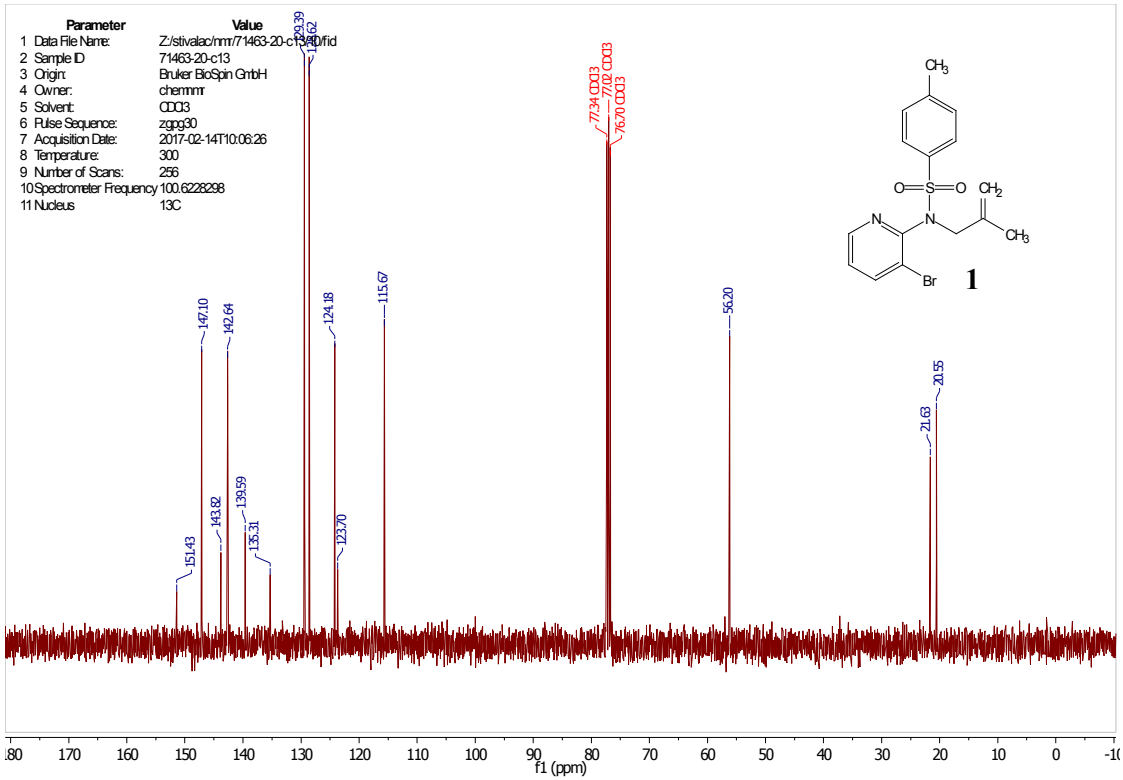
Entry[a]	Base	Ligand	% Conversion[b]	% ee[c]
1	Cs_2CO_3	(*R*)-(*S*)-BPPFA	0	-
2	Cs_2CO_3	(*R,R*)-Chiraphos	100	racemic
3	Cs_2CO_3	(*R*)-BINAP	100	racemic
4	Cs_2CO_3	(*S,S*)-DIOP	100	racemic
5	Cs_2CO_3	(*R*)-^{i}PrPHOX	100	racemic
6	Cs_2CO_3	(*R*)-BnBOX	100	racemic
7	K_2CO_3	(*R*)-(*S*)-BPPFA	100	racemic
8	K_2CO_3	(*R,R*)-Chiraphos	100	racemic
9	K_2CO_3	(*R*)-BINAP	100	racemic
10	K_2CO_3	(*S,S*)-DIOP	100	racemic
11	K_2CO_3	(*R*)-^{i}PrPHOX	100	racemic
12	K_2CO_3	(*R*)-BnBOX	100	racemic
13	Na_2CO_3	(*R*)-(*S*)-BPPFA	100	racemic
14	Na_2CO_3	(*R,R*)-Chiraphos	16	racemic
15	Na_2CO_3	(*R*)-BINAP	67	racemic
16	Na_2CO_3	(*S,S*)-DIOP	100	racemic
17	Na_2CO_3	(*R*)-^{i}PrPHOX	0	-
18	Na_2CO_3	(*R*)-BnBOX	100	racemic
19	K_3PO_4	(*R*)-(*S*)-BPPFA	100	racemic
20	K_3PO_4	(*R,R*)-Chiraphos	100	racemic
21	K_3PO_4	(*R*)-BINAP	100	racemic
22	K_3PO_4	(*S,S*)-DIOP	100	racemic
23	K_3PO_4	(*R*)-^{i}PrPHOX	100	racemic
24	K_3PO_4	(*R*)-BnBOX	100	racemic

[a]All reactions were performed on a 0.05 mmol scale (0.2 M) using 10 mol % Pd, 20 mol % ligand, 3 equiv base, 1 equiv phenylboronic acid, and heated at 100 °C for 18 h. [b]Conversion was determined by ^{1}H NMR. [c]%ee was determined by chiral HPLC (OD-3 column, 10 % isopropanol /heptane, 1.5 mL min^{-1}, enantiomers at RT = 9.00 min and 10.75 min).



Copies of NMR Spectra





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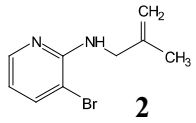
4	Owner:	chemnmr
5	Solvent:	CDCl3
6	Pulse Sequence:	zg30
7	Acquisition Date:	2016-06-30T10:11:58
8	Temperature:	300
9	Number of Scans:	16
10	Spectrometer Frequency	400.132470966543
11	Nucleus	1H



2

	Parameter	Value
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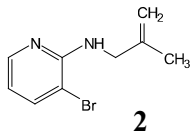
3	Origin:	Bruker BioSpin GmbH
4	Owner:	chemnmr
5	Solvent:	CDCl3
6	Pulse Sequence:	zgpg30
7	Acquisition Date:	2016-08-23T00:03:30
8	Temperature:	300
9	Number of Scans:	2048
10	Spectrometer Frequency	100.6228298
11	Nucleus	13C



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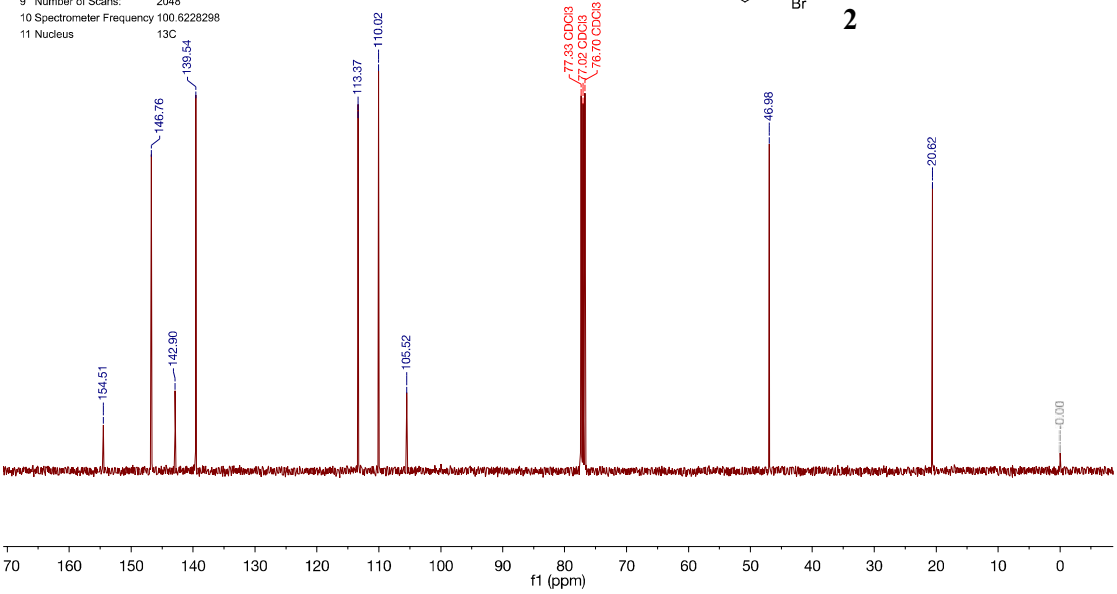

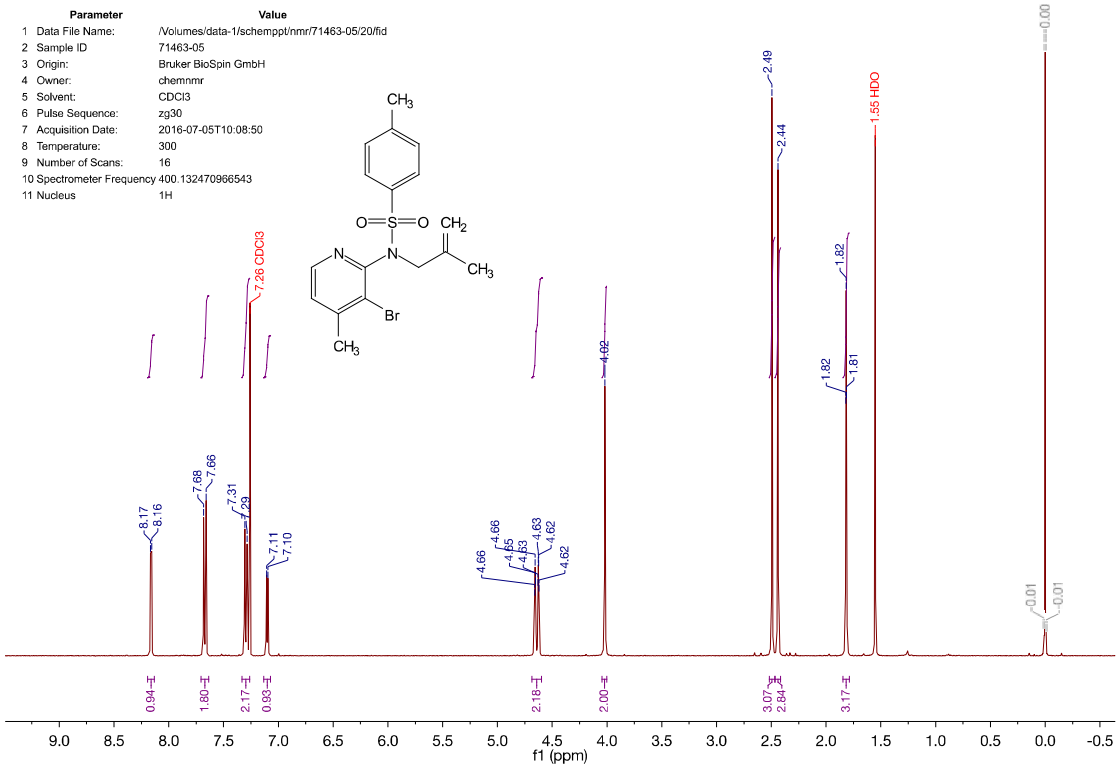
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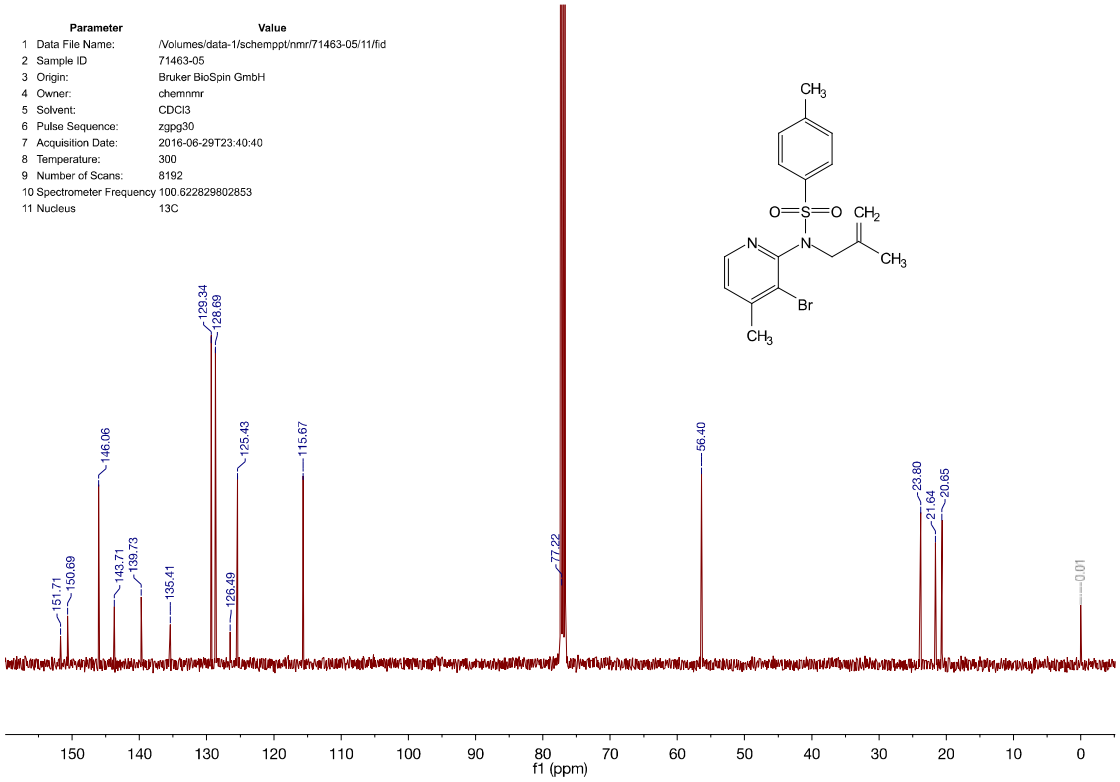
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-07-05T10:08:50
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
7.26 CDCl3
1.55 HDO
f1 (ppm)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6 Pulse Sequence: zgpg30
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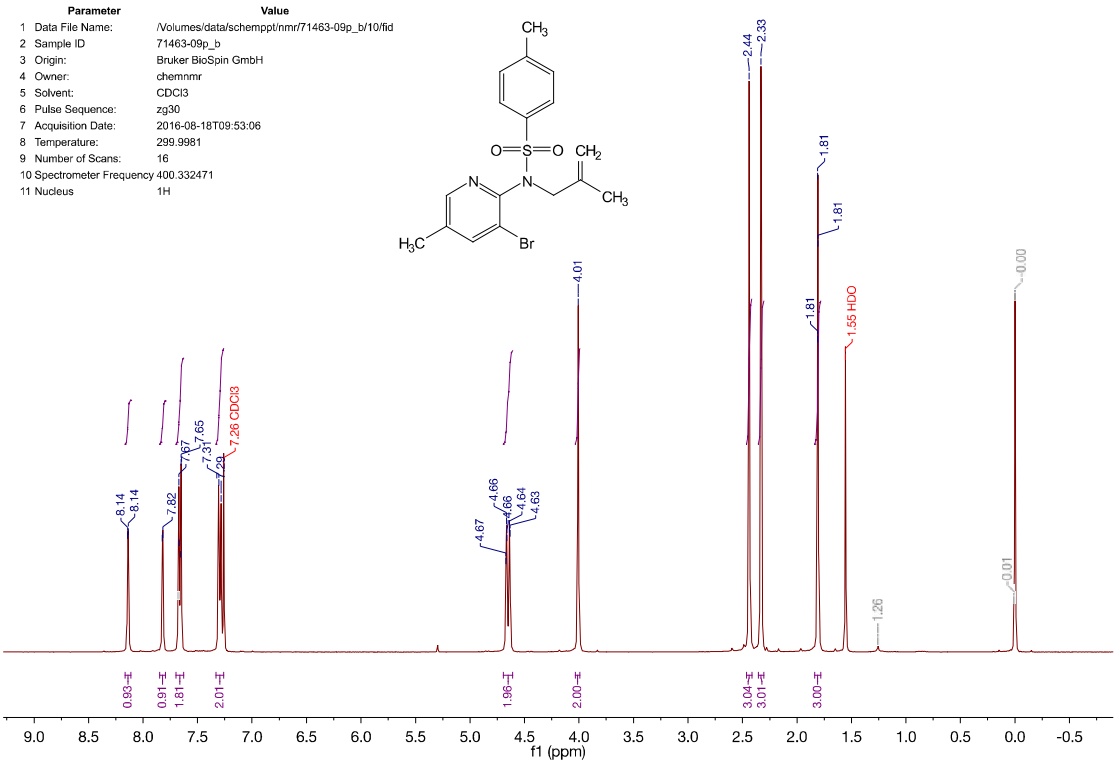
8 Temperature: 300
9 Number of Scans: 8192
10 Spectrometer Frequency 100.622829802853
11 Nucleus 13C
f1 (ppm)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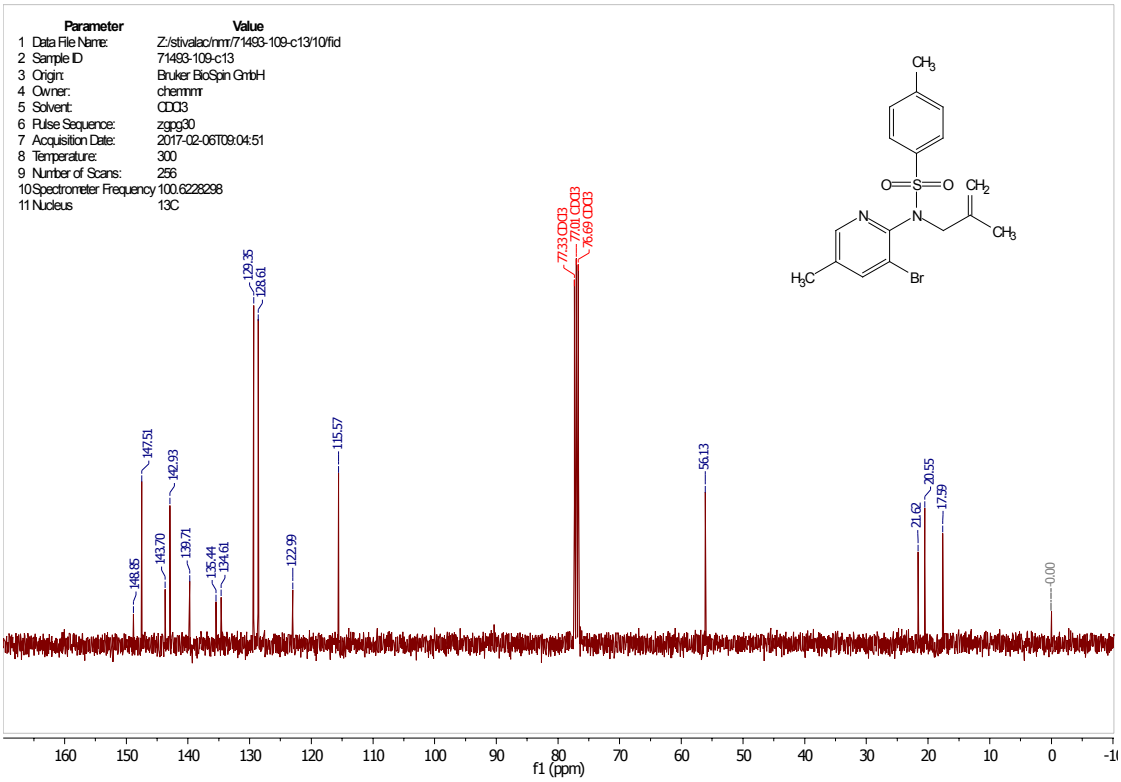
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-18T09:53:06
8 Temperature: 299.9981
9 Number of Scans: 16
10 Spectrometer Frequency 400.332471
11 Nucleus 1H
8.14
8.14
7.82
7.67
7.65
7.31
7.26 CDCl3
4.67
4.66
4.66
4.64
4.63
4.01
2.44
2.33
1.81
1.81
1.81
1.55 HDO
1.26
0.00
0.01
0.93
0.91
1.81
2.01
1.96
2.00
3.04
3.01
3.00
f1 (ppm)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3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-06T09:04:51
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
77.33 CDCl3
77.01 CDCl3
76.69 CDCl3
129.35
128.61
147.51
142.93
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122.99
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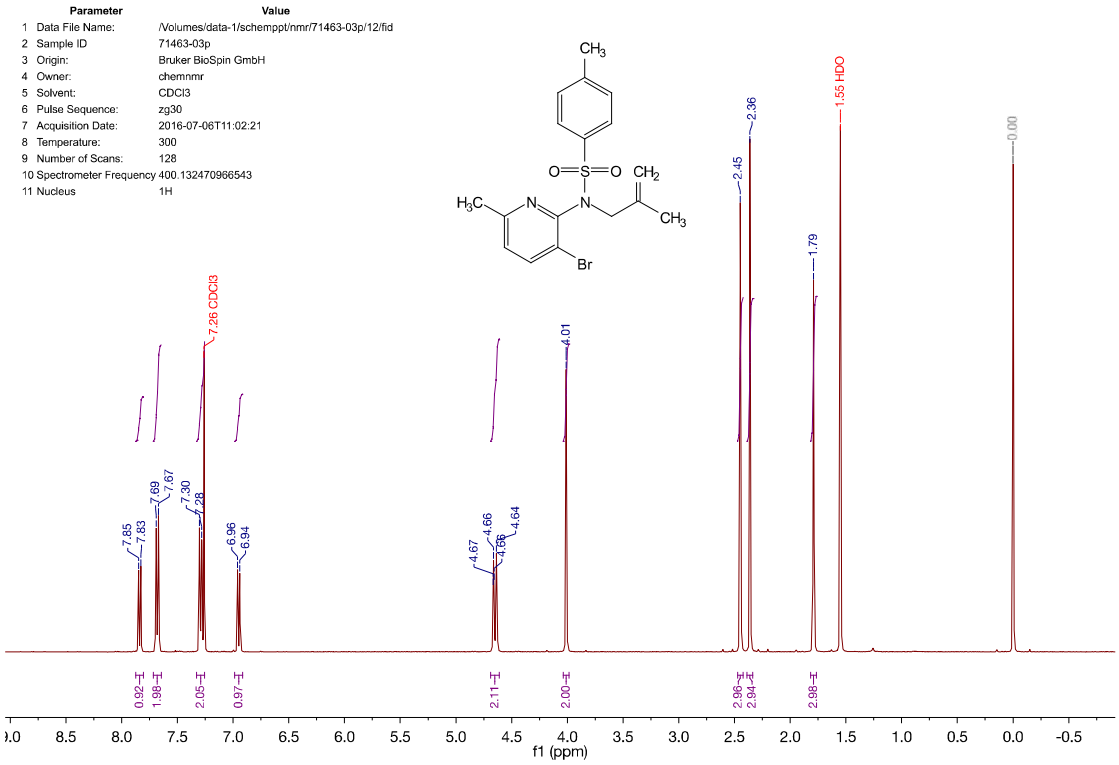
56.13
21.62
20.55
17.59
0.00
f1 (ppm)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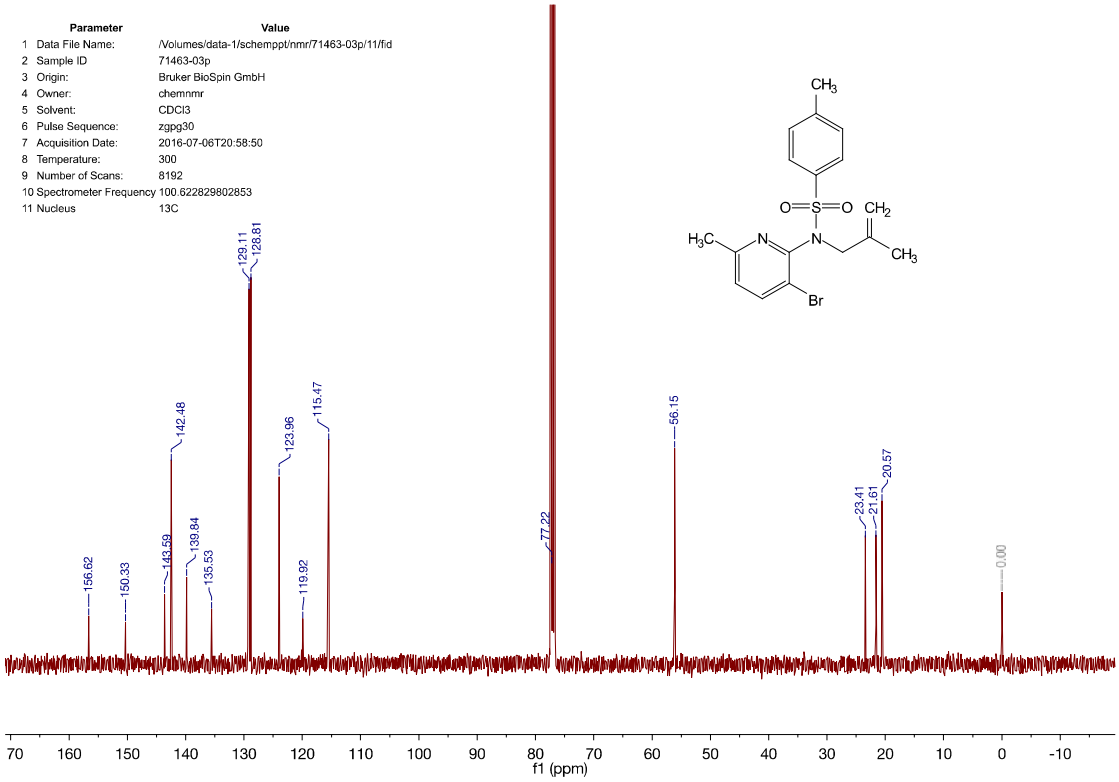
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-07-06T11:02:21
8 Temperature: 300
9 Number of Scans: 128
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
7.85
7.83
7.69
7.67
7.30
7.28
7.26 CDCl3
6.96
6.94
4.67
4.66
4.64
4.01
2.45
2.36
1.79
1.55 HDO
0.00
0.92
1.98
2.05
0.97
2.11
2.00
2.96
2.94
2.98
f1 (ppm)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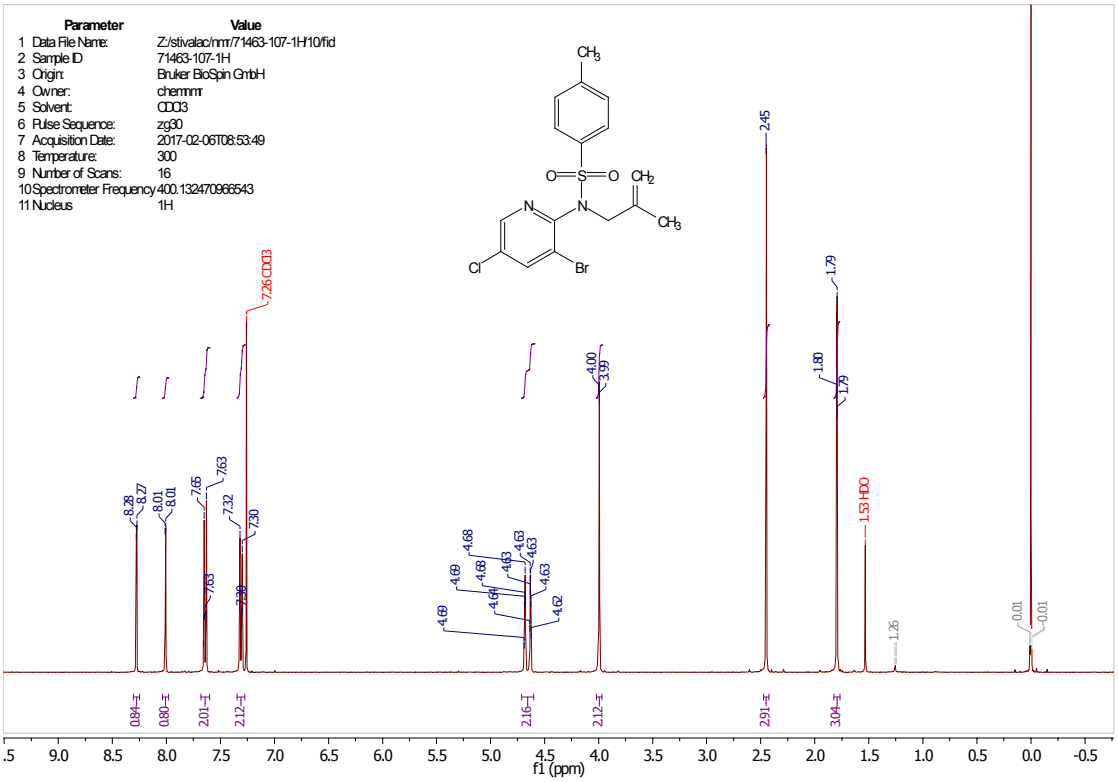
8 Temperature: 300
9 Number of Scans: 8192
10 Spectrometer Frequency 100.622829802853
11 Nucleus 13C
156.62
150.33
143.59
142.48
139.84
135.53
129.11
128.81
123.96
119.92
115.47
77.22
56.15
23.41
21.61
20.57
0.00
f1 (ppm)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4 Owner: chemmm
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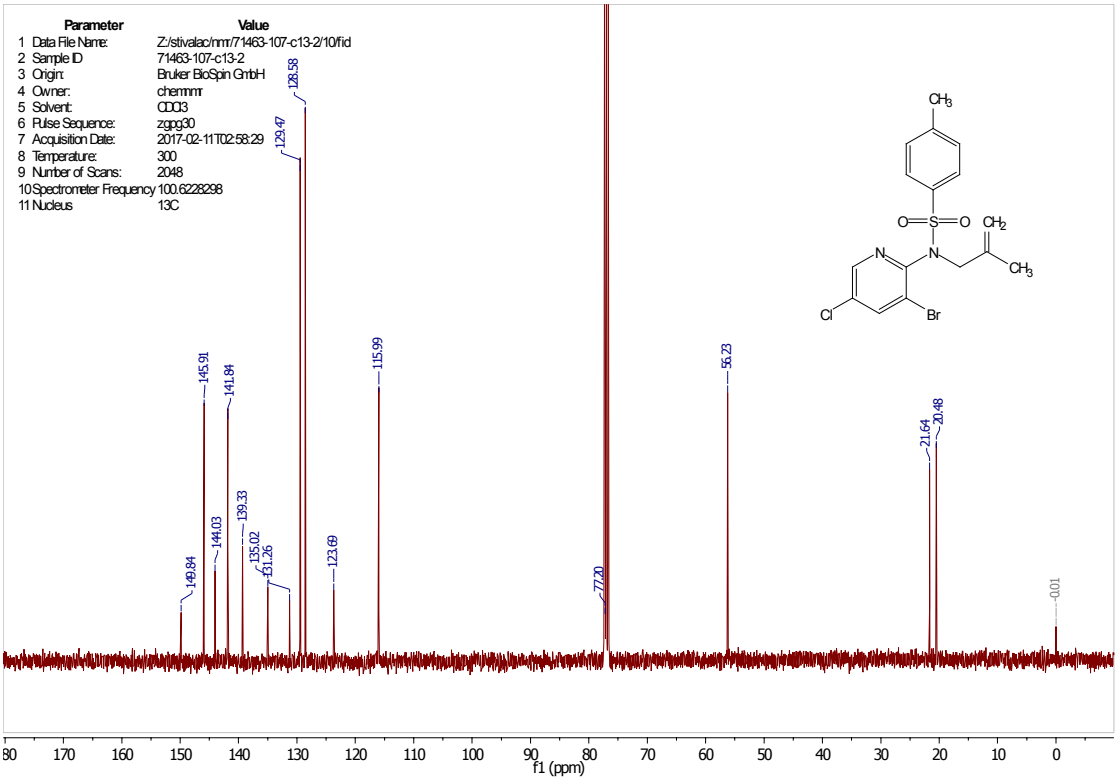
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T08:53:49
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
7.26 CDCl3
1.53 H2O
f1 (ppm)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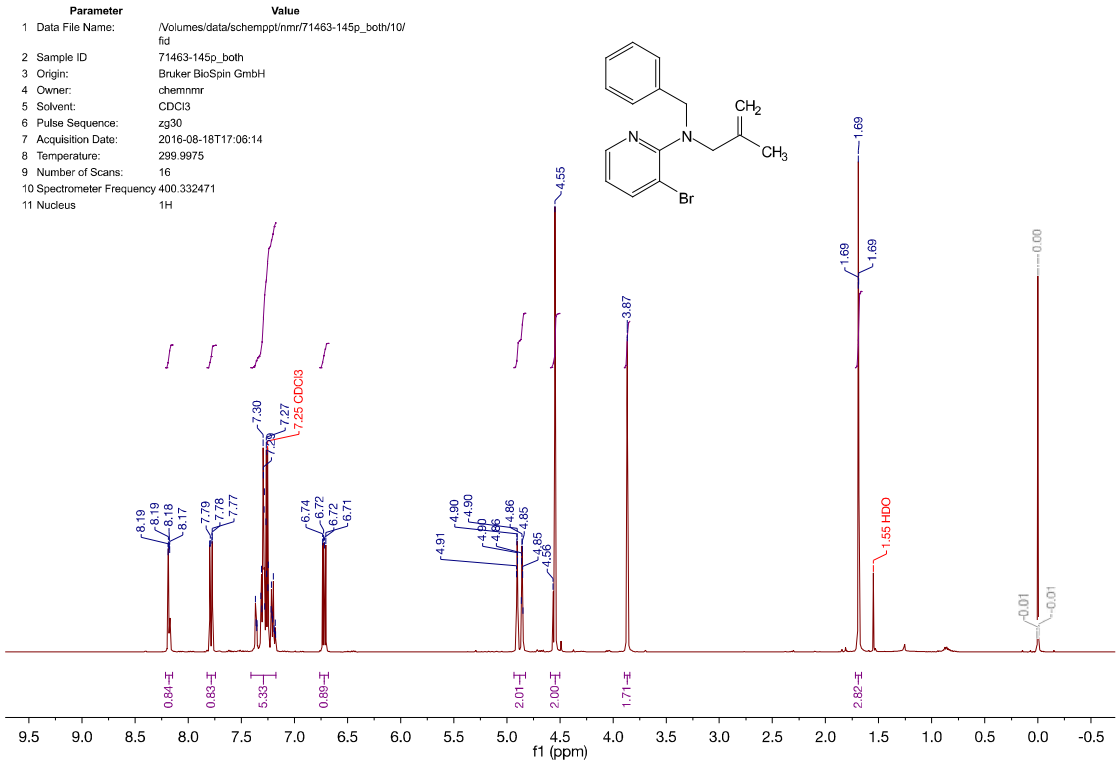
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-11T02:58:29
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
77.20
f1 (ppm)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6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-18T17:06:14
8 Temperature: 299.9975
9 Number of Scans: 16
10 Spectrometer Frequency 400.332471
11 Nucleus 1H
CH2
N
N
CH3
Br
4.55
1.69
1.69
1.69
3.87
0.00
7.30
7.27
7.25 CDCl3
7.28
8.19
8.19
8.18
8.17
7.79
7.78
7.77
6.74
6.72
6.72
6.71
4.91
4.90
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4.88
4.86
4.85
4.85
4.56
1.55 HDO
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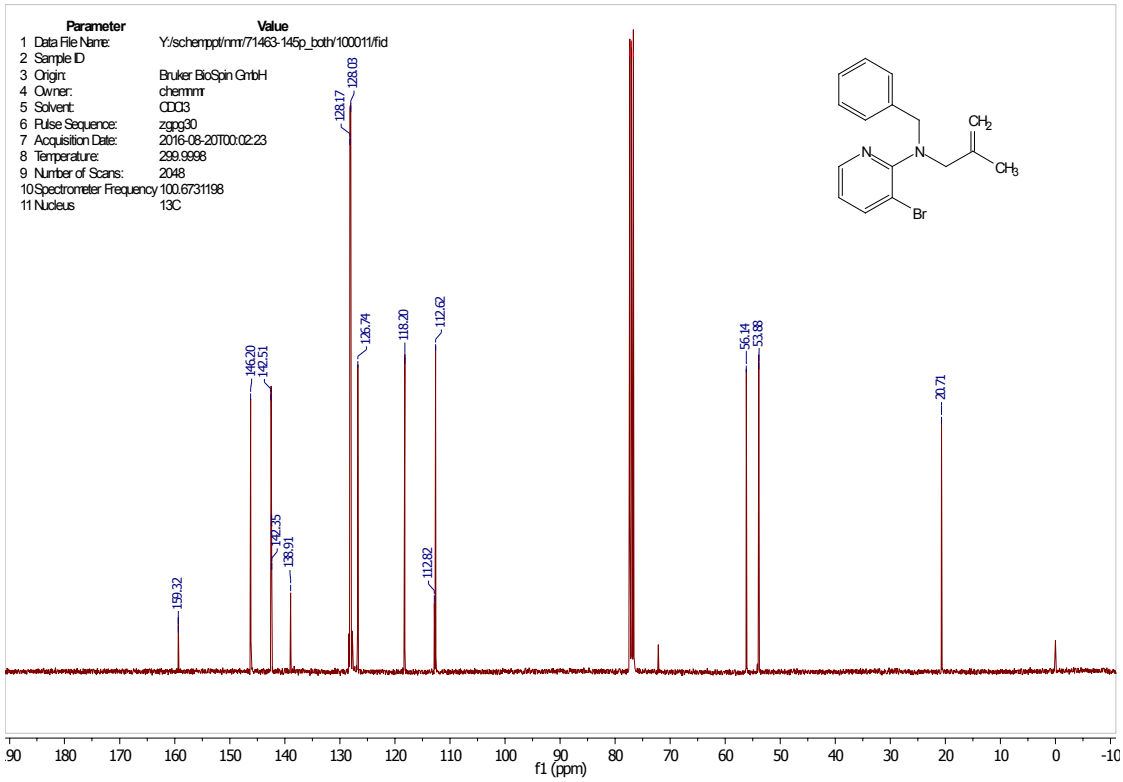
1.71
2.82
f1 (ppm)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6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-20T00:02:23
8 Temperature: 299.9998
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6731198
11 Nucleus 13C
CH2
N
N
CH3
Br
128.03
128.17
126.74
118.20
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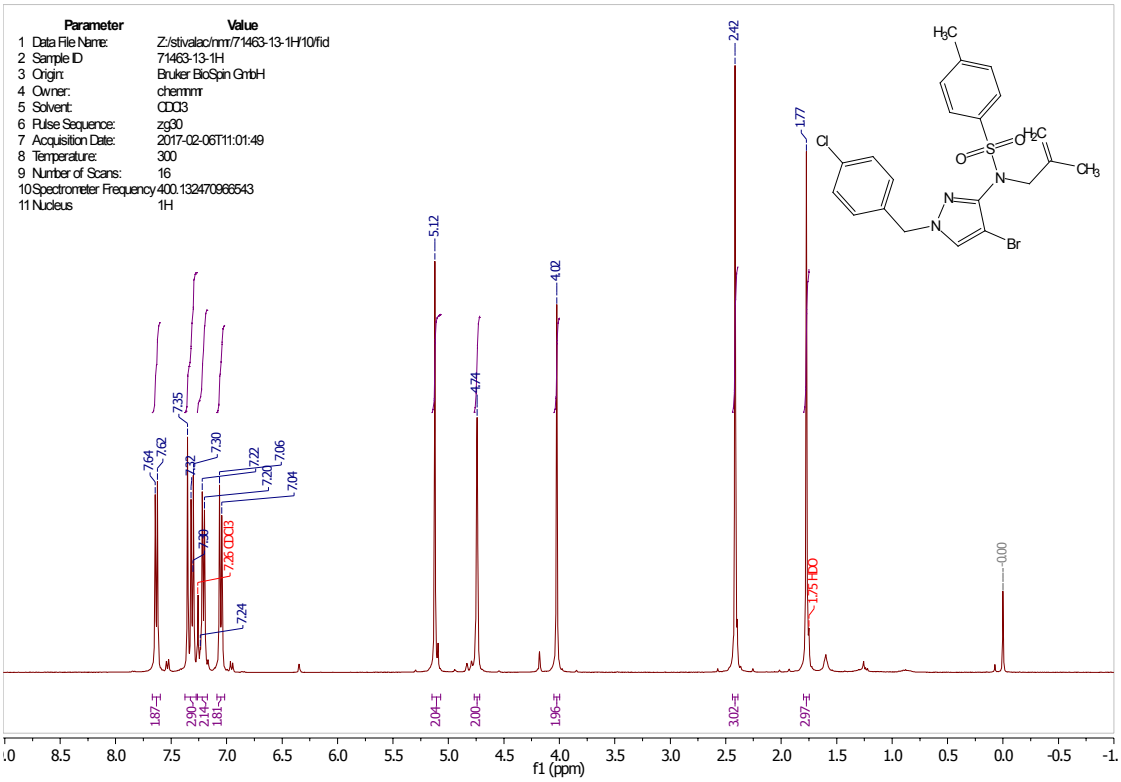
112.82
146.20
142.51
142.35
138.91
159.32
56.14
53.88
20.71
f1 (ppm)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9 Number of Scans: 16
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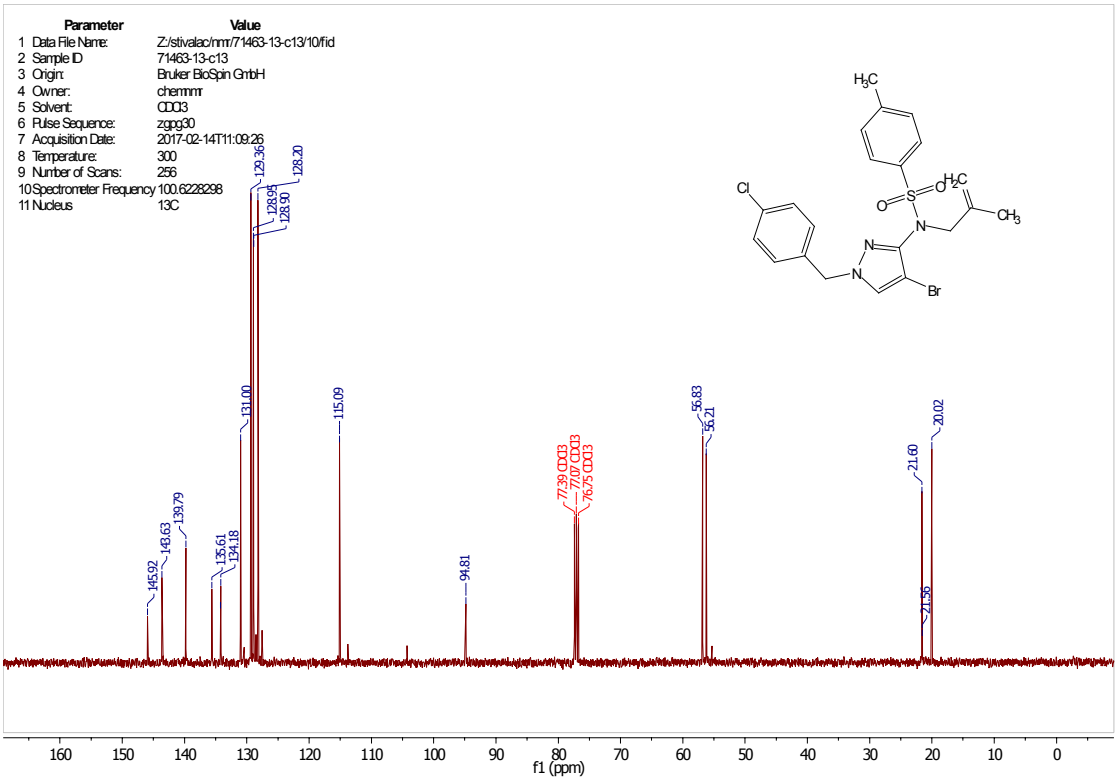
11 Nucleus 1H
f1 (ppm)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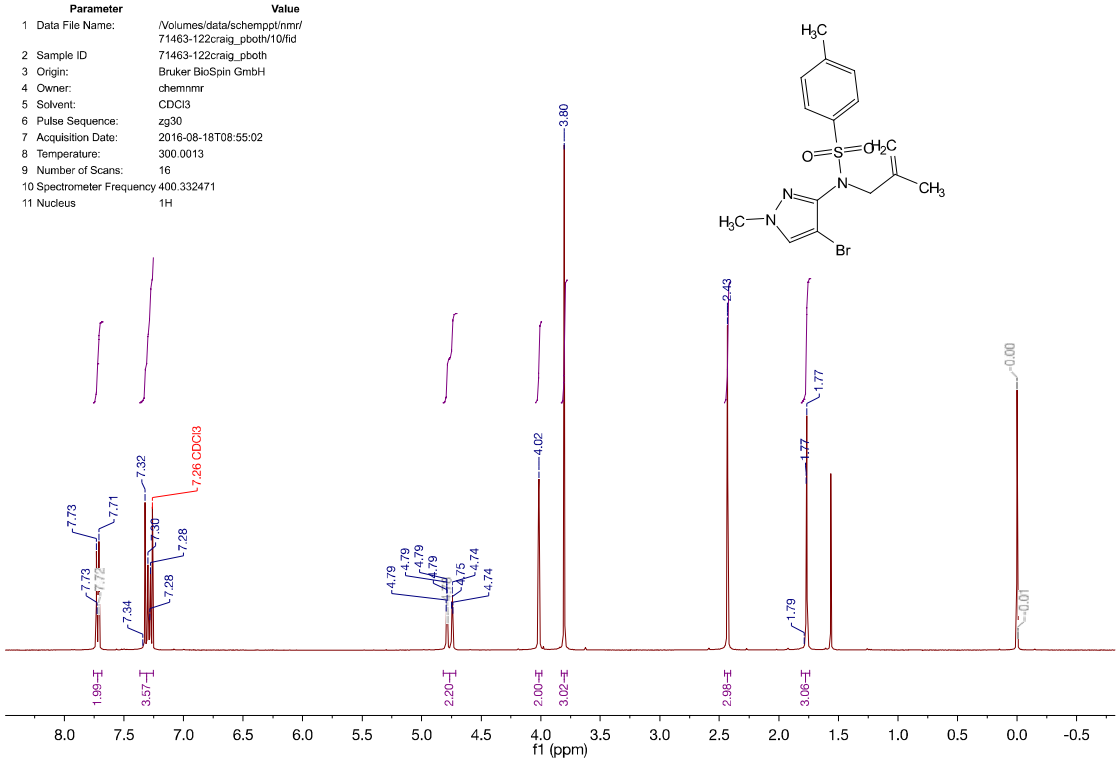
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
f1 (ppm)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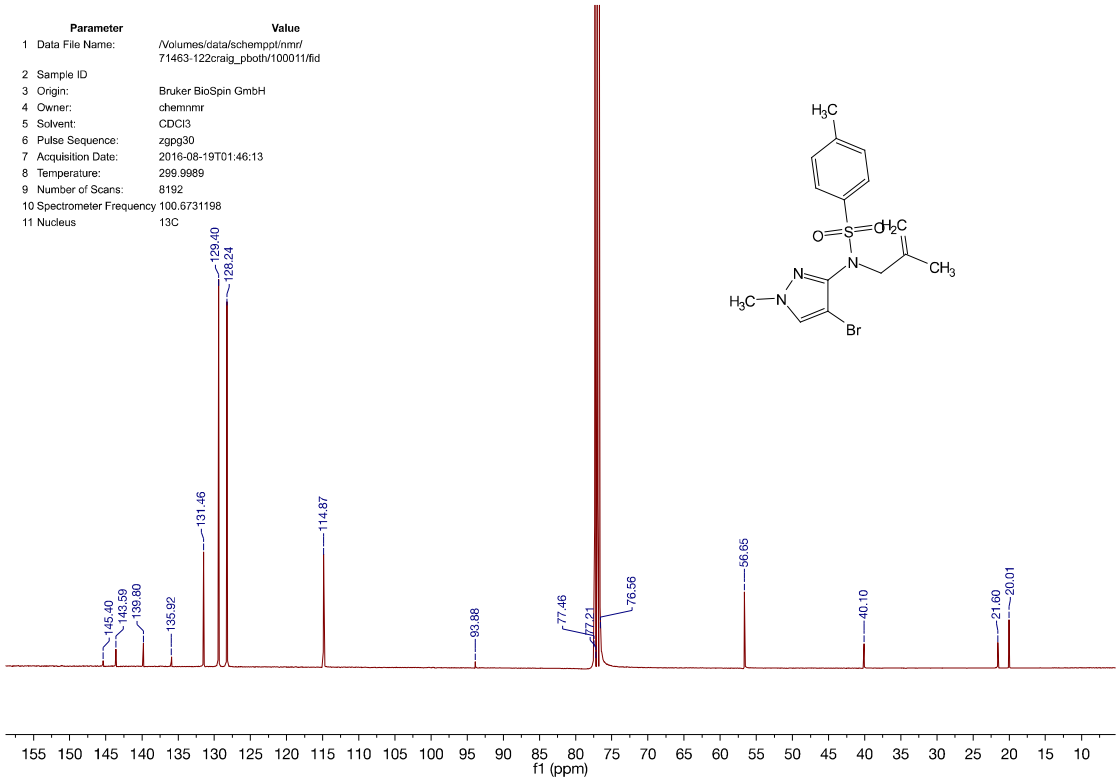
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-18T08:55:02
8 Temperature: 300.0013
9 Number of Scans: 16
10 Spectrometer Frequency 400.332471
11 Nucleus 1H
7.26 CDCl3
f1 (ppm)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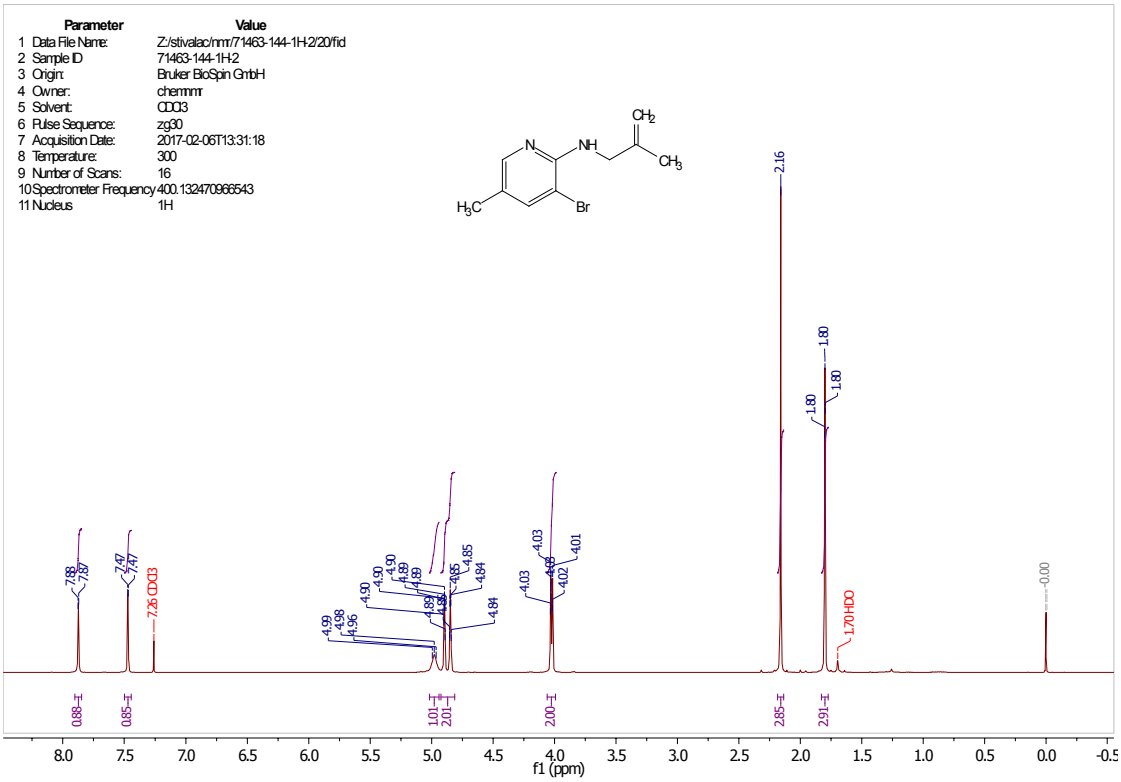
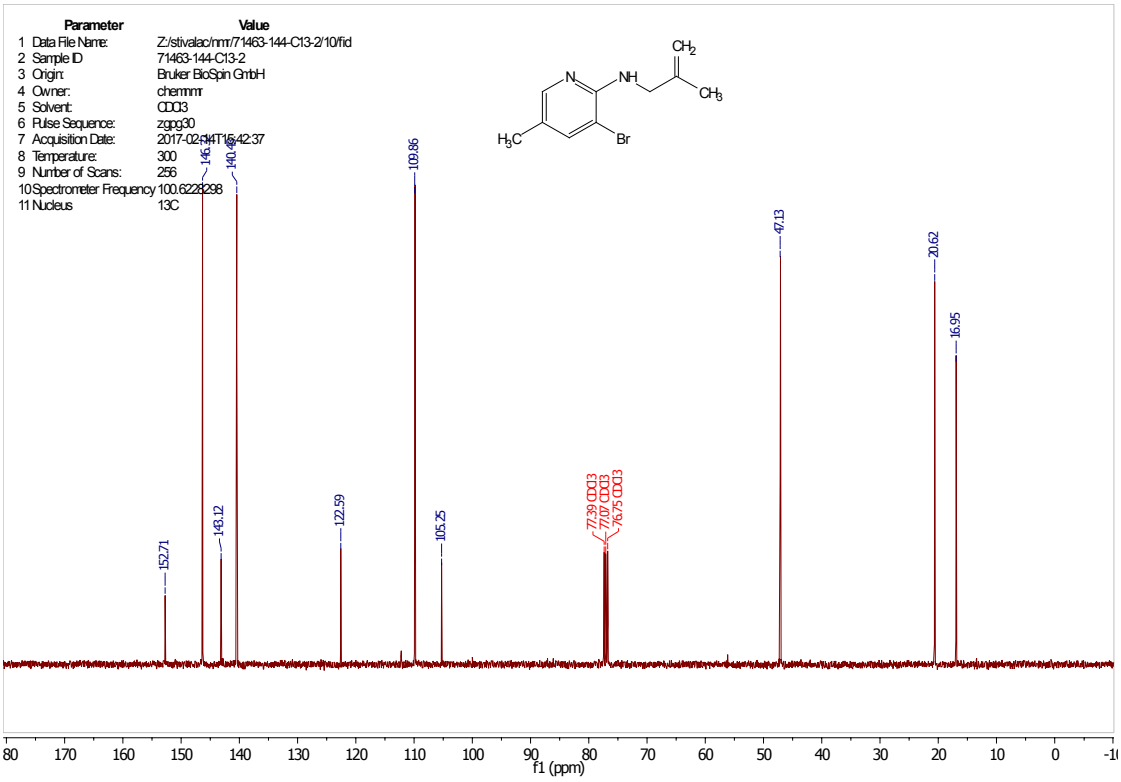
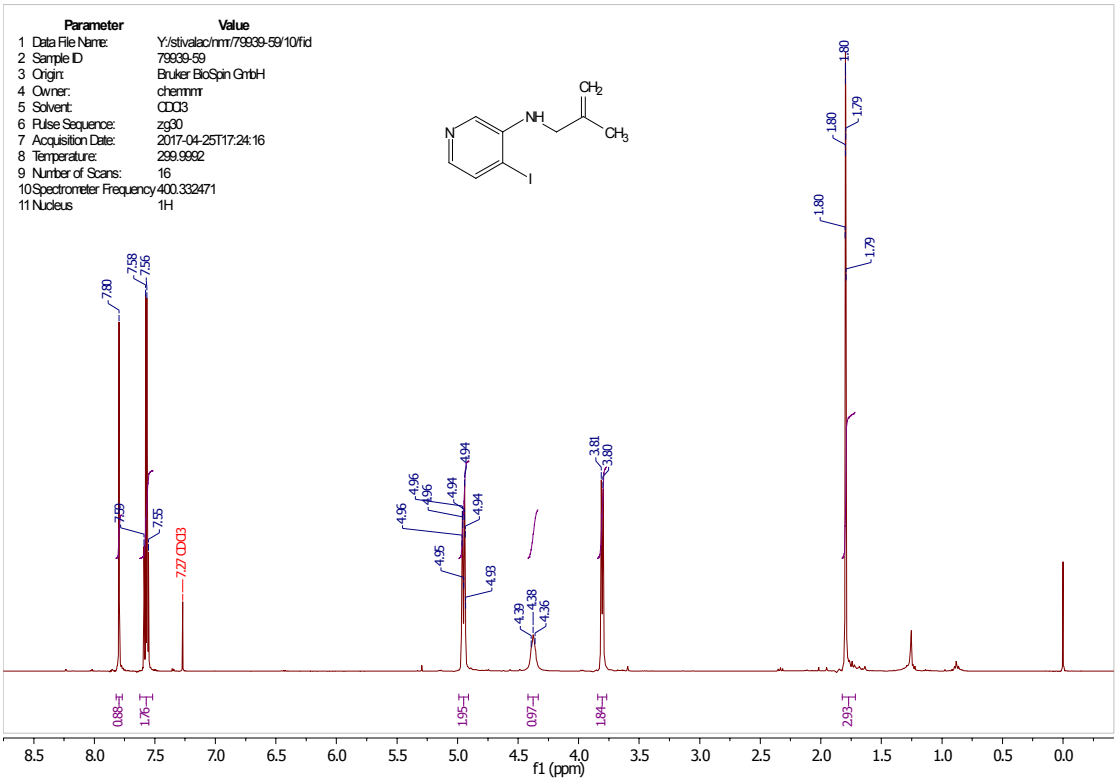
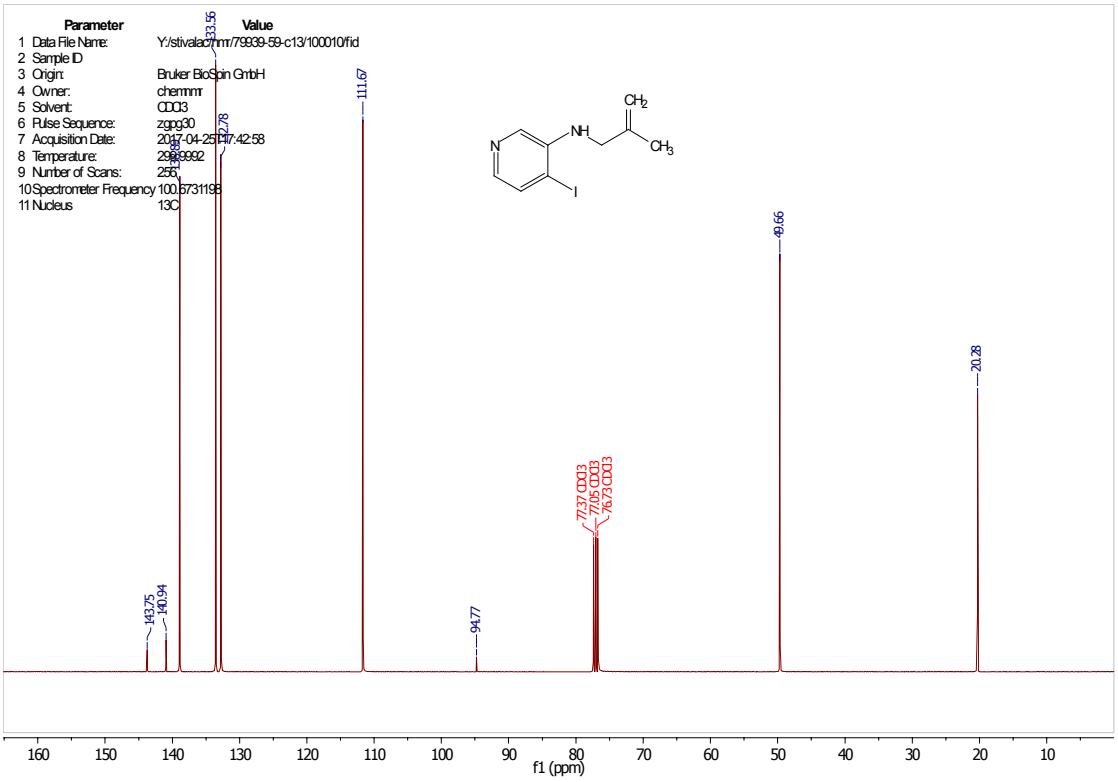
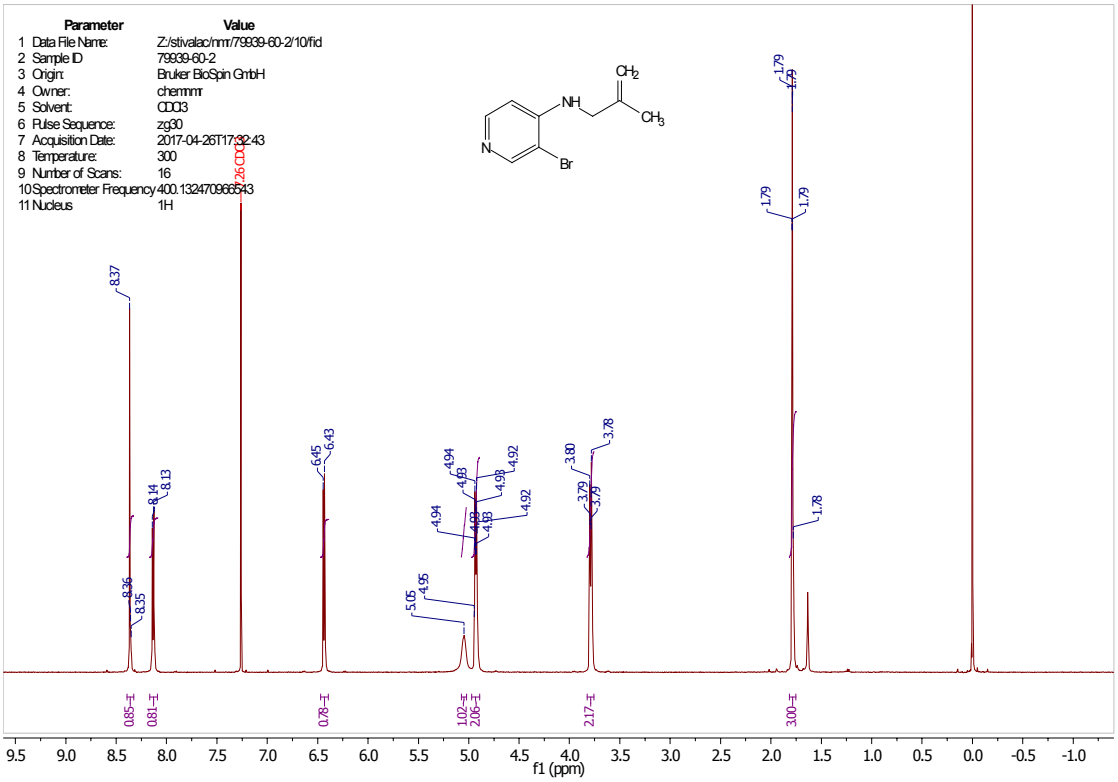
7 Acquisition Date: 2016-08-19T01:46:13
8 Temperature: 299.9989
9 Number of Scans: 8192
10 Spectrometer Frequency 100.6731198
11 Nucleus 13C
f1 (ppm)

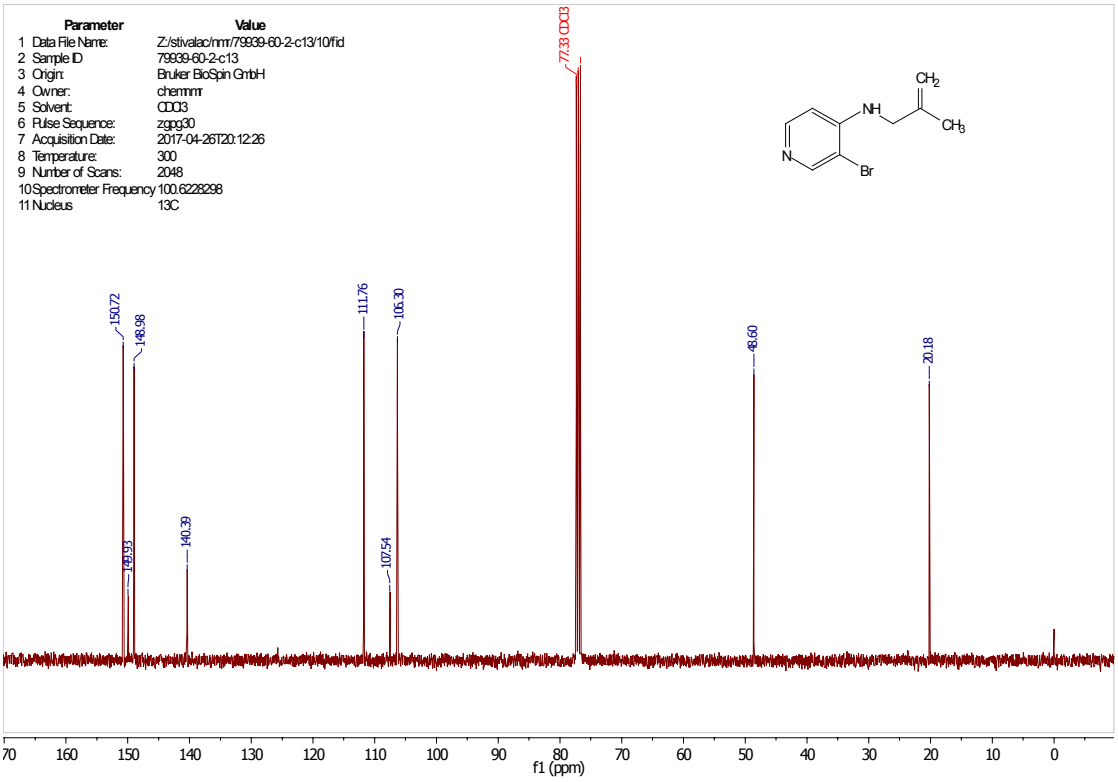

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-144-1H-2/20/fid
2 Sample ID 71463-144-1H-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T13:31:18
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
f1 (ppm)

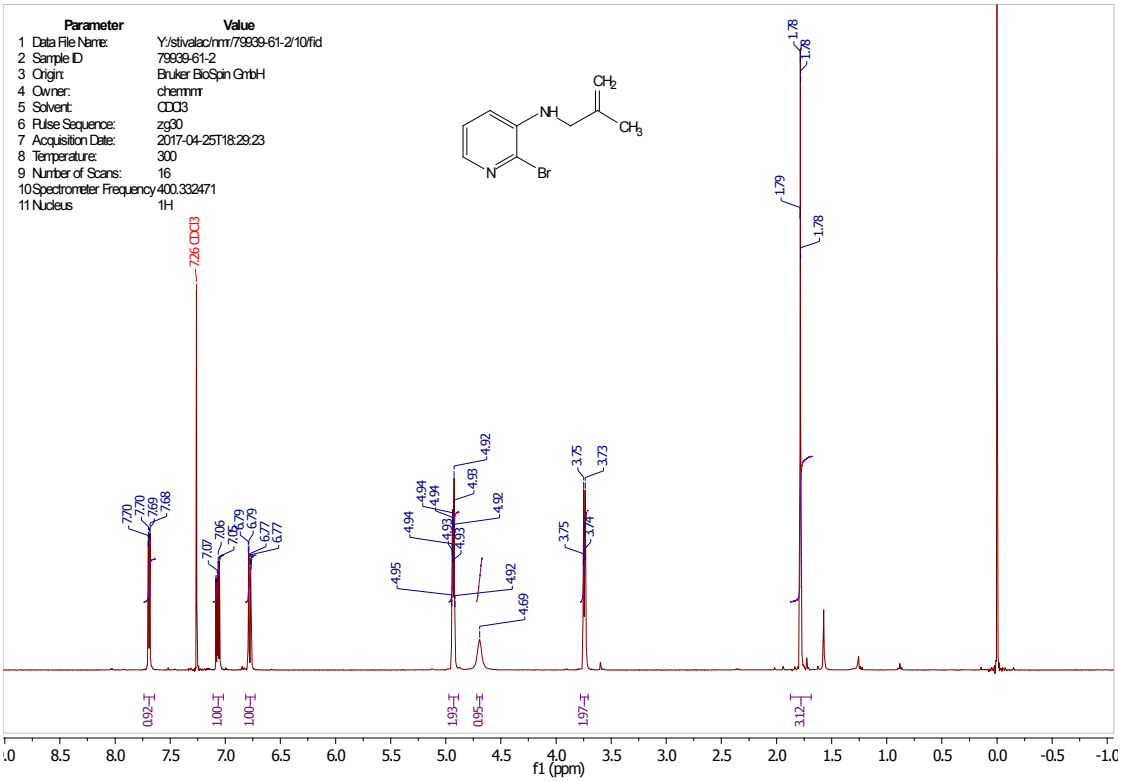

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-144-C13-2/10/fid
2 Sample ID 71463-144-C13-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-14T16:42:37
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
f1 (ppm)

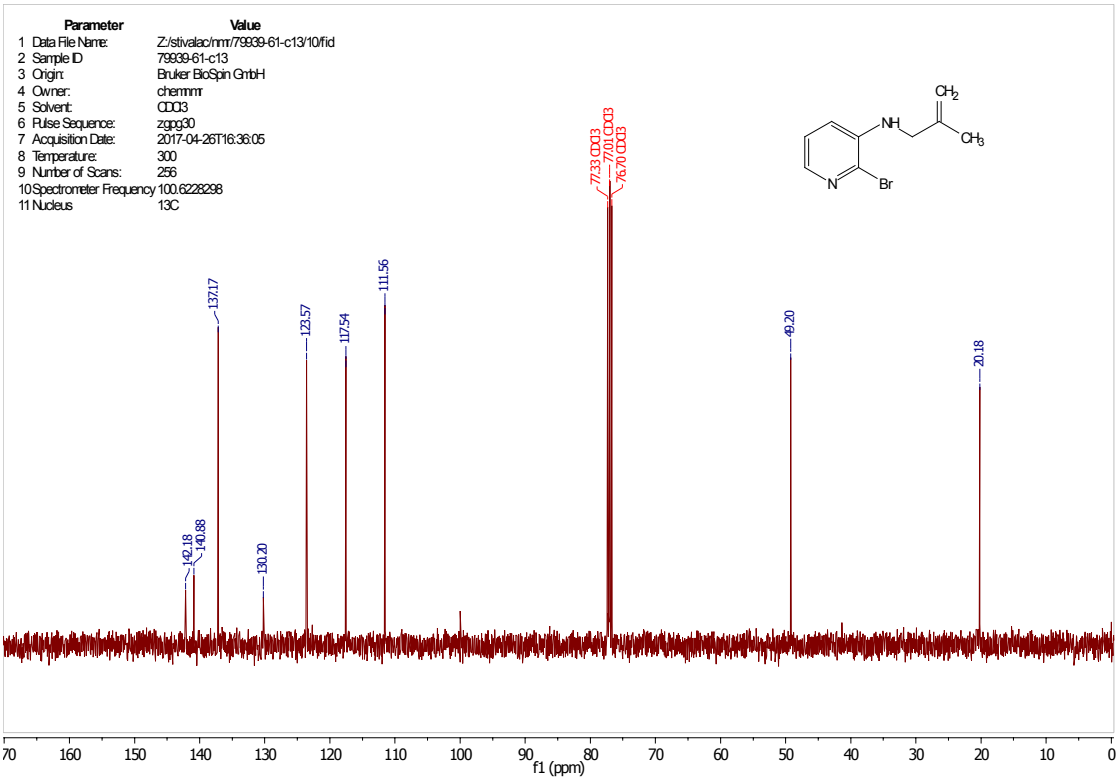

Parameter Value
1 Data File Name: Y:/stivalac/nmr/79939-59/10/fid
2 Sample ID 79939-59
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-04-25T17:24:16
8 Temperature: 299.9992
9 Number of Scans: 16
10 Spectrometer Frequency 400.332471
11 Nucleus 1H
NH
N
I
CH2
CH3
7.80
7.58
7.56
7.59
7.55
7.27 CDCl3
4.96
4.95
4.94
4.93
4.39
4.38
4.36
3.81
3.80
1.80
1.79
0.88
1.76
1.95
0.97
1.84
2.93
f1 (ppm)

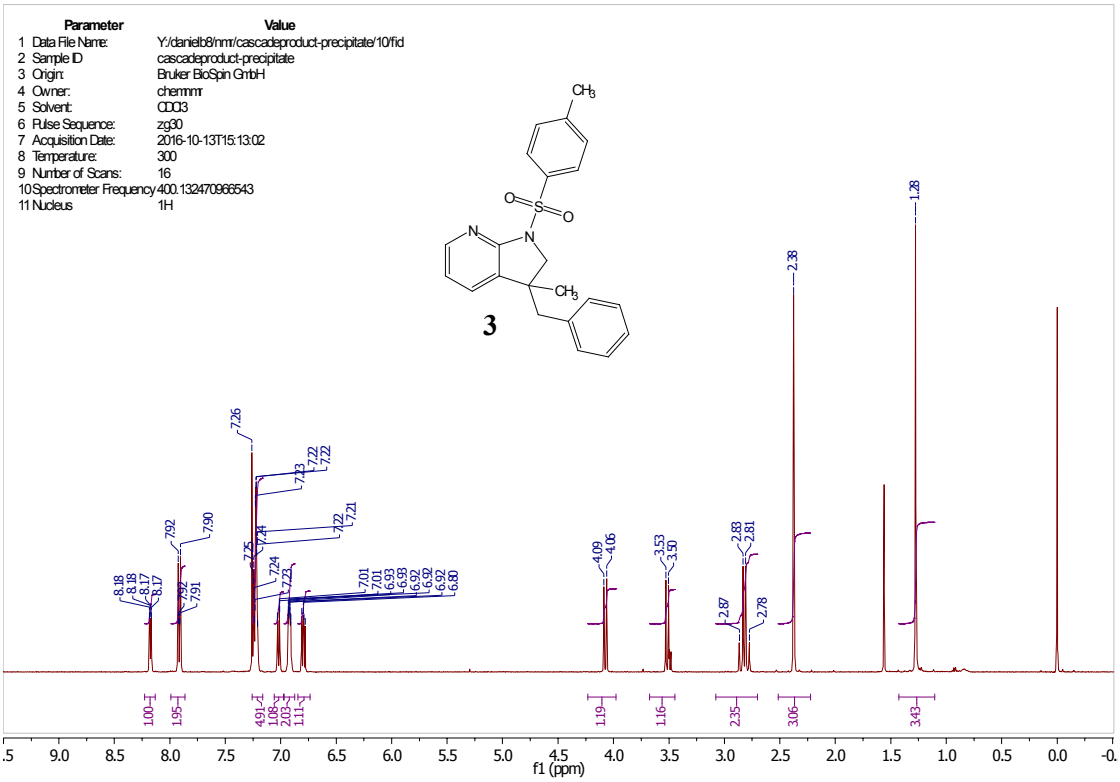

Parameter Value
1 Data File Name: Y:/stivalac/nmr/79939-59-c13/100010/fid
2 Sample ID
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-04-25T17:42:58
8 Temperature: 299.9992
9 Number of Scans: 256
10 Spectrometer Frequency 100.6731198
11 Nucleus 13C
NH
N
I
CH2
CH3
133.56
128.78
111.67
49.66
20.28
77.37 CDCl3
77.05 CDCl3
76.73 CDCl3
143.75
140.94
94.77
f1 (ppm)

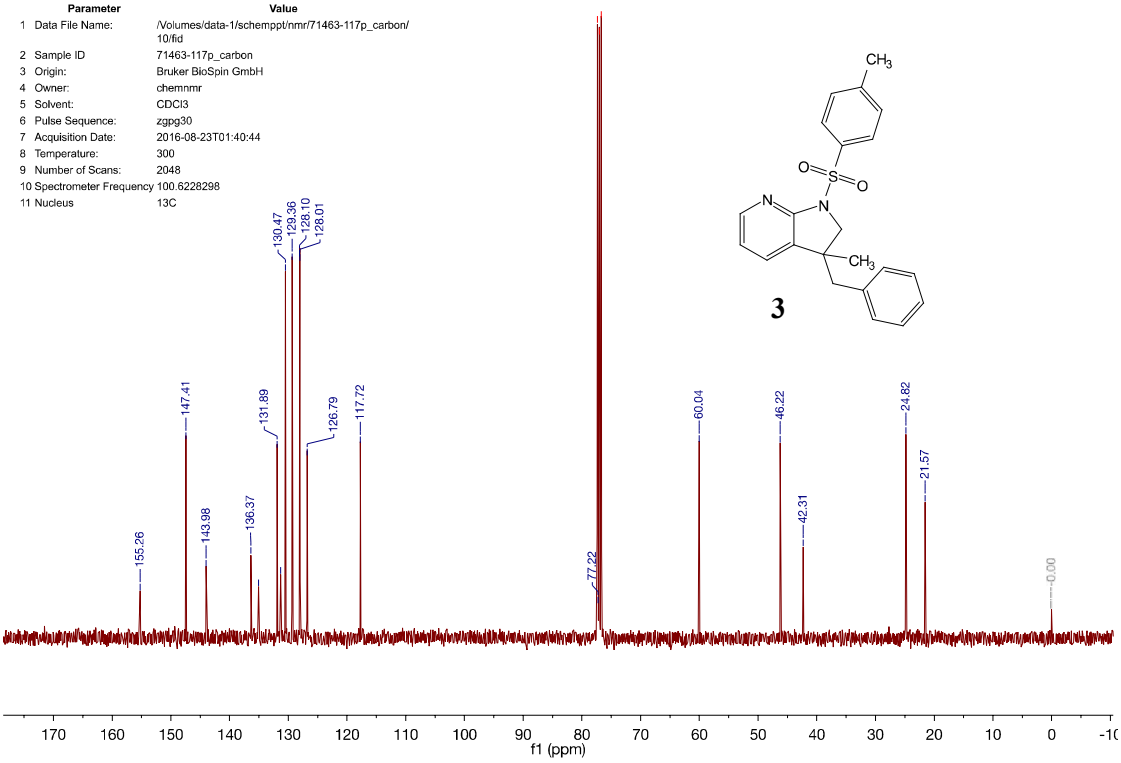

Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-60-2/10/fid
2 Sample ID 79939-60-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-04-26T17:32:43
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.1324709665 43
11 Nucleus 1H
NH
CH2
CH3
N
Br
8.37
8.36
8.35
8.14
8.13
7.26 CDCl3
6.45
6.43
4.94
4.93
4.92
4.98
4.83
4.95
5.05
3.80
3.79
3.78
1.79
1.78
0.85
0.81
0.78
1.02
2.06
2.17
3.00
f1 (ppm)

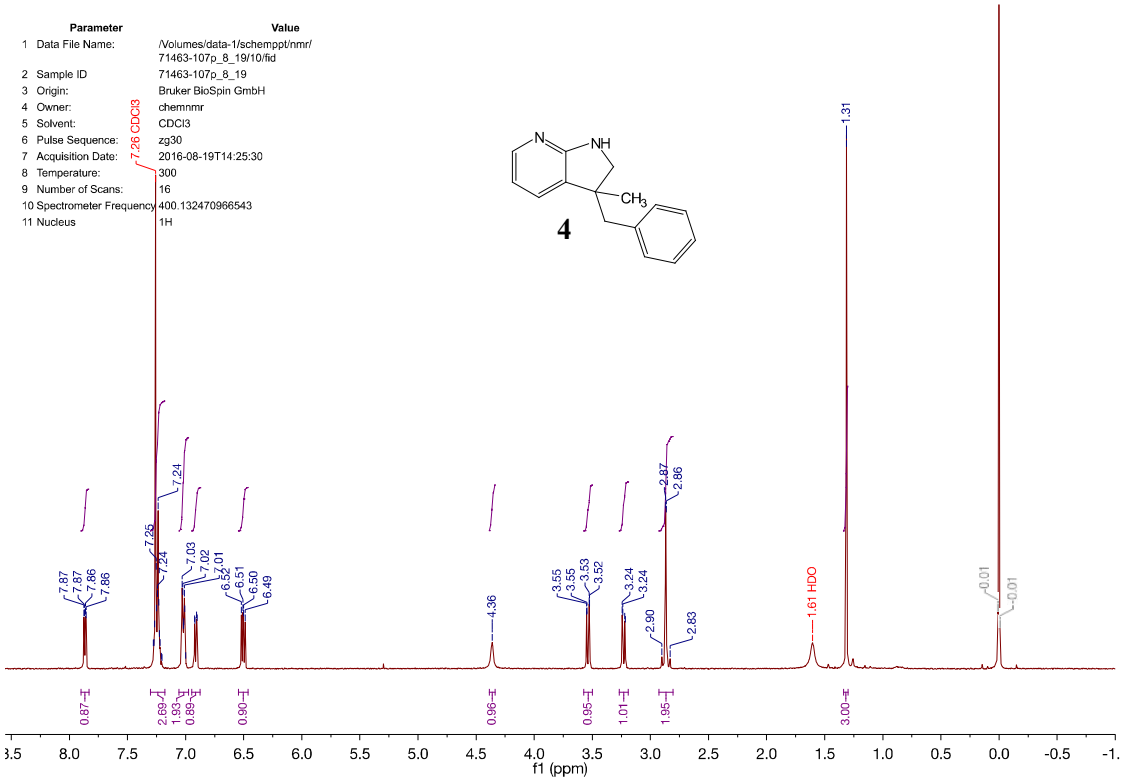

Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-60-2-c13/10/fid
2 Sample ID 79939-60-2-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-04-26T20:12:26
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
NH
CH2
CH3
N
Br
77.33 CDCl3
150.72
148.98
140.39
111.76
106.30
107.54
48.60
20.18
f1 (ppm)

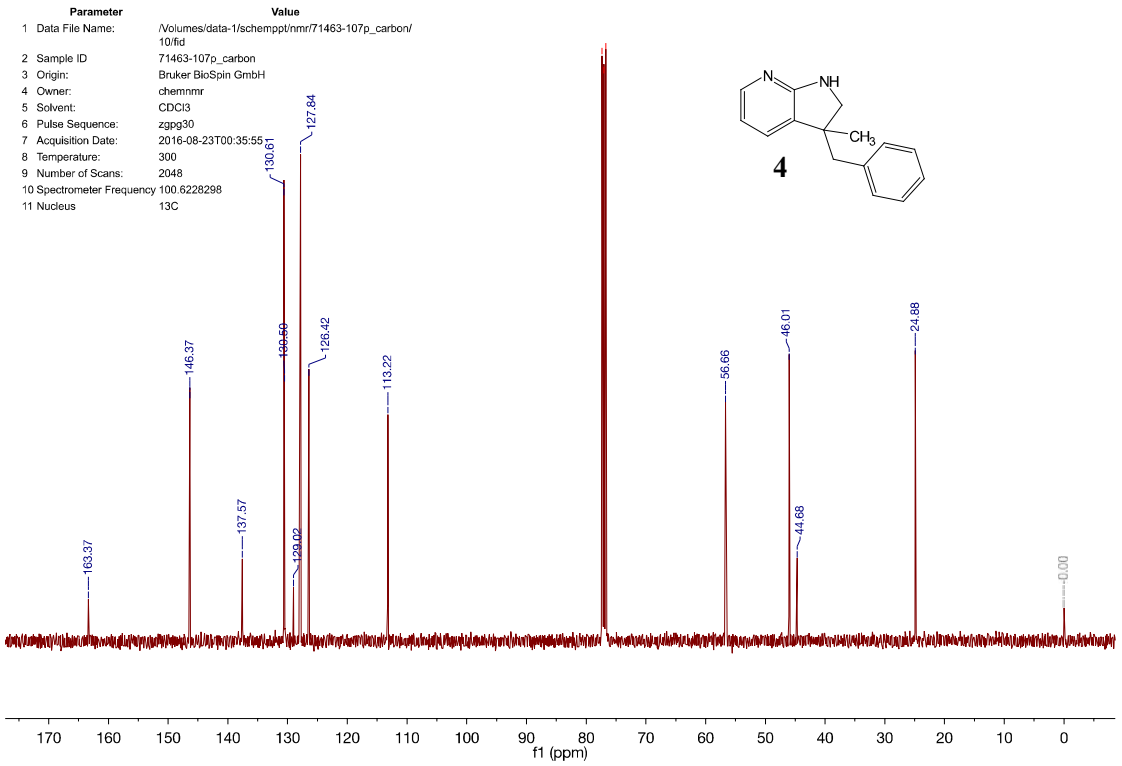

Parameter Value
1 Data File Name: Y:/stivalac/nmr/79939-61-2/10/fid
2 Sample ID 79939-61-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-04-25T18:29:23
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.332471
11 Nucleus 1H
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-61-c13/10/fid
2 Sample ID 79939-61-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-04-26T16:36:05
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
f1 (ppm)


Parameter Value
1 Data File Name: Y:/danielb8/nmr/cascadeproduct-precipitate/10/fid
2 Sample ID cascadeproduct-precipitate
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-10-13T15:13:02
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
3
f1 (ppm)


Parameter Value
1 Data File Name: /Volumes/data-1/schemppt/nmr/71463-117p_carbon/10/fid
2 Sample ID 71463-117p_carbon
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-23T01:40:44
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
3
f1 (ppm)


Parameter Value
1 Data File Name: /Volumes/data-1/schemppt/nmr/71463-107p_8_19/10/fid
2 Sample ID 71463-107p_8_19
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-19T14:25:30
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
4
f1 (ppm)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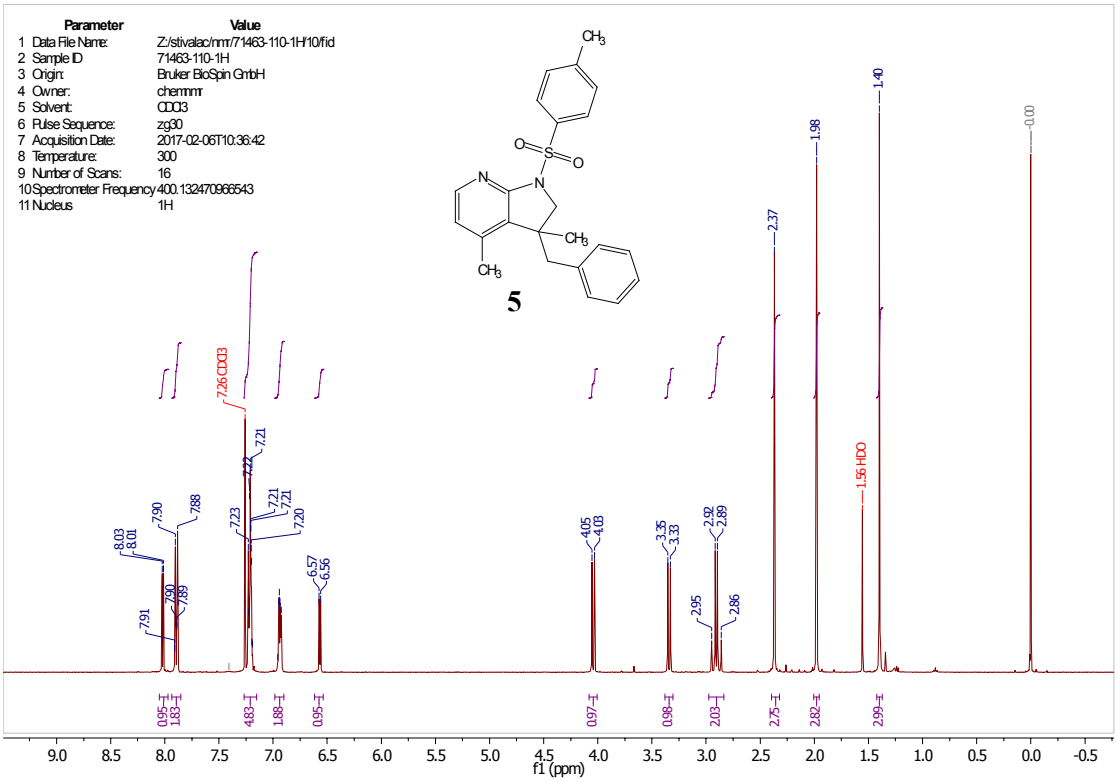
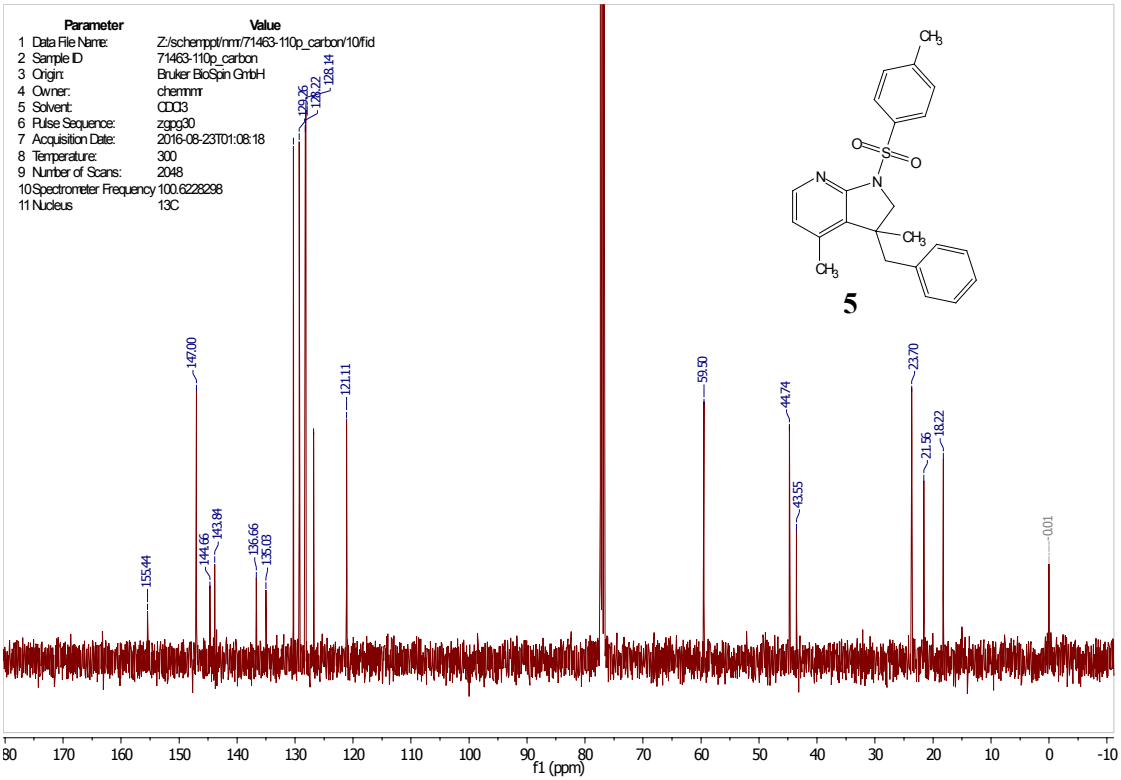
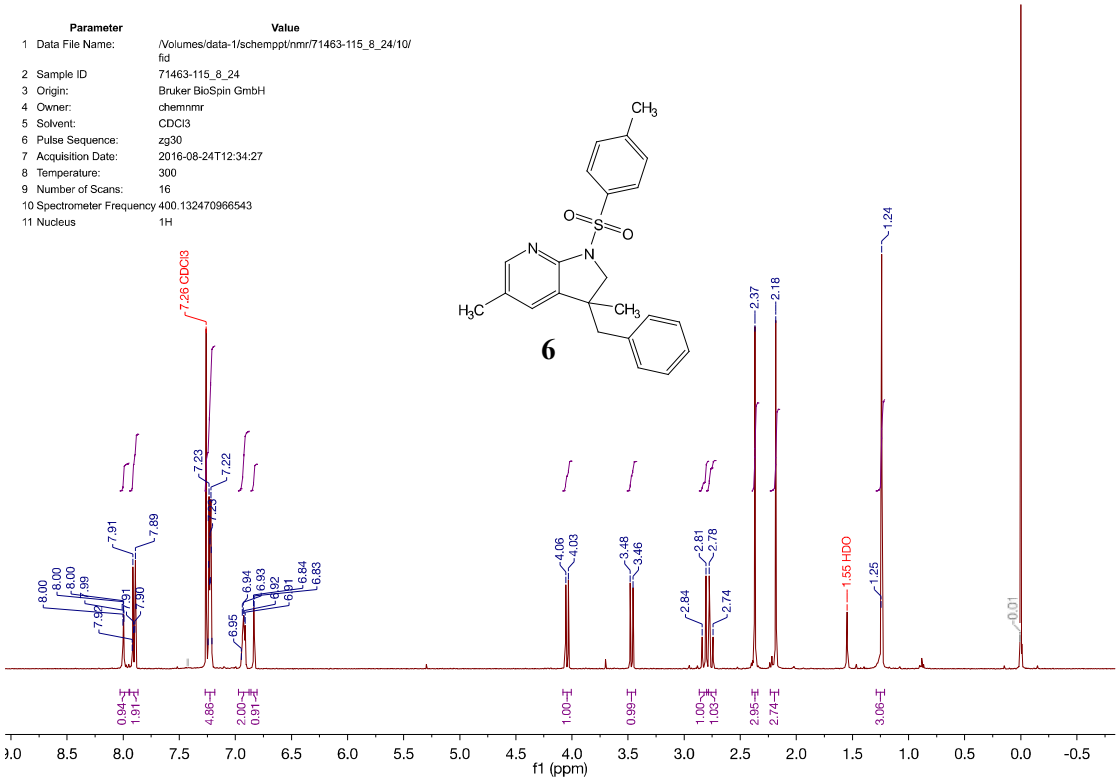
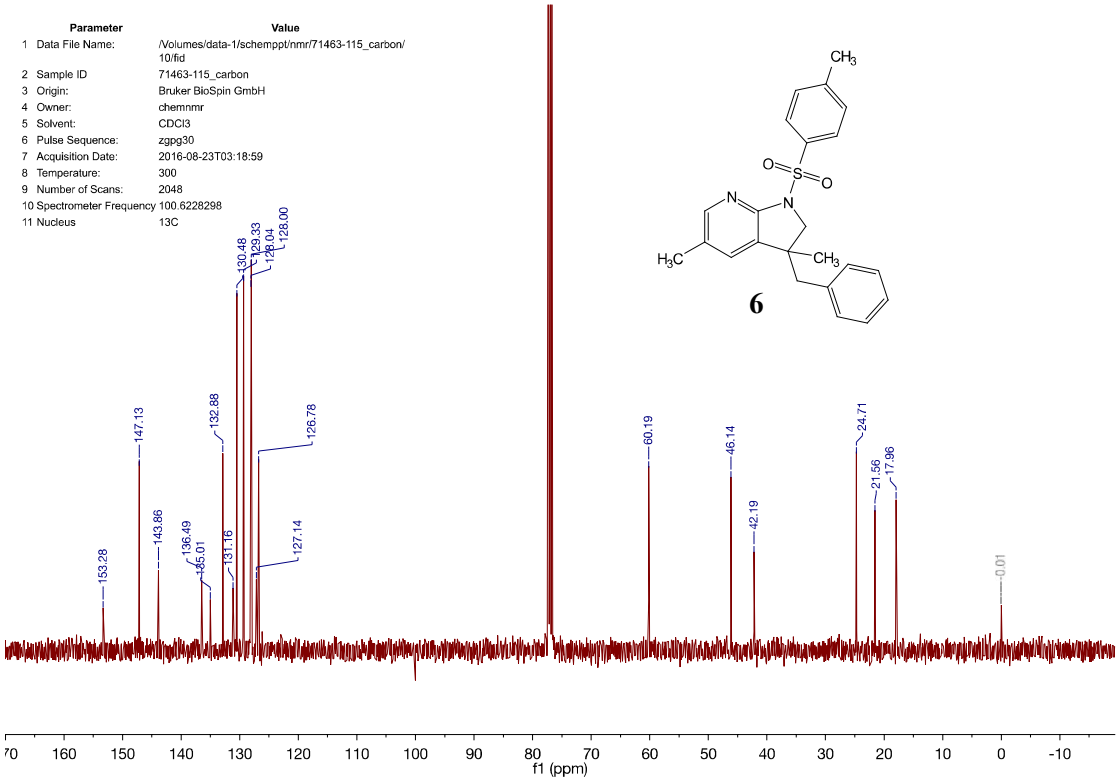
1 Data File Name: /Volumes/data-1/schemppt/nmr/71463-107p_carbon/10/fid
2 Sample ID 71463-107p_carbon
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-23T00:35:55
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
4
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-110-1H/10/fid
2 Sample ID 71463-110-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T10:36:42
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
5
7.26 CDCl3
1.56 HDO
f1 (ppm)


Parameter Value
1 Data File Name: Z:/schempbl/nmr/71463-110p_carbon/10/fid
2 Sample ID 71463-110p_carbon
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-23T01:08:18
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
5
f1 (ppm)


Parameter Value
1 Data File Name: /Volumes/data-1/schemppt/nmr/71463-115_8_24/10/fid
2 Sample ID 71463-115_8_24
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-24T12:34:27
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
7.26 CDCl3
1.55 HDO
f1 (ppm)
6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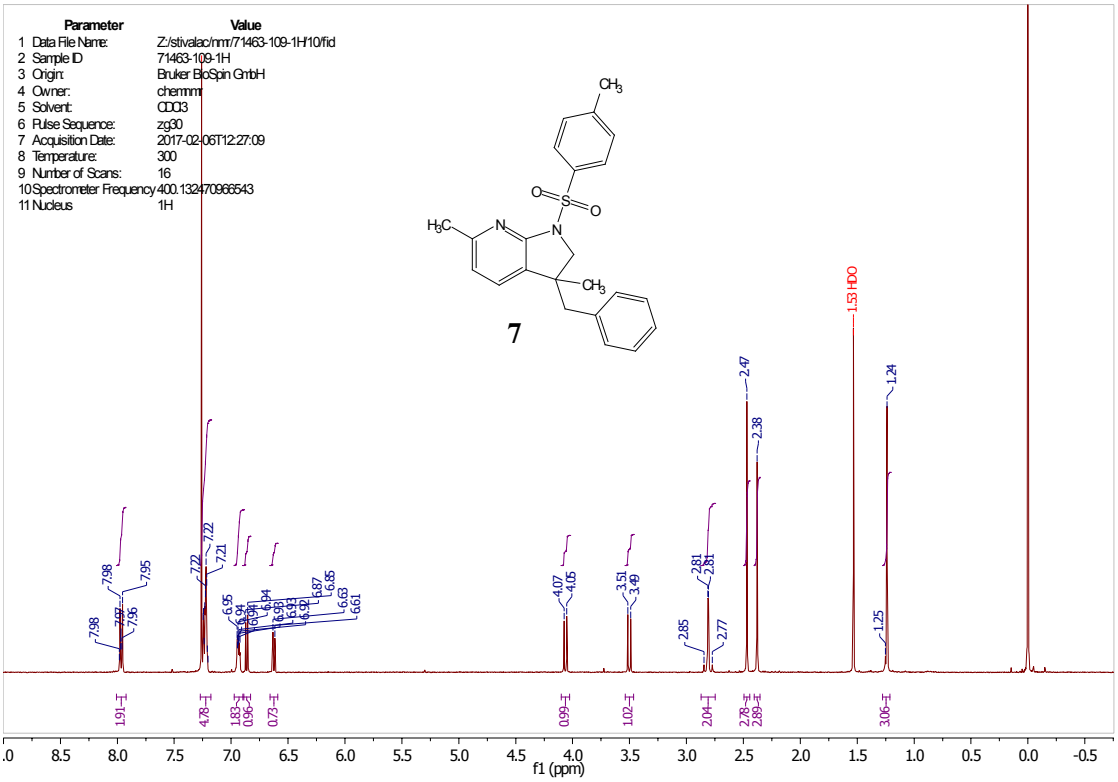
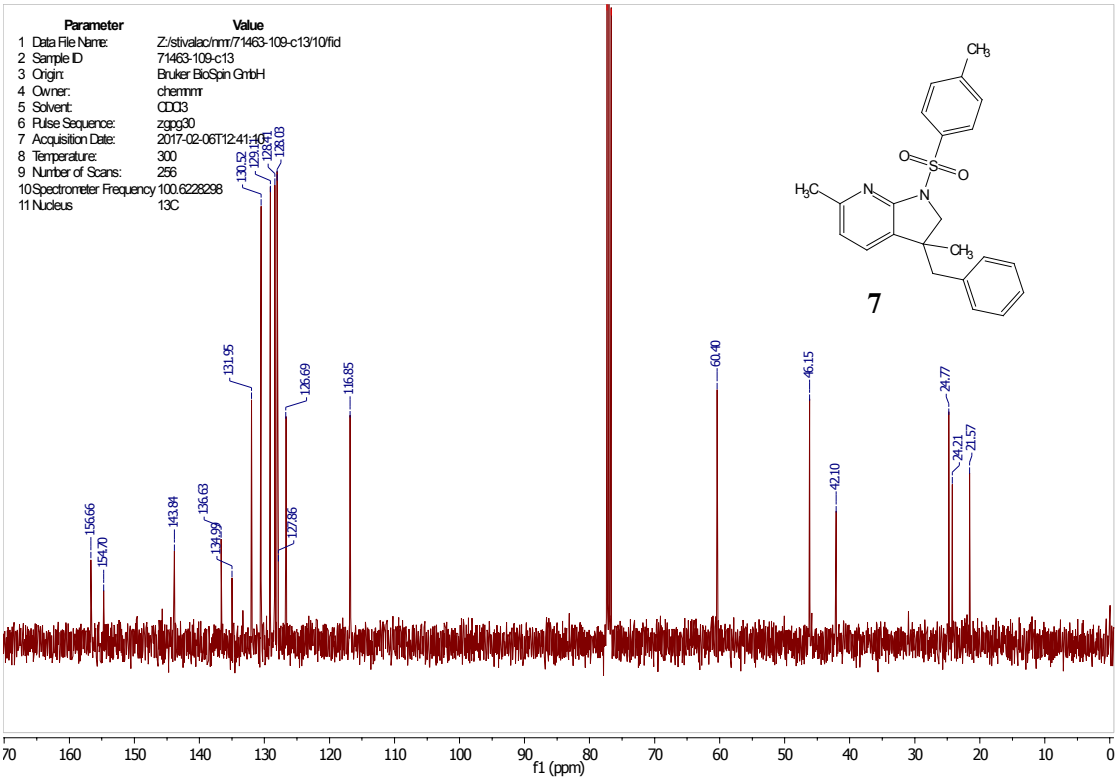
1 Data File Name: /Volumes/data-1/schemppt/nmr/71463-115_carbon/10/fid
2 Sample ID 71463-115_carbon
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-23T03:18:59
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
f1 (ppm)
6


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-109-1H/10/fid
2 Sample ID 71463-109-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T12:27:09
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.1324709666543
11 Nucleus 1H
7
f1 (ppm)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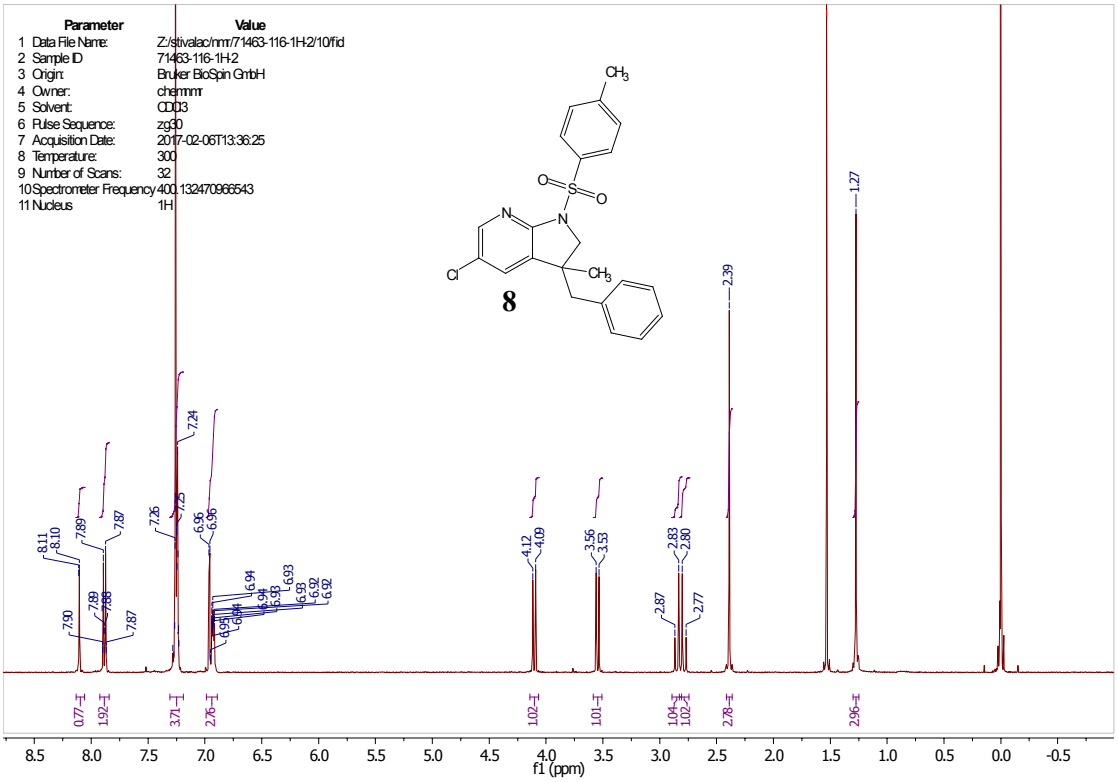
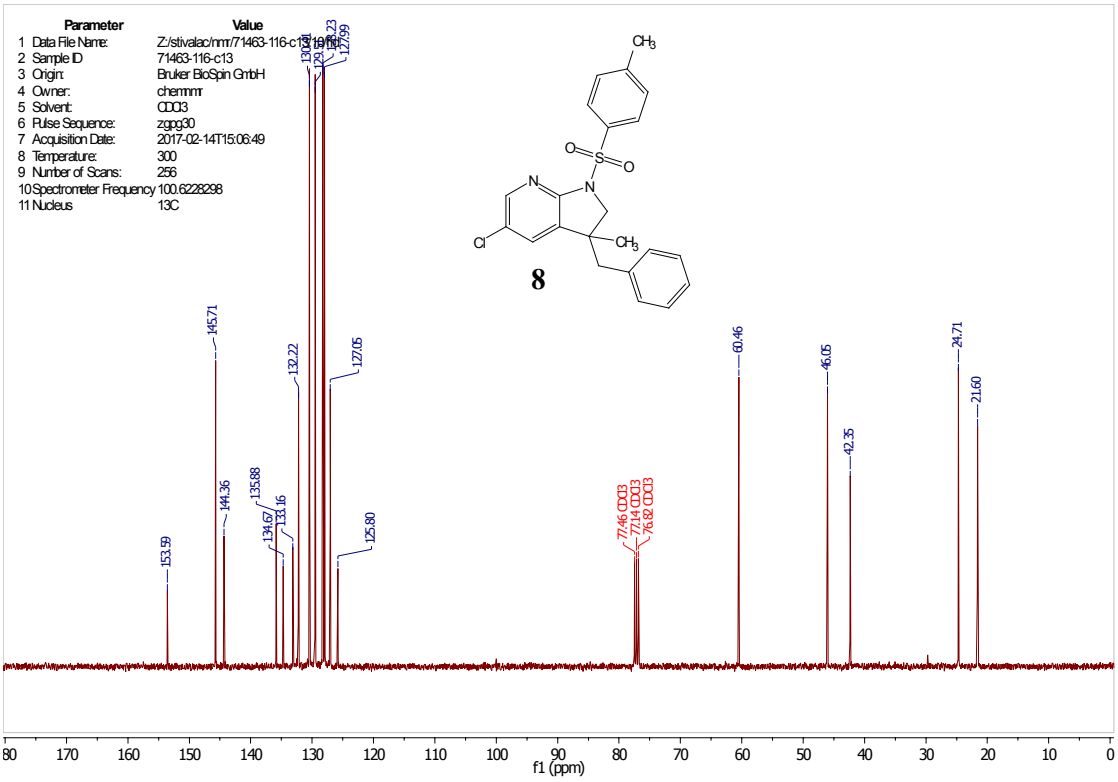
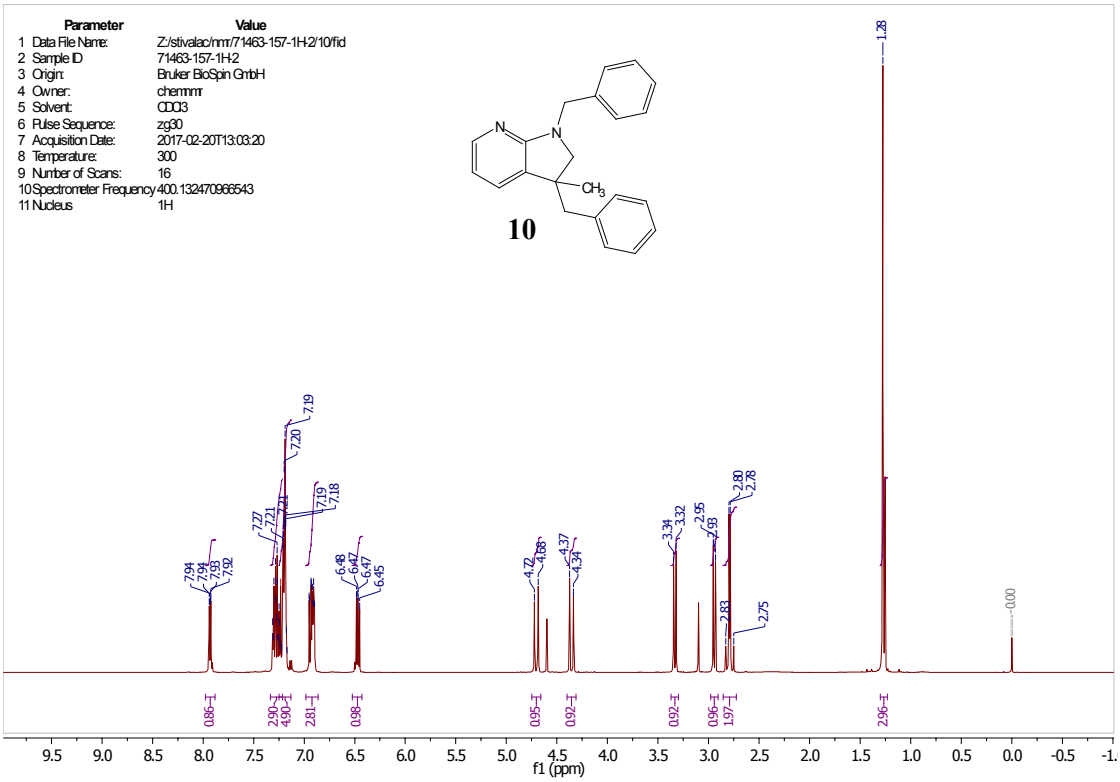
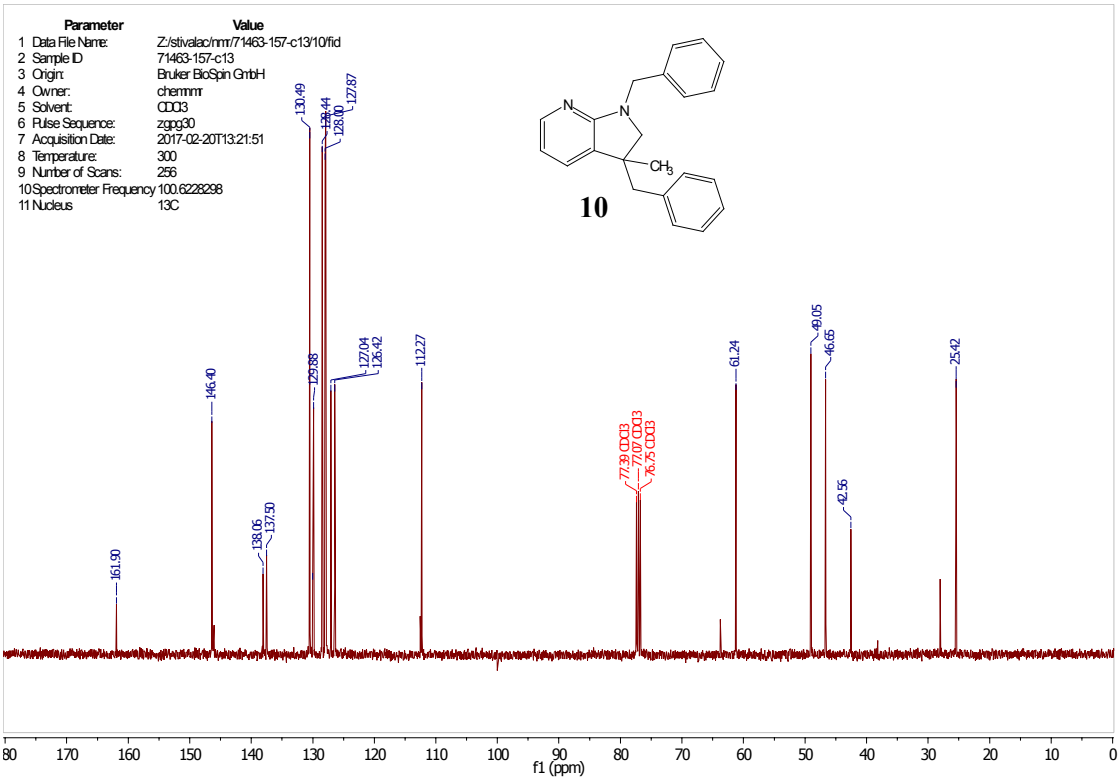
1 Data File Name: Z:/stivalac/nmr/71463-109-c13/10/fid
2 Sample ID 71463-109-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-06T12:41:40
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
7
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-116-1H-2/10/fid
2 Sample ID 71463-116-1H-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T13:36:25
8 Temperature: 300
9 Number of Scans: 32
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
8
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-116-c13/10/fid
2 Sample ID 71463-116-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-14T15:06:49
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
8
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-157-1H-2/10/fid
2 Sample ID 71463-157-1H-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-20T13:03:20
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
10
f1 (ppm)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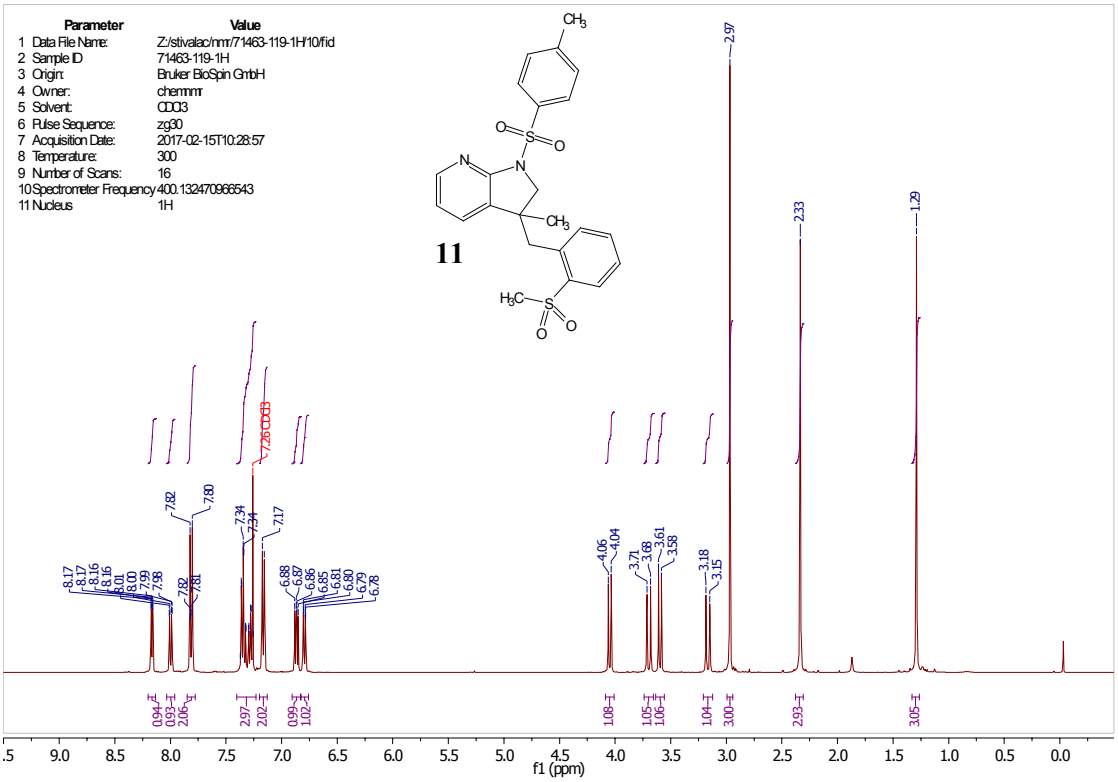
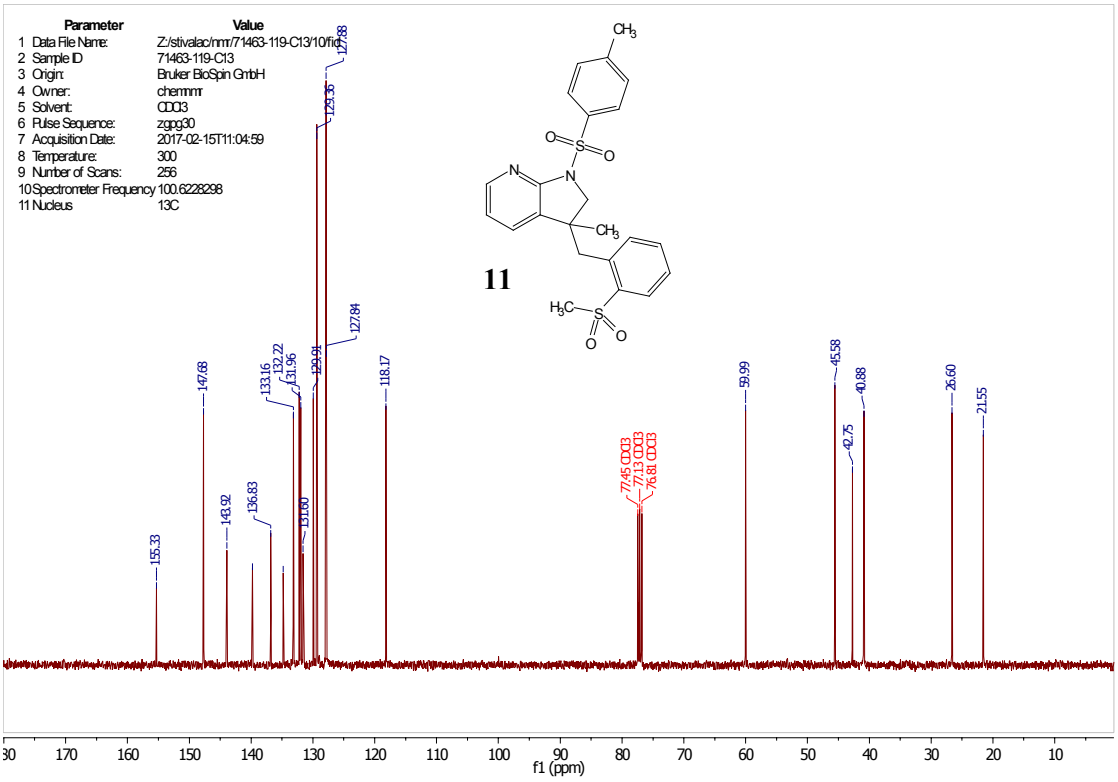
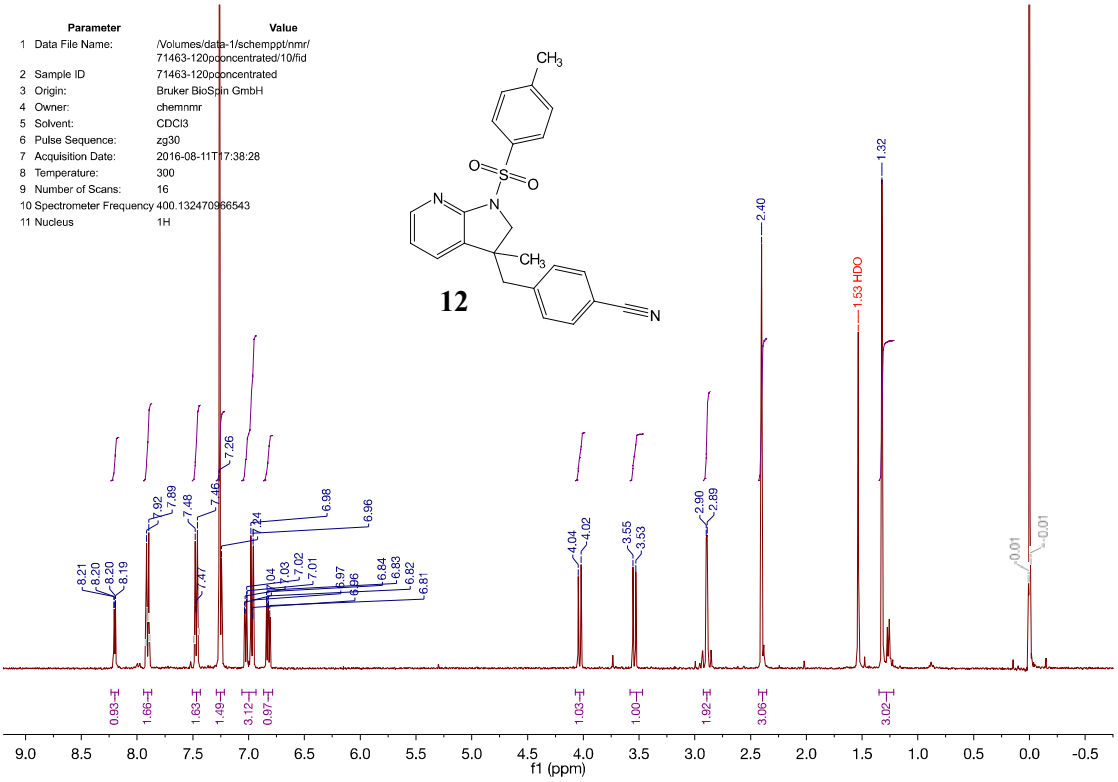
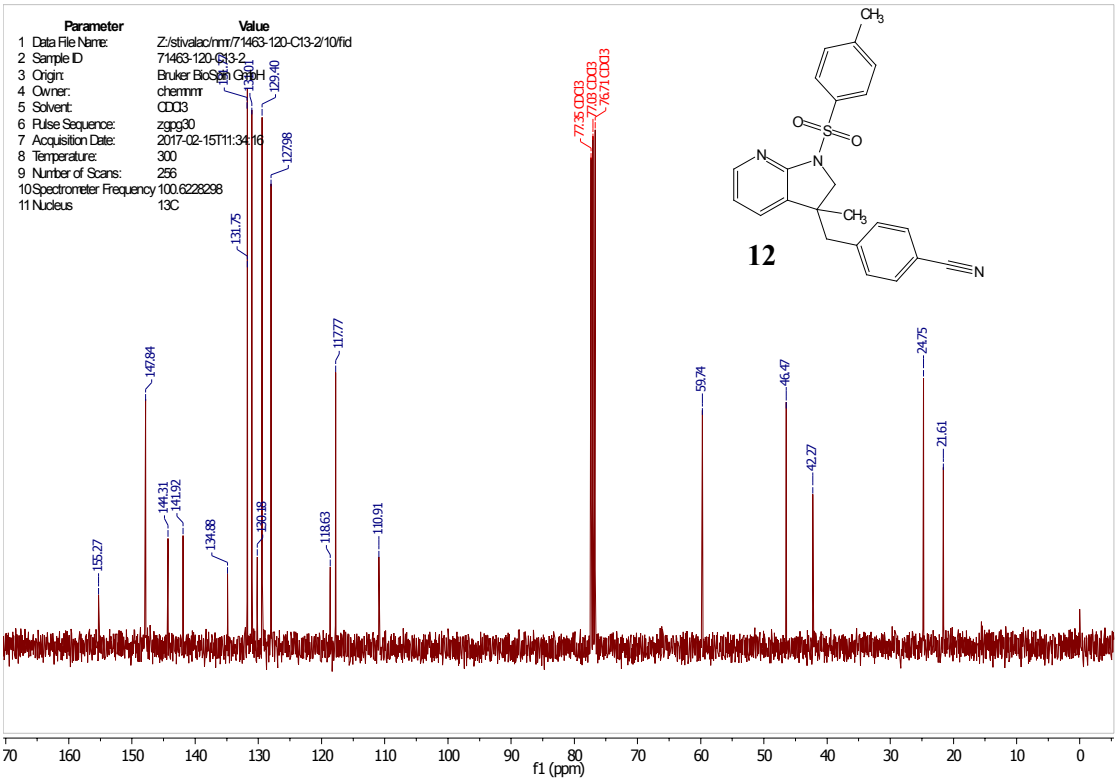
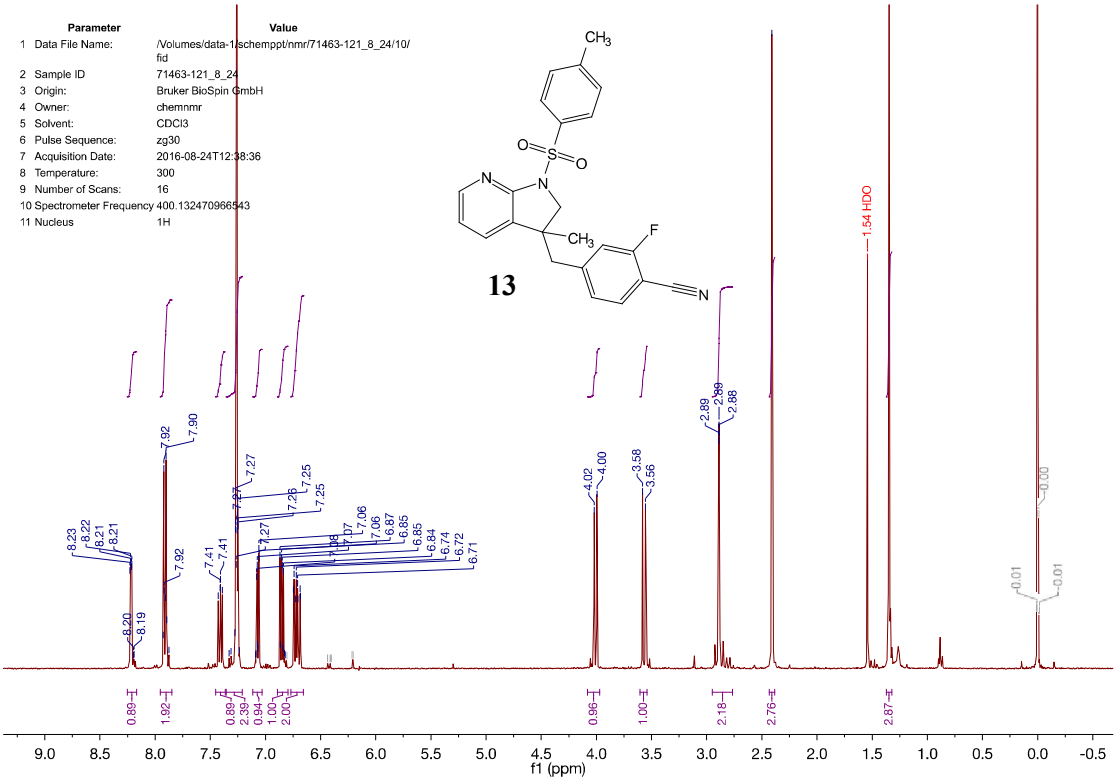
1 Data File Name: Z:/stivalac/nmr/71463-157-c13/10/fid
2 Sample ID 71463-157-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-20T13:21:51
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
10
f1 (ppm)

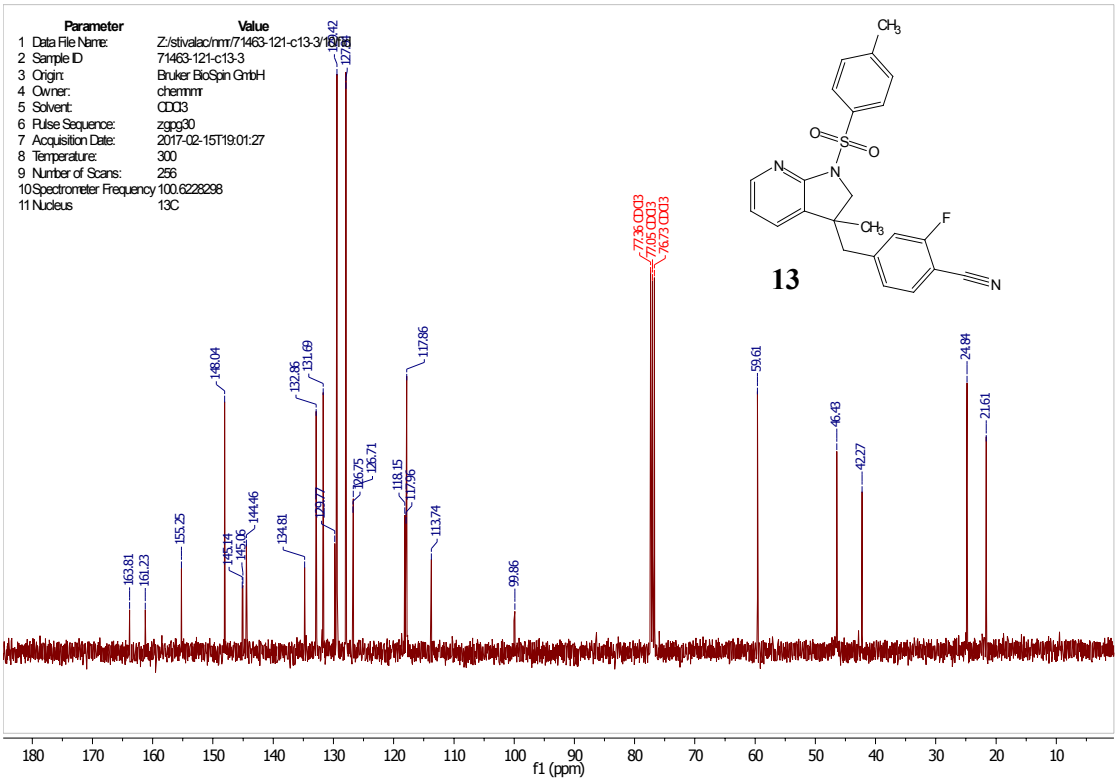

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-119-1H/10/fid
2 Sample ID 71463-119-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-15T10:28:57
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
11
f1 (ppm)

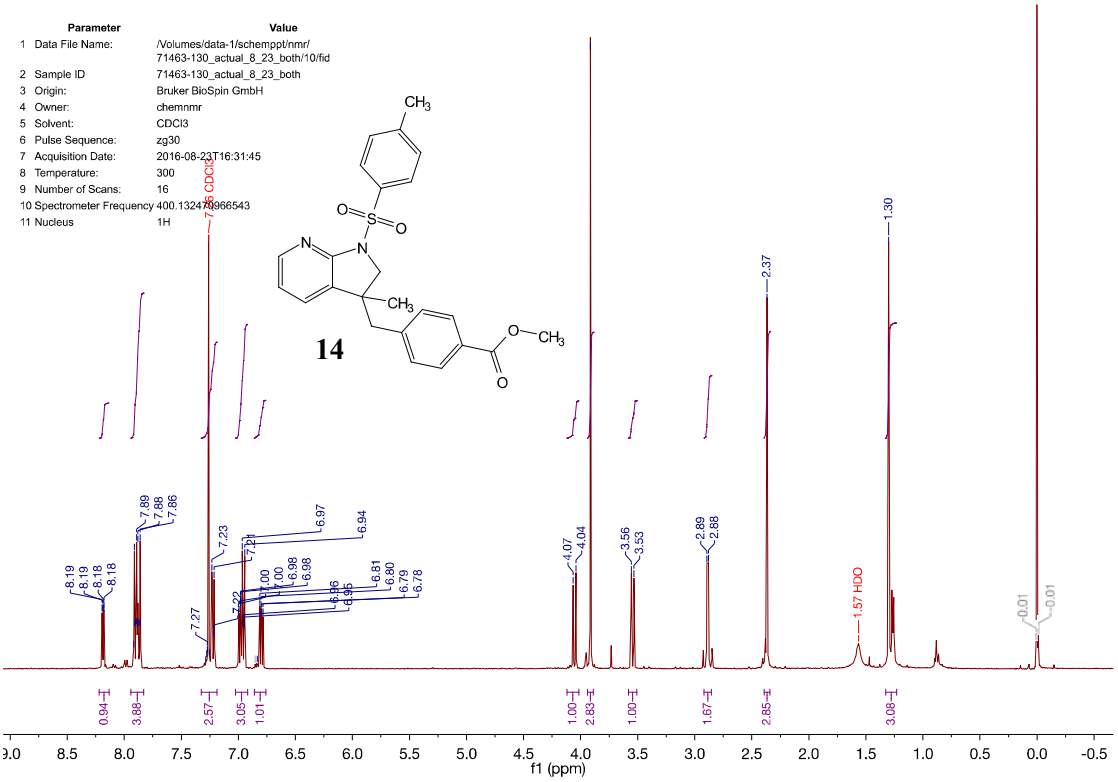

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-119-C13/10/fid
2 Sample ID 71463-119-C13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-15T11:04:59
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
11
f1 (ppm)

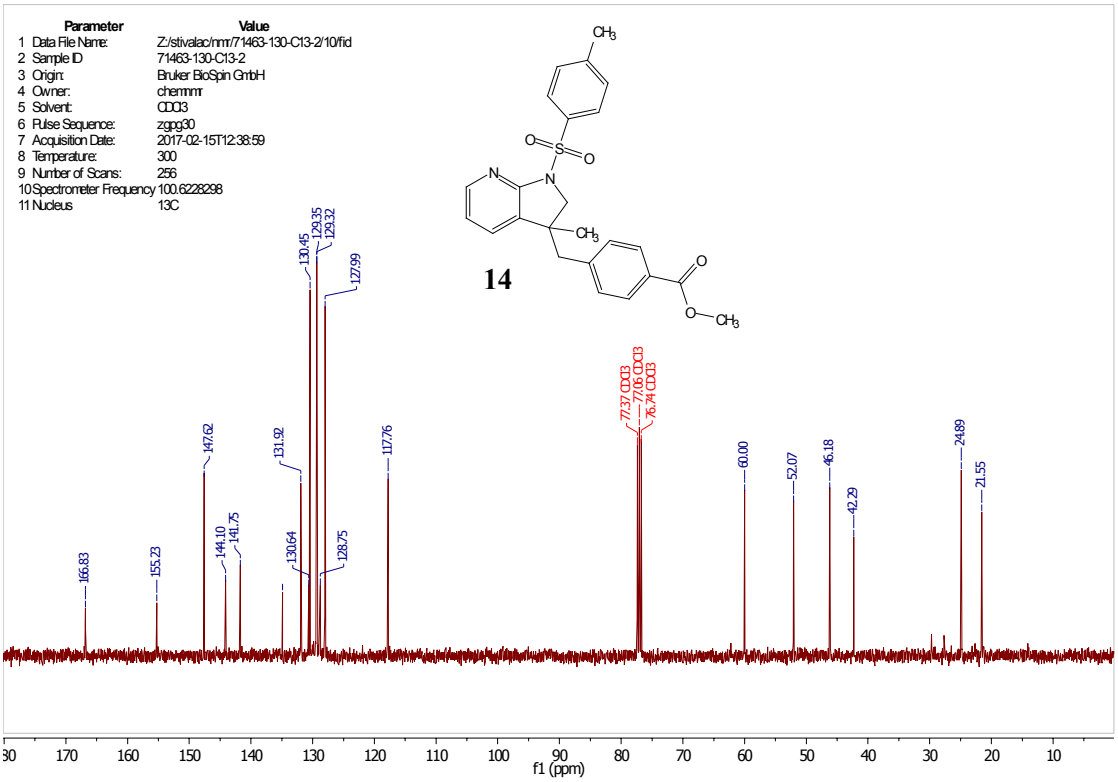

Parameter Value
1 Data File Name: /Volumes/data-1/schempt/nmr/71463-120pconcentrated/10/fid
2 Sample ID 71463-120pconcentrated
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-11T17:38:28
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.1324709666543
11 Nucleus 1H
12
1.53 HDO
f1 (ppm)

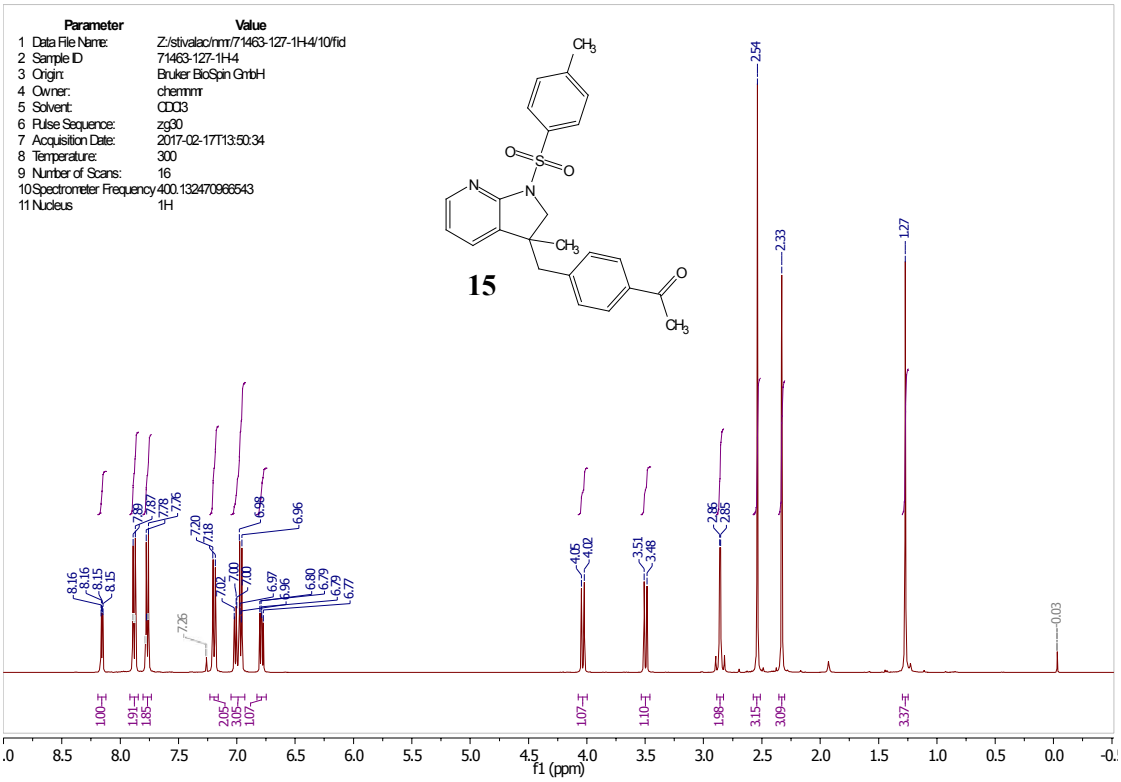

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-120-C13-2/10/fid
2 Sample ID 71463-120-C13-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-15T11:34:16
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
12
77.35 CDCl3
77.08 CDCl3
76.71 CDCl3
f1 (ppm)

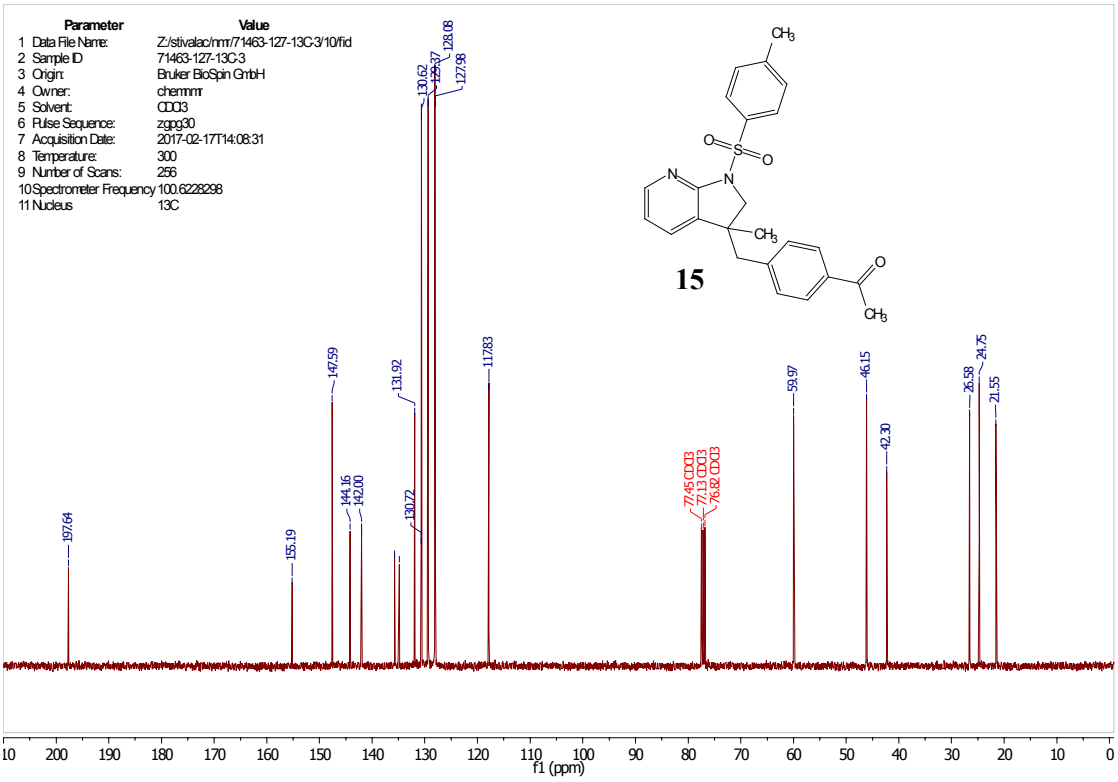

Parameter Value
1 Data File Name: /Volumes/data-1/schempt/nmr/71463-121_8_24/10/fid
2 Sample ID 71463-121_8_24
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-24T12:38:36
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
13
f1 (ppm)

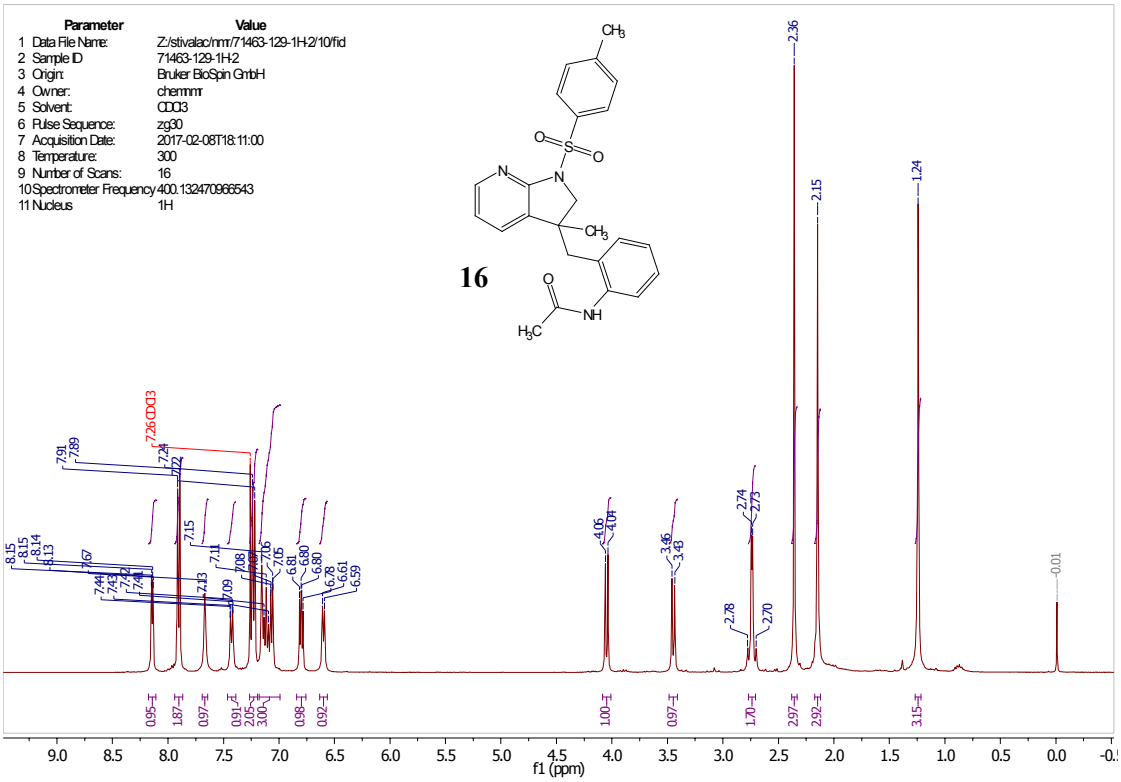

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-121-c13-3/10/fid
2 Sample ID 71463-121-c13-3
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-15T19:01:27
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
13
f1 (ppm)

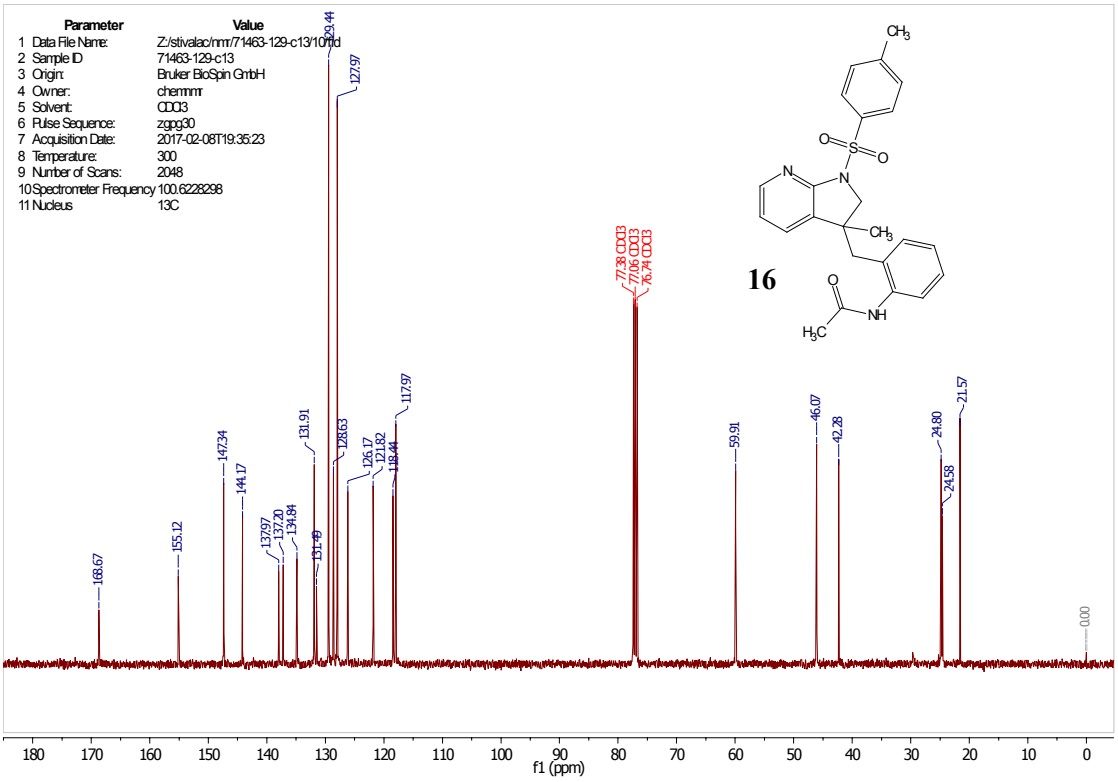

Parameter Value
1 Data File Name: /Volumes/data-1/schempt/nmr/71463-130_actual_8_23_both/10/fid
2 Sample ID 71463-130_actual_8_23_both
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-23T16:31:45
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.13247966543
11 Nucleus 1H
14
f1 (ppm)

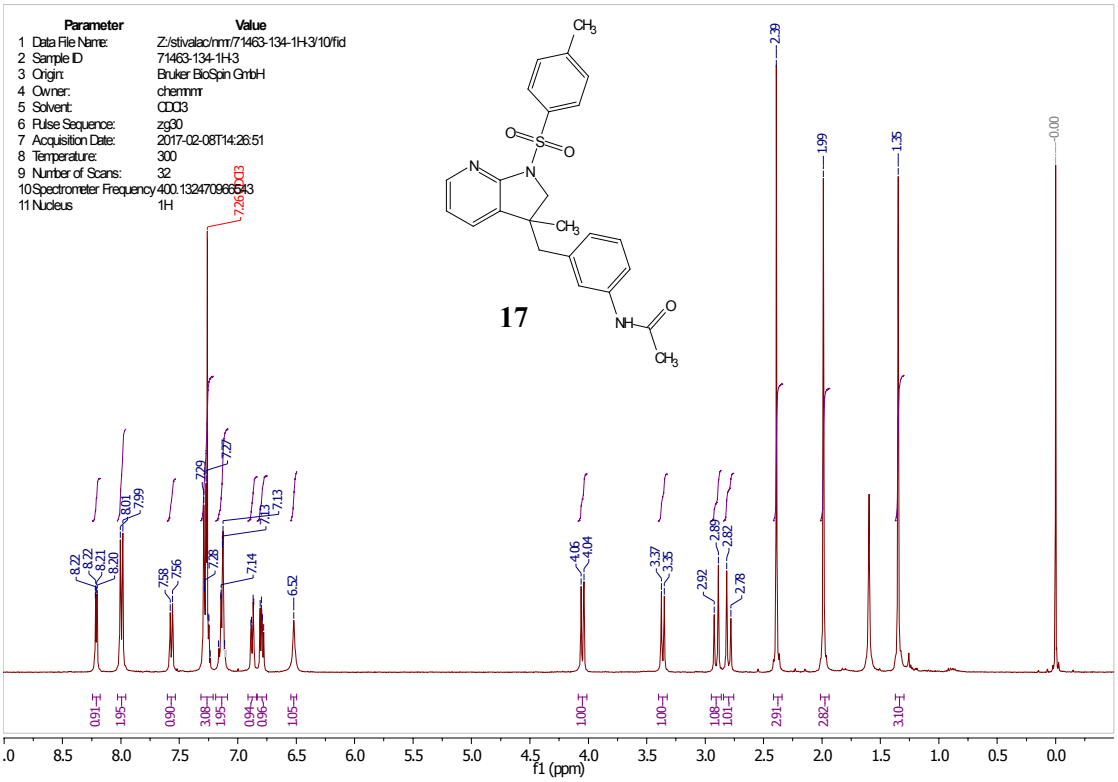

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-130-C13-2/10/fid
2 Sample ID 71463-130-C13-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-15T12:38:59
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
14
f1 (ppm)

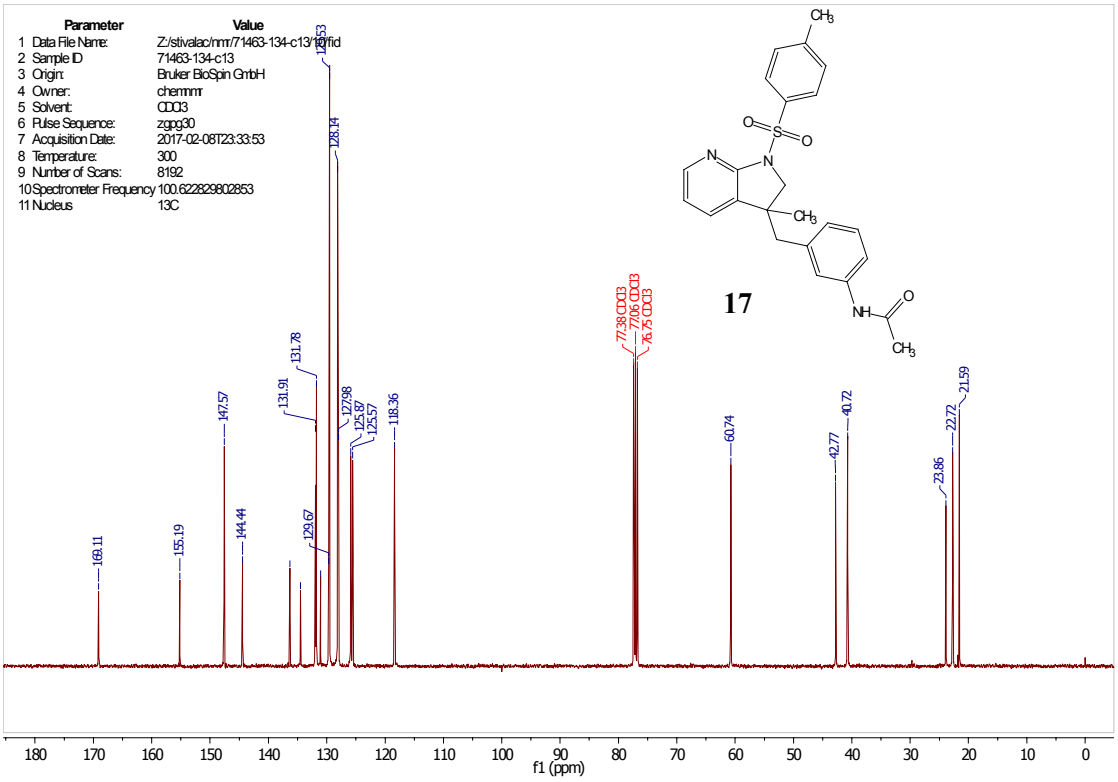

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-127-1H-4/10/fid
2 Sample ID 71463-127-1H-4
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-17T13:50:34
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
15
f1 (ppm)

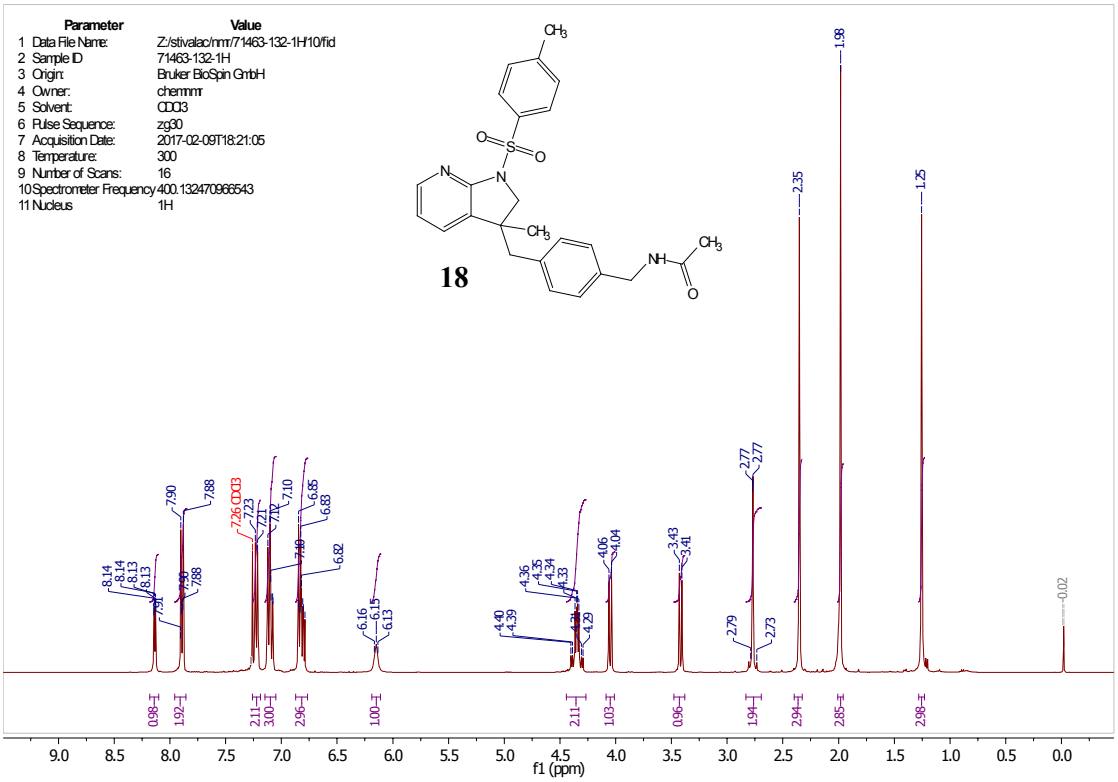

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-127-13C-3/10/fid
2 Sample ID 71463-127-13C-3
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-17T14:08:31
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
15
f1 (ppm)

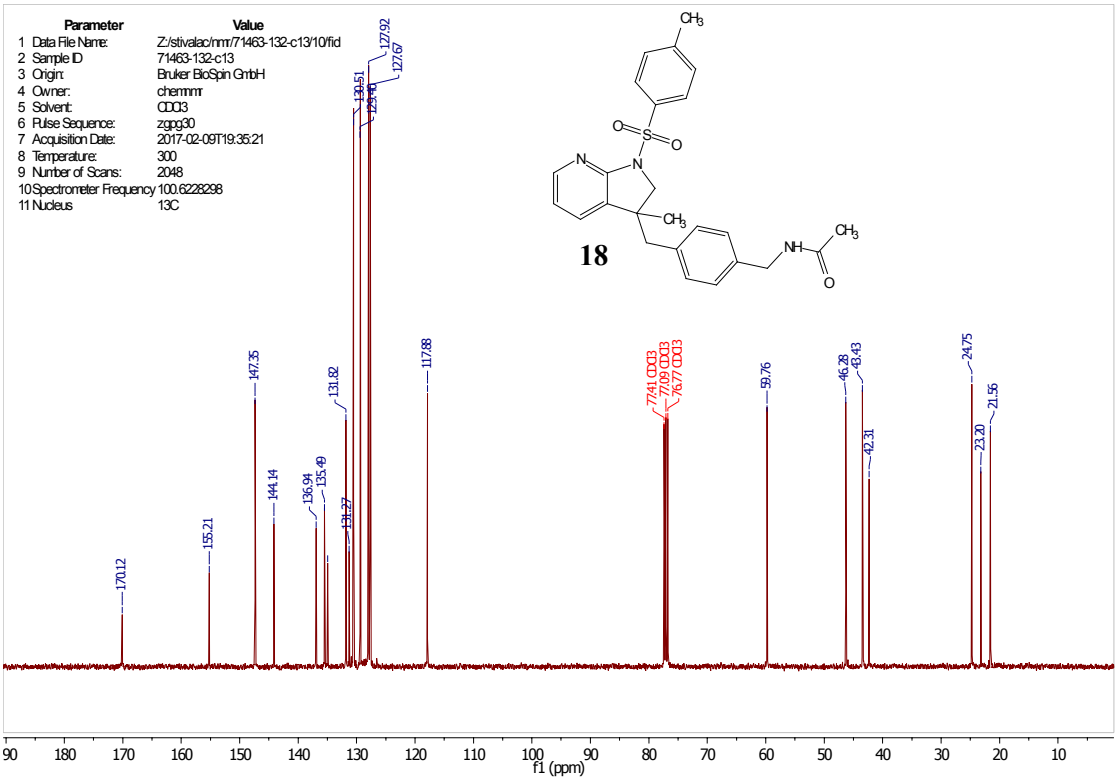

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-129-1H-2/10/fid
2 Sample ID 71463-129-1H-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-08T18:11:00
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
16
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-129-c13/10/fid
2 Sample ID 71463-129-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-08T19:35:23
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
16
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-134-1H-3/10/fid
2 Sample ID 71463-134-1H-3
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-08T14:26:51
8 Temperature: 300
9 Number of Scans: 32
10 Spectrometer Frequency 400.1324709666543
11 Nucleus 1H
17
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-134-c13/10/fid
2 Sample ID 71463-134-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-08T23:33:53
8 Temperature: 300
9 Number of Scans: 8192
10 Spectrometer Frequency 100.622829802853
11 Nucleus 13C
17
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-132-1H/10/fid
2 Sample ID 71463-132-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-09T18:21:05
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
18
f1 (ppm)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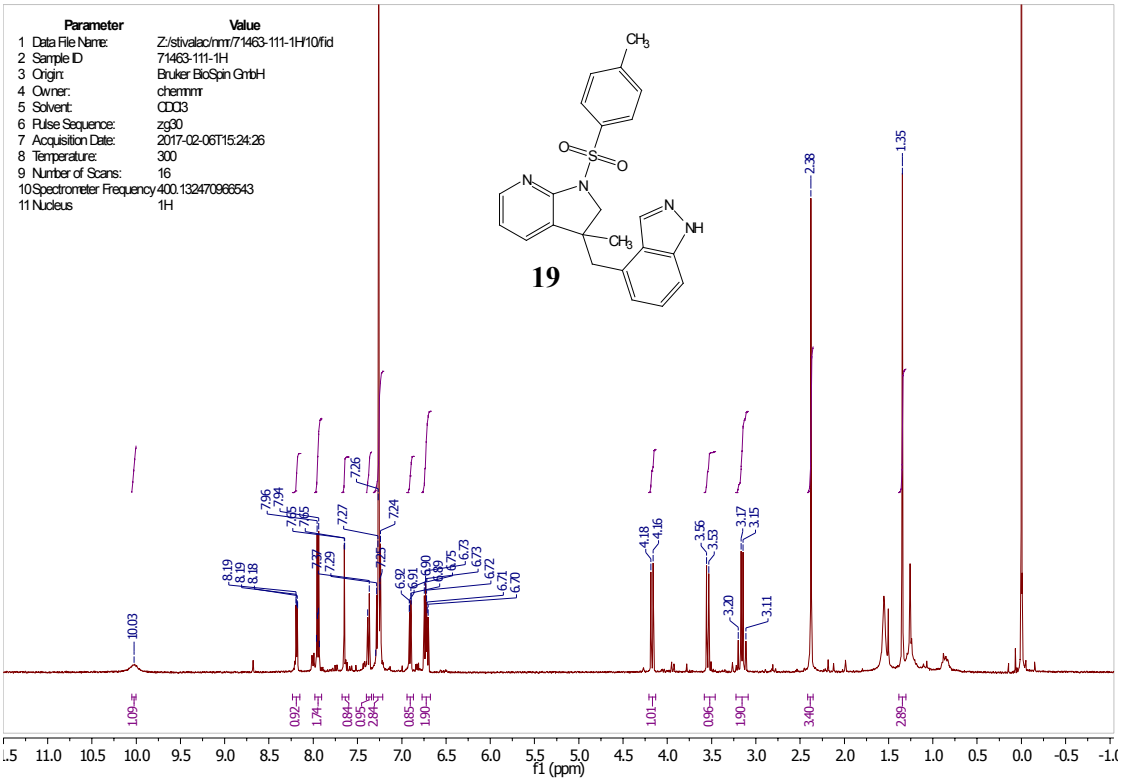
1 Data File Name: Z:/stivalac/nmr/71463-132-c13/10/fid
2 Sample ID 71463-132-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-09T19:35:21
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
18
f1 (ppm)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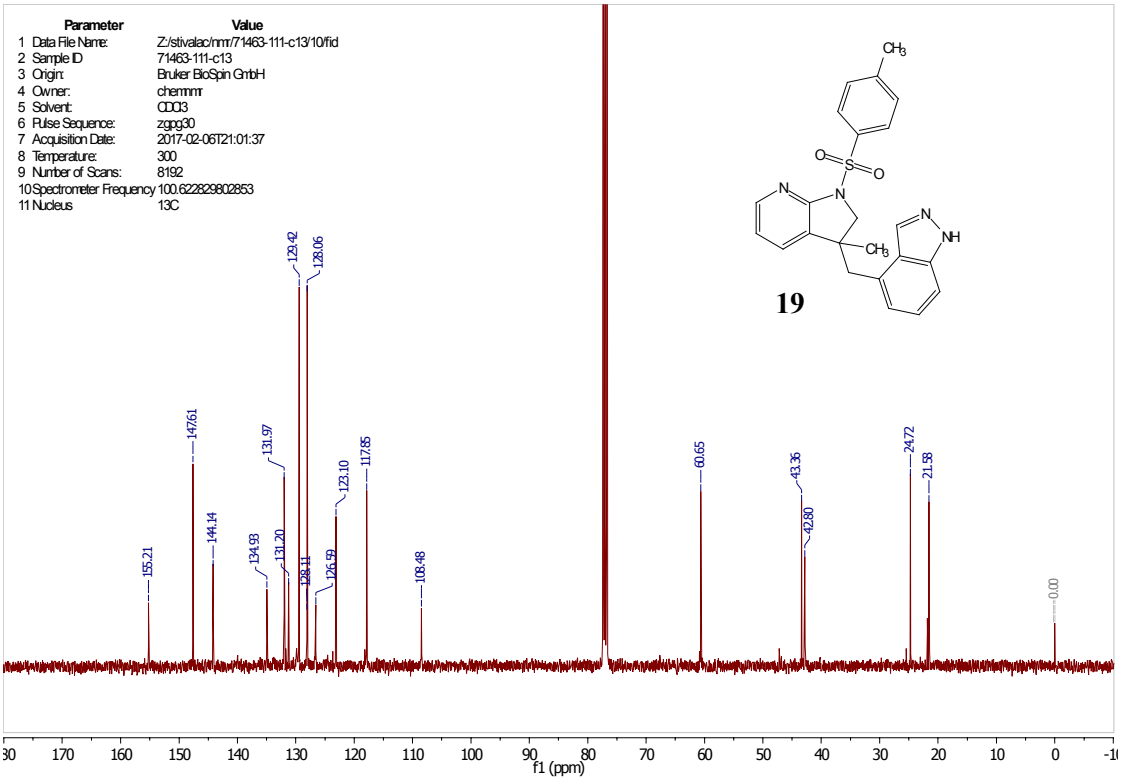
1 Data File Name: Z:/stivalac/nmr/71463-111-1H/10/fid
2 Sample ID 71463-111-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T15:24:26
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
19
f1 (ppm)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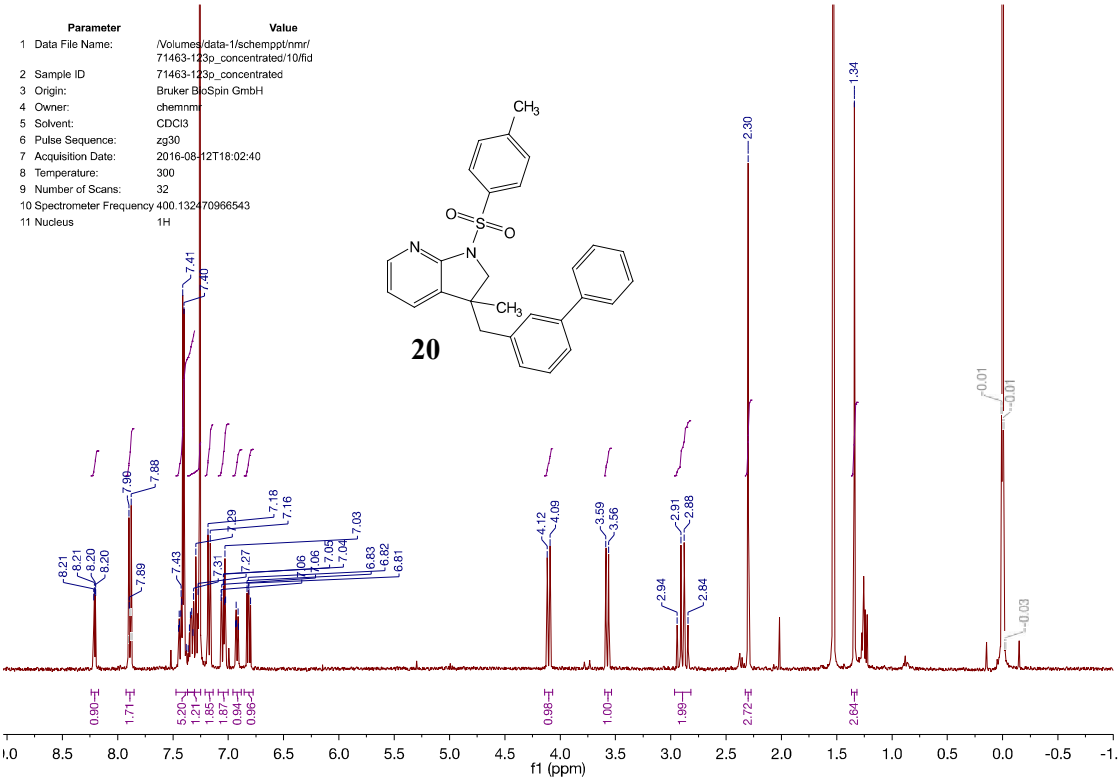
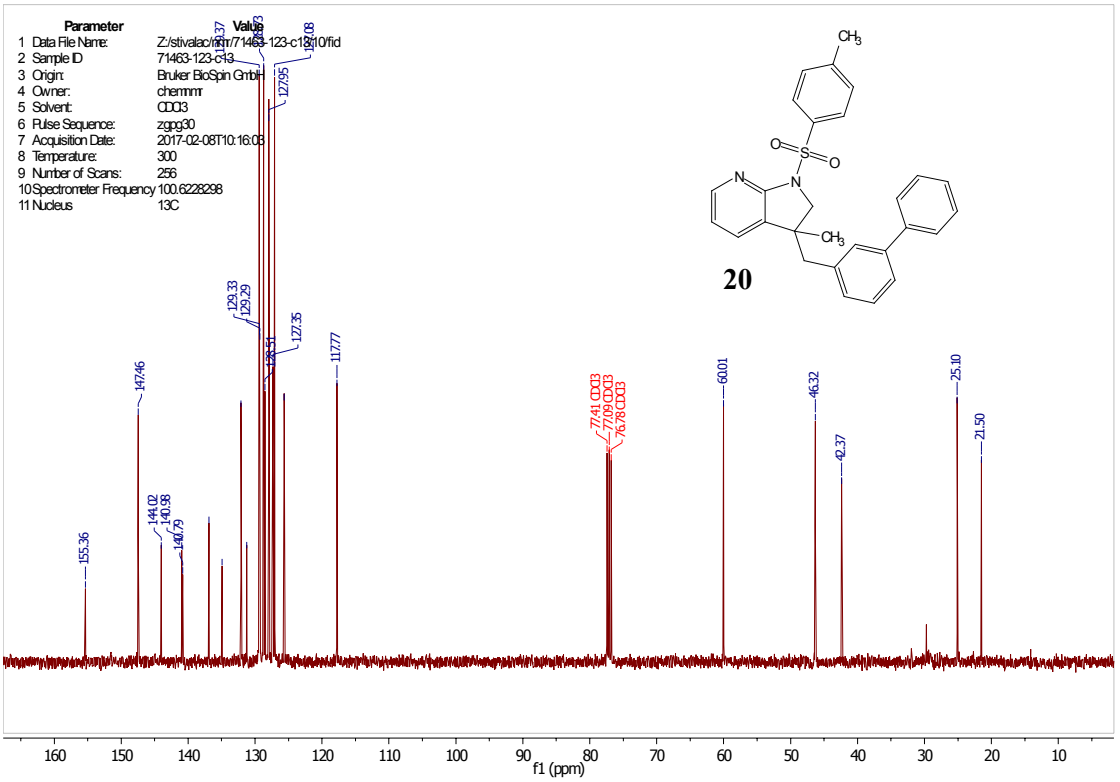
1 Data File Name: Z:/stivalac/nmr/71463-111-c13/10/fid
2 Sample ID 71463-111-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-06T21:01:37
8 Temperature: 300
9 Number of Scans: 8192
10 Spectrometer Frequency 100.622829802853
11 Nucleus 13C
19
f1 (ppm)


Parameter Value
1 Data File Name: /Volumes/data-1/schempt/nmr/71463-123p_concentrated/10/fid
2 Sample ID 71463-123p_concentrated
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-12T18:02:40
8 Temperature: 300
9 Number of Scans: 32
10 Spectrometer Frequency 400.1324709665 43
11 Nucleus 1H
20
f1 (ppm)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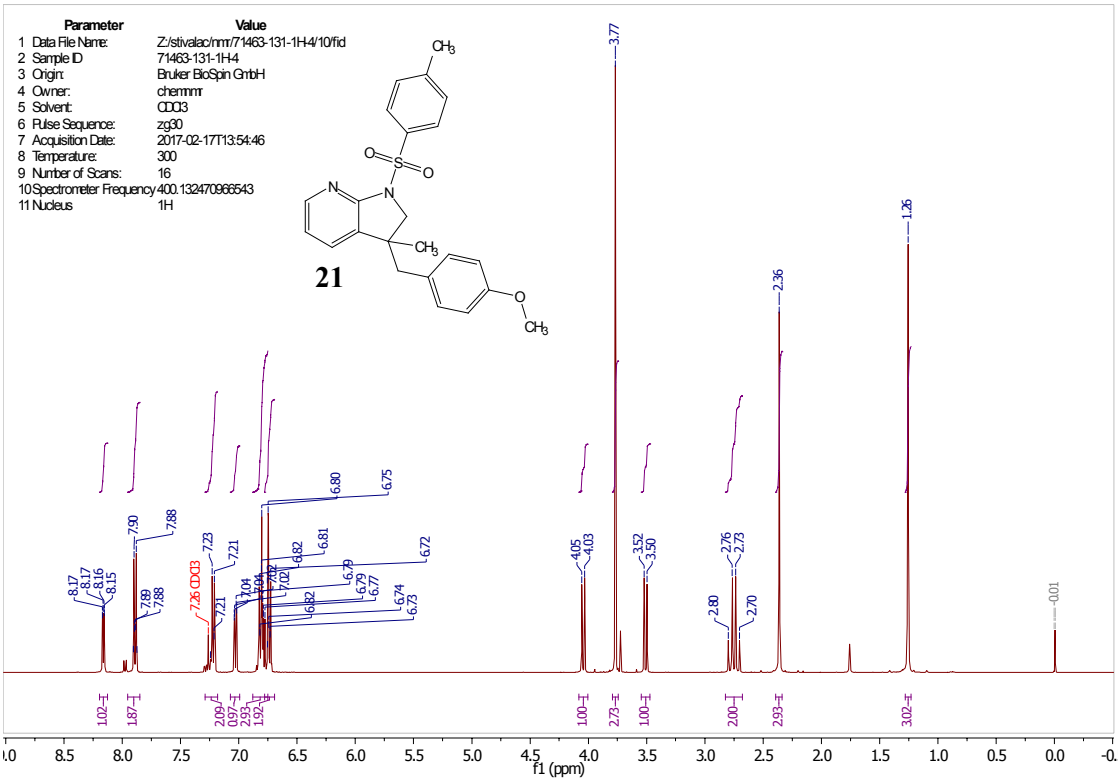
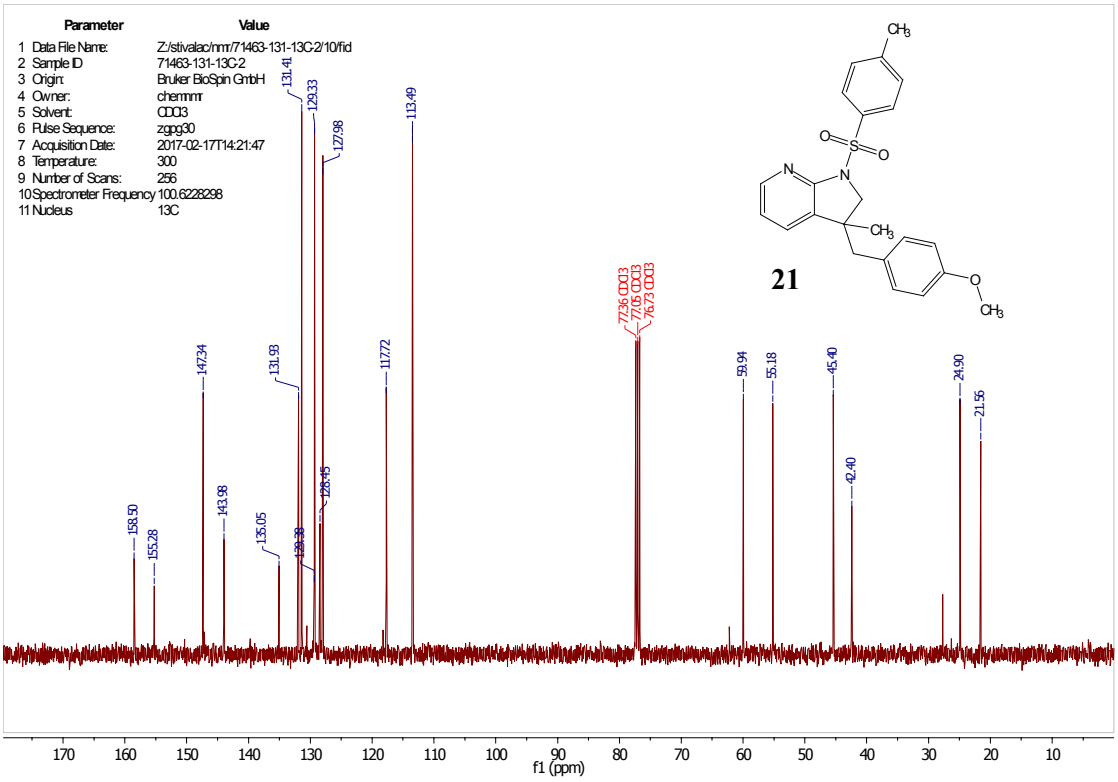
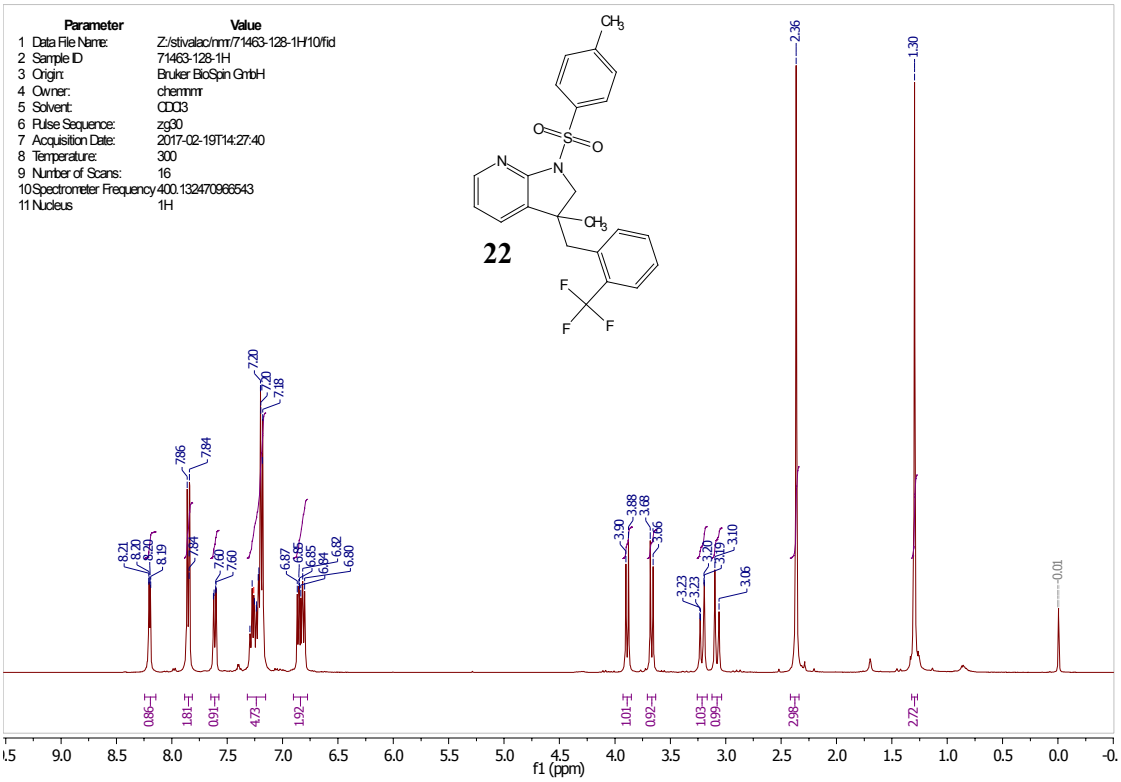
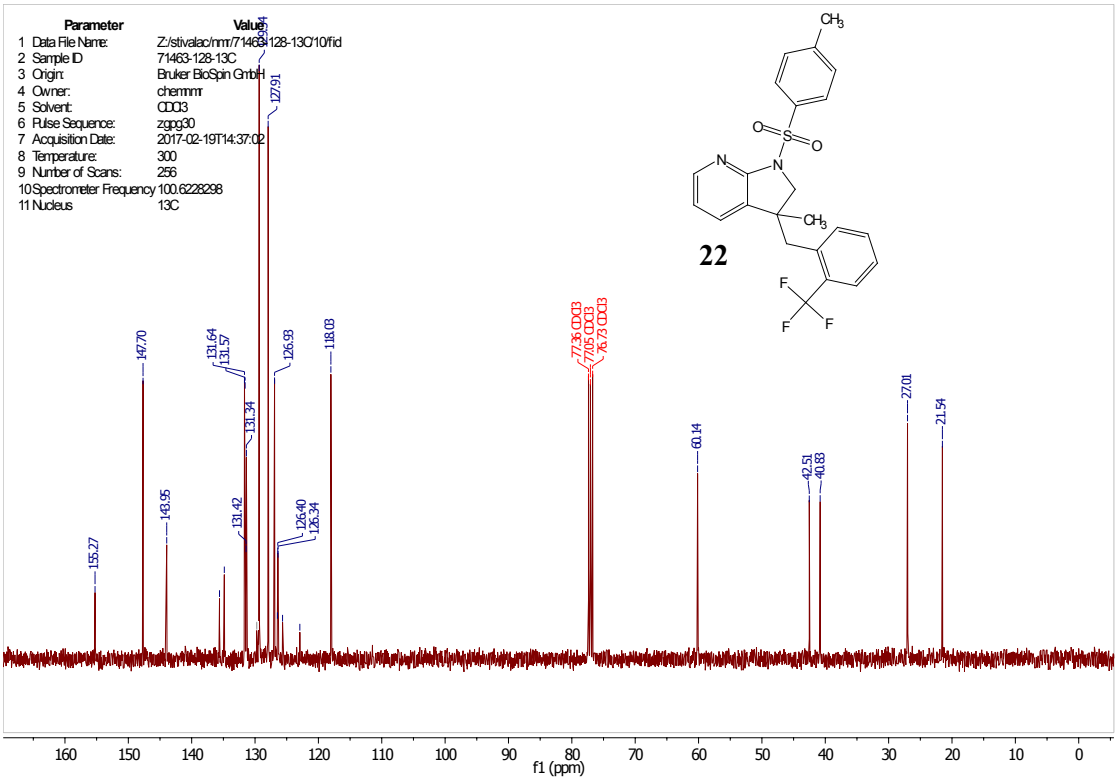
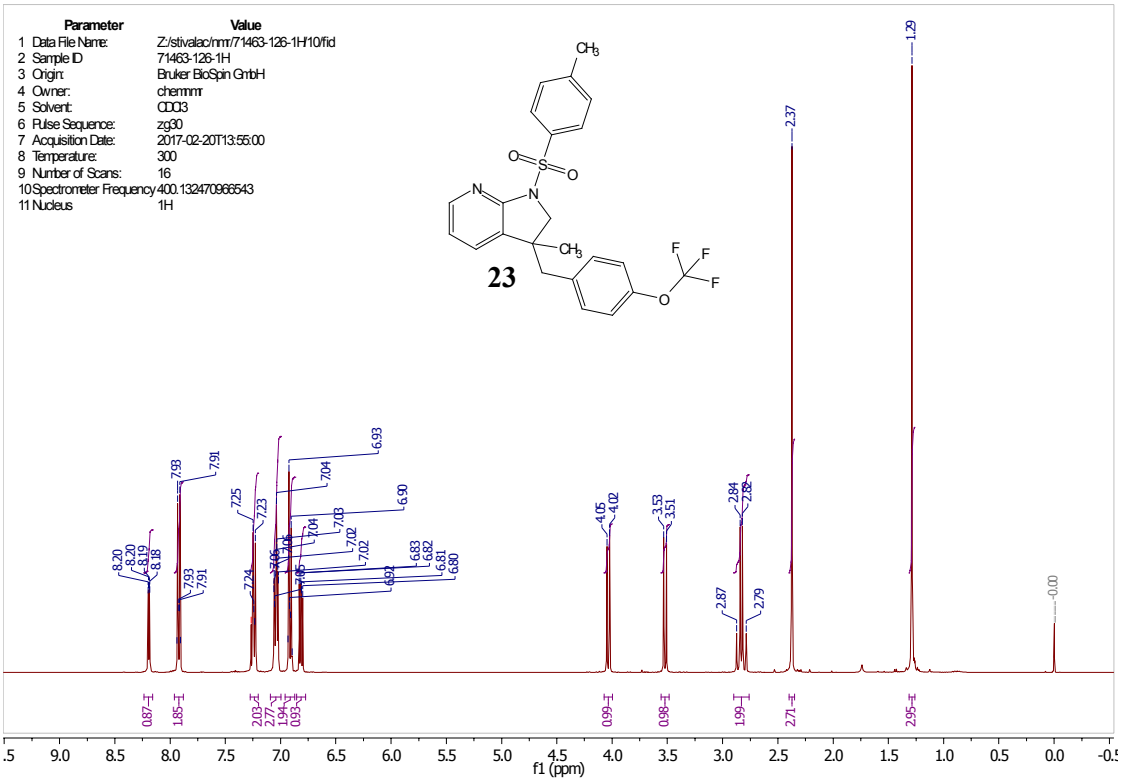
1 Data File Name: Z:/stivalac/nmr/71463-123-c13/10/fid
2 Sample ID 71463-123-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-08T10:16:03
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
20
f1 (ppm)

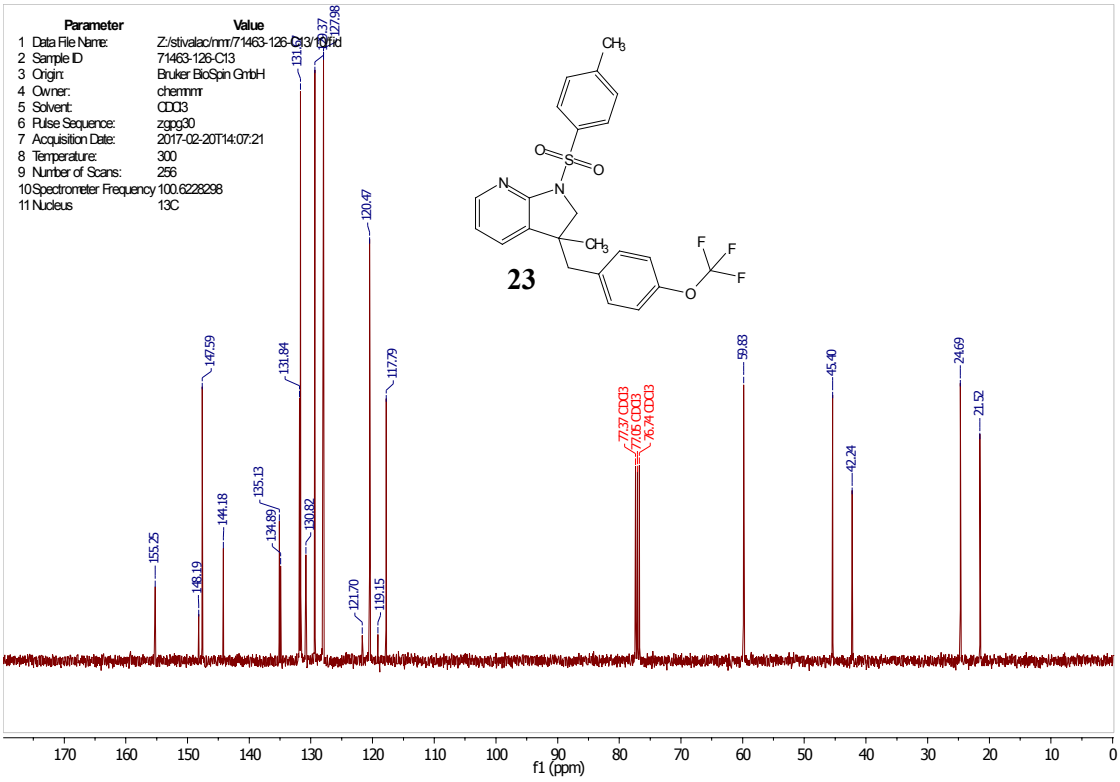

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-131-1H-4/10/fid
2 Sample ID 71463-131-1H-4
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-17T13:54:46
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
21
f1 (ppm)

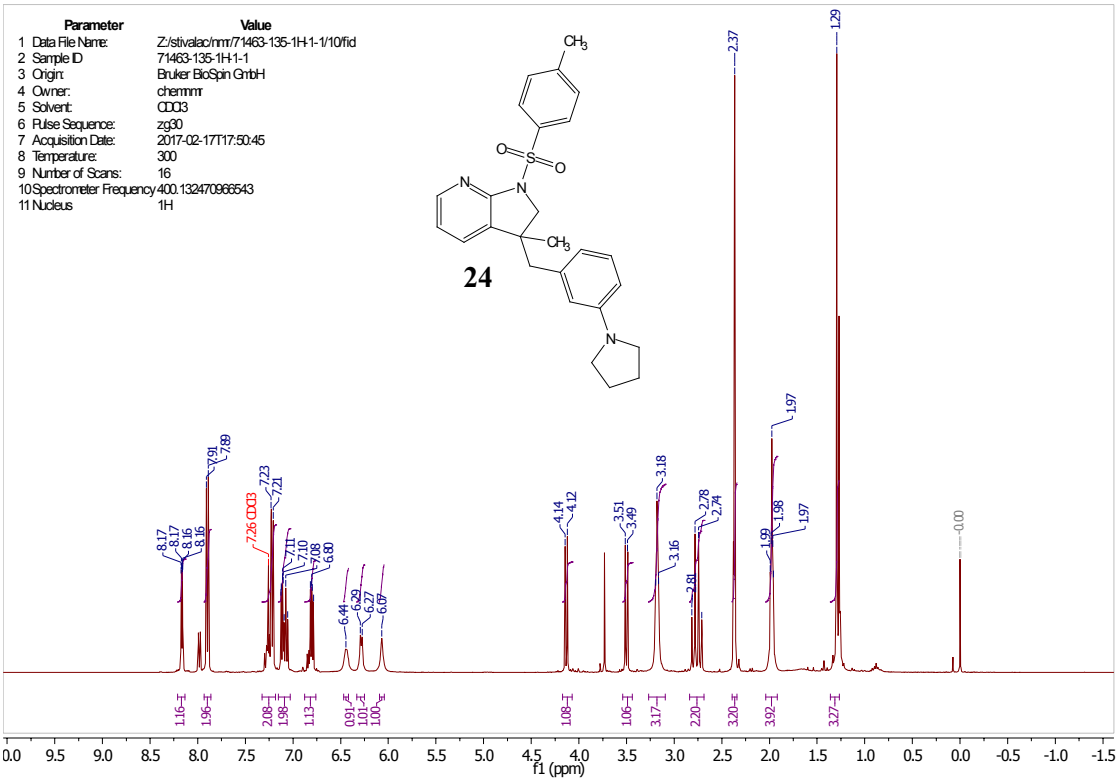

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-131-13C-2/10/fid
2 Sample ID 71463-131-13C-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-17T14:21:47
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
21
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-128-1H/10/fid
2 Sample ID 71463-128-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-19T14:27:40
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
22
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-128-13C/10/fid
2 Sample ID 71463-128-13C
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-19T14:37:02
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
22
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-126-1H/10/fid
2 Sample ID 71463-126-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-20T13:55:00
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
23
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-126-C13/10/fid
2 Sample ID 71463-126-C13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-20T14:07:21
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
23
f1 (ppm)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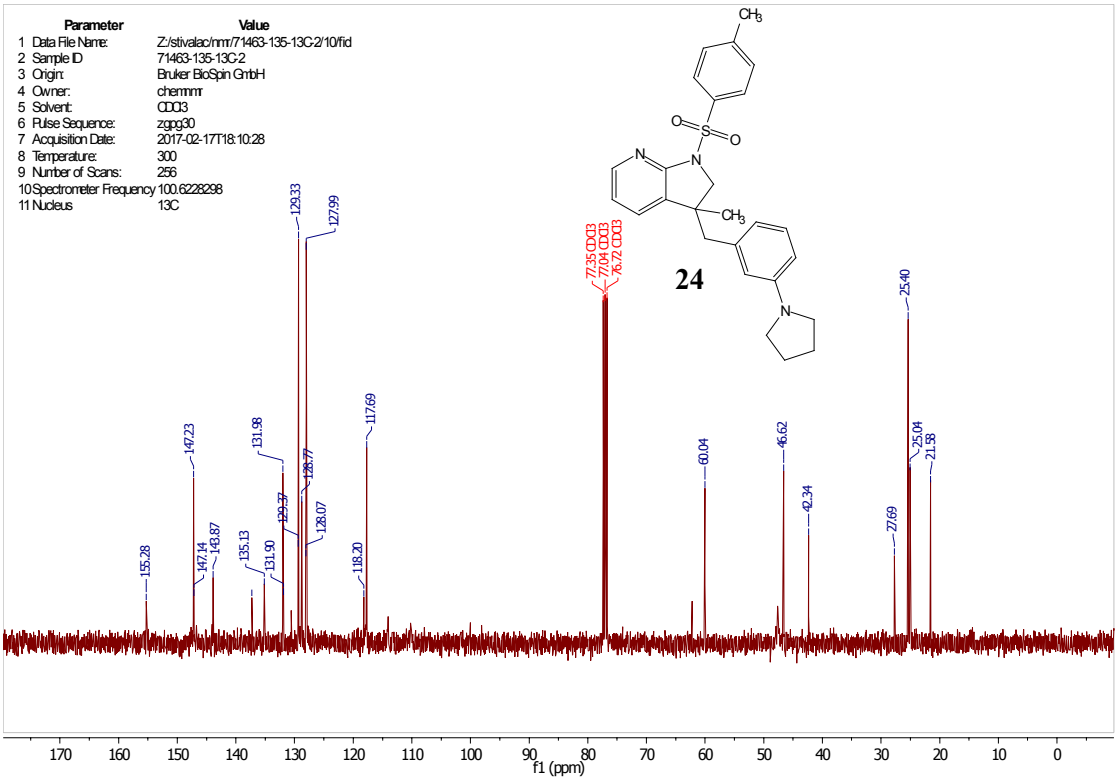
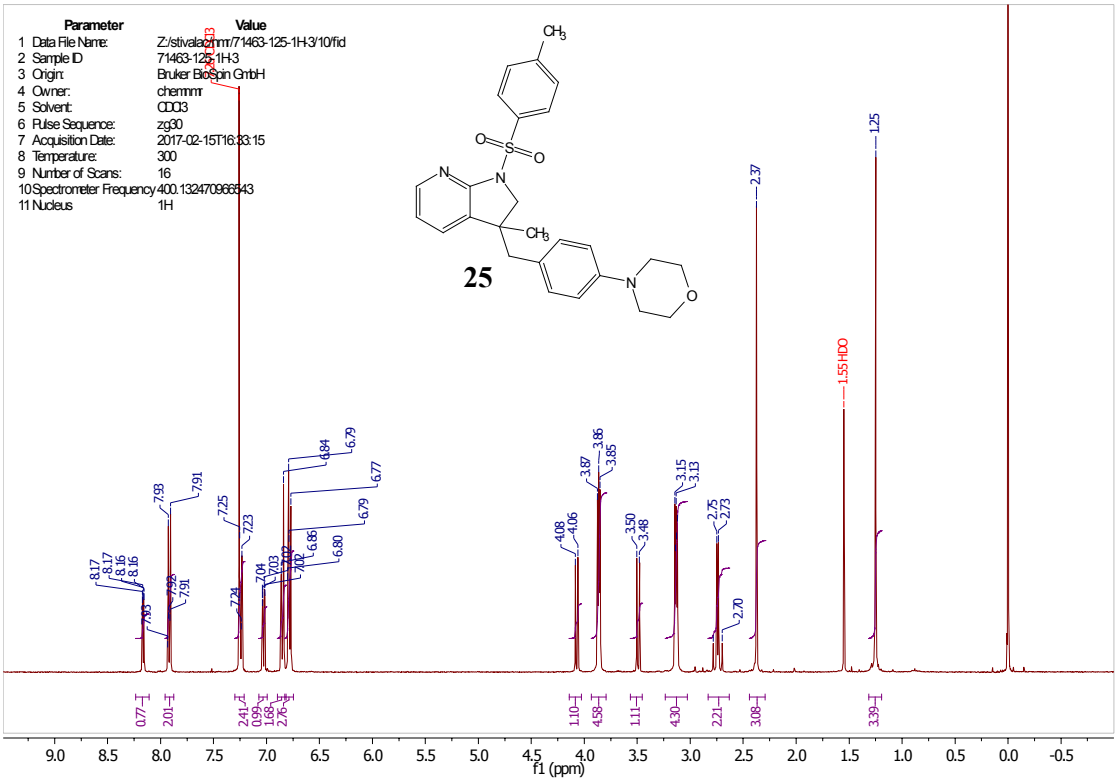
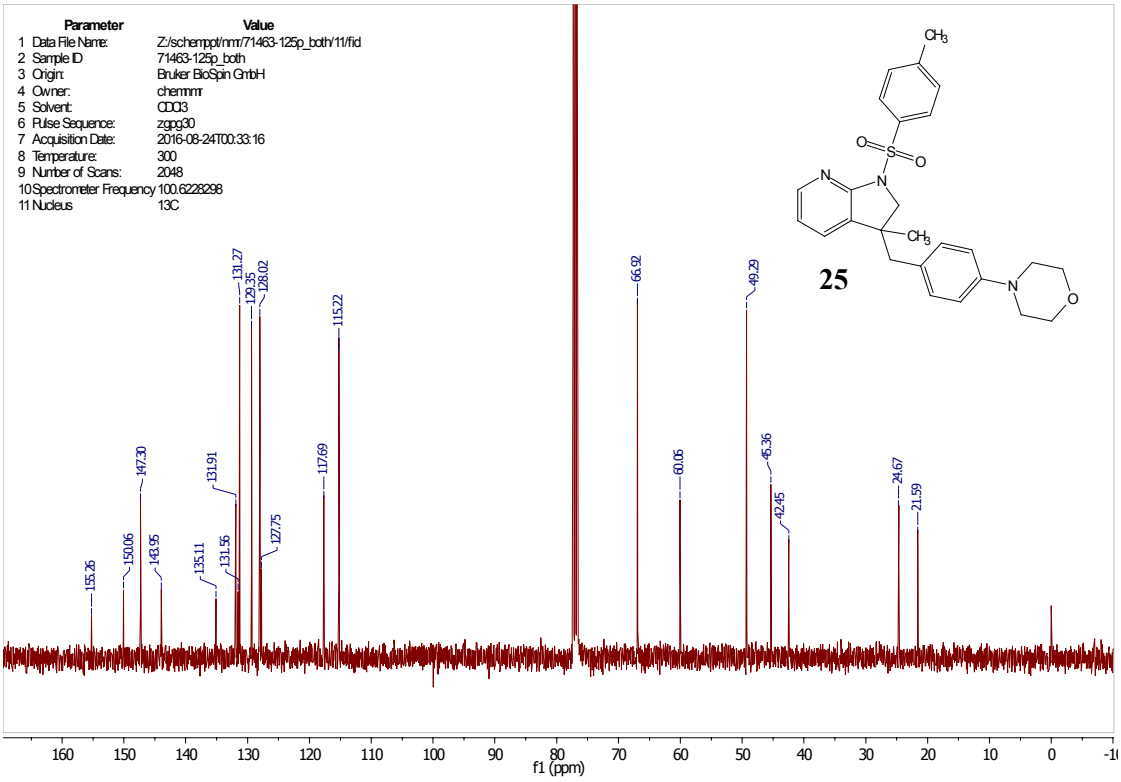
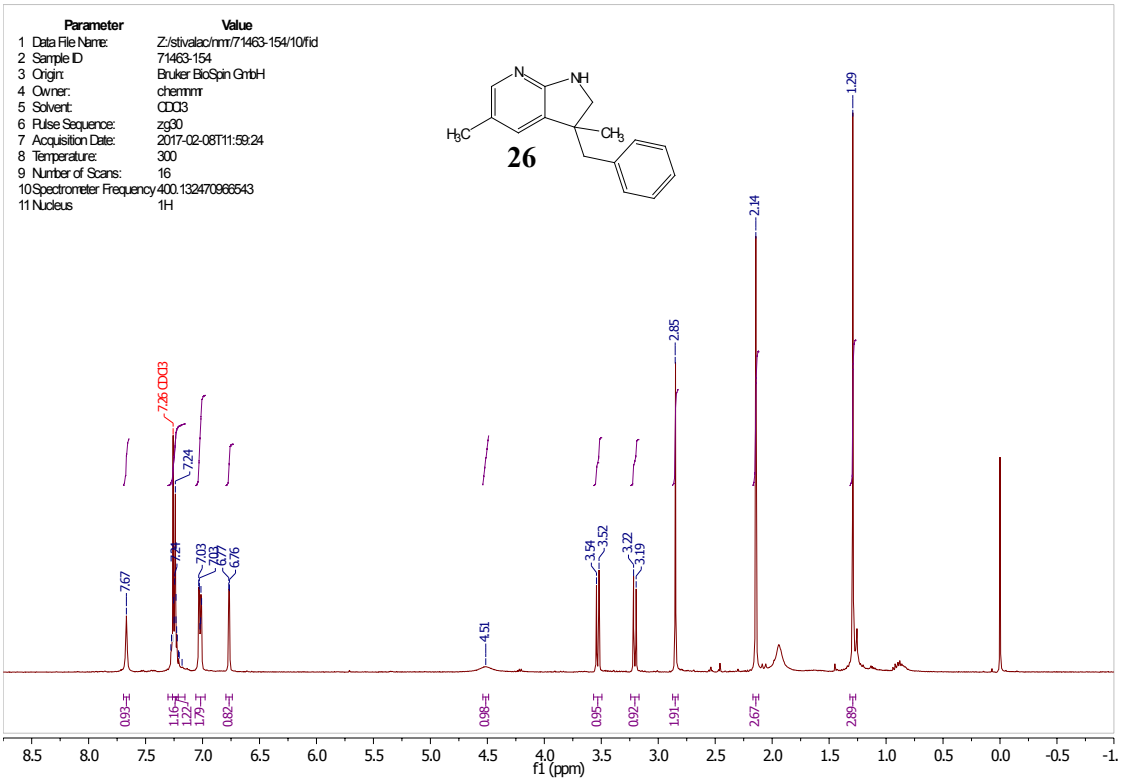
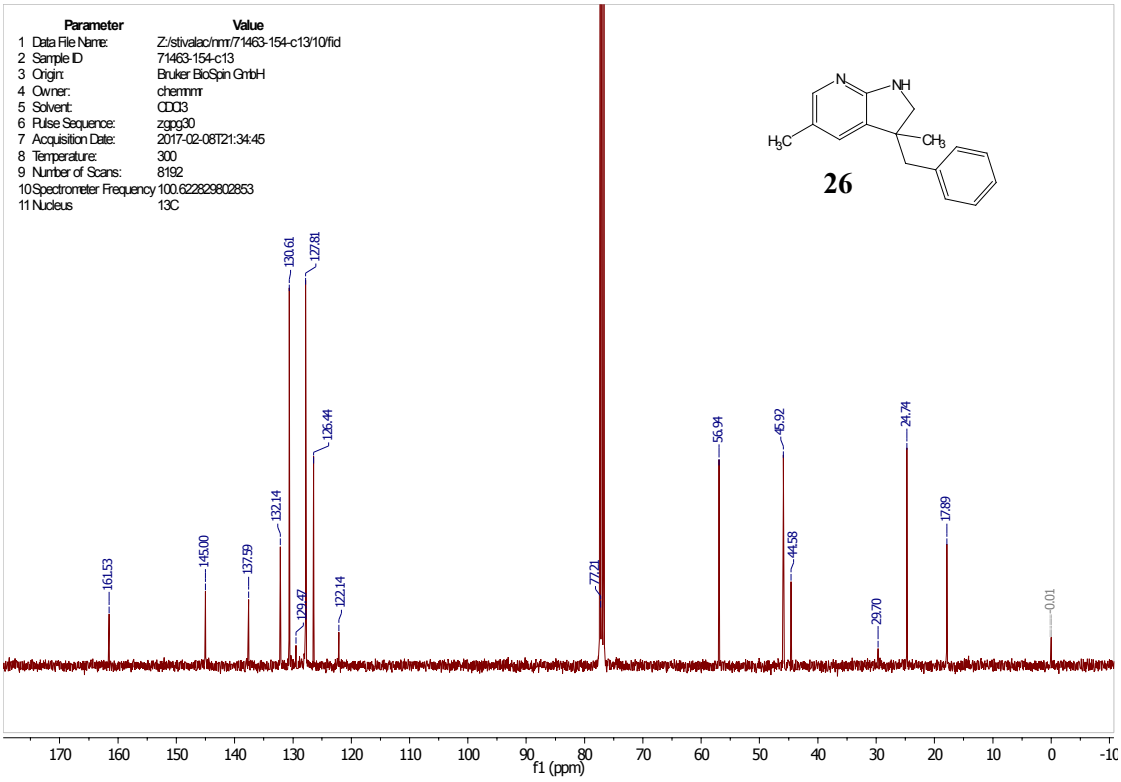
1 Data File Name: Z:/stivalac/nmr/71463-135-1H-1-1/10/fid
2 Sample ID 71463-135-1H-1-1
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-17T17:50:45
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
24
f1 (ppm)

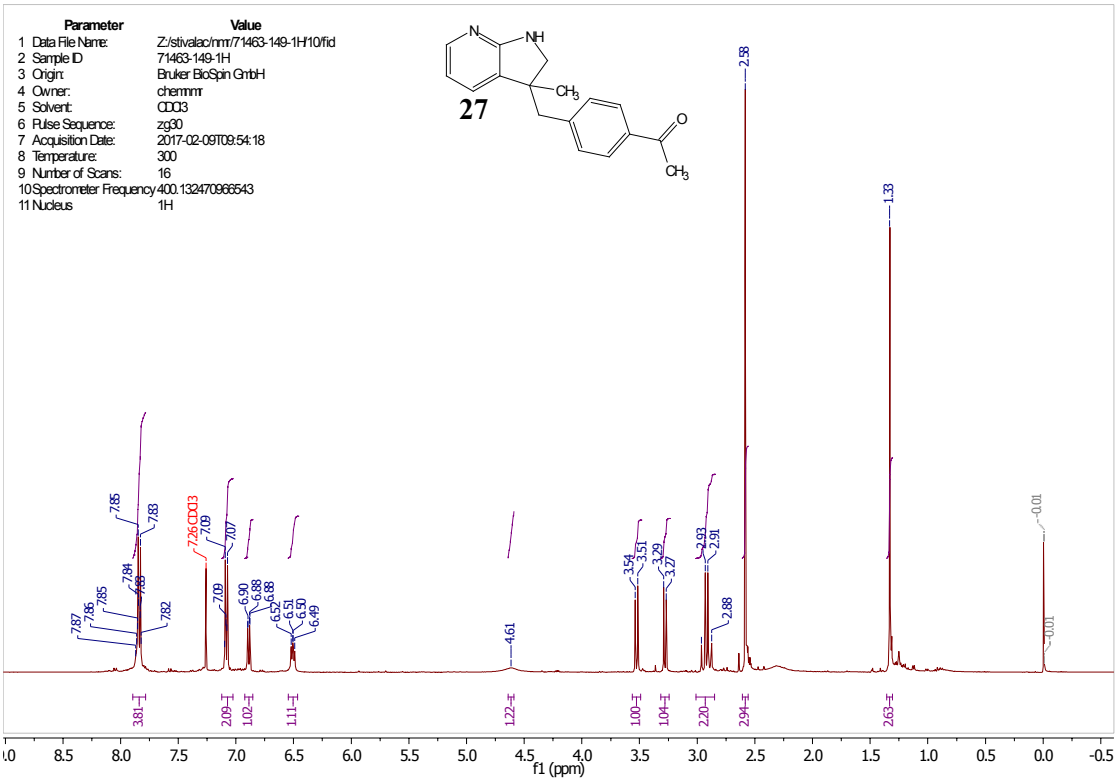

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-135-13C-2/10/fid
2 Sample ID 71463-135-13C-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-17T18:10:28
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
24
f1 (ppm)

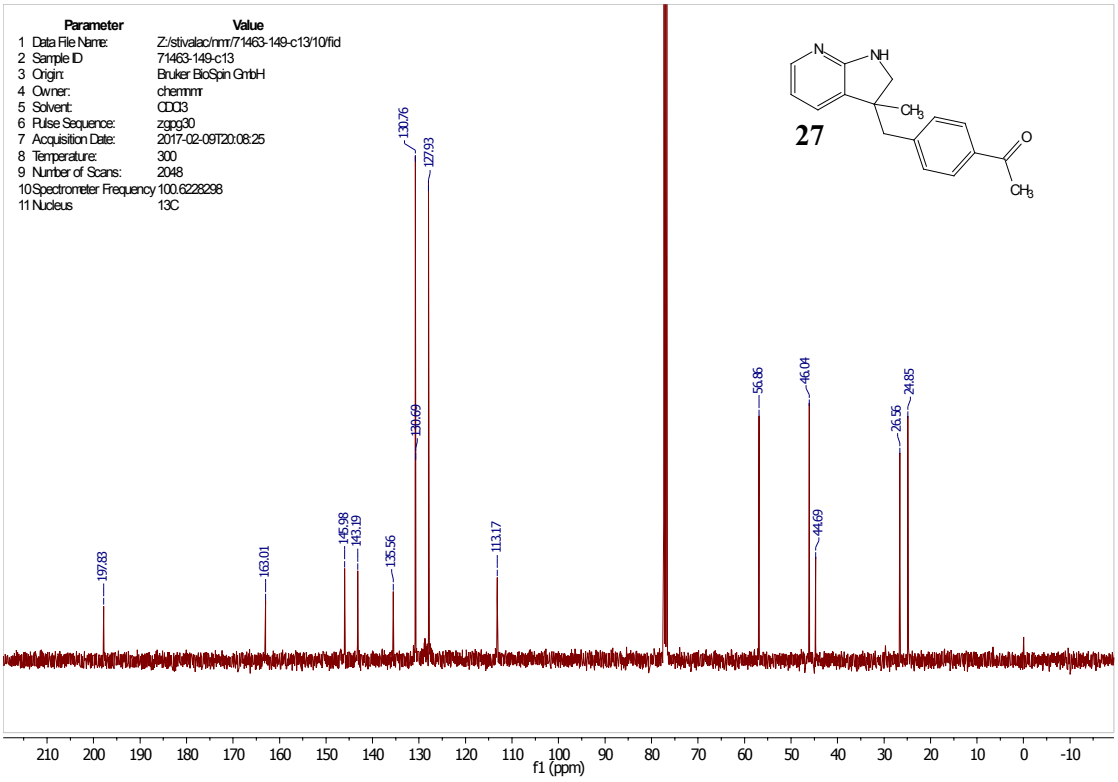

Parameter Value
1 Data File Name: Z:/stivala2/nmr/71463-125-1H-3/10/fid
2 Sample ID 71463-125-1H-3
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-15T16:33:15
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
25
f1 (ppm)

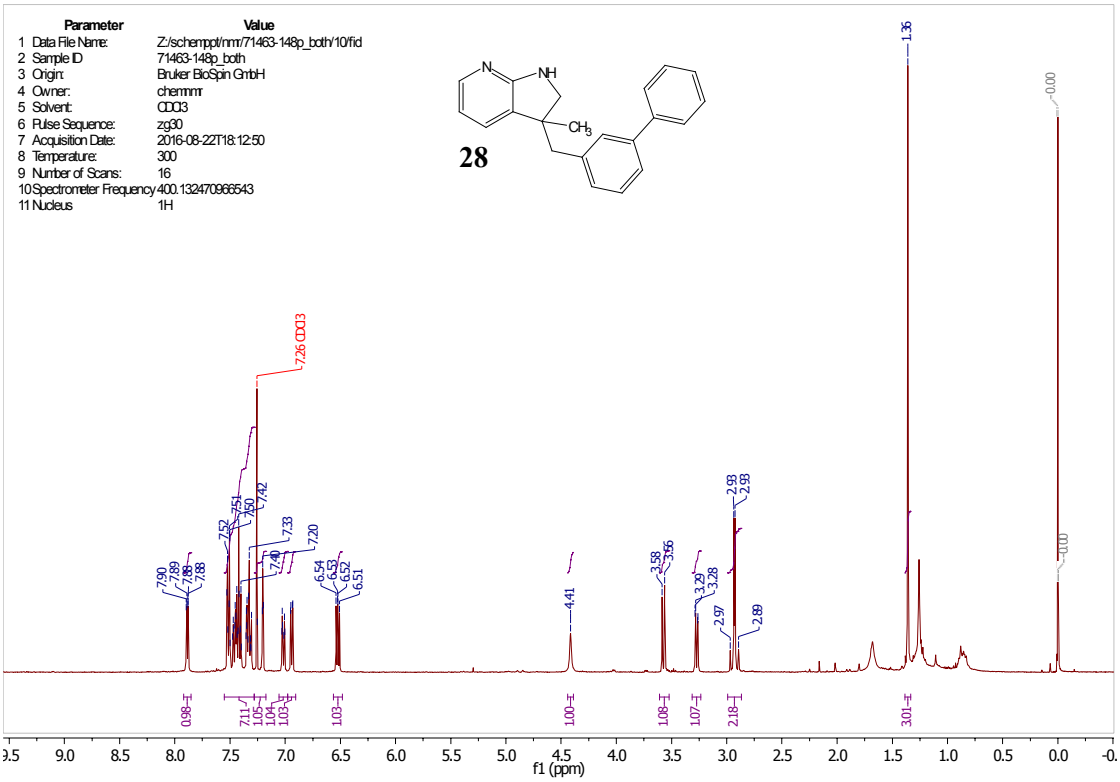

Parameter Value
1 Data File Name: Z:/schempbt/nmr/71463-125p_both/11/fid
2 Sample ID 71463-125p_both
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-24T00:33:16
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
25
f1 (ppm)

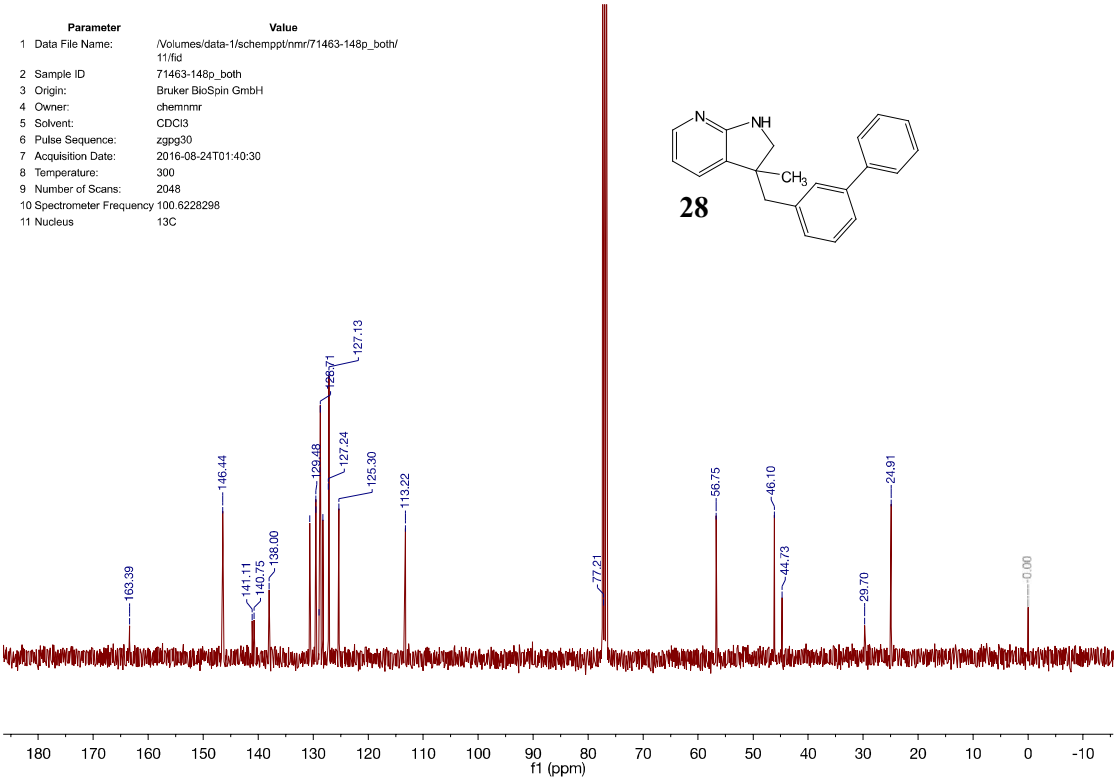

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-154/10/fid
2 Sample ID 71463-154
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-08T11:59:24
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
26
7.26 CDCl3
7.67
7.24
7.23
7.03
7.01
6.77
6.76
4.51
3.54
3.52
3.22
3.19
2.85
2.14
1.29
0.93
1.16
1.22
1.79
0.82
0.98
0.95
0.92
1.91
2.67
2.89
f1 (ppm)

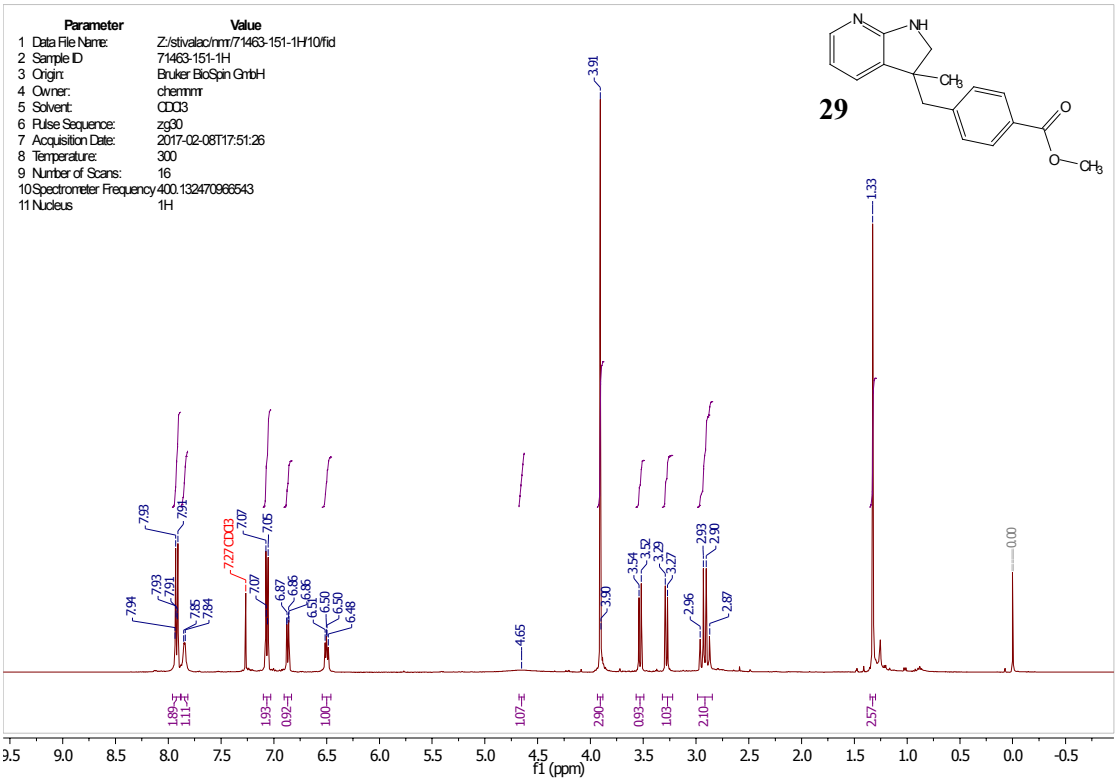

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-154-c13/10/fid
2 Sample ID 71463-154-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-08T21:34:45
8 Temperature: 300
9 Number of Scans: 8192
10 Spectrometer Frequency 100.622829802853
11 Nucleus 13C
26
161.53
145.00
137.59
132.14
130.61
129.47
127.81
126.44
122.14
77.21
56.94
45.92
44.58
29.70
24.74
17.89
0.01
f1 (ppm)

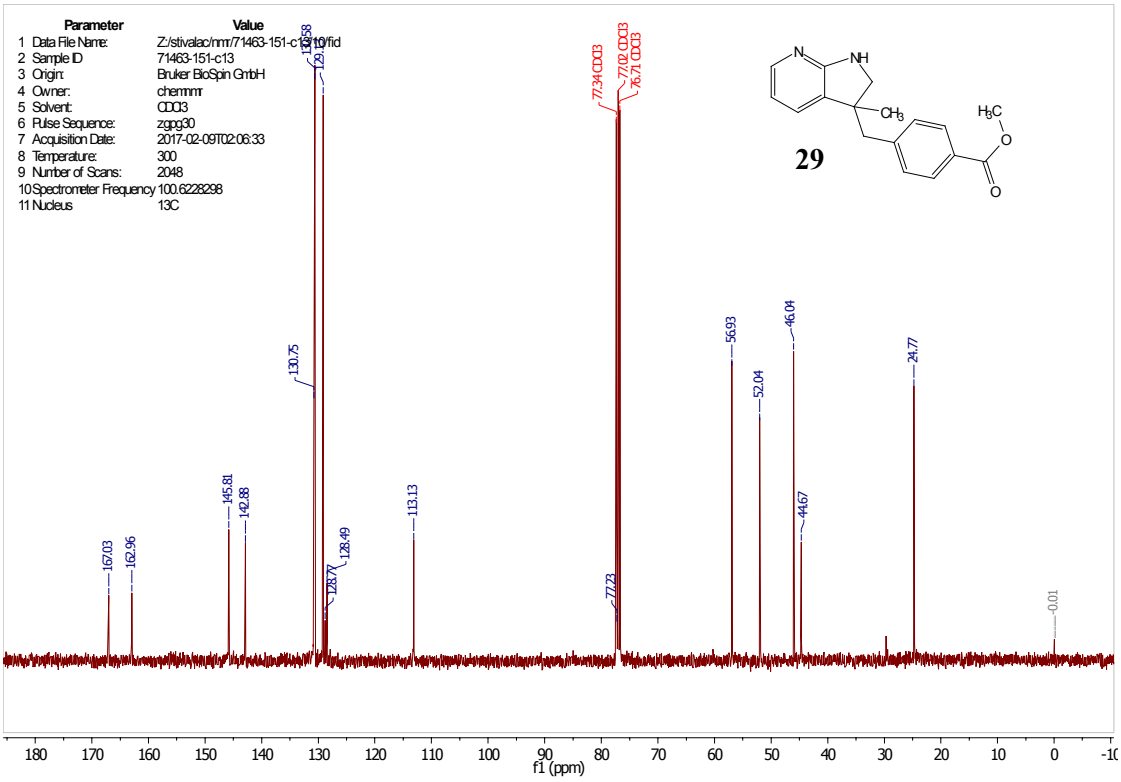

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-149-1H/10/fid
2 Sample ID 71463-149-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-09T09:54:18
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
27
f1 (ppm)

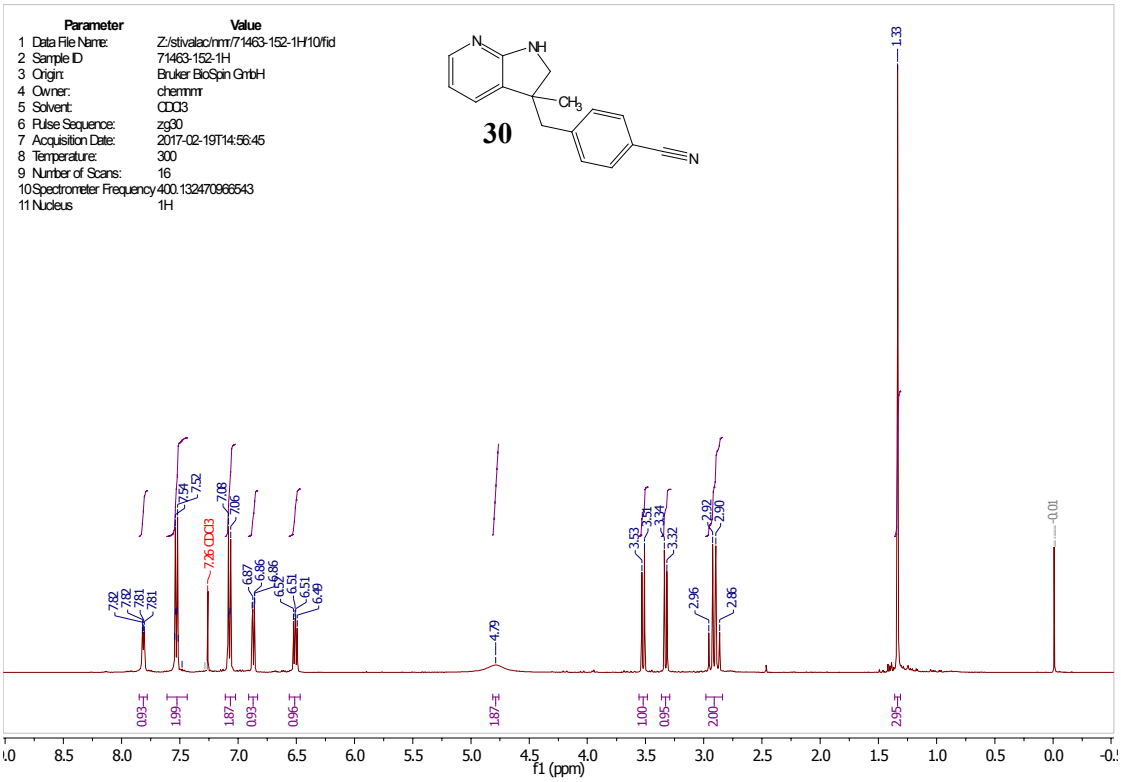

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-149-c13/10/fid
2 Sample ID 71463-149-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-09T20:08:25
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
27
f1 (ppm)

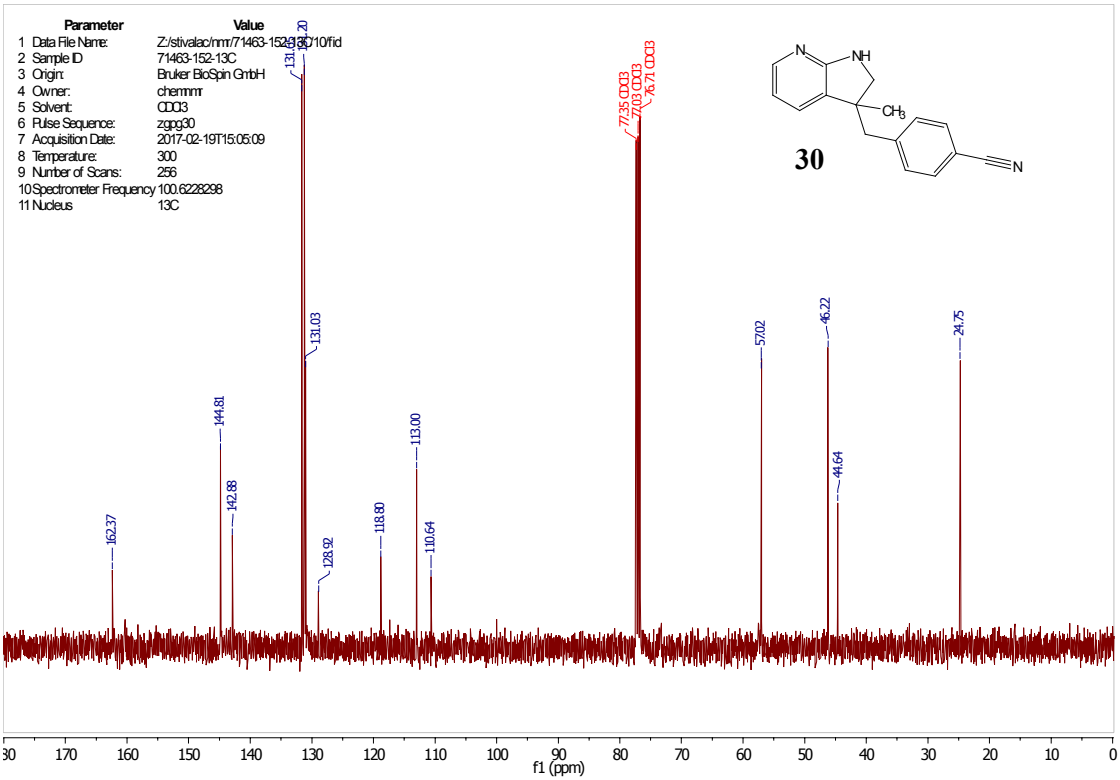

Parameter Value
1 Data File Name: Z:/schemppt/nmr/71463-148p_both/10/fid
2 Sample ID 71463-148p_both
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2016-08-22T18:12:50
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
28
7.26 CDCl3
f1 (ppm)

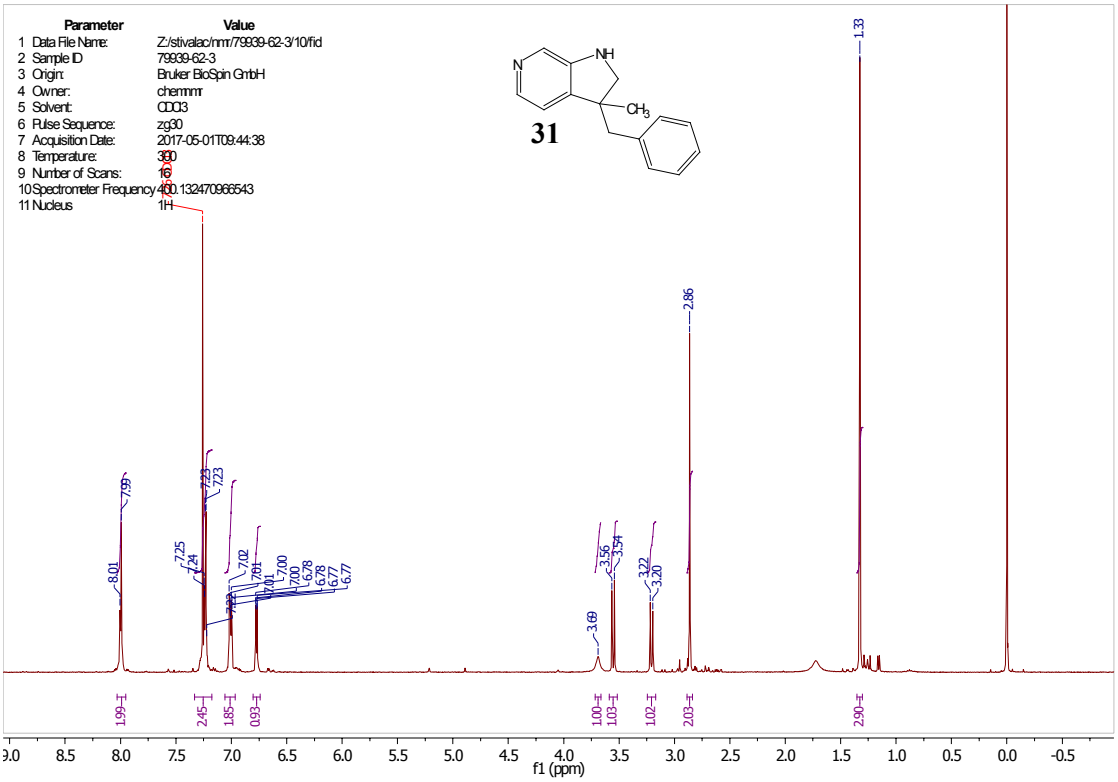

Parameter Value
1 Data File Name: /Volumes/data-1/schemppt/nmr/71463-148p_both/11/fid
2 Sample ID 71463-148p_both
3 Origin: Bruker BioSpin GmbH
4 Owner: chemnmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2016-08-24T01:40:30
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
28
f1 (ppm)

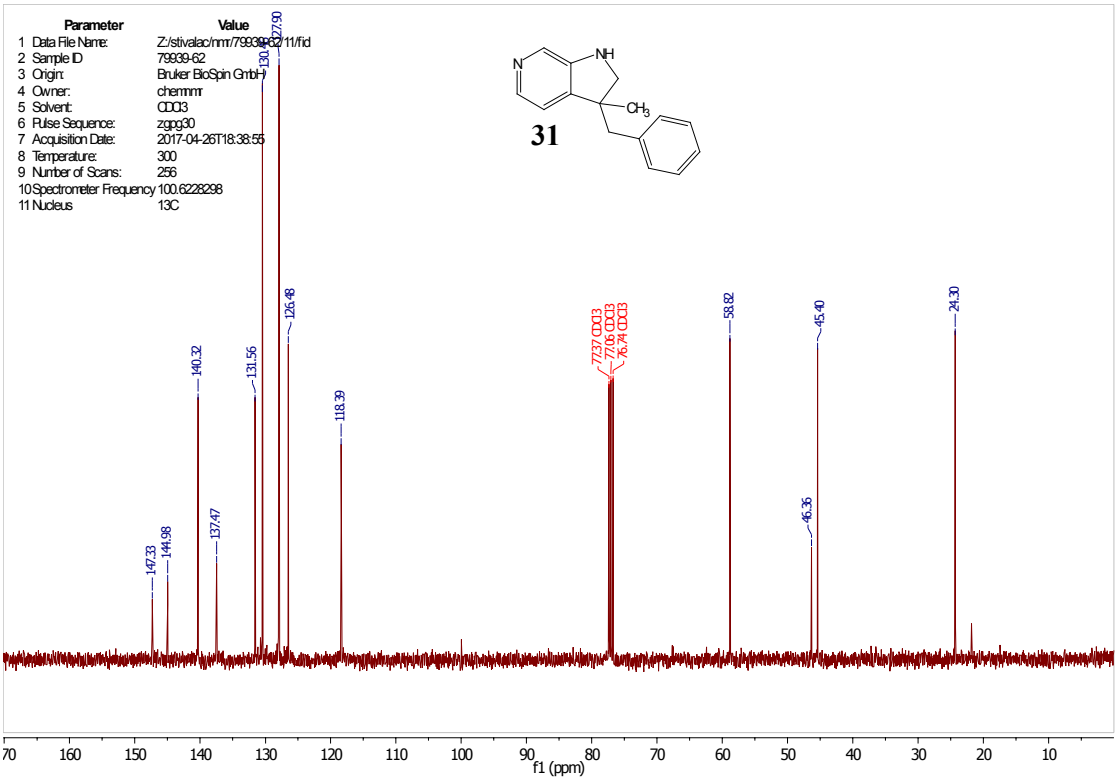

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-151-1H/10/fid
2 Sample ID 71463-151-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-08T17:51:26
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
29
f1 (ppm)

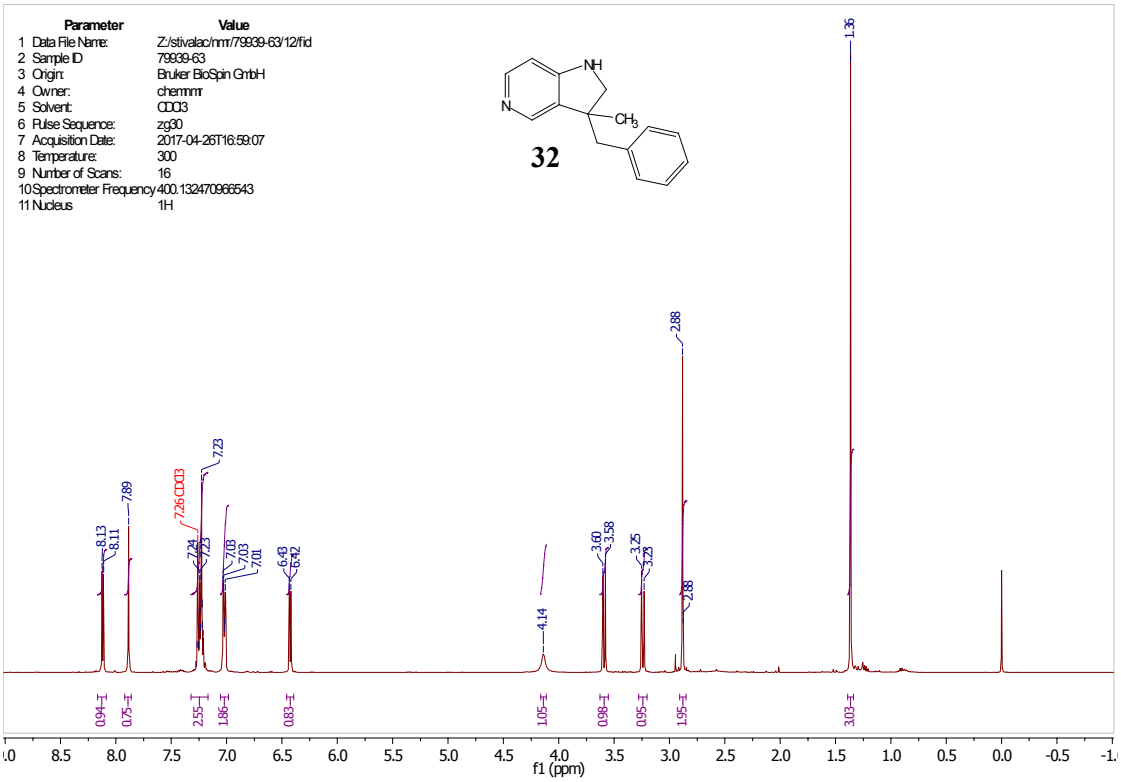

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-151-c13/10/fid
2 Sample ID 71463-151-c13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-09T02:06:33
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
29
f1 (ppm)

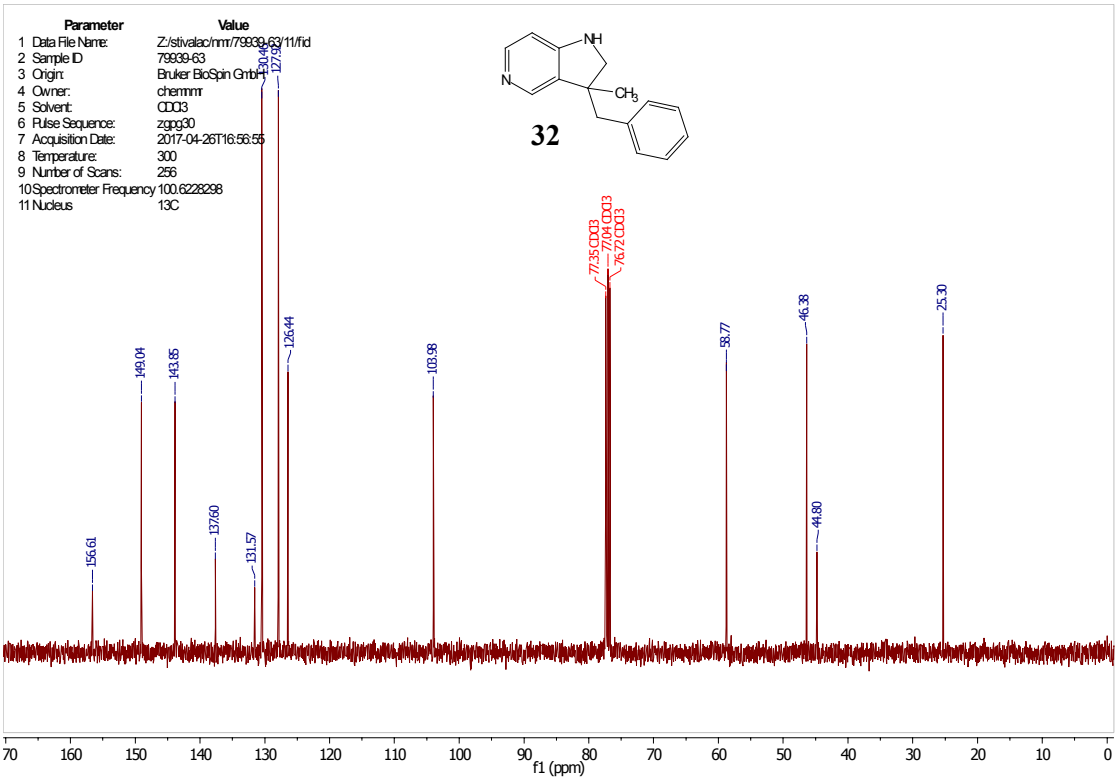

Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-152-1H/10/fid
2 Sample ID 71463-152-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-19T14:56:45
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
30
7.82
7.82
7.81
7.81
7.54
7.52
7.26 CDCl3
7.08
7.06
6.87
6.86
6.86
6.52
6.51
6.51
6.49
4.79
3.53
3.51
3.34
3.32
2.96
2.92
2.90
2.86
1.33
0.01
0.93
1.99
1.87
0.93
0.96
1.87
1.00
0.95
2.00
2.95
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-152-13C/10/fid
2 Sample ID 71463-152-13C
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-19T15:05:09
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
30
162.37
144.81
142.88
131.20
131.03
128.92
118.80
113.00
110.64
77.35 CDCl3
77.03 CDCl3
76.71 CDCl3
57.02
46.22
44.64
24.75
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-62-3/10/fid
2 Sample ID 79939-62-3
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-05-01T09:44:38
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
31
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-62-11/fid
2 Sample ID 79939-62
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-04-26T18:38:55
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
31
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-63/12/fid
2 Sample ID 79939-63
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-04-26T16:59:07
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
32
f1 (ppm)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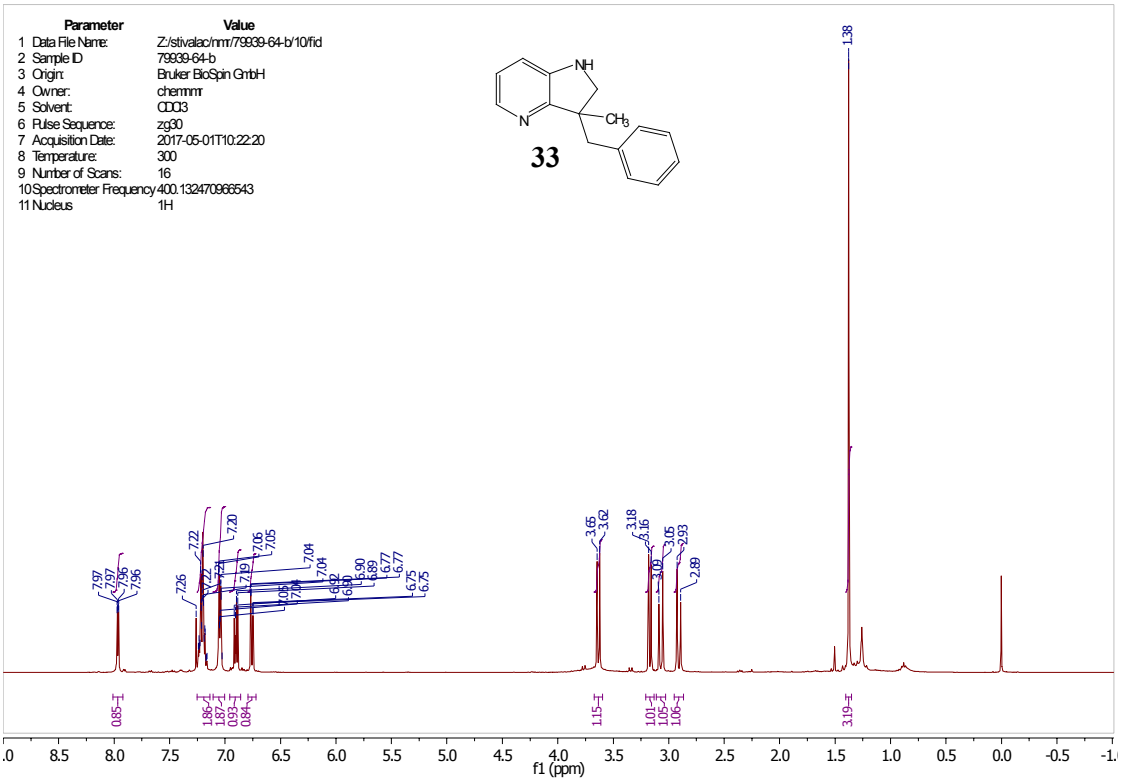
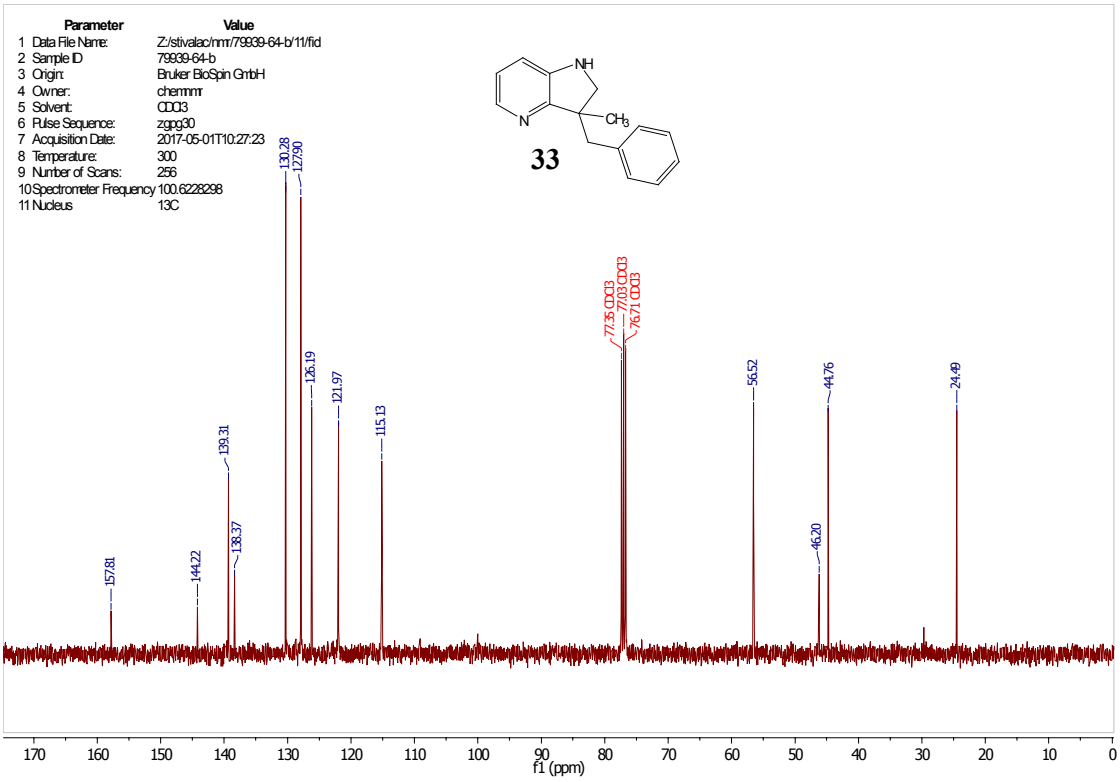
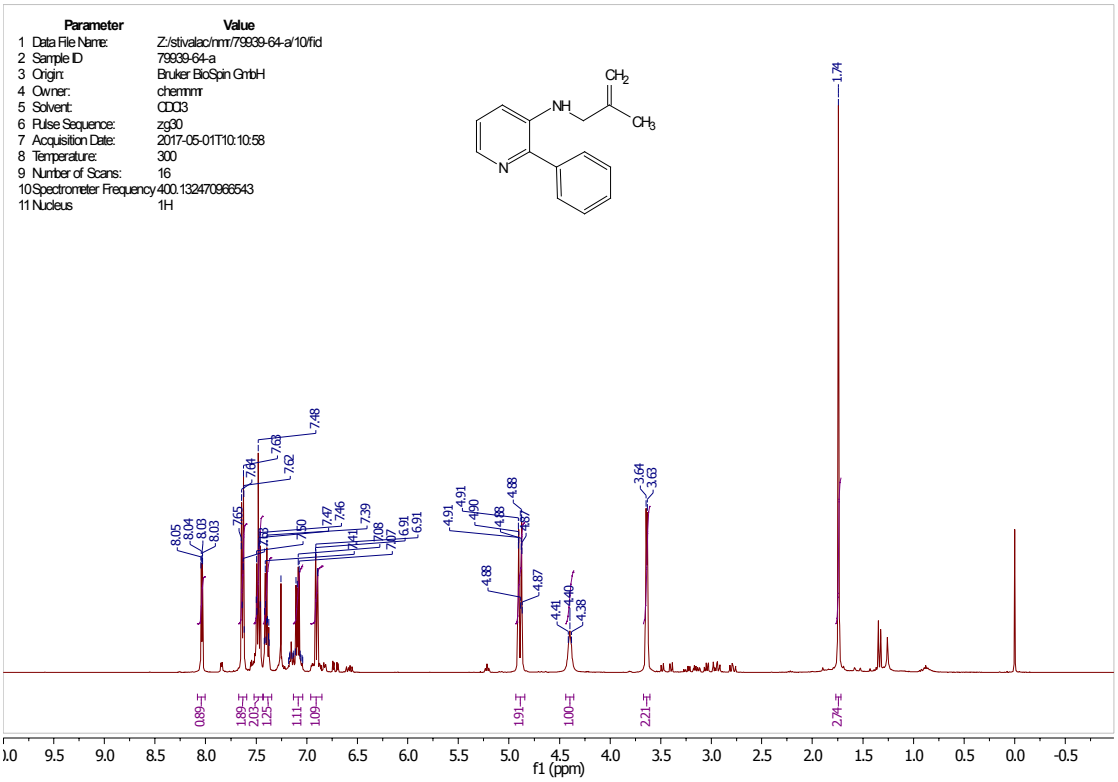
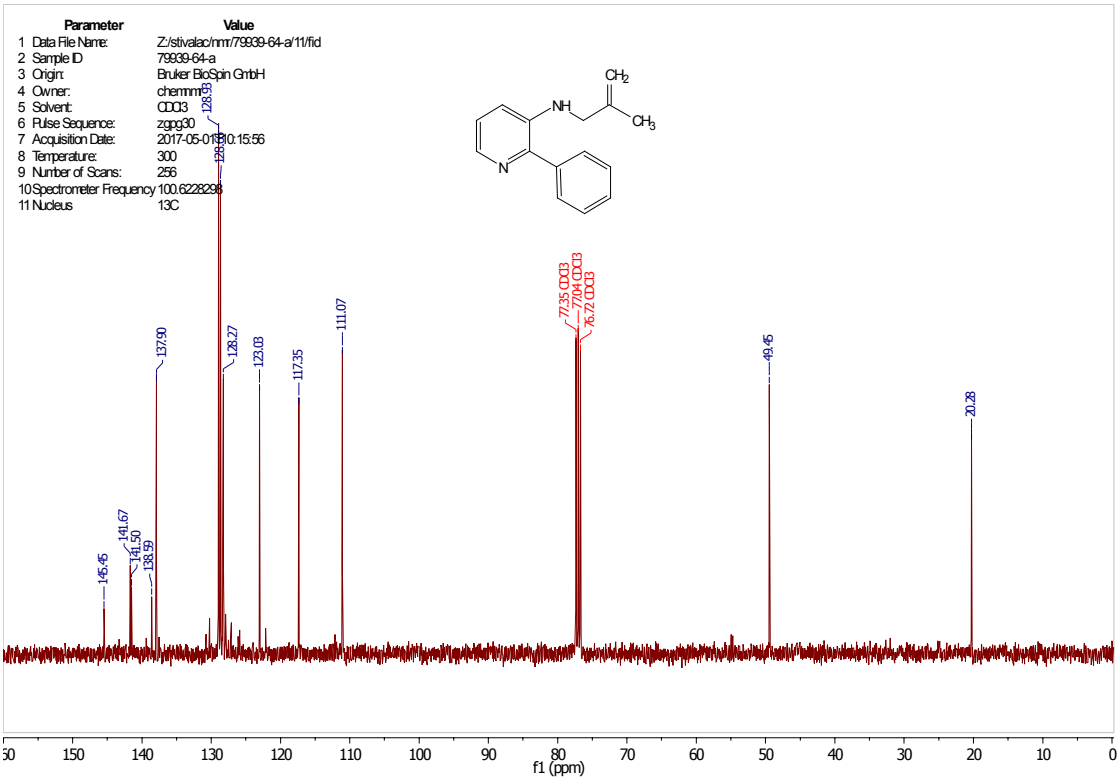
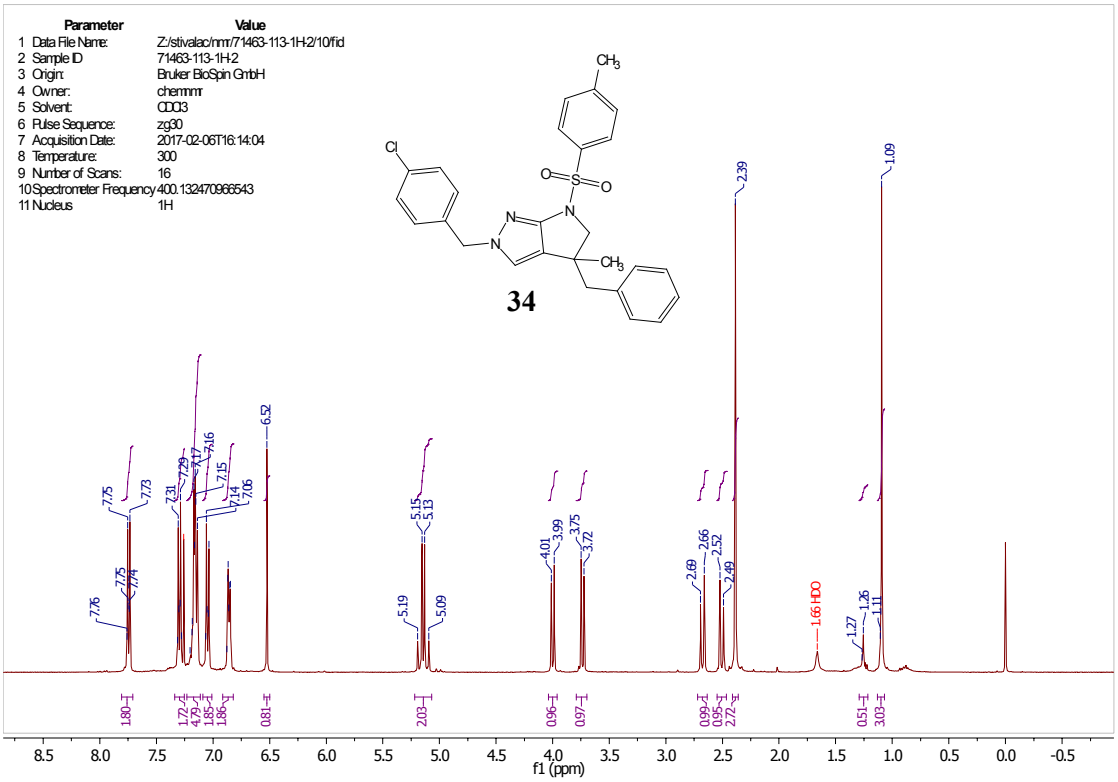
1 Data File Name: Z:/stivalac/nmr/79939-63/11/fid
2 Sample ID 79939-63
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-04-26T16:56:55
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
32
f1 (ppm)

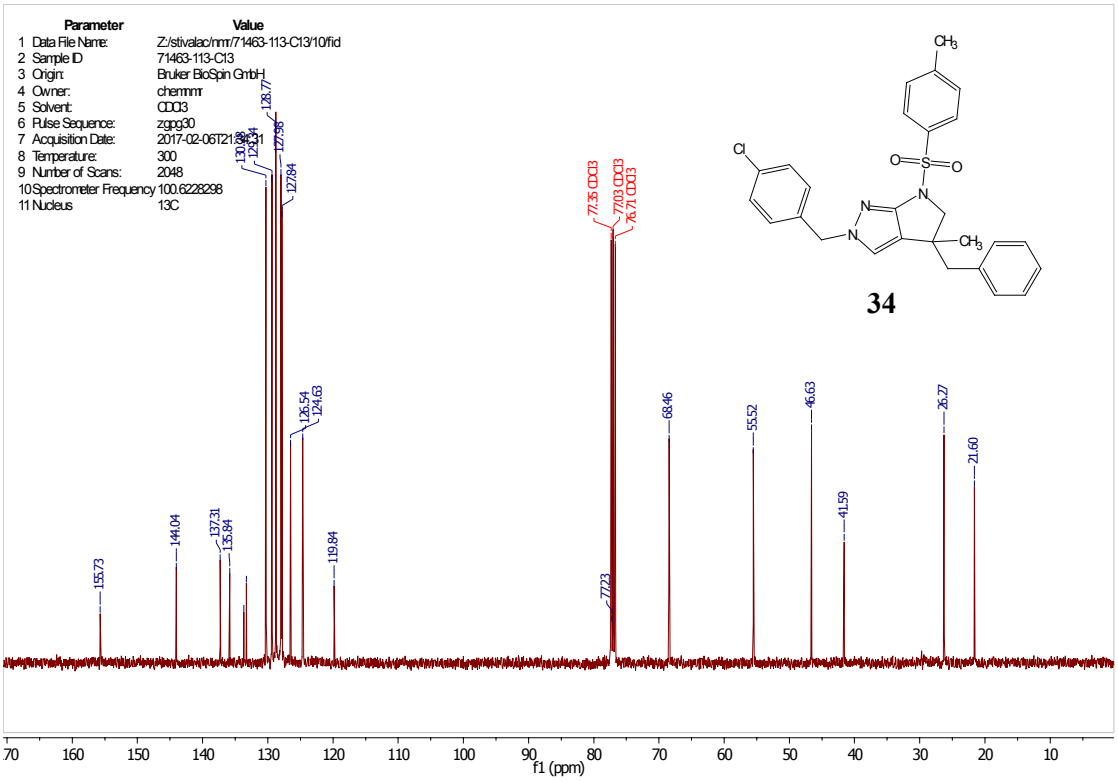

Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-64-b/10/fid
2 Sample ID 79939-64-b
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-05-01T10:22:20
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
NH
N
CH3
33
f1 (ppm)

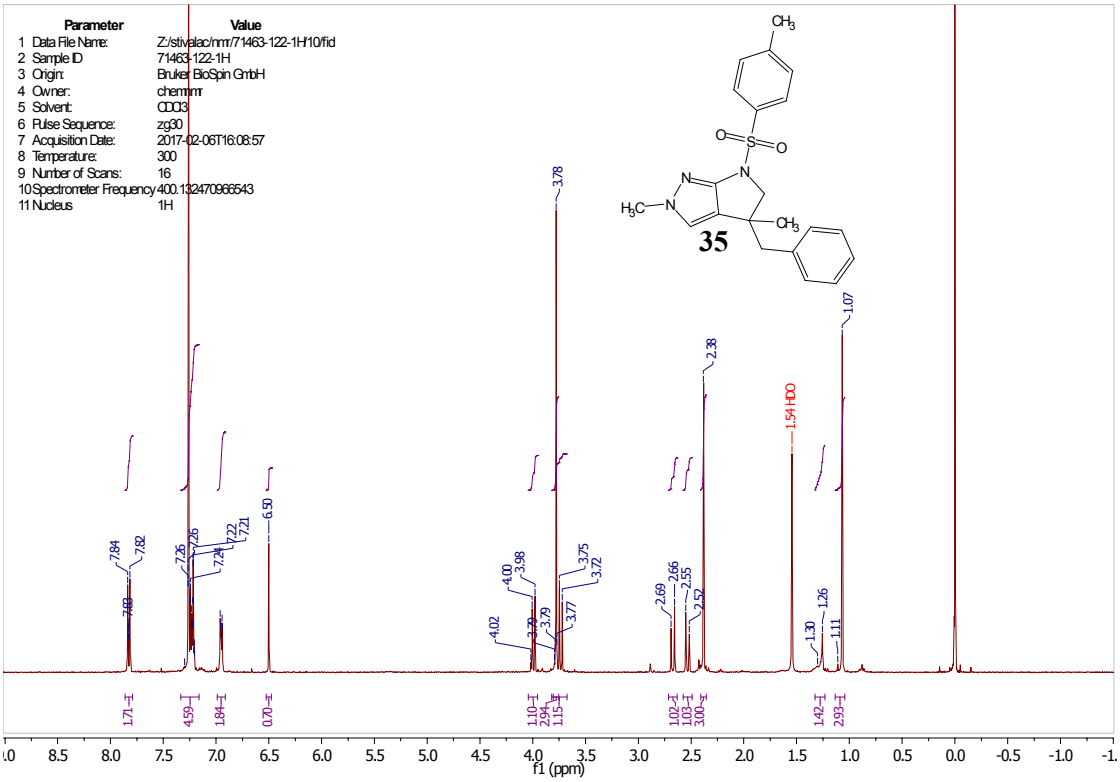

Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-64-b/11/fid
2 Sample ID 79939-64-b
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-05-01T10:27:23
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
NH
N
CH3
33
f1 (ppm)

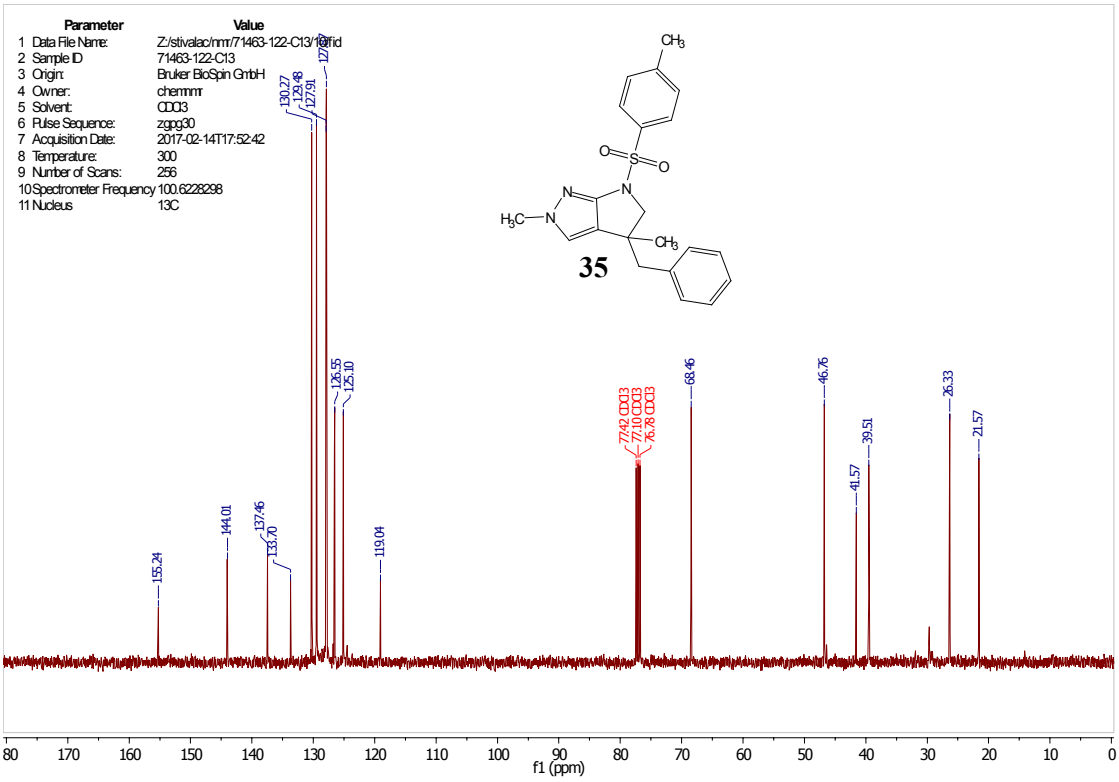

Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-64-a/10/fid
2 Sample ID 79939-64-a
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-05-01T10:10:58
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
NH
CH2
CH3
N
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/79939-64-a/11/fid
2 Sample ID 79939-64-a
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-05-01T10:15:56
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
NH
CH2
CH3
N
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-113-1H-2/10/fid
2 Sample ID 71463-113-1H-2
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T16:14:04
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
34
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-113-C13/10/fid
2 Sample ID 71463-113-C13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmm
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-06T21:
8 Temperature: 300
9 Number of Scans: 2048
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
34
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-122-1H/10/fid
2 Sample ID 71463-122-1H
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmmr
5 Solvent: CDCl3
6 Pulse Sequence: zg30
7 Acquisition Date: 2017-02-06T16:08:57
8 Temperature: 300
9 Number of Scans: 16
10 Spectrometer Frequency 400.132470966543
11 Nucleus 1H
35
f1 (ppm)


Parameter Value
1 Data File Name: Z:/stivalac/nmr/71463-122-C13/10/fid
2 Sample ID 71463-122-C13
3 Origin: Bruker BioSpin GmbH
4 Owner: chemmmr
5 Solvent: CDCl3
6 Pulse Sequence: zgpg30
7 Acquisition Date: 2017-02-14T17:52:42
8 Temperature: 300
9 Number of Scans: 256
10 Spectrometer Frequency 100.6228298
11 Nucleus 13C
35
f1 (ppm)