Nickel-Catalyzed Reductive Alkylation of Redox-Active Heteroaryl Imines

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Supporting Information

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1. General Information

Materials and Methods

Unless otherwise stated, reactions were performed under a N_2 atmosphere using freshly dried solvents. All reagents were purchased from commercial suppliers (Sigma Aldrich, Combi Blocks, TCI, Enamine, Strem) and used without further purifications unless mentioned otherwise. Tetrahydrofuran (THF), diethyl ether (Et_2O), methylene chloride (CH_2Cl_2), toluene (PhMe), hexane, and benzene (C_6H_6) were dried by passing through activated alumina columns. Anhydrous *N*-methylpyrrolidinone (NMP) were purchased from Aldrich and stored under N_2. $NiCl_2$·dme was purchased from Strem and stored in the glovebox. Manganese powder (~325 mesh, 99.3%) was purchased from Alfa Aesar. Zinc dust (97.5%) was purchased from Strem. Unless otherwise stated, chemicals and reagents were used as received. All reactions were monitored by thin-layer chromatography using EMD/Merck silica gel 60 F254 pre-coated plates (0.25 mm) and were visualized by UV, *p*-Anisaldehyde, Ninhydrin, or $KMnO_4$ staining. Flash column chromatography was performed as described by Still et al. using silica gel (230-400 mesh, Silicycle).[1] Purified compounds were dried on a high vacuum line (0.2 torr) to remove trace solvent. ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance III HD with Prodigy cryoprobe (at 400 MHz and 101 MHz, respectively), a Varian 400 MR (at 400 MHz and 101 MHz, respectively), or a Varian Inova 500 (at 500 MHz and 126 MHz, respectively). ^1H and ^{19}F NMR spectra were also recorded on a Varian Inova 300 (at 300 MHz and 282 MHz, respectively). NMR data is reported relative to internal $CHCl_3$ (^1H, δ = 7.26) and $CDCl_3$ (^{13}C, δ = 77.0). Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicity and qualifier abbreviations are as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. IR spectra were recorded on a Perkin Elmer Paragon 1000 spectrometer and are reported in frequency of absorption (cm^{-1}). HRMS were acquired from the Caltech Mass Spectral Facility using fast-atom bombardment (FAB), electrospray ionization (ESI-TOF), or electron impact (EI). Elemental analysis (EA) with ICP-MS on a commercial manganese sample was performed at the Resnick Sustainability Institute's Water and Environment Lab at the California Institute of Technology. X-ray diffraction was performed at the Caltech X-ray Crystal Facility. The computations presented here were conducted on the Caltech High Performance Cluster, partially supported by a grant from the Gordon and Betty Moore Foundation.

2. Optimization of Reaction Parameters (Table 1.)

General Procedure: To a 1-dram vial equipped with a stir bar was added 2-imino pyridine **1a** (0.3 mmol), benzyl bromide (0.36 mmol, 1.2 equiv), and Mn^0 (0.3 mmol, 1.0 equiv) on the benchtop. The vial was brought into a nitrogen-filled glovebox and a stock solution of $NiCl_2$·dme in NMP (0.75 ml, 0.02 M, 0.05 equiv [Ni]) and TMSCl (0.6 mmol, 2.0 equiv) was added. The vial was sealed with a Teflon cap, removed from the glovebox, and stirred at ambient temperature for 14 hours at 600 rpm. The resulting suspension was diluted with CH_2Cl_2 (0.5 ml) and extracted 3x with 1 N HCl (0.5 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased. The resulting aqueous solution was extracted 3x with EtOAc and the combined EtOAc layers were concentrated under reduced pressure and analyzed by ^1H NMR with 1,1,2,2-tetrachloroethane as an analytical standard to obtain the reaction yield.

3. Electrochemistry

3.1. Cyclic Voltammetry

Cyclic voltammograms were obtained at an analyte concentration of 10.0 mM and a supporting electrolyte concentration of 0.1 M $TBAPF_6$ in DMA. A glassy carbon working electrode, graphite counter electrode, and a silver wire pseudo-reference electrode were employed, and data were collected using a Biologic SP-300 potentiostat. All cyclic voltammograms were measured in the presence of 1 equiv of freshly-sublimed ferrocene and the reduction potentials are given versus the ½ wave potential of the Fc/Fc^+ peak. Yields reported are average of 2 runs from reactions of imine with benzyl bromide according to General Procedure 3.

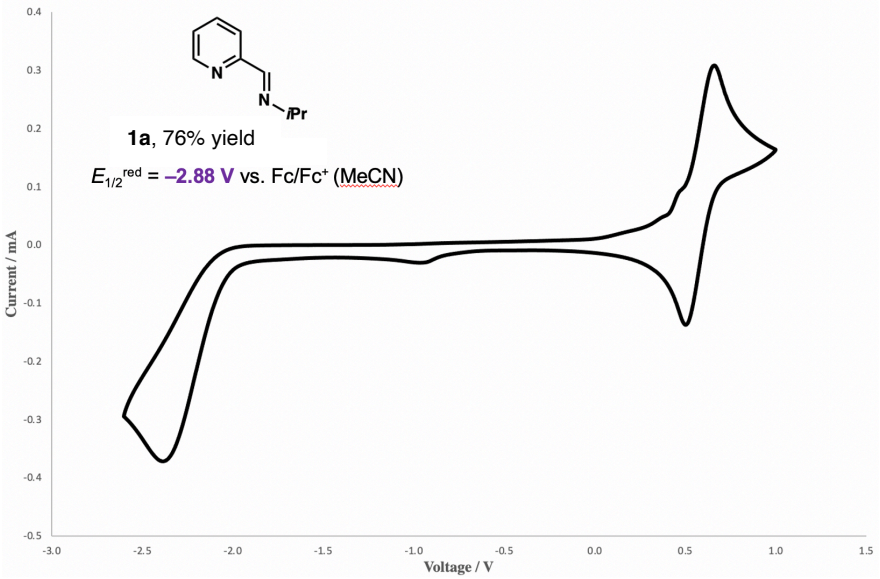


Figure S1: Cyclic voltammogram of **1a**, at a scan rate of 200 mV/s

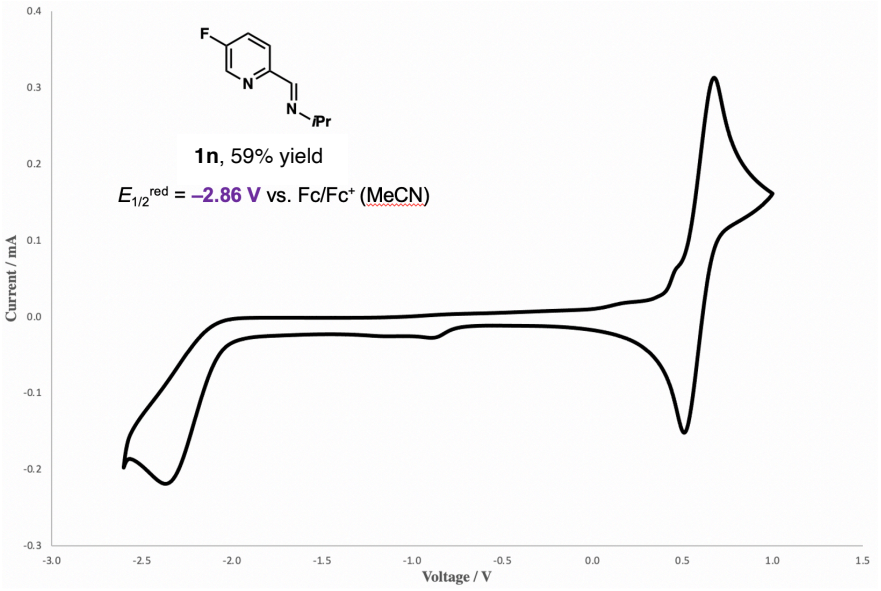


Figure S2: Cyclic voltammogram of **1n**, at a scan rate of 200 mV/s

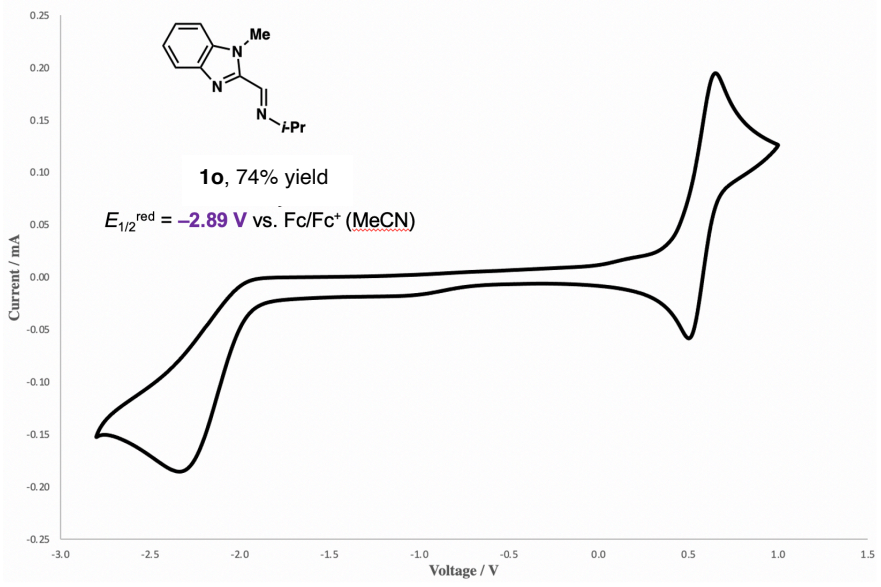


Figure S3: Cyclic voltammogram of **1o**, at a scan rate of 300 mV/s

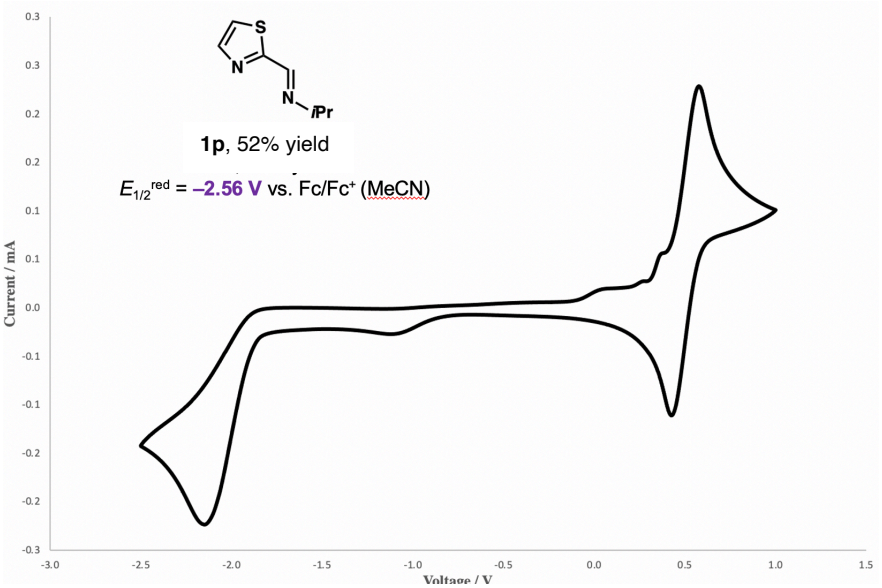


Figure S4: Cyclic voltammogram of **1p**, at a scan rate of 200 mV/s

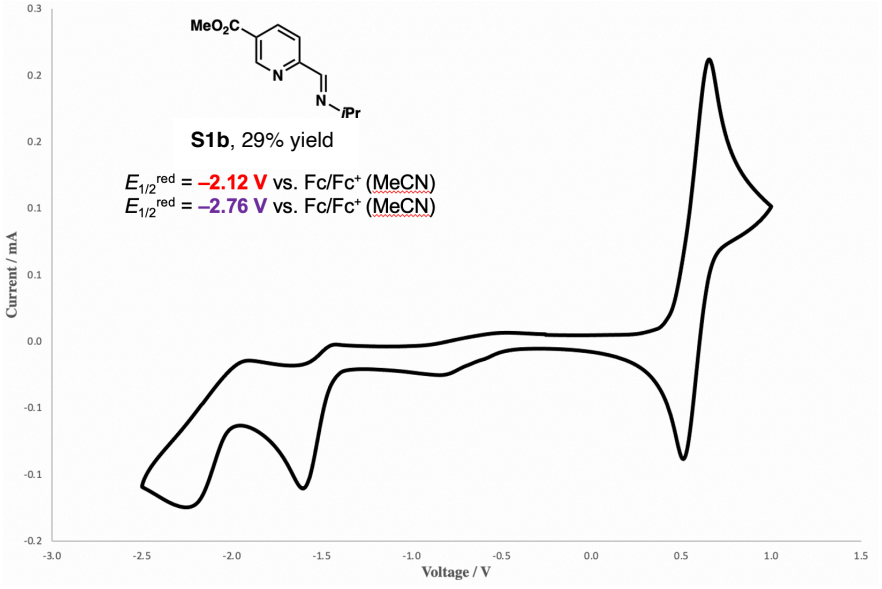


Figure S5: Cyclic voltammogram of **S1b**, at a scan rate of 200 mV/s

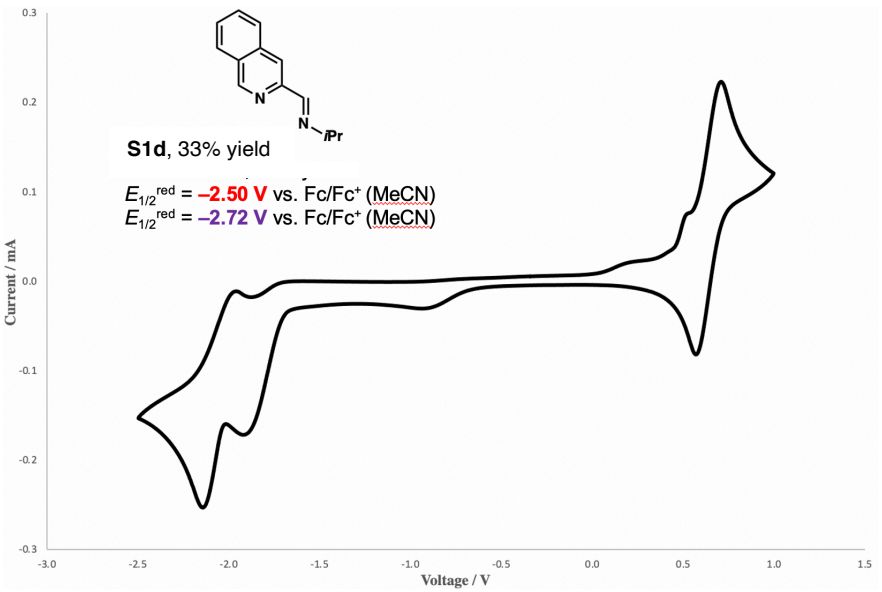


Figure S6: Cyclic voltammogram of **S1d**, at a scan rate of 200 mV/s

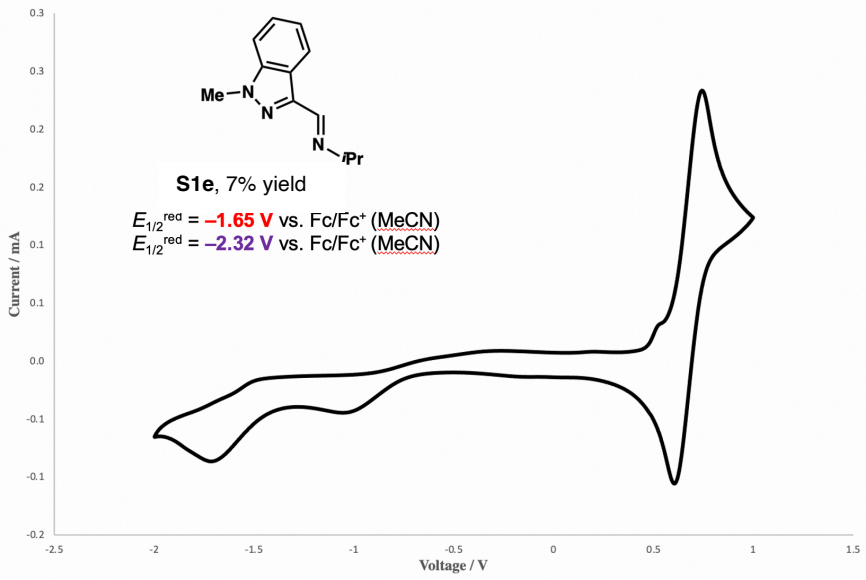


Figure S7: Cyclic voltammogram of **S1fe** at a scan rate of 200 mV/s.

The presence of an additional, earlier (–1.65 V to –2.50 V), irreversible reduction peak in imine substrates that did not perform well in the imine alkylation reaction (**S1b, S1d,** and **S1e**) suggests that there may be deleterious redox reactions happening under the reaction conditions. Selected heteroaryl imines (**1a, 1n,** and **1o**) perform well in the alkylation reaction that only have the quasi-reversible peaks at ~2.88 V. Further investigations into this correlation are ongoing in our laboratory.

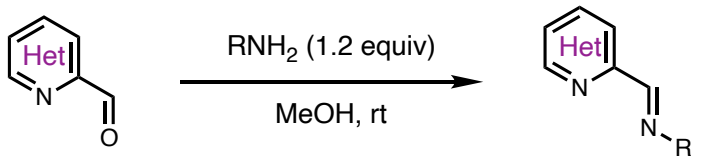
3.2. Electrochemical Alkylation Procedure

On the bench-top, a standard 2 mL ElectraSyn vial was charged with a stir bar, iminopyridine **1a** (44.5mg, 1.2 mmol, 1.0 equiv) and cyclohexyl iodide (378 mg, 1.8 mmol, 1.2 equiv). The vial was brought into a N_2-filled glovebox and a stock-solution of $NiCl_2$·dme in NMP (3.0 ml, 0.04 M, 0.1 equiv [Ni]) was added. The vial was sealed with a septum and brought out of the glove box. IKA **Zn** (anode) and **RVC** (cathode) plate electrodes were connected to an ElectraSyn vial cap. The cap was installed under N_2-flow and fit into the ElectraSyn and the following setup was employed: *New exp. -> Constant current -> 10 mA -> no ref. electrode -> no alternating polarity -> start.* The reaction was stirred at room temperature for 5 hours. The resulting dark solution was diluted with CH_2Cl_2 (2 ml) and extracted 3x with 1N HCl (2 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased. The resulting aqueous solution was extracted 3x with EtOAc and the combined organic phases were concentrated under reduced pressure at 40 °C until most of the NMP was removed. The crude material was purified by column chromatography (1:1 hexanes:EtOAc w/ 1% Et_3N) to afford the desired product **4o** (162 mg, 0.70 mmol, 58%).

4. Substrate Preparation

4.1. Synthesis of Heteroaryl Imines

a. General Procedure 1: Heteroaryl Imine Synthesis using Volatile Amines



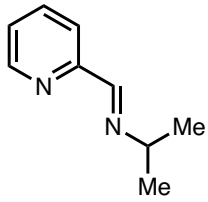
A 1-dram vial equipped with a stir bar was charged with MeOH (0.7 M), heteroaryl aldehyde (1.0 equiv), and primary amine RNH_2 (1.2 equiv). The resulting solution was stirred at room temperature for 2 hours, followed by concentration in vacuo. The resulting 2-imino-heteroarene was obtained in pure form and used without further purification.

b. General Procedure 2: Heteroaryl Imine Synthesis using Non-volatile Amines

A 1-dram vial equipped with a stir bar was charged with CH_2Cl_2 (0.7 M), heteroaryl aldehyde (1.05 equiv), $MgSO_4$ (1.5 equiv) and primary amine RNH_2 (1.0 equiv). The resulting solution

was stirred at room temperature for 18 hours. The resulting suspension was filtered and concentrated in vacuo. The resulting 2-imino-heteroaryl was obtained in pure form and used without further purification.

(*E*)-*N*-isopropyl-1-(pyridin-2-yl)methanimine (1a)



Prepared from 2-pyridine carboxaldehyde (2.30 g, 21.5 mmol) and isopropylamine (1.59 g, 26.8 mmol) following General Procedure 1. After concentration in vacuo, **1a** (2.68 g, 18.1 mmol, 84%) was obtained as a yellow oil.

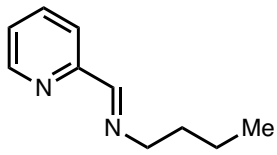
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (d, *J* = 3.1 Hz, 1H), 8.39 (s, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.73 (td, *J* = 7.9, 2.2 Hz, 1H), 7.29 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 3.69 – 3.60 (m, 1H), 1.29 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.5, 155.0, 149.6, 136.7, 124.8, 121.6, 61.7, 24.2.

FTIR (NaCl, thin film, cm^{-1}): 3056, 2968, 2929, 2865, 1647, 1588, 1568, 1466, 1437, 1362, 1316, 1139, 993, 973, 945, 775, 744, 615.

HRMS (FAB, m/z): calc'd for $C_9H_{11}N_2$ $[M+H]^+$ $-H_2$: 147.0922; found 147.0922.

(*E*)-*N*-butyl-1-(pyridin-2-yl)methanimine (1b)



Prepared from 2-pyridine carboxaldehyde (1.07 g, 10.0 mmol) and *n*-butylamine (878 mg, 12.0 mmol) following General Procedure 1. After concentration in vacuo, **1b** (1.30 g, 8.00 mmol, 80%) was obtained as a yellow oil.

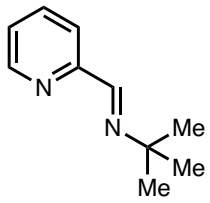
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.64 (d, *J* = 4.8 Hz, 1H), 8.37 (s, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.73 (td, *J* = 7.7, 1.7 Hz, 1H), 7.30 (dd, *J* = 7.5, 4.8 Hz, 1H), 3.68 (t, *J* = 6.8 Hz, 2H), 1.71 (p, *J* = 7.1 Hz, 2H), 1.40 (h, *J* = 7.4 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 161.9, 154.8, 149.6, 136.8, 124.8, 121.4, 61.5, 33.0, 20.6, 14.1.

FTIR (NaCl, thin film, cm^{-1}): 3053, 3009, 2958, 2938, 2872, 1649, 1587, 1567, 1468, 1436, 1377, 1332, 1292, 1227, 1145, 1117, 1066, 1044, 992, 978, 939, 898, 864, 775, 743, 654, 617.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1235; found 163.1256.

(*E*)-*N*-*tert*-butyl-1-(pyridin-2-yl)methanimine (1c)



Prepared from 2-pyridine carboxaldehyde (225 mg, 2.10 mmol) and *tert*-butlyamine (185 mg, 2.52 mmol) following General Procedure 1. After concentration in vacuo, **1c** (398 mg, 2.0 mmol, 95%) was obtained as a yellow oil.

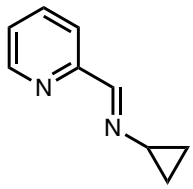
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.66 – 8.58 (m, 1H), 8.35 (s, 1H), 8.01 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.76 – 7.67 (m, 1H), 7.28 (ddd, *J* = 7.5, 4.9, 1.3 Hz, 1H), 1.31 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 156.6, 155.7, 149.5, 136.7, 124.6, 121.2, 58.0, 29.8.

FTIR (NaCl, thin film, cm^{-1}): 3056, 2969, 2931, 1646, 1588, 1568, 1467, 1436, 1228, 1209, 1044, 994, 972, 908, 860, 775, 744, 616.

HRMS (ESI-TOF, m/z): calc'd for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1235; found 163.1210.

(*E*)-*N*-cyclopropyl-1-(pyridin-2-yl)methanimine (1d)



Prepared from 2-pyridine carboxaldehyde (225 mg, 2.10 mmol) and cyclopropylamine (144 mg, 2.52 mmol following General Procedure 1. After concentration in vacuo, **1d** (200 mg, 1.37 mmol, 65%) was obtained as a yellow oil.

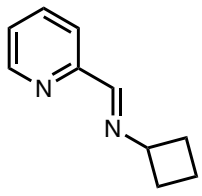
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.88 (d, *J* = 9.0 Hz, 1H), 7.71 (td, *J* = 7.7, 1.7 Hz, 1H), 7.31 – 7.24 (m, 1H), 3.13 (hept, *J* = 6.8, 3.4 Hz, 1H), 1.09 – 1.04 (m, 2H), 1.03 – 0.97 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.3, 154.8, 149.6, 136.6, 124.4, 121.3, 42.2, 9.5.

FTIR (NaCl, thin film, cm^{-1}): 3420, 3055, 3010, 2962, 2878, 1635, 1583, 1568, 1470, 1436, 1381, 1320, 1174, 1146, 1090, 1042, 956, 887, 812, 773, 743, 612.

HRMS (FAB, m/z): calc'd for $C_9H_{11}N_2$ $[M+H]^+$: 147.0922; found 147.0922.

(*E*)-*N*-cyclobutyl-1-(pyridin-2-yl)methanimine (1e)



Prepared from 2-pyridine carboxaldehyde (225 mg, 2.10 mmol) and cyclobutylamine (179 mg, 2.52 mmol) following General Procedure 1. After concentration in vacuo, **1e** (243 mg, 1.51 mmol, 72%) was obtained as a yellow oil.

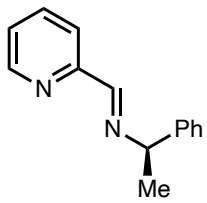
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.6 (d, *J* = 4.8 Hz, 1H), 8.3 (d, *J* = 1.7 Hz, 1H), 8.0 (d, *J* = 7.9 Hz, 1H), 7.7 (td, *J* = 7.7, 1.7 Hz, 1H), 7.3 (dd, *J* = 6.4, 4.8 Hz, 1H), 4.3 – 4.2 (m, 1H), 2.4 – 2.3 (m, 2H), 2.3 – 2.1 (m, 2H), 1.9 – 1.8 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.4, 154.9, 149.6, 136.7, 124.8, 121.4, 62.9, 30.5, 15.8.

FTIR (NaCl, thin film, cm^{-1}): 3055, 2980, 2939, 2868, 1642, 1589, 1567, 1469, 1436, 1374, 1319, 1228, 1140, 1080, 1042, 992, 972, 861, 773, 743.

HRMS (FAB, m/z): calc'd for $C_{10}H_{13}N_2$ $[M+H]^+$: 161.1079; found 161.1086.

(*R*,*E*)-*N*-(1-phenylethyl)-1-(pyridin-2-yl)methanimine (1f)



Prepared from 2-pyridine carboxaldehyde (176 mg, 1.65 mmol) and (R)-(+)-1-phenethylamine (190 mg, 1.57 mmol) following General Procedure 2. After concentration in vacuo, **1f** (82.4 mg, 0.39 mmol, 25%) was obtained as tan solid.

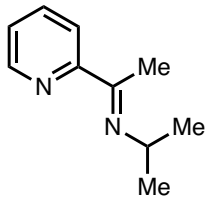
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.64 (ddd, *J* = 4.9, 1.7, 0.9 Hz, 1H), 8.47 (s, 1H), 8.10 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.78 – 7.67 (m, 1H), 7.46 – 7.41 (m, 2H), 7.38 – 7.32 (m, 2H), 7.30 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 7.28 – 7.22 (m, 1H), 4.65 (q, *J* = 6.4 Hz, 1H), 1.61 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 160.6, 155.0, 149.5, 144.8, 136.7, 128.7, 127.2, 126.9, 124.9, 121.7, 69.8, 24.8.

FTIR (NaCl, thin film, cm^{-1}): 3059, 3027, 2972, 2927, 2861, 1646, 1586, 1568, 1491, 1466, 1456, 1436, 1373, 1338, 1304, 1080, 993, 973, 908, 763, 700.

HRMS (FAB, m/z): calc'd for $C_{14}H_{15}N_2$ $[M+H]^+$: 211.1235; found 211.1217.

(*E*)-*N*-isopropyl-1-(pyridin-2-yl)ethan-1-imine (1g)



Prepared from 2-acetylpyridine (162 mg, 1.34 mmol) and isopropylamine (95.2 mg, 1.61 mmol following General Procedure 1 modified to allow the reaction to run for 48 hours. After concentration in vacuo, **1g** (126 mg, 0.78 mmol, 58%) was obtained as a yellow oil.

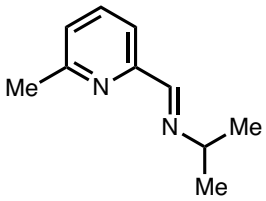
^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.46 (ddd, J = 4.8, 1.8, 1.0 Hz, 1H), 7.98 (dt, J = 8.0, 1.1 Hz, 1H), 7.60 (ddd, J = 8.0, 7.4, 1.8 Hz, 1H), 7.18 (ddd, J = 7.4, 4.8, 1.3 Hz, 1H), 3.83 (hept, J = 6.3 Hz, 1H), 2.25 (s, 3H), 1.11 (d, J = 6.2 Hz, 6H).

^{13}C NMR (101 MHz, CD_2Cl_2): δ 163.19, 158.28, 148.07, 135.98, 123.76, 120.63, 51.46, 23.20, 12.98.

FTIR (NaCl, thin film, cm^{-1}): 3050, 2967, 2929, 2869, 1638, 1585, 1565, 1464, 1433, 1368, 1297, 1134, 1098, 1043, 991, 783, 743.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1235; found: 163.1231.

(E)-*N*-isopropyl-1-(6-methylpyridin-2-yl)methanimine (1h)



Prepared from 6-methylpicolinaldehyde (200 mg, 1.65 mmol) and isopropylamine (117 mg, 1.98 mmol) following General Procedure 1. After concentration in vacuo, **1h** (174 mg, 1.07 mmol, 65%) was obtained as a yellow oil.

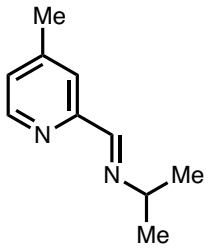
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (s, 1H), 7.81 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 3.62 (hept, *J* = 6.3 Hz, 1H), 2.59 (s, 3H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.9, 158.2, 154.5, 137.0, 124.4, 118.5, 61.6, 24.6, 24.2.

FTIR (NaCl, thin film, cm^{-1}): 3061, 2968, 2927, 2863, 1646, 1591, 1574, 1455, 1378, 1361, 1308, 1250, 1224, 1141, 1086, 990, 967, 948, 9191, 863, 792, 762, 738, 636.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1235; found 163.1236.

(E)-*N*-isopropyl-1-(4-methylpyridin-2-yl)methanimine (1i)



Prepared from 6-methylpicolinaldehyde (200 mg, 1.65 mmol) and isopropylamine (117 mg, 1.98 mmol) following General Procedure 1. After concentration in vacuo, **1i** (268 mg, 1.37 mmol, 83%) was obtained as a yellow oil.

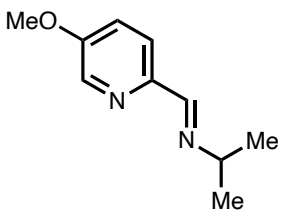
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.48 (d, *J* = 5.0 Hz, 1H), 8.37 (s, 1H), 7.82 (s, 1H), 7.12 (d, *J* = 3.2 Hz, 1H), 3.63 (hept, *J* = 6.3 Hz, 1H), 2.38 (s, 3H), 1.29 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.8, 154.7, 149.4, 148.0, 125.8, 122.1, 61.7, 24.2, 21.2.

FTIR (NaCl, thin film, cm^{-1}): 2968, 2925, 2864, 1647, 1602, 1558, 1466, 1380, 1362, 1315, 1155, 994, 945, 850, 826, 768, 650.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1235; found 163.1257.

(E)-*N*-isopropyl-1-(5-methoxypyridin-2-yl)methanimine (1j)



Prepared from 5-methoxypicolinaldehyde (250 mg, 1.82 mmol) and isopropylamine (129 mg, 2.19 mmol) following General Procedure 1. After concentration in vacuo, **1j** (195 mg, 1.09 mmol, 60%) was obtained as a yellow oil.

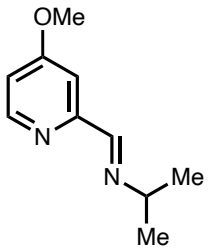
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.34 (s, 1H), 8.30 (d, *J* = 2.9 Hz, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.22 (dd, *J* = 8.7, 2.9 Hz, 1H), 3.89 (s, 3H), 3.60 (hept, *J* = 6.3 Hz, 1H), 1.27 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 158.8, 156.7, 147.9, 137.2, 122.4, 120.9, 61.6, 55.9, 24.3.

FTIR (NaCl, thin film, cm^{-1}): 2967, 2867, 1644, 1588, 1571, 1491, 1379, 1363, 1302, 1278, 1251, 1217, 1142, 1030, 1142, 1030, 972, 886, 838.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2O$ $[M+H]^+$: 179.1184; found 179.1187.

(E)-*N*-isopropyl-1-(4-methoxypyridin-2-yl)methanimine (1k)



Prepared from 4-methoxypicolinaldehyde (250 mg, 1.82 mmol) and isopropylamine (129 mg, 2.19 mmol) following General Procedure 1. After concentration in vacuo, **1k** (310 mg, 1.73 mmol, 95%) was obtained as a yellow oil.

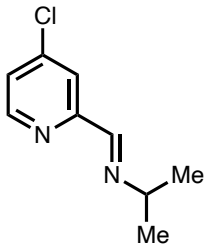
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (d, *J* = 5.8 Hz, 1H), 8.33 (s, 1H), 7.49 (s, 1H), 6.81 (d, *J* = 5.9 Hz, 1H), 3.88 (s, 3H), 3.62 (hept, *J* = 6.5 Hz, 1H), 1.27 (d, *J* = 4.9 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 166.4, 159.4, 156.9, 150.6, 112.1, 106.1, 61.5, 55.5, 24.1.

FTIR (NaCl, thin film, cm^{-1}): 2968, 2866, 1648, 1592, 1560, 1477, 1364, 1303, 1252, 1142, 1037, 993, 969, 944, 850, 767.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2O$ $[M+H]^+$: 179.1184; found 179.1181.

(*E*)-1-(4-chloropyridin-2-yl)-*N*-isopropylmethanimine (1l)



Prepared from 4-chloropicolinaldehyde (200 mg, 1.41 mmol) and isopropylamine (91.9 mg, 1.55 mmol) following General Procedure 1. After concentration in vacuo, **1l** (224 mg, 1.22 mmol, 87%) was obtained as a yellow oil.

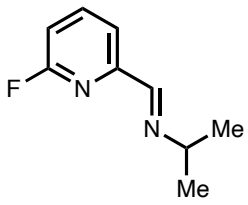
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.51 (d, *J* = 7.0 Hz, 1H), 8.35 (s, 1H), 8.02 (s, 1H), 7.30 (d, *J* = 5.4 Hz, 1H), 3.65 (hept, *J* = 6.2 Hz, 1H), 1.28 (d, *J* = 5.7 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 158.3, 156.5, 150.4, 145.1, 125.0, 121.7, 61.6, 24.1.

FTIR (NaCl, thin film, cm^{-1}): 2969, 2924, 2864, 1648, 1575, 1553, 1458, 1398, 1362, 1313, 1264, 1230, 1145, 1090, 945, 827, 709.

HRMS (FAB, m/z): calc'd for $C_9H_{12}N_2Cl$ $[M+H]^+$: 183.0689; found 183.0662.

(*E*)-1-(6-fluoropyridin-2-yl)-*N*-isopropylmethanimine (1m)



Prepared from 6-fluoropicolinaldehyde (177 mg, 1.41 mmol) and ispropylamine (91.9 mg, 1.55 mmol) following General Procedure 1. After concentration in vacuo, **1m** (202 mg, 1.21 mmol, 86%) was obtained as a yellow oil.

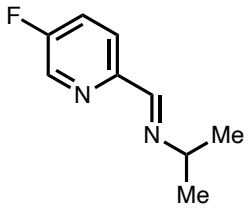
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (s, 1H), 7.88 (d, *J* = 7.3 Hz, 1H), 7.85 – 7.78 (m, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 3.63 (hept, *J* = 6.3 Hz, 1H), 1.27 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.4 (d, *J* = 240.1 Hz), 158.0, 153.7 (d, *J* = 12.5 Hz), 141.6 (d, *J* = 7.4 Hz), 118.6 (d, *J* = 4.1 Hz), 110.7 (d, *J* = 36.9 Hz), 61.6, 24.1.

FTIR (NaCl, thin film, cm^{-1}): 2970, 2930, 2868, 1650, 1598, 1578, 1455, 1380, 1362, 1309, 1262, 1228, 1139, 1071, 994, 974, 937, 865, 804, 771, 731, 630.

HRMS (FAB, m/z): calc'd for $C_9H_{12}N_2F$ $[M+H]^+$: 167.0985; found 167.0963.

(*E*)-1-(5-fluoropyridin-2-yl)-*N*-isopropylmethanimine (1n)



Prepared from 5-fluoropicolinaldehyde (177 mg, 1.41 mmol) and isopropylamine (91.9 mg, 1.55 mmol) following General Procedure 1. After concentration in vacuo, **1n** (162 mg, 0.98 mmol, 69%) was obtained as a yellow oil.

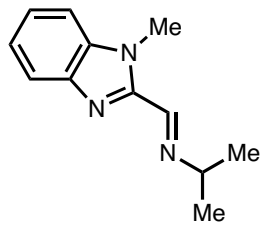
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 (s, 1H), 8.35 (s, 1H), 8.02 (dd, *J* = 8.5, 4.9 Hz, 1H), 7.43 (t, *J* = 8.4 Hz, 1H), 3.62 (hept, *J* = 7.1 Hz, 1H), 1.27 (d, *J* = 6.5 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 160.2 (d, *J* = 259.2 Hz), 158.0, 151.5 (d, *J* = 3.9 Hz), 137.8 (d, *J* = 24.1 Hz), 123.6 (d, *J* = 18.5 Hz), 122.8 (d, *J* = 5.0 Hz), 61.6, 24.2.

FTIR (NaCl, thin film, cm^{-1}): 2970, 2933, 2865, 1647, 1593, 1579, 1478, 1380, 1363, 1312, 1253, 1232, 1143, 1281, 1232, 1143, 1019, 961, 886, 841.

HRMS (FAB, m/z): calc'd for $C_9H_{12}FN_2$ $[M+H]^+$: 167.0985; found 167.0980.

(E)-*N*-isopropyl-1-(1-methyl-1H-benzo[d]imidazol-2-yl)methanimine (1o)



Prepared from 1-methyl-1H-benzo[d]imidazole-2-carbaldehyde (200 mg, 1.25 mmol) and isopropylamine (81.2 mg, 1.37 mmol) following General Procedure 1. After concentration in vacuo, **1o** (227 mg, 1.13 mmol, 91%) was obtained as a yellow oil.

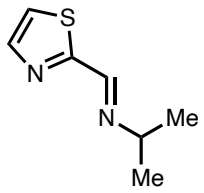
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.53 (s, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.32 (m, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 4.18 (s, 3H), 3.65 – 3.56 (m, 1H), 1.30 (d, *J* = 8.1 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 151.6, 147.8, 142.6, 137.0, 124.2, 122.7, 120.6, 109.8, 62.4, 31.9, 24.1.

FTIR (NaCl, thin film, cm^{-1}): 2968, 2861, 1471, 1405, 1359, 1336, 1143, 931, 882, 748.

HRMS (ESI-TOF, m/z): calc'd for $C_{12}H_{16}N_3$ $[M+H]^+$: 202.1344; found 202.1315.

(E)-*N*-isopropyl-1-(thiazol-2-yl)methanimine (1p)



Prepared from thiazole-2-carbaldehyde (200 mg, 1.77 mmol) and isopropylamine (115 mg, 1.94 mmol) following General Procedure 1. After concentration in vacuo, **1p** (251 mg, 1.63 mmol, 92%) was obtained as a yellow oil.

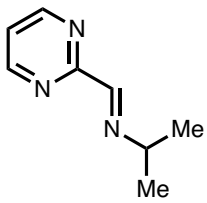
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 (s, 1H), 7.89 (d, *J* = 3.5 Hz, 1H), 7.38 (s, 1H), 3.65 (hept, *J* = 6.4 Hz, 1H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 167.7, 152.6, 144.0, 121.4, 61.4, 23.9.

FTIR (NaCl, thin film, cm^{-1}): 3080, 2969, 2966, 1636, 1507, 1490, 1458, 1418, 1362, 1294, 1235, 1132, 1058, 945, 853, 775, 733, 691, 629.

HRMS (FAB, m/z): calc'd for $C_7H_{11}N_2S$ $[M+H]^+$: 155.0643; found 155.0652.

(E)-*N*-isopropyl-1-(pyrimidin-2-yl)methanimine (1q)



Prepared from pyrimidine-2-carbaldehyde (120 mg, 1.11 mmol) and isopropylamine (72.2 mg, 1.22 mmol) following General Procedure 1. After concentration in vacuo, **1q** (75.1 mg, 0.50 mmol, 45%) was obtained as a yellow oil.

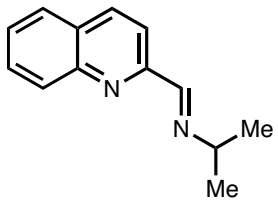
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.84 (d, *J* = 4.9 Hz, 1H), 8.43 (s, 1H), 7.29 (t, *J* = 5.4 Hz, 1H), 3.72 (hept, *J* = 6.4 Hz, 1H), 1.33 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.3, 158.3, 157.8, 121.2, 62.0, 24.0.

FTIR (NaCl, thin film, cm^{-1}): 3041, 2969, 3938, 3867, 1651, 1561, 1423, 1382, 1365, 1319, 1246, 1144, 994, 964, 944, 898, 818, 793, 634.

HRMS (FAB, m/z): calc'd for $C_8H_{12}N_3$ $[M+H]^+$: 150.1031; found 150.1043.

(E)-N-isopropyl-1-(quinolin-2-yl)methanimine (1r)



Prepared from quinoline-2-carbaldehyde (250 mg, 1.59 mmol) and isopropylamine (113 mg, 1.91 mmol) following General Procedure 1. After concentration in vacuo, **1r** (296 mg, 1.50 mmol, 94%) was obtained as a yellow oil.

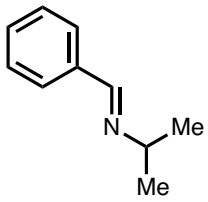
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.17 (s, 2H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.73 (t, *J* = 7.7 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 3.73 (hept, *J* = 6.2 Hz, 1H), 1.33 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 160.1, 155.3, 148.0, 136.7, 130.0, 129.7, 128.9, 127.9, 127.5, 118.7, 61.7, 24.2.

FTIR (NaCl, thin film, cm^{-1}): 3061, 2968, 2929, 2865, 1716, 1939, 1596, 1559, 1540, 1505, 1457, 1363, 1338, 1302, 1142, 966, 893, 833, 752, 620.

HRMS (FAB, m/z): calc'd for $C_{13}H_{15}N_{12}$ $[M+H]^+$: 199.1235; found 199.1210.

(*E*)-*N*-isopropyl-1-phenylmethanimine (7)



Prepared from benzaldehyde (157 mg, 1.48 mmol) and isopropylamine (105 mg, 1.77 mmol) following General Procedure 1. After concentration in vacuo, **7** (215 mg, 1.46 mmol, 99%) was obtained as a yellow oil.

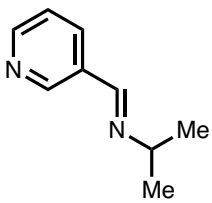
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (s, 1H), 7.77 – 7.69 (m, 2H), 7.40 (t, *J* = 3.9 Hz, 3H), 3.55 (hept, *J* = 6.3 Hz, 1H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 158.5, 136.7, 130.6, 128.7, 128.2, 61.9, 24.4.

FTIR (NaCl, thin film, cm^{-1}): 3061, 3026, 2967, 2931, 2836, 1647, 1581, 1450, 1382, 1306, 1159, 1141, 967, 881, 755, 693.

HRMS (FAB, m/z): calc'd for $C_{10}H_{13}N$ $[M+H]^+$: 148.1126; found 148.1125

(*E*)-*N*-isopropyl-1-(pyridin-3-yl)methanimine (8)



Prepared from nicotinaldehyde (151 mg, 1.41 mmol) and isopropylamine (91.9 mg, 1.55 mmol) following General Procedure 1. After concentration in vacuo, **8** (199 mg, 1.34 mmol, 95%) was obtained as a yellow oil.

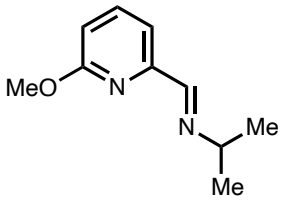
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.62 (d, *J* = 4.7 Hz, 1H), 8.33 (s, 1H), 8.11 (d, *J* = 5.9 Hz, 1H), 7.36 – 7.29 (m, 1H), 3.57 (hept, *J* = 12.6, 6.3 Hz, 1H), 1.27 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 155.6, 151.5, 150.4, 134.6, 132.2, 123.8, 24.2.

FTIR (NaCl, thin film, cm^{-1}): 2969, 2931, 2864, 1646, 1591, 1575, 1558, 1419, 1385, 1315, 1188, 1142, 1026, 975, 944, 882, 806, 708.

HRMS (FAB, m/z): calc'd for $C_9H_{13}N_2$ $[M+H]^+$: 149.1079; found 149.1086.

((E)-N-isopropyl-1-(6-methoxypyridin-2-yl)methanimine (S1a)



Prepared from 6-methoxypicolinaldehyde (250 mg, 1.82 mmol) and isopropylamine (129 mg, 2.19 mmol) following General Procedure 1. After concentration in vacuo, **S1a** (246 mg, 1.38 mmol, 76%) was obtained as a yellow oil.

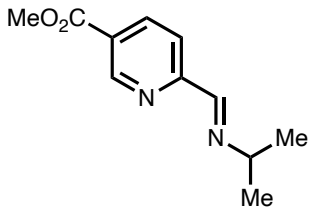
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (s, 1H), 7.64 – 7.56 (m, 2H), 6.75 (dd, *J* = 6.0, 3.0 Hz, 1H), 3.97 (s, 3H), 3.62 (p, *J* = 6.3 Hz, 1H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.0, 159.7, 152.7, 139.1, 114.1, 112.0, 61.6, 53.6, 24.2.

FTIR (NaCl, thin film, cm^{-1}): 2968, 2862, 1648, 1592, 1574, 1469, 1434, 1414, 1362, 1324, 1305, 1266, 1139, 1073, 1034, 988, 966, 866, 805, 765, 734, 631.

HRMS (FAB, m/z): calc'd for $C_{10}H_{15}N_2O$ $[M+H]^+$: 179.1184; found 179.1155.

Methyl (E)-6-((isopropylimino)methyl)nicotinate (S1b)



Prepared from methyl-6-formylnicotinate (237 mg, 1.43 mmol) and isopropylamine (127 mg, 2.15 mmol) following General Procedure 1. After concentration in vacuo, **S1b** (294 mg, 1.43 mmol, 99%) was obtained as a brown solid.

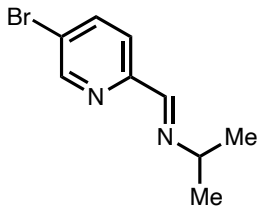
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.22 (s, 1H), 8.43 (s, 1H), 8.32 (d, *J* = 8.2 Hz, 1H), 8.08 (d, *J* = 9.7 Hz, 1H), 3.97 (s, 3H), 3.68 (hept, *J* = 6.4 Hz, 1H), 1.30 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 165.8, 158.7, 158.2, 150.8, 137.8, 126.6, 121.1, 61.9, 52.7, 24.1.

FTIR (NaCl, thin film, cm^{-1}): 2968, 2863, 1721, 1596, 1456, 1388, 1360, 1287, 1194, 1112, 1021, 965, 862, 776.

HRMS (FAB, m/z): calc'd for $C_{11}H_{15}N_2O_2$ $[M+H]^+$: 207.1134; found 207.1131.

(*E*)-1-(5-bromopyridin-2-yl)-*N*-isopropylmethanimine (S1c)



Prepared from 5-bromopicolinaldehyde (247 mg, 1.33 mmol) and isopropylamine (118 mg, 2.00 mmol) following General Procedure 1. After concentration in vacuo, **S1c** (282 mg, 1.24 mmol, 93%) was obtained as a colorless oil.

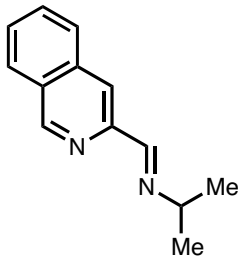
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (dd, J = 2.2, 0.8 Hz, 1H), 8.33 (d, J = 0.7 Hz, 1H), 7.94 – 7.80 (m, 2H), 3.64 (pd, J = 6.3, 0.8 Hz, 1H), 1.27 (d, J = 6.3 Hz, 5H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 158.34, 153.43, 150.59, 139.34, 122.61, 122.08, 61.60, 24.05.

FTIR (NaCl, thin film, cm^{-1}): 3046, 2969, 2926, 2867, 1645, 1570, 1553, 1462, 1380, 1363, 1314, 1141, 1087, 1006, 963, 945, 881, 837, 630.

HRMS (FAB, m/z): calc'd for $C_9H_{12}N_2Br$ $[M+H]^+$: 227.0184; found 227.0201.

(E)-N-isopropyl-1-(isoquinolin-3-yl)methanimine (S1d)



Prepared from isoquinoline-2-carbaldehyde (300 mg, 1.91 mmol) and isopropylamine (135 mg, 2.29 mmol) following General Procedure 1. After concentration in vacuo, **S1d** (370 mg, 1.87 mmol, 98%) was obtained as a yellow oil.

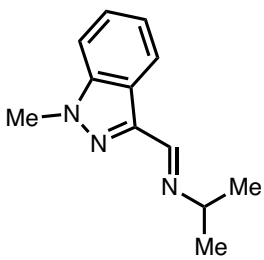
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.28 (s, 1H), 8.57 (s, 1H), 8.26 (s, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 8.3 Hz, 1H), 3.69 (hept, *J* = 5.9 Hz, 1H), 1.34 (d, *J* = 4.8 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.5, 152.8, 148.5, 136.2, 130.9, 129.3, 128.3, 127.8, 127.7, 119.5, 61.9, 24.3.

FTIR (NaCl, thin film, cm^{-1}): 2967, 2924, 2864, 1646, 1624, 1508, 1490, 1379, 1362, 1309, 1272, 1148, 970, 945, 894, 751.

HRMS (FAB, m/z): calc'd for $C_{13}H_{15}N_{12}$ $[M+H]^+$: 199.1235; found 199.1245.

(E)-N-isopropyl-1-(1-methyl-1H-indazol-3-yl)methanimine (S1e)

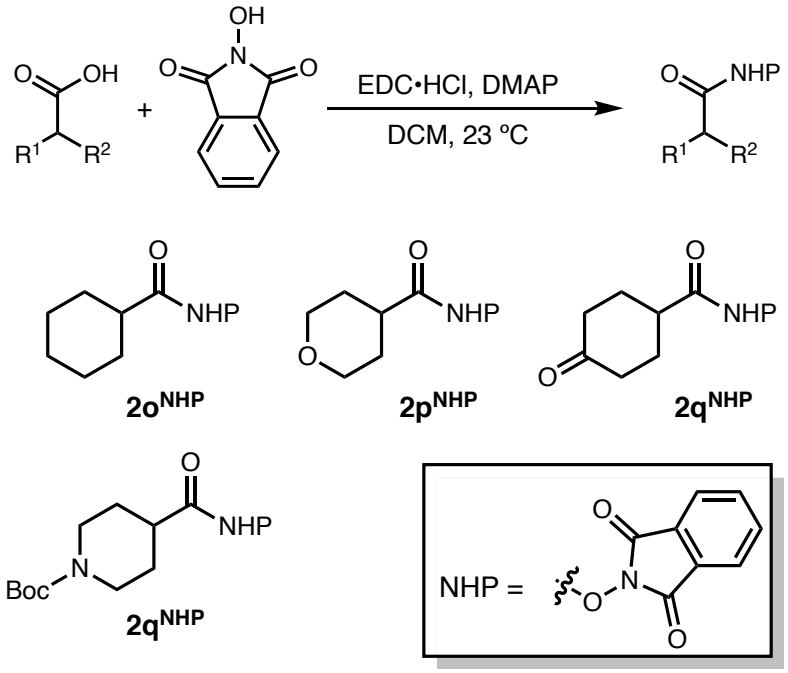


Prepared from 1-methyl-1H-indazole-3-carbaldehyde (200 mg, 1.25 mmol) and isopropylamine (88.6 mg, 1.50 mmol) following General Procedure 1. After concentration in vacuo, **S1e** (208 mg, 1.03 mmol, 83%) was obtained as a yellow oil.

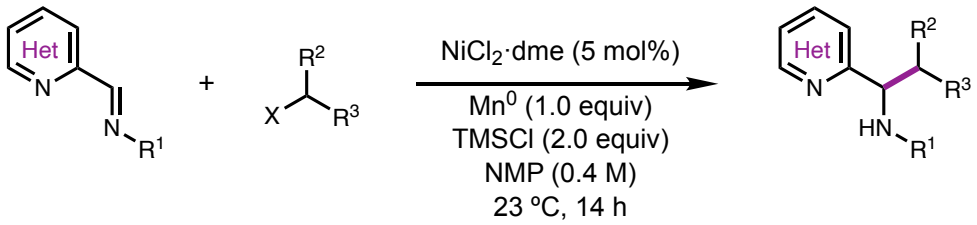
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (d, *J* = 0.8 Hz, 1H), 8.39 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.47 – 7.34 (m, 2H), 7.28 – 7.20 (m, 1H), 4.10 (s, 3H), 3.66 – 3.51 (m, 1H), 1.31 (d, *J* = 6.3 Hz, 6H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 152.4, 142.1, 141.2, 126.8, 123.2, 122.3, 121.9, 108.8, 62.1, 35.8, 24.4.
FTIR (NaCl, thin film, cm^{-1}): 3056, 2966, 2936, 2852, 1644, 1618, 1576, 1487, 1456, 1401, 1377, 1360, 1346, 1294, 1247, 1142, 1062, 1004, 961, 944, 864, 795, 768, 746, 660.
HRMS (FAB, m/z): calc'd for $C_{12}H_{16}N_3$ $[M+H]^+$: 202.1344; found 202.1320.

4.2. Synthesis of *N*-hydroxyphthalimide (NHP) Ester Substrates

NHP esters **2o^{NHP}-2r^{NHP}** were prepared according to procedure reported and referenced by Reisman and coworkers.[2] The NMR spectra of **2o^{NHP}** [3], **2p^{NHP}** [4], **2q^{NHP}** [5], and **2r^{NHP}** [5] matched those reported in the literature.



5. Nickel-Catalyzed Addition of Alkyl Electrophiles to Heteroaryl Imines



5.1. General procedure 3: Reaction on 0.3 mmol scale

On the bench-top, an oven-dried 1 dram vial, equipped with a stir bar, was charged with heteroarylimine (0.3 mmol, 1.0 equiv), alkyl halide (if non-volatile, 0.36 mmol, 1.2 equiv), and Mn^0 (16.5 mg, 0.3 mmol, 1.0 equiv). The vial was brought into a N_2-filled glovebox and a stock-solution of $NiCl_2$·dme in NMP (0.75 ml, 0.02 M, 0.05 equiv [Ni]), TMSCl (76 µl, 0.6 mmol, 2.0 equiv) and alkyl halide (if volatile, 0.36 mmol, 1.2 equiv) was added consecutively. The vial was sealed with a Teflon cap and taken out of the glove box. The vial was sealed with electrical tape and stirred at room temperature for 14 hours at 600 rpm. The resulting suspension was diluted with CH_2Cl_2 (0.5 ml) and extracted 3x with 1N HCl (0.5 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased. The resulting aqueous solution was extracted 3x with EtOAc and the combined organic phases were concentrated under reduced pressure at 40 °C until most of the NMP was removed. The crude material was purified by column chromatography to afford the desired product.

5.2. Challenging Substrates

Substrates not featured in the main text which undergo alkylation under the optimized conditions in poor yields. Products **S3a-S3e** were prepared from imines **S1a-S1e** reacted under standard conditions with 1.2 equivalents of benzyl bromide. Product **S4a** was prepared from reacting **1b** under standard reaction conditions with 1.2 equivalents of 4-iodo-1-tosylpiperidine. Yields are reported as the average of 2 runs based on isolated product on 0.3 mmol scale.

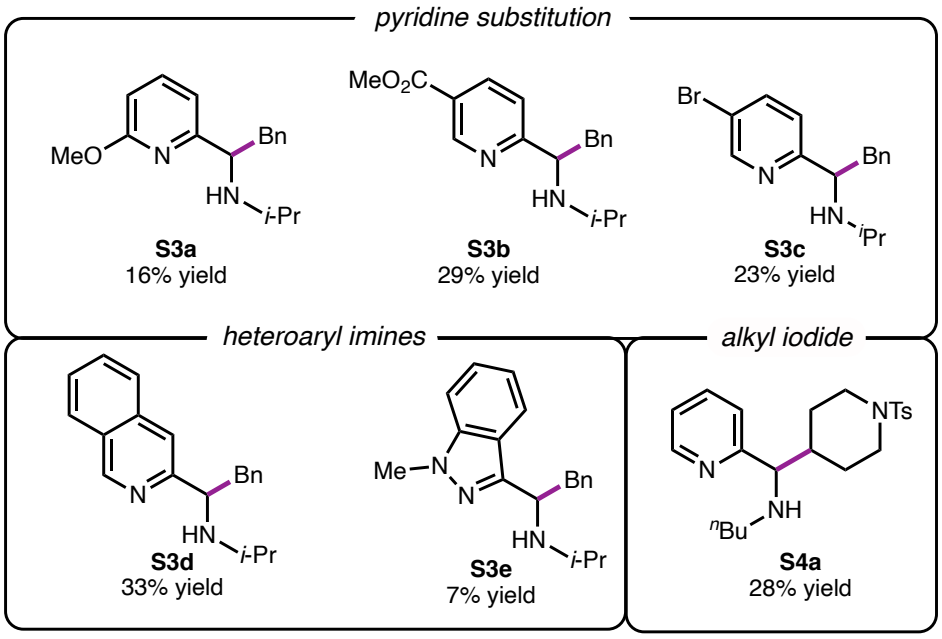
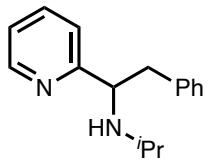


Figure S8: Imine and halide coupling partners that did not perform well in the alkylation reaction.

5.3. Characterization of Reaction Products: Scheme 1

***N*-(2-phenyl-1-(pyridin-2-yl)ethyl)propan-2-amine (3a)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3a** (56.0 mg, 0.23 mmol, 78%) as a colorless oil. Yield for duplicate run: 54.0 mg, 0.23 mmol, 75% – 76 % average yield.

Reaction was also performed on 1.0 mmol scale to afford **3a** (184 mg, 0.77 mmol, 77 %). Yield for duplicate run: 168 mg, 0.70 mmol, 70% – 74% average yield.

R_f = 0.27 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

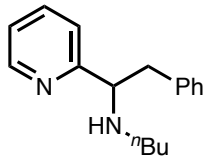
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.58 (d, *J* = 4.7 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 7.3 Hz, 2H), 7.18 – 7.08 (m, 2H), 7.05 (dd, *J* = 17.7, 7.6 Hz, 3H), 4.06 (t, *J* = 7.2 Hz, 1H), 3.04 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.98 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.57 (hept, *J* = 6.3 Hz, 1H), 1.77 (s, 1H), 0.96 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.5, 149.6, 139.0, 136.2, 129.4, 128.4, 126.4, 122.8, 122.1, 63.2, 46.2, 43.9, 24.2, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3328, 3062, 3038, 3005, 2964, 2928, 2868, 1682, 1590, 1572, 1556, 1494, 1470, 1454, 1434, 1379, 1368, 1337, 1295, 1266, 1175, 1148, 1126, 1083, 1049, 1030, 996, 775, 748, 701.

HRMS (ESI-TOF, m/z): calc'd for $C_{16}H_{21}N_2$ $[M+H]^+$: 241.1705; found 241.1693.

***N*-(2-phenyl-1-(pyridin-2-yl)ethyl)butan-1-amine (3b)**



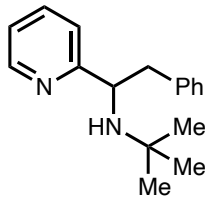
Prepared from imine **1b** (48.7 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3b** (56.0 mg, 0.22 mmol, 73%) as a colorless oil. Yield for duplicate run: 57.5 mg, 0.23 mmol, 75% – 74% average yield.

Also prepared from imine **1b** (48.7 mg, 0.3 mmol) and benzyl chloride (41.4 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3b** (54.6 mg, 0.21 mmol, 74%) as a colorless oil. Yield for duplicate run: 53.9 mg, 0.21 mmol, 71% – 72% average yield.

R_f = 0.30 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.58 (d, *J* = 4.9 Hz, 1H), 7.56 (td, *J* = 7.6, 1.8 Hz, 1H), 7.22 (t, *J* = 7.3 Hz, 2H), 7.20 – 7.10 (m, 3H), 7.09 (d, *J* = 7.0 Hz, 2H), 3.95 (t, *J* = 7.4 Hz, 1H), 3.07 (dd, *J* = 13.3, 6.5 Hz, 1H), 2.95 (dd, *J* = 13.3, 7.8 Hz, 1H), 2.45 – 2.32 (m, 2H), 1.83 (s, 1H), 1.42 – 1.32 (m, 2H), 1.27 – 1.14 (m, 2H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3, 149.5, 139.0, 136.4, 128.5, 126.5, 122.4, 122.2, 66.1, 47.8, 43.7, 32.4, 20.5, 14.1.
FTIR (NaCl, thin film, cm^{-1}): 3062, 3027, 2956, 2927, 2859, 1589, 1570, 1495, 1456, 1433, 1120, 996, 774, 748, 700, 668.
HRMS (ESI-TOF, m/z): calc'd for $C_{17}H_{23}N_2$ $[M+H]^+$: 255.1861; found 255.1859.

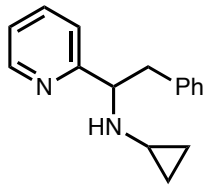
2-methyl-*N*-(2-phenyl-1-(pyridin-2-yl)ethyl)propan-2-amine (3c)



Prepared from imine **1c** (48.7 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3c** (60.0 mg, 0.24 mmol, 79%) as a colorless oil. Yield for duplicate run: 55.0 mg, 0.22 mmol, 72% – 76% average yield.

R_f = 0.42 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (d, *J* = 4.8 Hz, 1H), 7.58 (td, *J* = 7.6, 1.8 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.31 – 7.24 (m, 3H), 7.25 – 7.18 (m, 1H), 7.17 (d, *J* = 6.9 Hz, 2H), 7.12 (dd, *J* = 6.3, 4.9 Hz, 1H), 4.13 (dd, *J* = 8.9, 5.7 Hz, 1H), 3.06 (dd, *J* = 13.3, 5.7 Hz, 1H), 2.76 (dd, *J* = 13.3, 8.9 Hz, 1H), 1.84 (s, 1H), 0.86 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 166.6, 149.0, 139.2, 136.2, 129.6, 128.5, 126.5, 122.3, 121.7, 60.6, 51.3, 45.6, 29.6.
FTIR (NaCl, thin film, cm^{-1}): 3063, 3027, 2961, 2928, 1590, 1570, 1495, 1472, 1456, 1434, 1388, 1364, 1229, 1108, 1030, 995, 774, 746, 700.
HRMS (ESI-TOF, m/z): calc'd for $C_{17}H_{23}N_2$ $[M+H]^+$: 255.1861; found 255.1848.

***N*-(2-phenyl-1-(pyridin-2-yl)ethyl)cyclopropanamine (3d)**



Prepared from imine **1d** (43.9 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3d** (50.0 mg, 0.21 mmol, 70%) as a colorless oil. Yield for duplicate run: 46.0 mg, 0.19 mmol, 64% – 67% average yield.

R_f = 0.27 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

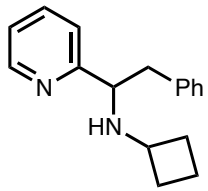
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.60 (d, *J* = 5.0 Hz, 1H), 7.52 (td, *J* = 7.6, 1.8 Hz, 1H), 7.19 (t, *J* = 7.2 Hz, 2H), 7.17 – 7.10 (m, 2H), 7.06 – 7.00 (m, 3H), 4.05 (t, *J* = 7.2 Hz, 1H), 3.10 – 2.97 (m, 2H), 2.20 (s, 1H), 1.96 – 1.88 (m, 1H), 0.35 – 0.25 (m, 3H), 0.25 – 0.19 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.2, 149.6, 139.0, 136.1, 129.5, 128.4, 126.3, 123.1, 122.2, 66.1, 43.2, 29.3, 7.1, 6.1.

FTIR (NaCl, thin film, cm^{-1}): 3325, 2084, 3006, 2928, 1684, 1590, 1570, 1496, 1472, 1455, 1434, 1369, 1338, 1216, 1148, 1088, 1015, 773, 747, 700.

HRMS (FAB, m/z): calc'd for $C_{16}H_{19}N_2$ $[M+H]^+$: 239.1548; found 239.1555.

***N*-(2-phenyl-1-(pyridin-2-yl)ethyl)cyclobutanamine (3e)**



Prepared from imine **1e** (48.1 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3e** (54.0 mg, 0.21 mmol, 71%) as a colorless oil. Yield for duplicate run: 52.0 mg, 0.21 mmol, 69% – 70% average yield.

R_f = 0.21 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

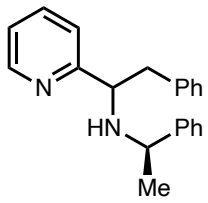
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.57 (d, *J* = 3.4 Hz, 1H), 7.55 (td, *J* = 7.7, 1.8 Hz, 1H), 7.23 (t, *J* = 7.3 Hz, 2H), 7.20 – 7.10 (m, 3H), 7.09 (d, *J* = 7.0 Hz, 2H), 3.95 (dt, *J* = 1627.0, 7.3 Hz, 1H), 3.12 – 3.02 (m, 2H), 2.93 (dd, *J* = 13.3, 8.0 Hz, 2H), 2.15 – 2.07 (m, 1H), 2.02 (s, 1H), 1.91 – 1.79 (m, 1H), 1.58 – 1.39 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3, 149.4, 138.9, 129.4, 128.5, 126.5, 122.4, 122.2, 63.8, 52.6, 43.6, 31.6, 31.6, 14.8.

FTIR (NaCl, thin film, cm^{-1}): 3321, 3061, 3026, 2968, 2932, 2853, 1590, 1570, 1495, 1472, 1455, 1434, 1340, 1237, 1161, 1119, 1076, 1049, 996, 774, 747, 700.

HRMS (FAB, m/z): calc'd for $C_{17}H_{21}N_2$ $[M+H]^+$: 253.1705; found 253.1691.

2-phenyl-*N*-((*S*)-1-phenylethyl)-1-(pyridin-2-yl)ethan-1-amine (3f)



Prepared from imine **1f** (63.1 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded a 1.8:1 mixture of diastereomers of **3f** (55.0 mg, 0.18 mmol, 61%) as a colorless oil. Yield for duplicate run: 43.0 mg, 0.14 mmol, 47% – 54% average yield.

R_f = 0.39 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

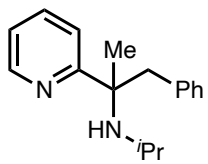
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.66 (d, *J* = 6.5 Hz, 1H, *minor*), 8.59 (d, *J* = 4.9 Hz, 1H, *major*), 7.57 (td, *J* = 7.6, 1.8 Hz, 1H, *minor*), 7.46 (td, *J* = 7.6, 1.8 Hz, 1H, *major*), 7.28 – 7.16 (m, 17H), 7.11 (dd, *J* = 7.6, 4.8 Hz, 1H, *major*), 7.01 (q, *J* = 9.9, 8.7 Hz, 5H, *major*), 6.93 (d, *J* = 6.6 Hz, 1H, *major*), 4.03 (t, *J* = 7.0 Hz, 1H, *major*), 3.77 (q, *J* = 6.5 Hz, 1H, *major*), 3.71 (dd, *J* = 8.2, 6.4 Hz, 1H, *minor*), 3.46 (q, *J* = 6.6 Hz, 1H, *minor*), 3.15 (dd, *J* = 13.2, 6.6 Hz, 1H, *major*), 3.08 (dd, *J* = 13.2, 7.4 Hz, 1H, *major*), 3.03 (dd, *J* = 13.4, 6.4 Hz, 1H, *minor*), 2.94 (dd, *J* = 13.4, 8.3 Hz, 1H, *minor*), 1.98 (s, 2H), 1.34 (d, *J* = 6.5 Hz, 6H, *major*), 1.27 (d, *J* = 6.6 Hz, 6H, *minor*).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.4 (*minor*), 163.0 (*major*), 149.8 (*minor*), 149.4 (*major*), 145.9 (*major*), 145.5 (*minor*), 138.99 (*major*), 138.96 (*minor*), 136.2 (*minor*), 136.1 (*major*), 129.54 (*minor*), 129.50 (*major*), 128.49 (*minor*), 128.45 (*major*), 128.35 (*major*), 128.32 (*minor*), 126.93 (*minor*), 126.91 (*major*), 126.8, 126.32 (*minor*), 126.29 (*major*), 122.9 (*minor*), 122.8 (*major*), 122.1 (*minor*), 122.0 (*major*), 63.4 (*major*), 62.6 (*minor*), 55.7, 43.9 (*minor*), 42.9 (*major*), 25.4 (*minor*), 23.2 (*major*).

FTIR (NaCl, thin film, cm^{-1}): 3060, 3026, 3963, 2922, 2860, 1589, 1570, 1493, 1472, 1455, 1435, 1369, 1207, 1127, 748, 700.

HRMS (FAB, m/z): calc'd for $C_{21}H_{23}N_2$ $[M+H]^+$: 303.1861; found 303.1848.

***N*-isopropyl-1-phenyl-2-(pyridin-2-yl)propan-2-amine (3g)**



Prepared from imine **3g** (48.7 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3g** (28.0 mg, 0.11 mmol, 37%) as a colorless oil. Yield for duplicate run: 28.0 mg, 0.11 mmol, 37% – 37% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.65 (d, *J* = 4.7 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.15 – 7.09 (m, 1H), 7.06 (dt, *J* = 14.6, 7.6 Hz, 4H), 6.65 (d, *J* = 6.9 Hz, 2H), 3.17 (d, *J* = 12.7 Hz, 1H),

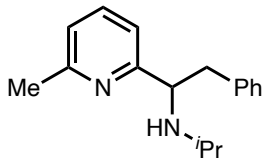
2.95 (d, *J* = 12.7 Hz, 1H), 2.66 (hept, *J* = 6.4 Hz, 1H), 1.50 (s, 3H), 1.08 (d, *J* = 6.1 Hz, 3H), 0.84 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 165.8, 148.8, 137.9, 135.7, 130.6, 127.7, 126.2, 121.9, 121.6, 62.1, 50.6, 44.4, 26.3, 25.3, 22.4.

FTIR (NaCl, thin film, cm^{-1}): 3337, 3061, 3028, 2960, 2866, 1698, 1587, 1570, 1496, 1456, 1431, 1376, 1339, 1168, 1093, 993, 794, 749, 703, 633.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2$ $[M+H]^+$: 255.1861; found 255.1843.

***N*-(1-(6-methylpyridin-2-yl)-2-phenylethyl)propan-2-amine (3h)**



Prepared from imine **1h** (48.7 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3h** (39.0 mg, 0.15 mmol, 51%) as a colorless oil. Yield for duplicate run: 38.0 mg, 0.15 mmol, 50% – 50% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

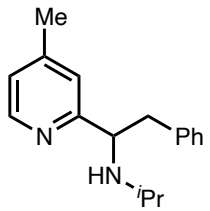
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.18 (m, 2H), 7.17 – 7.13 (m, 1H), 7.08 – 7.02 (m, 2H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 4.05 (t, *J* = 7.1 Hz, 1H), 3.06 (dd, *J* = 13.3, 7.0 Hz, 1H), 2.96 (dd, *J* = 13.6, 7.2 Hz, 1H), 2.63 – 2.57 (m, 1H), 2.56 (s, 3H), 0.97 (dd, *J* = 6.2, 1.8 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.9, 158.1, 139.1, 136.3, 129.5, 128.4, 126.3, 121.6, 119.5, 63.1, 46.2, 43.8, 24.8, 24.2, 22.3.

FTIR (NaCl, thin film, cm^{-1}): 3325, 3061, 3026, 2961, 2927, 2866, 1592, 1576, 1559, 1456, 1377, 1339, 1170, 1085, 1031, 996, 792, 746, 700.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2$ $[M+H]^+$: 255.1861; found 255.1865.

N-(1-(4-methylpyridin-2-yl)-2-phenylethyl)propan-2-amine (3i)



Prepared from imine **1i** (48.7 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3i** (57.0 mg, 0.23 mmol, 75%) as a colorless oil. Yield for duplicate run: 55.0 mg, 0.14 mmol, 72% – 74% average yield.

R_f = 0.16 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

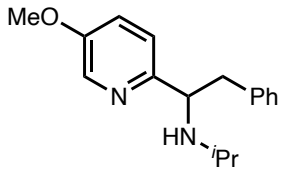
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (d, *J* = 5.0 Hz, 1H), 7.05 (d, *J* = 7.1 Hz, 2H), 6.96 – 6.90 (m, 2H), 4.02 (t, *J* = 7.2 Hz, 1H), 3.04 (dd, *J* = 13.3, 7.0 Hz, 1H), 2.94 (dd, *J* = 13.3, 7.4 Hz, 1H), 2.57 (hept, *J* = 6.2 Hz, 1H), 2.26 (s, 3H), 1.87 (s, 1H), 0.95 (t, *J* = 6.6 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.2, 149.2, 147.3, 139.1, 129.4, 128.4, 126.3, 123.5, 123.1, 63.1, 46.2, 43.8, 24.2, 22.2, 21.2.

FTIR (NaCl, thin film, cm^{-1}): 3307, 3059, 3026, 2962, 2924, 2865, 1604, 1559, 1455, 1378, 1339, 1174, 1084, 1030, 998, 823, 743, 700.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2$ $[M+H]^+$: 255.1861; found 255.1859.

***N*-(1-(5-methoxypyridin-2-yl)-2-phenylethyl)propan-2-amine (3j)**



Prepared from imine **1j** (53.5 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3j** (54.0 mg, 0.20 mmol, 67%) as a colorless oil. Yield for duplicate run: 51.0 mg, 0.019 mmol, 63% – 65% average yield.

R_f = 0.16 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

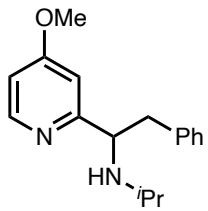
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (d, *J* = 2.9 Hz, 1H), 7.23 – 7.16 (m, 2H), 7.17 – 7.11 (m, 1H), 7.07 – 7.00 (m, 3H), 6.97 (d, *J* = 8.5 Hz, 1H), 4.02 (t, *J* = 7.2 Hz, 1H), 3.84 (s, 3H), 3.05 – 2.93 (m, 2H), 2.55 (hept, *J* = 6.2 Hz, 1H), 1.83 (s, 1H), 0.95 (dd, *J* = 6.2, 2.6 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 155.3, 154.6, 139.1, 137.1, 129.4, 128.4, 126.3, 122.9, 120.6, 62.4, 55.8, 46.1, 43.9, 24.2, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3026, 2961, 2837, 1574, 1491, 1475, 1396, 1339, 1266, 1176, 1125, 1078, 1032, 831, 749, 700.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2O$ $[M+H]^+$: 271.1810; found 271.1804.

***N*-(1-(4-methoxypyridin-2-yl)-2-phenylethyl)propan-2-amine (3k)**



Prepared from imine **1k** (53.5 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3k** (60.0 mg, 0.22 mmol, 74%) as a colorless oil. Yield for duplicate run: 56.0 mg, 0.21 mmol, 69% – 72% average yield.

R_f = 0.13 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

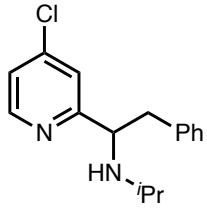
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 – 8.36 (m, 1H), 7.24 – 7.18 (m, 2H), 7.18 – 7.12 (m, 1H), 7.07 (d, *J* = 7.0 Hz, 2H), 6.68 – 6.62 (m, 2H), 4.01 (t, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 3.04 (dd, *J* = 13.3, 6.9 Hz, 1H), 2.92 (dd, *J* = 13.3, 7.5 Hz, 1H), 2.57 (hept, *J* = 6.2 Hz, 1H), 1.92 (s, 1H), 0.96 (d, *J* = 6.3 Hz, 3H), 0.94 (d, *J* = 6.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 166.0, 165.5, 150.6, 139.0, 129.4, 128.4, 126.4, 108.6, 108.2, 63.3, 55.2, 46.3, 43.7, 24.2, 22.2.

FTIR (NaCl, thin film, cm^{-1}): δ 3025, 2963, 1596, 1569, 1479, 1457, 1367, 1302, 1166, 1039, 994, 820, 742, 700.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2O$ $[M+H]^+$: 271.1810; found 271.1796.

***N*-(1-(4-chloropyridin-2-yl)-2-phenylethyl)propan-2-amine (3l)**



Prepared from imine **1l** (54.8 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3l** (35.0 mg, 0.13 mmol, 42%) as a colorless oil. Yield for duplicate run: 34.0 mg, 0.12 mmol, 41% – 42% average yield.

R_f = 0.32 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

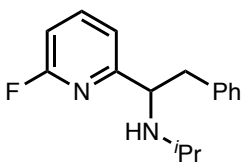
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 (d, *J* = 5.3 Hz, 1H), 7.26 – 7.16 (m, 4H), 7.14 (dd, *J* = 5.3, 2.0 Hz, 1H), 7.09 – 7.04 (m, 2H), 4.09 – 4.02 (m, 1H), 3.04 (dd, *J* = 13.4, 6.6 Hz, 1H), 2.90 (dd, *J* = 13.4, 7.7 Hz, 1H), 2.55 (hept, *J* = 6.3 Hz, 1H), 1.71 (s, 1H), 0.94 (dd, *J* = 10.9, 6.2 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 165.9, 150.3, 144.4, 138.5, 129.4, 128.6, 126.6, 122.8, 122.5, 63.1, 46.5, 43.7, 24.2, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3027, 2963, 2928, 2865, 1697, 1574, 1557, 1457, 1389, 1367, 1339, 1174, 1127, 1096, 826, 745, 700.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2Cl$ $[M+H]^+$: 275.1315; found 275.1330.

***N*-(1-(6-fluoropyridin-2-yl)-2-phenylethyl)propan-2-amine (3m)**



Prepared from imine **1m** (49.9 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3m** (35.0 mg, 0.14 mmol, 45%) as a colorless oil. Yield for duplicate run: 34.0 mg, 0.13 mmol, 44% – 44% average yield.

R_f = 0.35 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

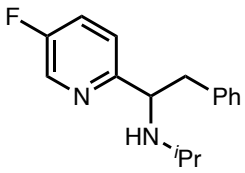
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.59 (q, *J* = 7.9 Hz, 1H), 7.23 – 7.11 (m, 3H), 7.02 (d, *J* = 6.7 Hz, 2H), 6.92 (dd, *J* = 7.3, 2.5 Hz, 1H), 6.75 (dd, *J* = 8.0, 2.8 Hz, 1H), 4.00 (t, *J* = 7.2 Hz, 1H), 3.00 (qd, *J* = 13.3, 7.2 Hz, 2H), 2.56 (hept, *J* = 6.2 Hz, 1H), 1.85 (s, 1H), 0.97 (dd, *J* = 11.7, 6.2 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.8 (d, *J* = 216.9 Hz), 162.8 (d, *J* = 10.6 Hz), 141.1 (d, *J* = 7.7 Hz), 138.6, 129.4, 128.5, 126.5, 120.0 (d, *J* = 3.9 Hz), 107.6 (d, *J* = 37.1 Hz), 62.5, 46.2, 43.4, 24.2, 22.1.

FTIR (NaCl, thin film, cm^{-1}): 3322, 3063, 3028, 2964, 2926, 2866, 1603, 1575, 1494, 1445, 1380, 1368, 1338, 1269, 1222, 1174, 1147, 1070, 995, 943, 916, 894, 845, 802, 744, 701.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2F$ $[M+H]^+$: 259.1611; found 259.1598.

***N*-(1-(5-fluoropyridin-2-yl)-2-phenylethyl)propan-2-amine (3n)**



Prepared from imine **1n** (49.9 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3n** (48.9 mg, 0.19 mmol, 63%) as a colorless oil. Yield for duplicate run: 43.0 mg, 0.17 mmol, 55% – 59% average yield.

R_f = 0.29 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

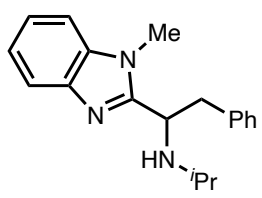
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.43 (s, 1H), 7.26 – 7.12 (m, 4H), 7.07 (dd, *J* = 8.7, 4.5 Hz, 1H), 7.02 (d, *J* = 7.3 Hz, 2H), 4.08 (t, *J* = 7.2 Hz, 1H), 3.03 – 2.92 (m, 2H), 2.55 (hept, *J* = 6.3 Hz, 1H), 1.85 (s, 1H), 0.95 (d, *J* = 6.1 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.48 (d, *J* = 3.7 Hz), 158.5 (d, *J* = 254 Hz), 157.5, 138.7, 137.6 (d, *J* = 23.5 Hz), 129.4, 128.5, 126.5, 123.4 (d, *J* = 3.9 Hz), 122.9 (d, *J* = 17.8 Hz), 62.6, 46.3, 43.9, 24.2, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3062, 3027, 2963, 3928, 2867, 1683, 1584, 1480, 1455, 1388, 1368, 1340, 1225, 1171, 1112, 1020, 956, 909, 838, 750, 700.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2F$ $[M+H]^+$: 259.1611; found 259.1610.

***N*-(1-(1-methyl-1H-benzo[d]imidazol-2-yl)-2-phenylethyl)propan-2-amine (3o)**



Prepared from imine **1o** (60.4 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3o** (67.0 mg, 0.23 mmol, 76%) as a colorless oil. Yield for duplicate run: 64.0 mg, 0.22 mmol, 73% – 74% average yield.

R_f = 0.09 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

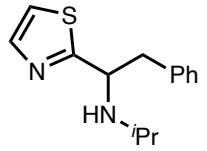
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.5 Hz, 1H), 7.32 – 7.13 (m, 6H), 6.98 (d, *J* = 4.6 Hz, 2H), 4.30 (dd, *J* = 9.1, 5.9 Hz, 1H), 3.33 (dd, *J* = 12.9, 5.7 Hz, 1H), 3.27 (s, 3H), 3.19 – 3.11 (m, 1H), 2.72 (hept, *J* = 6.0 Hz, 1H), 2.20 (s, 1H), 1.04 (dd, *J* = 14.3, 6.2 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 156.8, 142.6, 138.1, 135.7, 129.4, 128.6, 126.8, 122.3, 122.1, 119.5, 109.4, 55.5, 46.2, 43.2, 29.3, 23.9, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3322, 3028, 2963, 1670, 1472, 1406, 1338, 1281, 1239, 1175, 1084, 1007, 852, 745, 702, 681.

HRMS (FAB, m/z): calc'd for $C_{19}H_{24}N_3$ $[M+H]^+$: 294.1970; found 294.1973.

***N*-(2-phenyl-1-(thiazol-2-yl)ethyl)propan-2-amine (3p)**



Prepared from imine **1p** (61.6 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3p** (40.0 mg, 0.16 mmol, 54%) as a colorless oil. Yield for duplicate run: 37.0 mg, 0.15 mmol, 50% – 52% average yield.

R_f = 0.41 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

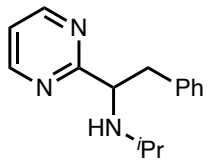
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.76 (d, *J* = 3.3 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.28 – 7.23 (m, 2H), 7.23 – 7.19 (m, 2H), 4.41 (dd, *J* = 9.0, 5.1 Hz, 1H), 3.28 (dd, *J* = 13.6, 5.1 Hz, 1H), 2.91 (dd, *J* = 13.6, 9.0 Hz, 1H), 2.71 (hept, *J* = 6.3 Hz, 1H), 1.64 (s, 1H), 1.01 (d, *J* = 6.4 Hz, 3H), 0.89 (d, *J* = 6.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 178.1, 142.7, 137.8, 129.4, 128.8, 127.0, 118.9, 59.8, 47.3, 44.3, 24.1, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3064, 3028, 2961, 2925, 2864, 1698, 1497, 1473, 1456, 1381, 1368, 1319, 1177, 1124, 1056, 773, 726, 700.

HRMS (FAB, m/z): calc'd for $C_{16}H_{21}N_2$ $[M+H]^+$: 247.1269; found 247.1244.

***N*-(2-phenyl-1-(pyrimidin-2-yl)ethyl)propan-2-amine (3q)**



Prepared from imine **1q** (44.8 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3q** (36.0 mg, 0.15 mmol, 50%) as a colorless oil. Yield for duplicate run: 34.0 mg, 0.14 mmol, 47% – 48% average yield.

R_f = 0.10 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

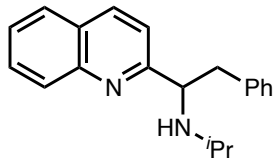
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (d, *J* = 6.7 Hz, 2H), 7.20 – 7.07 (m, 4H), 7.01 (d, *J* = 7.2 Hz, 2H), 4.27 (t, *J* = 7.2 Hz, 2H), 3.15 (dd, *J* = 13.4, 6.6 Hz, 1H), 3.06 (dd, *J* = 13.4, 7.7 Hz, 1H), 2.58 (hept, *J* = 6.1 Hz, 1H), 1.94 (s, 1H), 1.01 (d, *J* = 6.2 Hz, 3H), 0.96 (d, *J* = 6.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 172.8, 157.0, 138.4, 129.3, 128.4, 126.3, 119.2, 63.8, 46.5, 42.9, 24.0, 22.4.

FTIR (NaCl, thin film, cm^{-1}): 3420, 3029, 2965, 2866, 1561, 1541, 1496, 1455, 1437, 1418, 1380, 1339, 1174, 1085, 1030, 995, 805, 751, 700.

HRMS (FAB, m/z): calc'd for $C_{15}H_{20}N_3$ $[M+H]^+$: 242.1657; found 242.1662.

***N*-(2-phenyl-1-(quinolin-2-yl)ethyl)propan-2-amine (3r)**



Prepared from imine **1r** (59.5 mg, 0.3 mmol) and benzyl bromide (42.8 μL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **3r** (44.0 mg, 0.15 mmol, 51%) as a colorless oil. Yield for duplicate run: 43.5 mg, 0.15 mmol, 50% – 50% average yield.

R_f = 0.31 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

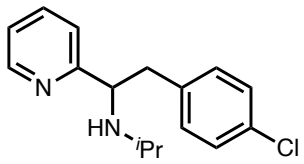
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.25 – 7.11 (m, 5H), 4.31 (t, *J* = 7.2 Hz, 1H), 3.15 (dd, *J* = 13.5, 6.4 Hz, 1H), 3.00 (dd, *J* = 13.5, 8.0 Hz, 1H), 2.61 (hept, *J* = 5.9 Hz, 1H), 1.80 (s, 1H), 0.96 (dd, *J* = 14.4, 4.7 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.8, 148.0, 138.8, 136.2, 129.5, 129.4, 129.3, 128.5, 127.8, 127.7, 126.5, 126.1, 120.6, 64.0, 46.8, 43.9, 24.3, 22.4.

FTIR (NaCl, thin film, cm^{-1}): 3028, 2961, 2928, 1618, 1600, 1558, 1540, 1506, 1473, 1456, 1379, 1169, 826, 750, 700.

HRMS (FAB, m/z): calc'd for $C_{20}H_{23}N_2$ $[M+H]^+$: 291.1861; found 291.1876.

***N*-(2-(4-chlorophenyl)-1-(pyridin-2-yl)ethyl)propan-2-amine (4a)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1-(bromomethyl)-4-chlorobenzene (74.0 mg, 0.36 mmol) and following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4a** (64.1 mg, 0.23 mmol, 78%) as a colorless oil. Yield for duplicate run: 53.3 mg, 0.20 mmol, 65% – 72% average yield.

R_f = 0.24 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

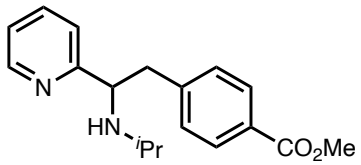
^{1}H NMR (400 MHz, $CDCl_3$): 8.50 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.44 (td, J = 7.6, 1.8 Hz, 1H), 7.11 – 7.01 (m, 3H), 6.95 (dt, J = 7.8, 1.1 Hz, 1H), 6.89 – 6.83 (m, 2H), 3.93 (t, J = 7.2 Hz, 1H), 2.90 (dd, J = 7.2, 1.6 Hz, 2H), 2.48 (p, J = 6.3 Hz, 1H), 1.84 (s, 1H), 0.88 (dd, J = 6.2, 1.3 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.83, 149.46, 137.30, 136.03, 131.91, 130.57, 128.28, 122.64, 122.00, 62.81, 45.94, 42.90, 23.99, 22.04.

FTIR (NaCl, thin film, cm^{-1}): 3309, 3005, 2962, 2925, 2865, 1589, 1570, 1490, 1469, 1433, 1379, 1367, 1338, 1174, 1092, 1015, 812, 776, 748.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2Cl$ $[M+H]^+$: 275.1315; found: 275.1328.

Methyl 4-(2-(isopropylamino)-2-(pyridin-2-yl)ethyl)benzoate (4b)



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and methyl 4-(bromomethyl)benzoate (82.5 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4b** (68.1 mg, 0.23 mmol, 76%) as a white solid. Yield for duplicate run: 55.7 mg, 0.19 mmol, 62% – 69% average yield.

R_f = 0.21 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

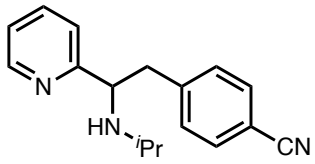
^{1}H NMR (400 MHz, $CDCl_3$): 8.48 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.88 – 7.66 (m, 2H), 7.39 (td, J = 7.6, 1.8 Hz, 1H), 7.09 – 6.93 (m, 3H), 6.89 (dt, J = 7.8, 1.1 Hz, 1H), 3.95 (t, J = 7.2 Hz, 1H), 3.77 (s, 3H), 2.96 (d, J = 7.2 Hz, 2H), 2.46 (p, J = 6.2 Hz, 1H), 1.86 (s, 2H), 0.85 (d, J = 6.3 Hz, 7H).

^{13}C NMR (101 MHz, $CDCl_3$): 162.22, 149.64, 144.73, 136.12, 131.91, 130.04, 122.62, 122.20, 119.02, 109.97, 62.46, 45.84, 43.61, 23.96, 22.05.

FTIR (NaCl, thin film, cm^{-1}): 3311**,** 2960, 2867, 1721, 1609, 1589, 1570, 1469, 1434, 1414, 1309, 1280, 1178, 1111, 765, 749, 706.

HRMS (FAB, m/z): calc'd for $C_{18}H_{23}N_2O_2$ $[M+H]^+$: 299.1760; found: 299.1767.

4-(2-(isopropylamino)-2-(pyridin-2-yl)ethyl)benzonitrile (4c)



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 4-(bromomethyl)benzonitrile (70.6 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4c** (55.2mg, 0.21 mmol, 69%) as a white solid. Yield for duplicate run: 51.4 mg, 0.20 mmol, 65% – 67% average yield.

R_f = 0.15 (silica, EtOAc, UV).

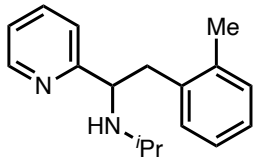
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.67 – 8.51 (m, 1H), 7.52 (td, *J* = 7.6, 1.8 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.14 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 7.7 Hz, 1H), 4.02 (t, *J* = 7.2 Hz, 1H), 3.15 – 2.95 (m, 2H), 2.56 (hept, *J* = 6.1 Hz, 1H), 1.26 (d, *J* = 3.1 Hz, 1H), 0.98 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$):δ 162.22, 149.64, 144.73, 136.12, 131.91, 130.04, 122.62, 122.20, 119.02, 109.97, 62.46, 45.84, 43.61, 23.96, 22.05.

FTIR (NaCl, thin film, cm^{-1}): 3316, 3049, 2962, 2929, 2866, 2226, 1606, 1589, 1570, 1505, 1470, 1433, 1379, 1337, 1175, 1147, 996, 823, 780, 751.

HRMS (FAB, m/z): calc'd for $C_{17}H_{20}N_3$ $[M+H]^+$: 266.1657; found: 266.1677.

***N*-(1-(pyridin-2-yl)-2-(*o*-tolyl)ethyl)propan-2-amine (4d)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1-(bromomethyl)-2-methylbenzene (66.6 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4d** (60.0 mg, 0.24 mmol, 79%) as a white solid. Yield for duplicate run: 56.3 mg, 0.22 mmol, 74% – 76% average yield.

R_f = 0.18 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

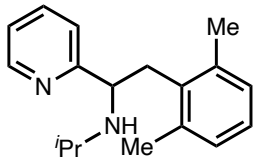
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.35 (td, *J* = 7.6, 1.8 Hz, 1H), 7.02 – 6.92 (m, 3H), 6.92 – 6.86 (m, 1H), 6.83 (dt, *J* = 7.8, 1.1 Hz, 1H), 6.81 – 6.76 (m, 1H), 3.93 (dd, *J* = 8.0, 6.5 Hz, 1H), 3.04 – 2.77 (m, 2H), 2.46 (p, *J* = 6.2 Hz, 1H), 2.08 (s, 3H), 2.03 – 1.90 (s, 1H), 0.96 – 0.79 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.33, 149.40, 137.07, 136.54, 135.83, 130.15, 129.95, 126.21, 125.62, 122.74, 121.89, 61.89, 46.03, 40.99, 24.04, 22.12, 19.42.

FTIR (NaCl, thin film, cm^{-1}): 3317, 3061, 3009, 2961, 2928, 2864, 1681, 1589, 1569, 1468, 1432, 1378, 1365, 1339, 1169, 1147, 1125, 1049, 995, 841, 781, 741.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2$ $[M+H]^+$: 255.1861; found: 255.1864.

***N*-(2-(2,6-dimethylphenyl)-1-(pyridin-2-yl)ethyl)propan-2-amine (4e)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 2-(bromomethyl)-1,3-dimethylbenzene (71.6 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4e** (58.5 mg, 0.22 mmol, 73 %) as a white solid. Yield for duplicate run: 55.0 mg, 0.20 mmol, 68% – 70% average yield.

R_f = 0.16 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

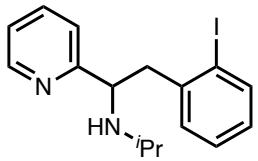
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.40 (td, *J* = 7.6, 1.8 Hz, 1H), 7.09 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 6.94 (dd, *J* = 8.3, 6.5 Hz, 1H), 6.88 (d, *J* = 7.4 Hz, 2H), 6.69 (dt, *J* = 7.7, 1.1 Hz, 1H), 3.95 (dd, *J* = 9.2, 5.3 Hz, 1H), 3.10 (dd, *J* = 13.4, 5.3 Hz, 1H), 2.96 (dd, *J* = 13.5, 9.3 Hz, 1H), 2.53 (hept, *J* = 6.2 Hz, 1H), 2.04 (s, 6H), 1.95 (brs, 4H), 0.99 (dd, *J* = 11.6, 6.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.06, 149.42, 137.13, 135.74, 128.04, 125.97, 123.07, 121.97, 60.95, 45.97, 37.92, 24.10, 22.07, 20.02.

FTIR (NaCl, thin film, cm^{-1}): 3308, 3065, 3007, 2961, 2867, 1687, 1588, 1569, 1468, 1432, 1378, 1366, 1171, 1146, 1096, 995, 769, 749.

HRMS (FAB, m/z): calc'd for $C_{18}H_{25}N_2$ $[M+H]^+$: 269.2018; found: 269.2020.

***N*-(2-(2-iodophenyl)-1-(pyridin-2-yl)ethyl)propan-2-amine (4f)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1-(bromomethyl)-2-iodobenzene (107 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4f** (77.3 mg, 0.21 mmol, 70%) as a pale yellow oil.

R_f = 0.22 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N). Yield for duplicate run: 69.6 mg, 0.19 mmol, 63% – 67% average yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.62 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.79 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.47 (td, *J* = 7.6, 1.8 Hz, 1H), 7.13 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 7.07 (td, *J* = 7.4, 1.3 Hz, 1H), 6.93 (dt, *J* = 7.7, 1.1 Hz, 1H), 6.83 (td, *J* = 7.6, 1.7 Hz, 1H), 6.78 (dd, *J* = 7.6, 1.7 Hz,

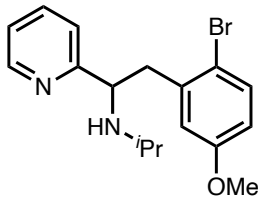
1H), 4.19 (dd, *J* = 8.5, 6.2 Hz, 1H), 3.25 (dd, *J* = 13.2, 6.2 Hz, 1H), 3.12 – 3.06 (m, 1H), 2.64 (hept, *J* = 6.3 Hz, 1H), 2.09 (s, 2H), 1.04 (dd, *J* = 7.1, 6.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.60, 149.55, 141.71, 139.39, 135.81, 130.95, 127.91, 127.78, 123.05, 121.99, 100.90, 60.83, 48.04, 46.02, 24.00, 22.40.

FTIR (NaCl, thin film, cm^{-1}): 3051, 2960, 1693, 1588, 1568, 1466, 1433, 1366, 1170, 1010, 748.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2I$ $[M+H]^+$: 367.0671; found: 367.0677.

***N*-(2-(2-bromo-5-methoxyphenyl)-1-(pyridin-2-yl)ethyl)propan-2-amine (4g)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1-bromo-2-(bromomethyl)-4-methoxybenzene (101 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4g** (77.2 mg, 0.22 mmol, 74 %) as an off-white solid. Yield for duplicate run: 68.1 mg, 0.19 mmol, 65% – 70% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

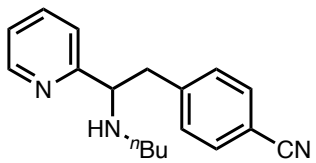
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.41 (td, *J* = 7.6, 1.8 Hz, 1H), 7.29 (d, *J* = 8.7 Hz, 1H), 7.05 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 6.88 (dt, *J* = 7.7, 1.1 Hz, 1H), 6.50 (dd, *J* = 8.8, 3.1 Hz, 1H), 6.27 (d, *J* = 3.1 Hz, 1H), 4.10 (dd, *J* = 8.4, 6.3 Hz, 1H), 3.52 (s, 3H), 3.18 (dd, *J* = 13.1, 6.3 Hz, 1H), 2.91 (dd, *J* = 13.1, 8.4 Hz, 1H), 2.57 (p, *J* = 6.2 Hz, 1H), 1.70 (brs, 3H), 0.94 (t, *J* = 6.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.75, 158.41, 149.49, 139.30, 135.93, 133.09, 123.08, 121.99, 116.62, 115.22, 114.22, 60.65, 55.30, 46.01, 43.87, 23.88, 22.38.

FTIR (NaCl, thin film, cm^{-1}): 3069, 3003, 2960, 1589, 1570,1471, 1433, 1378, 1292, 1278, 1241, 1164, 1129, 1056, 1015, 996, 801, 749.

HRMS (FAB, m/z): HRMS (ESI-TOF, m/z): calc'd for $C_{17}H_{22}N_2OBr$ $[M+H]^+$: 349.0915; found: 349.0917.

4-(2-(butylamino)-2-(pyridin-2-yl)ethyl)benzonitrile (4h)



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and 4-(bromomethyl)benzonitrile (70.6 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4h** (61.4 mg, 0.22 mmol,

73%) as a yellow-orange solid. Yield for duplicate run: 59.0 mg, 0.18 mmol, 70% – 72% average yield.

R_f = 0.22 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

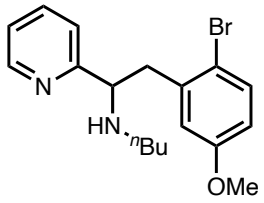
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 – 8.50 (m, 1H), 7.53 (td, J = 7.6, 1.8 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.13 (ddd, J = 7.7, 4.9, 1.2 Hz, 3H), 7.02 (dt, J = 7.8, 1.1 Hz, 1H), 3.90 (t, J = 7.1 Hz, 1H), 3.07 (d, J = 7.1 Hz, 2H), 2.50 – 2.30 (m, 2H), 2.00 – 1.77 (m, 2H), 1.43 – 1.31 (m, 2H), 1.27 – 1.15 (m, 2H), 0.80 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.83, 149.36, 144.45, 136.00, 131.74, 129.82, 122.21, 122.04, 118.78, 109.81, 65.16, 47.21, 43.18, 32.03, 20.10, 13.67.

FTIR (NaCl, thin film, cm^{-1}): 2955, 2926, 2869, 2226, 1606, 1589, 1570, 1504, 1469, 1433, 1121, 995, 824, 779, 750.

HRMS (FAB, m/z): calc'd for $C_{18}H_{22}N_3$ $[M+H]^+$: 280.1814; found: 280.1822.

4-(2-(butylamino)-2-(pyridin-2-yl)ethyl)benzonitrileN-(2-(2-bromo-5-methoxyphenyl)-1-(pyridin-2-yl)ethyl)butan-1-amine (4i)



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and 1-bromo-2-(bromomethyl)-4-methoxybenzene (101 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4i** (51.2 mg, 0.14 mmol, 47%) as a yellow oil. Yield for duplicate run: 49.5 mg, 0.14 mmol, 45% – 46% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

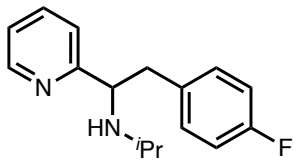
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.52 (td, J = 7.6, 1.8 Hz, 1H), 7.37 (d, J = 8.8 Hz, 1H), 7.13 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 7.05 (dt, J = 7.7, 1.1 Hz, 1H), 6.58 (dd, J = 8.8, 3.1 Hz, 1H), 6.45 (d, J = 3.1 Hz, 1H), 4.05 (t, J = 7.2 Hz, 1H), 3.62 (s, 3H), 3.21 (dd, J = 13.3, 6.9 Hz, 1H), 3.03 (dd, J = 13.3, 7.5 Hz, 1H), 2.57 – 2.33 (m, 2H), 1.52 – 1.30 (m, 2H), 1.30 – 1.16 (m, 2H), 0.83 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.08, 158.95, 149.92, 139.69, 136.52, 133.62, 123.27, 122.51, 117.08, 115.74, 114.70, 64.10, 55.77, 47.96, 44.04, 32.73, 20.81, 14.39.

FTIR (NaCl, thin film, cm^{-1}): 3004, 2955, 2927, 2857, 1589, 1570, 1471, 1433, 1291, 1240, 1163, 1112, 1048, 1015, 995, 782, 749.

HRMS (FAB, m/z): calc'd for $C_{18}H_{24}N_2OBr$ $[M+H]^+$: 363.1072; found: 363.1083.

***N*-(2-(4-fluorophenyl)-1-(pyridin-2-yl)ethyl)propan-2-amine (4j)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1-(chloromethyl)-4-fluorobenzene (52.0 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4j** (61.5 mg, 0.24 mmol, 79%) as a pale yellow oil. Yield for duplicate run: 57.2 mg, 0.22 mmol, 74% – 76% average yield.

R_f = 0.13 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.50 (td, *J* = 7.6, 1.8 Hz, 1H), 7.10 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 7.00 (dt, *J* = 7.8, 1.1 Hz, 1H), 6.96 – 6.91 (m, 2H), 6.89 – 6.82 (m, 2H), 3.99 (t, *J* = 7.2 Hz, 1H), 3.02 – 2.91 (m, 2H), 2.54 (hept, *J* = 6.2 Hz, 1H), 1.80 – 1.69 (m, 3H), 0.95 (dd, *J* = 6.2, 1.4 Hz, 6H).

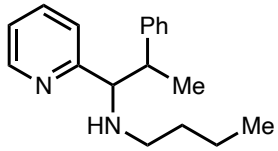
^{13}C NMR (101 MHz, $CDCl_3$): δ 163.00, 160.24, 149.44, 136.02, 134.47, 130.64, 122.65, 121.97, 115.07, 114.86, 63.02, 45.98, 42.76, 24.02, 22.03.

^{19}F NMR (282 MHz, $CDCl_3$): δ -117.15

FTIR (NaCl, thin film, cm^{-1}): 3046, 3005, 2962, 2927, 2865, 1684, 1589, 1570, 1508, 1469, 1433, 1379, 1367, 1338, 1221, 1168, 1157, 1094, 830, 748.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2F$ $[M+H]^+$: 259.1611; found 259.1622.

***N*-(2-phenyl-1-(pyridin-2-yl)propyl)butan-1-amine (4k)**



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and (1-chloroethyl)benzene (50.6 mg, 0.36 mmol) and (E)-*N*-butyl-1-(pyridin-2-yl)methanimine (48.7 mg, 0.30 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4k** (36.4 mg, 0.14 mmol, 46%) as a 1.4:1 mixture of diastereomers as a brown oil. Yield for duplicate run: 34.4 mg, 0.13 mmol, 43% – 44% average yield.

R_f = 0.39 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.57 (d, *J* = 4.9 Hz, 1H, *major*), 8.51 – 8.46 (d, *J* = 4.6 Hz,, 1H, *minor*), 7.61 (td, *J* = 7.6, 1.8 Hz, 1H, *major*), 7.41 (td, *J* = 7.6, 1.8 Hz, 1H, *major*), 7.33 (d, *J* = 8.4 Hz, 2H, *minor*), 7.29 (d, *J* = 7.3 Hz, 2H, *major*), 7.24 (m, *J* = 4.6 Hz, 1H, *major*), 7.21 (t, *J* = 7.1 Hz, 1H, *minor*), 7.15 (t, *J* = 7.6 Hz, 3H, *major*), 7.10 – 7.04 (m, 3H, *minor*), 7.01 (dd, *J* = 7.5, 4.9 Hz, 1H, *minor*), 6.95 (d, *J* = 7.8 Hz, 1H, *minor*), 3.81 (d, *J* = 9.3 Hz, 1H, *minor*), 3.79 – 3.73 (m, 1H, *major*), 3.17 (p, *J* = 7.1 Hz, 1H, *minor*), 3.01 (p, *J* = 7.1 Hz, 1H, *major*), 2.37 – 2.27 (m, 2H, *minor*), 2.27 – 2.17 (m, 2H, *major*), 1.64 (br s, 2H), 1.39 – 1.33

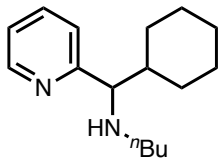
(m, 2H, *minor*), 1.31 (d, *J* = 7.1 Hz, 3H, *minor*), 1.20 (m, 4H, *major*+*minor*), 1.04 (dt, *J* = 14.9, 7.4 Hz, 2H, *major*), 0.98 (d, *J* = 7.1 Hz, 3H, *major*), 0.79 (t, *J* = 7.3 Hz, 3H, *minor*), 0.70 (t, *J* = 7.3 Hz, 3H, *major*).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.22 (*major)*, 162.71 (*minor)*, 149.15 (*minor)*, 149.02 (*major)*, 144.65 (*major)*, 144.52 (*minor)*, 136.35 (*major)*, 135.54 (*minor)*, 128.71 (*major)*, 128.11 (*minor)*, 127.94 (*minor)*, 127.83 (*major)*, 126.74 (*major)*, 126.15 (*minor)*, 123.13 (*minor)*, 122.64 (*major)*, 122.19 (*major)*, 121.62 (*minor)*, 70.68 (*major)*, 70.09 (*minor)*, 47.88 (*minor)*, 47.71 (*major)*, 46.51 (*major)*, 45.47 (*minor)*, 32.34 (*minor)*, 31.91 (*major)*, 20.41 (*minor)*, 20.21 (*major)*, 19.34 (*major)*, 16.63 (*minor)*, 14.04 (*minor)*, 13.91 (*major)*.

FTIR (NaCl, thin film, cm^{-1}): 3026, 2957, 2926, 2871, 1589, 1569, 1453, 1432, 1376, 1125, 994, 763,748, 700.

HRMS (FAB, m/z): calc'd for $C_{18}H_{25}N_2$ $[M+H]^+$: 269.2018; found: 269.2028.

***N*-(cyclohexyl(pyridin-2-yl)methyl)butan-1-amine (4l)**



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and iodocyclohexane (75.6 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4l** (42.9 mg, 0.17 mmol, 58%) as a yellow oil. Yield for duplicate run: 41.3 mg, 0.17 mmol, 56% – 57% average yield.

Also prepared from imine **1b** (48.7 mg, 0.3 mmol) and bromocyclohexane (58.7 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4l** (25.6 mg, 0.10 mmol, 35%) as a yellow oil. Yield for duplicate run: 21.5 mg, 0.087 mmol, 29% – 32% average yield.

Also prepared from imine **1b** (48.7 mg, 0.3 mmol) and 1,3-dioxoisoindolin-2-yl cyclohexanecarboxylate (98.4 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4l** (32.7 mg, 0.13 mmol, 44%) as a yellow oil. Yield for duplicate run: 21.7 mg, 0.11 mmol, 37% – 41% average yield.

R_f = 0.26 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

^{1}H NMR (400 MHz, $CDCl_3$):δ 8.54 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.59 (td, J = 7.6, 1.8 Hz, 1H), 7.22 (dt, J = 7.8, 1.1 Hz, 1H), 7.11 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.42 (d, J = 6.9 Hz,

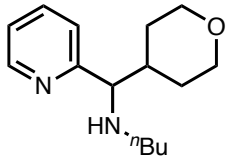
1H), 2.42 – 2.23 (m, 2H), 1.91 (ddq, J = 12.3, 4.0, 2.1 Hz, 2H), 1.83 (d, J = 7.5 Hz, 1H), 1.74 – 1.53 (m, 2H), 1.47 – 1.01 (m, 6H), 1.01 – 0.89 (m, 2H), 0.83 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.28, 148.87, 135.50, 122.68, 121.37, 69.50, 47.67, 43.50, 32.22, 29.80, 29.72, 26.36, 26.15, 26.11, 20.24, 13.78.

FTIR (NaCl, thin film, cm^{-1}): 3311,3068, 2923, 2851, 1588, 1569, 1467, 1431, 1375, 1342, 1117, 994, 838, 777, 747.

HRMS (FAB, m/z): calc'd for $C_{16}H_{27}N_2$ $[M+H]^+$: 247.2174; found: 247.2186.

***N*-(pyridin-2-yl(tetrahydro-2H-pyran-4-yl)methyl)butan-1-amine (4m)**



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and 4-iodotetrahydro-2H-pyran (76.3 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4m** (63.9 mg, 0.26 mmol, 86%) as a yellow oil. Yield for duplicate run: 54.3 mg, 0.22 mmol, 73% – 80% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

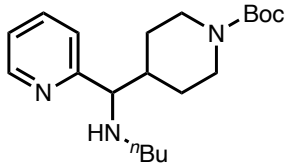
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.60 (td, J = 7.6, 1.9 Hz, 1H), 7.18 (dt, J = 7.8, 1.1 Hz, 1H), 7.12 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.90 (dddd, J = 47.4, 11.5, 4.5, 2.5 Hz, 2H), 3.38 (d, J = 7.4 Hz, 1H), 3.29 (dtd, J = 33.0, 11.9, 2.1 Hz, 2H), 2.43 – 2.23 (m, 2H), 1.96 – 1.72 (m, 4H), 1.48 – 1.17 (m, 6H), 1.10 (ddq, J = 13.2, 4.3, 2.3 Hz, 1H), 0.82 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.96, 149.89, 136.27, 123.58, 122.30, 69.52, 68.59, 68.31, 48.10, 41.39, 32.82, 30.74, 30.42, 20.81, 14.37.

FTIR (NaCl, thin film, cm^{-1}): 3317, 3067, 3004, 2928, 2839, 2755, 1588, 1569, 1468, 1432, 1385, 1264, 1237, 1122, 1093, 1015, 994, 983, 876, 782, 749.

HRMS (FAB, m/z): calc'd for $C_{15}H_{25}N_2O$ $[M+H]^+$: 249.1967; found: 249.1973.

***tert*-butyl 4-((butylamino)(pyridin-2-yl)methyl)piperidine-1-carboxylate (4n)**



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and tert-butyl 4-iodopiperidine-1-carboxylate (112 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4n** (33.8 mg, 0.10 mmol, 32%) as a yellow oil. Yield for duplicate run: 28.9 mg, 0.083 mmol, 29% – 30% average yield.

R_f = 0.18 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

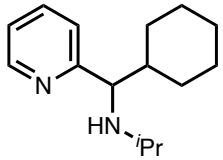
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.60 (td, J = 7.6, 1.8 Hz, 1H), 7.21 – 7.09 (m, 2H), 4.04 (d, J = 38.7 Hz, 2H), 3.39 (d, J = 7.4 Hz, 1H), 2.59 (dt, J = 25.7, 11.8 Hz, 2H), 2.40 – 2.25 (m, 2H), 2.03 – 1.86 (m, 1H), 1.77 (ddt, J = 19.0, 11.3, 3.1 Hz, 3H), 1.41 (s, 9H), 1.39 – 0.98 (m, 1H), 0.82 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.96, 155.23, 149.89, 136.31, 123.55, 122.33, 79.60, 69.17, 48.14, 42.46, 32.80, 28.86, 20.80, 14.37.

FTIR (NaCl, thin film, cm^{-1}): 2954, 2929, 2853, 1732, 1692, 1651, 1588, 1424, 1365, 1276, 1247, 1171, 872, 750.

HRMS (FAB, m/z): calc'd for $C_{20}H_{34}N_3O_2$ $[M+H]^+$: 348.2651; found: 348.2646.

***N*-(cyclohexyl(pyridin-2-yl)methyl)propan-2-amine (4o)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1,3-dioxoisoindolin-2-yl cyclohexanecarboxylate (98.4 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4o** (34.2 mg, 0.15 mmol, 49%) as a colorless oil. Yield for duplicate run: 28.0 mg, 0.12 mmol, 40% – 44% average yield.

R_f = 0.26 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

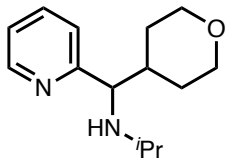
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.73 (td, J = 7.6, 1.8 Hz, 1H), 7.35 (dt, J = 7.8, 1.1 Hz, 1H), 7.25 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.66 (d, J = 6.8 Hz, 1H), 2.60 (hept, J = 6.2 Hz, 1H), 2.08 (dtt, J = 12.1, 3.6, 1.7 Hz, 1H), 1.95 – 1.82 (m, 3H), 1.75 (dddd, J = 13.4, 11.5, 6.7, 3.3 Hz, 3H), 1.54 – 1.42 (m, 1H), 1.37 – 1.19 (m, 2H), 1.17 – 1.02 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.81, 149.09, 135.61, 123.04, 121.50, 66.70, 46.26, 43.80, 30.08, 29.96, 26.59, 26.37, 26.32, 24.27, 22.18.

FTIR (NaCl, thin film, cm^{-1}): 2920, 2851, 1693, 1588, 1432, 1364, 1174, 749.

HRMS (FAB, m/z): calc'd for $C_{15}H_{25}N_2$ $[M+H]^+$: 233.2018; found: 233.2027.

***N*-(pyridin-2-yl(tetrahydro-2H-pyran-4-yl)methyl)propan-2-amine (4p)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1,3-dioxoisoindolin-2-yl tetrahydro-2H-pyran-4-carboxylate (99.1 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column

chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4p** (36.2 mg, 0.15 mmol, 51%) as a yellow oil. Yield for duplicate run: 36.1 mg, 0.15 mmol, 51% – 51% average yield.

R_f = 0.23 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

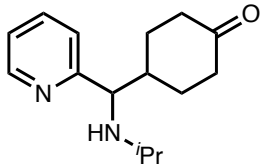
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.58 (dt, J = 4.7, 1.2 Hz, 1H), 7.60 (td, J = 7.6, 1.8 Hz, 1H), 7.23 – 7.08 (m, 2H), 4.04 – 3.78 (m, 2H), 3.48 (d, J = 7.5 Hz, 1H), 3.30 (dtd, J = 25.5, 11.8, 2.1 Hz, 2H), 2.46 (p, J = 6.2 Hz, 1H), 1.98 – 1.75 (m, 4H), 1.41 – 1.22 (m, 2H), 1.15 – 1.03 (m, 1H), 0.96 (dd, J = 15.9, 6.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.30, 149.95, 136.22, 123.68, 122.26, 68.67, 68.34, 66.57, 46.53, 41.54, 30.93, 30.48, 24.73, 22.59.

FTIR (NaCl, thin film, cm^{-1}): 3315, 2957, 2929, 2841, 1588,1569, 1469, 1433, 1366,1262, 1236, 1176, 1127, 1093, 877, 750.

HRMS (FAB, m/z): calc'd for $C_{14}H_{23}N_2O$ $[M+H]^+$: 235.1810; found: 235.1805.

4-((isopropylamino)(pyridin-2-yl)methyl)cyclohexan-1-one (4q)



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1,3-dioxoisoindolin-2-yl 4-oxocyclohexane-1-carboxylate (103 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4q** (49.0 mg, 0.20 mmol, 66%) as a yellow oil. Yield for duplicate run: 38.2 mg, 0.16 mmol, 52% – 59% average yield.

R_f = 0.20 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

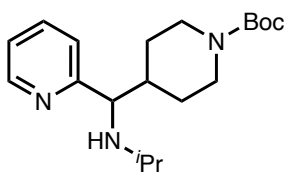
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (ddd, J = 4.8, 1.8, 1.0 Hz, 1H), 7.60 (td, J = 7.6, 1.9 Hz, 1H), 7.22 – 7.06 (m, 2H), 3.55 (d, J = 7.3 Hz, 1H), 2.45 (p, J = 6.2 Hz, 1H), 2.40 – 2.18 (m, 4H), 2.06 (dddd, J = 14.6, 11.5, 6.6, 3.2 Hz, 1H), 1.95 (s, 2H), 1.64 (ddq, J = 12.4, 6.4, 3.2 Hz, 1H), 1.56 – 1.32 (m, 2H), 0.96 (dd, J = 18.3, 6.2 Hz, 6H).

^{13}C NMR (101 MHz, CD_2Cl_2): δ 212.10, 149.99, 136.30, 123.59, 122.38, 65.34, 46.77, 42.53, 41.29, 30.12, 24.56, 22.42.

FTIR (NaCl, thin film, cm^{-1}): 3314, 2960, 2866, 1714, 1589, 1469, 1432, 1378, 1337, 1168, 753.

HRMS (FAB, m/z): calc'd for $C_{15}H_{23}N_2O$ $[M+H]^+$: 247.1810; found: 247.1805.

***tert*-butyl 4-((isopropylamino)(pyridin-2-yl)methyl)piperidine-1-carboxylate (4r)**



Prepared from imine **1a** (44.5 mg, 0.3 mmol) and 1-(tert-butyl) 4-(1,3-dioxoisoindolin-2-yl) piperidine-1,4-dicarboxylate (135 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **4r** (55.9 mg, 0.17 mmol, 56%) as a white solid. Yield for duplicate run: 47.7 mg, 0.14 mmol, 48% – 52% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

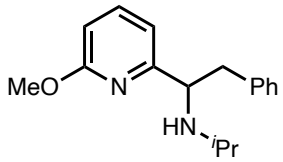
^{1}H NMR (400 MHz, $CDCl_3$): δ δ 8.56 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.59 (td, J = 7.6, 1.8 Hz, 1H), 7.21 – 7.01 (m, 2H), 4.04 (d, J = 37.9 Hz, 2H), 3.46 (d, J = 7.4 Hz, 1H), 2.71 – 2.49 (m, 2H), 2.44 (p, J = 6.2 Hz, 1H), 2.02 – 1.91 (m, 2H), 1.73 (tdt, J = 11.3, 7.4, 3.7 Hz, 1H), 1.40 (s, 9H), 1.22 – 1.03 (m, 3H), 0.94 (dd, J = 18.2, 6.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.98, 154.92, 149.61, 135.91, 123.29, 121.94, 79.27, 65.89, 46.21, 42.26, 29.23, 28.56, 24.38, 22.23.

FTIR (NaCl, thin film, cm^{-1}): 2964, 1861, 2724, 1772, 1735, 1689, 1589, 1569, 1469, 1424, 1365, 1278, 1250, 1168, 1119, 1050, 871, 750, 718.

HRMS (FAB, m/z): calc'd for $C_{19}H_{32}N_3O_2$ $[M+H]^+$: 334.2495; found: 334.2469.

***N*-(1-(6-methoxypyridin-2-yl)-2-phenylethyl)propan-2-amine (S3a)**



Prepared from imine **S1a** (53.5 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **S3a** (14.0 mg, 0.051 mmol, 17%) as a colorless oil. Yield for duplicate run: 12.0 mg, 0.044 mmol, 15% – 16% average yield.

R_f = 0.29 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

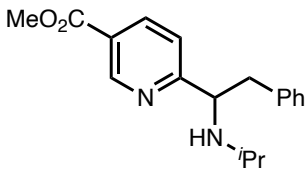
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (t, *J* = 7.7 Hz, 1H), 7.20 – 7.09 (m, 3H), 6.97 (d, *J* = 7.4 Hz, 2H), 6.55 (d, *J* = 7.4 Hz, 1H), 6.48 (d, *J* = 7.1 Hz, 1H), 3.95 – 3.86 (m, 4H), 3.02 (t, *J* = 6.3 Hz, 2H), 2.58 (hept, *J* = 6.3 Hz, 1H), 1.89 (s, 1H), 1.00 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.1, 160.5, 139.3, 138.5, 129.5, 128.2, 126.2, 115.8, 108.7, 62.5, 45.9, 43.5, 24.3, 22.1.

FTIR (NaCl, thin film, cm^{-1}): 3063, 3026, 2962, 2857, 1599, 1578, 1466, 1436, 1416, 1310, 1288, 1173, 1147, 1073, 1032, 988, 803, 770, 743, 699.

HRMS (FAB, m/z): calc'd for $C_{17}H_{23}N_2O$ $[M+H]^+$: 271.1810; found 271.1806.

Methyl 6-(1-(isopropylamino)-2-phenylethyl)nicotinate (S3b)



Prepared from imine **S1b** 61.9 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **S3b** (26.0 mg, 0.087 mmol, 29%) as a colorless oil. Yield for duplicate run: 26.0 mg, 0.087 mmol, 29% – 29% average yield.

R_f = 0.23 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

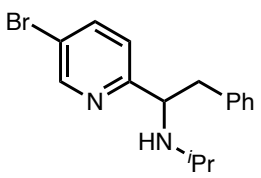
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.17 (d, *J* = 2.1 Hz, 1H), 8.12 (dd, *J* = 8.1, 2.2 Hz, 1H), 7.23 – 7.13 (m, 4H), 7.02 (d, *J* = 6.8 Hz, 2H), 4.13 (t, *J* = 7.2 Hz, 1H), 3.94 (s, 3H), 3.04 (dd, *J* = 13.3, 7.2 Hz, 1H), 2.98 (dd, *J* = 13.3, 7.2 Hz, 1H), 2.58 – 2.49 (m, 1H), 1.78 (s, 1H), 0.95 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.5, 166.1, 157.1, 150.9, 138.4, 137.3, 129.4, 128.5, 126.6, 124.5, 122.3, 63.3, 52.5, 46.5, 43.7, 24.2, 22.2.

FTIR (NaCl, thin film, cm^{-1}): 3063, 3027, 2960, 2866, 1729, 1597, 1586, 1456, 1436, 1381, 1339, 1289, 1194, 1176, 1118, 1024, 960, 777, 738, 701.

HRMS (FAB, m/z): calc'd for $C_{18}H_{23}N_2O_2$ $[M+H]^+$: 299.1760; found 299.1755.

N-(1-(5-bromopyridin-2-yl)-2-phenylethyl)propan-2-amine (S3c)



Prepared from imine **S1c** (68.1 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **S3c** (22.0 mg, 0.069 mmol, 23%) as a colorless oil. Yield for duplicate run: 22.0 mg, 0.069 mmol, 23% – 23% average yield.

R_f = 0.35 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

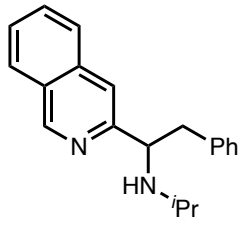
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (dd, *J* = 2.4, 0.7 Hz, 1H), 7.64 (dd, *J* = 8.3, 2.4 Hz, 1H), 7.26 – 7.12 (m, 3H), 7.07 – 6.94 (m, 3H), 4.05 (t, *J* = 7.2 Hz, 1H), 3.05 – 2.90 (m, 2H), 2.54 (hept, *J* = 6.3 Hz, 1H), 2.07 (s, 1H), 0.95 (dd, *J* = 6.3, 2.9 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.2, 150.6, 138.8, 138.5, 129.4, 128.6, 126.6, 124.0, 118.8, 62.8, 46.5, 43.7, 24.1, 22.1.

FTIR (NaCl, thin film, cm^{-1}): 3083, 3027, 2925, 1863, 1710, 1602, 1572, 1494, 1463, 1367, 1173, 1091, 1006, 839, 744, 628.

HRMS (FAB, m/z): calc'd for $C_{16}H_{20}N_2Br$ $[M+H]^+$: 319.0810; found 319.0825.

***N*-(1-(isoquinolin-3-yl)-2-phenylethyl)propan-2-amine (S3d)**



Prepared from imine **S1d** (59.5 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **S3d** (30.5 mg, 0.11 mmol, 35%) as a colorless oil. Yield for duplicate run: 27.0 mg, 0.093 mmol, 31% – 33% average yield.

R_f = 0.19 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

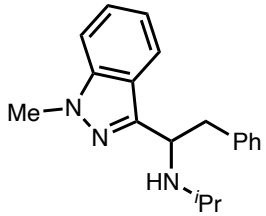
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.27 (s, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.69 (d, *J* = 9.5 Hz, 1H), 7.64 (ddd, *J* = 8.2, 6.7, 1.2 Hz, 1H), 7.55 (ddd, *J* = 8.1, 6.7, 1.3 Hz, 1H), 7.38 (s, 1H), 7.20 – 7.09 (m, 3H), 7.04 (d, *J* = 4.5 Hz, 2H), 4.19 (t, *J* = 7.1 Hz, 1H), 3.20 (dd, *J* = 13.3, 7.5 Hz, 1H), 3.08 (dd, *J* = 13.3, 6.8 Hz, 1H), 2.58 (hept, *J* = 6.2 Hz, 1H), 2.09 (s, 1H), 0.99 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 156.0, 152.7, 139.2, 136.2, 130.5, 129.4, 128.4, 128.0, 127.7, 126.9, 126.7, 126.3, 118.8, 63.0, 46.1, 43.6, 24.3, 22.1.

FTIR (NaCl, thin film, cm^{-1}): 3308, 3057, 3026, 2963, 2927, 2862, 1684, 1647, 1628, 1582, 1558, 1490, 1456, 1379, 1339, 1271, 1174, 1127, 1080, 945, 883, 750, 689, 668.

HRMS (FAB, m/z): calc'd for $C_{20}H_{23}N_2$ $[M+H]^+$: 291.1861; found 291.1858.

N-(1-(1-methyl-1H-indazol-3-yl)-2-phenylethyl)propan-2-amine (S3e)



Prepared from imine **S1e** (60.4 mg, 0.3 mmol) and benzyl bromide (42.8 µL, 0.36 mmol, 1.2 equiv) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **S3e** (6.0 mg, 0.021 mmol, 7%) as a colorless oil.

R_f = 0.19 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

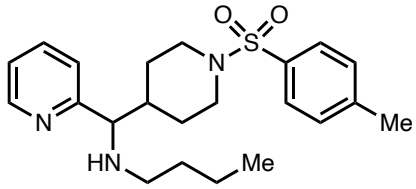
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.2 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.23 – 7.11 (m, 5H), 7.11 – 7.03 (m, 1H), 4.53 (t, *J* = 7.1 Hz, 1H), 4.01 (s, 3H), 3.18 (dd, *J* = 7.1, 2.7 Hz, 2H), 2.68 (hept, *J* = 6.3 Hz, 1H), 1.71 (s, 1H), 0.96 (dd, *J* = 10.7, 6.2 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 141.0, 138.8, 129.3, 128.2, 126.2, 126.1, 121.1, 119.7, 108.9, 55.7, 46.1, 43.3, 35.3, 23.9, 22.0.

FTIR (NaCl, thin film, cm^{-1}): 3444, 3025, 2956, 2928, 2864, 1684, 1615, 1506, 1456, 1369, 1294, 1236, 1171, 768, 746, 702.

HRMS (FAB, m/z): calc'd for $C_{19}H_{24}N_3$ $[M+H]^+$: 294.1970; found 294.1961.

***N*-(pyridin-2-yl(1-tosylpiperidin-4-yl)methyl)butan-1-amine (S4a)**



Prepared from imine **1b** (48.7 mg, 0.3 mmol) and tert-butyl 4-iodo-1-tosylpiperidine (131 mg, 0.36 mmol) following General Procedure 3. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) afforded **S4a** (36.2 mg, 0.090 mmol, 30%) as a white solid. Yield for duplicate run: 31.1 mg, 0.077 mmol, 26% – 28% average yield.

R_f = 0.22 (silica, Hex/EtOAc 1:1, UV w/ 1% Et_3N).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54 (d, J = 4.8 Hz, 1H), 7.60 (m, 3H), 7.28 (d, J = 7.9 Hz, 2H), 7.14 (m, 2H), 3.81 (d, J = 11.6 Hz, 1H), 3.70 (d, J = 11.4 Hz, 1H), 3.37 (d, J = 14.4 Hz, 1H), 2.42 (s, 3H), 2.40 – 2.25 (m, 1H), 2.18 (td, J = 11.9, 2.6 Hz, 1H), 2.11 (td, J = 11.3, 7.2 Hz, 1H), 2.05 (dd, J = 13.5, 3.2 Hz, 1H), 1.47 – 1.34 (m, 3H), 1.34 – 1.18 (m, 8H), 0.84 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 149.63, 143.35, 135.94, 133.00, 129.52, 127.72, 123.25, 122.05, 68.21, 47.64, 46.63, 46.40, 41.08, 32.32, 28.65, 28.40, 21.52, 20.36, 13.94.

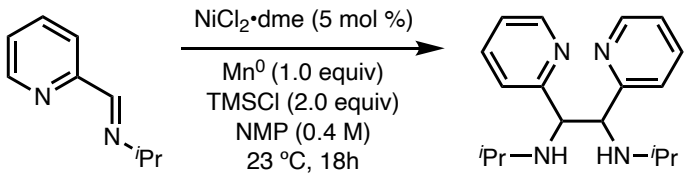
FTIR (NaCl, thin film, cm^{-1}): 3323, 2952, 2921, 2856, 2361, 1588, 1467, 1351, 1338, 1163, 1093, 929, 752, 728.

HRMS (FAB, m/z): calc'd for $C_{22}H_{32}N_3O_2S$ $[M+H]^+$: 402.2215; found: 402.2218.

6. Mechanistic Experiments

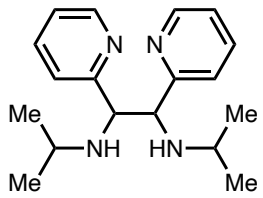
6.1. Independent synthesis of diamine 1a':

N1,N2-diisopropyl-1,2-di(pyridin-2-yl)ethane-1,2-diamine (1a')



On the bench-top, to a 1 dram vial, equipped with a stir bar, was charged with (*E*)-*N*-isopropyl-1-(pyridin-2-yl)methanimine **1a** (44.5 mg 0.3 mmol, 1.0 equiv) and Mn^0 (16.5 mg, 0.3 mmol, 1.0 equiv). The vial was brought into a N_2-filled glovebox and a stock-solution of $NiCl_2$·dme

in NMP (0.75 ml, 0.02 M, 0.05 equiv [Ni]) and TMSCl (76 µl, 0.6 mmol, 2.0 equiv) was added consecutively. The vial was sealed with a Teflon cap and electrical tape and stirred at room temperature for 18 hours at 600 rpm. The resulting suspension was diluted with CH_2Cl_2 (0.5 ml) and extracted 3x with 1N HCl (0.5 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased. The resulting aqueous solution was extracted 3x with EtOAc and the combined organic phases were concentrated under reduced pressure at 40 °C until most of the NMP was removed. The crude material was purified by column chromatography (Hex/EtOAc 1:1 w/ 1% Et_3N) to afford **1a'** (11.2 mg, 0.038 mmol, 25%) as a colorless crystalline solid.



R_f = 0.26 (silica, Hex/EtOAc 1:1, UV).

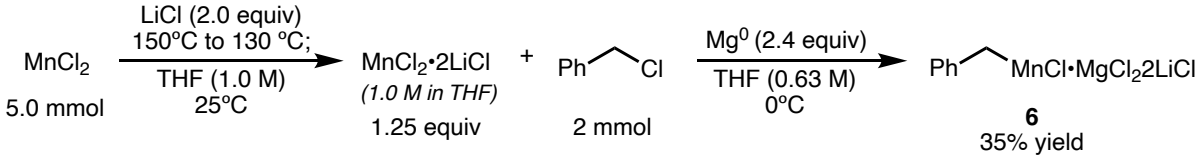
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (dddd, J = 5.0, 3.3, 1.8, 0.9 Hz, 4H), 7.46 (td, J = 7.6, 1.8 Hz, 2H), 7.33 (td, J = 7.6, 1.8 Hz, 2H), 7.05 (ddd, J = 7.5, 4.9, 1.2 Hz, 2H), 7.01 – 6.93 (m, 4H), 6.88 (dt, J = 7.8, 1.1 Hz, 2H), 4.16 (s, 2H), 3.93 (s, 2H), 2.52 (dh, J = 25.0, 6.2 Hz, 4H), 0.97 (d, J = 6.2 Hz, 2H), 0.94 – 0.82 (m, 18H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 206.96, 162.16, 161.91, 149.03, 148.74, 135.59, 135.39, 123.32, 123.10, 121.64, 121.54, 67.00, 65.85, 65.09, 46.91, 46.13, 30.93, 24.28, 23.86, 22.45, 22.41.

FTIR (NaCl, thin film, cm^{-1}): 3298, 3051, 2960, 2926, 2866, 1693, 1589, 1568, 1469, 1433, 1379, 1337, 1173, 1146, 995, 748.

HRMS (FAB, m/z): calc'd for $C_{18}H_{27}N_4$ $[M+H]^+$: 348.2651; found: 348.2646.

6.2. Probing Intermediacy of Organomanganese Intermediate:

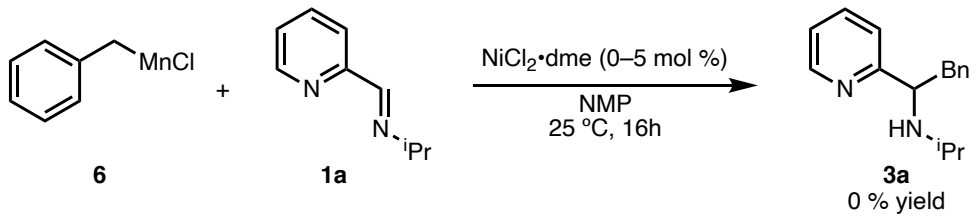


Benzyl organomanganese reagent **6** was prepared according to a procedure from Knochel and coworkers.[6]

Preparation of $MnCl_2$•2LiCl: To an oven-dried 10 mL Schlenk flask charged with a stir bar and cooled under an atmosphere of N_2 was added LiCl (424 mg, 10.0 mmol). The flask was then placed under vacuum (~0.2 mmHg) and heated to 150 ºC in an oil bath for 3 hours. The flask was then backfilled with N_2 and removed from the oil bath. After cooling to room

temperature, $MnCl_2$ (629 mg, 5.0 mmol) was added. The flask was then resealed and the mixture of solids was reheated under vacuum at 130 ºC for 3 hours. The flask was then refilled with N_2 and cooled to room temperature followed by the addition of 5mL of THF was added to the flask. The solution was then stirred for 24 hours at 25 ºC to give a transparent, light-yellow solution of 1.0 M $MnCl_2$•2LiCl in THF.

Preparation of 6: A 50 mL round-bottom flask charged with a stir bar was flame-dried under vacuum and allow to cool to 25 ºC under an atmosphere of N_2 then charged with activated Mg^0 turnings (117 mg, 4.80 mmol, 2.4 equiv). The flask was then evacuated and backfilled with N_2 three times before 0.67 mL of THF was added to the flask followed by 2.5 mL of the $MnCl_2$•2LiCl solution (1.0 M in THF, 2.50 mmol). The mixture was then cooled to 0 ºC in an ice bath and stirred. Once cooled, benzyl chloride (253 mg, 2.0 mmol) was added neat to the reaction and the solution was allowed to stir at 0 ºC for 1.5 hours. The solution was then transferred to a flame-dried Schlenk flask with a filter cannula. The resulting solution was then titrated with I_2 in triplicate to give an average concentration of 0.22 M of **6** in THF (35% yield).

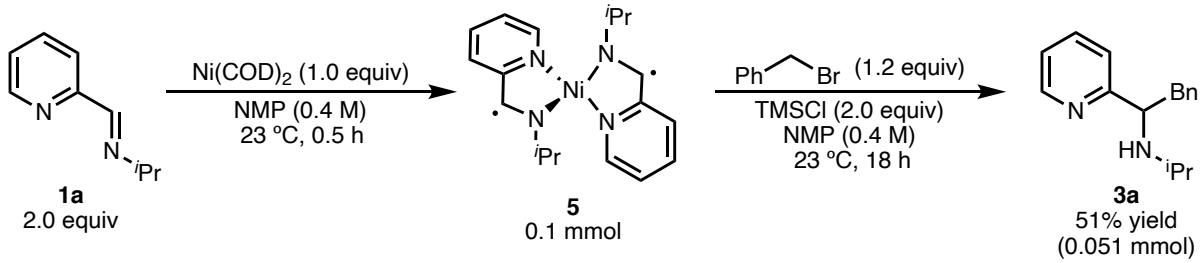


6 **1a** **3a**
0 % yield

1,2-addition with Organomanganese Reagent 6: To an oven-dried 1 dram vial with a new stir bar was added **1a** (14.8 mg, 0.10 mmol). The vial was then pumped into a N_2-filled glovebox where (if applicable) $NiCl_2$•dme (1.1 mg, 5µmol, 5 mol %) was added and dissolved in 750 µL of NMP. This solution was allowed to stir for 15 min at 27ºC causing it to turn green (in the presence of Ni). To the solution was then added the 0.22 M solution of **6** via syringe. The vial was then sealed with a teflon-lined cap and isolation tape then removed from the glovebox and stirred on the bench at 600 rpm for 16 hours. The resulting suspension was diluted with CH_2Cl_2 (0.5 ml) and extracted 3x with 1N HCl (0.5 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased. The resulting aqueous solution was extracted 3x with EtOAc and the combined organic phases were concentrated under reduced pressure and analyzed by ^1H NMR to obtain the reaction yield. In the case of 0 % Nickel catalyst only starting material was recovered with no product formed. Likewise with 5 mol % $NiCl_2$•dme no product **3a** was formed but a significant amount of **1a'** (57% yield) was recovered. Given that the formation of **1a'** had been observed in our other experiments with **1a**, Ni catalyst, and

reductant in the absence of electrophile, we propose the organomanganese intermediate is reducing the nickel catalyst to facilitate the imine homocoupling.

6.3. Stoichiometric Ni^0 Alkylation:



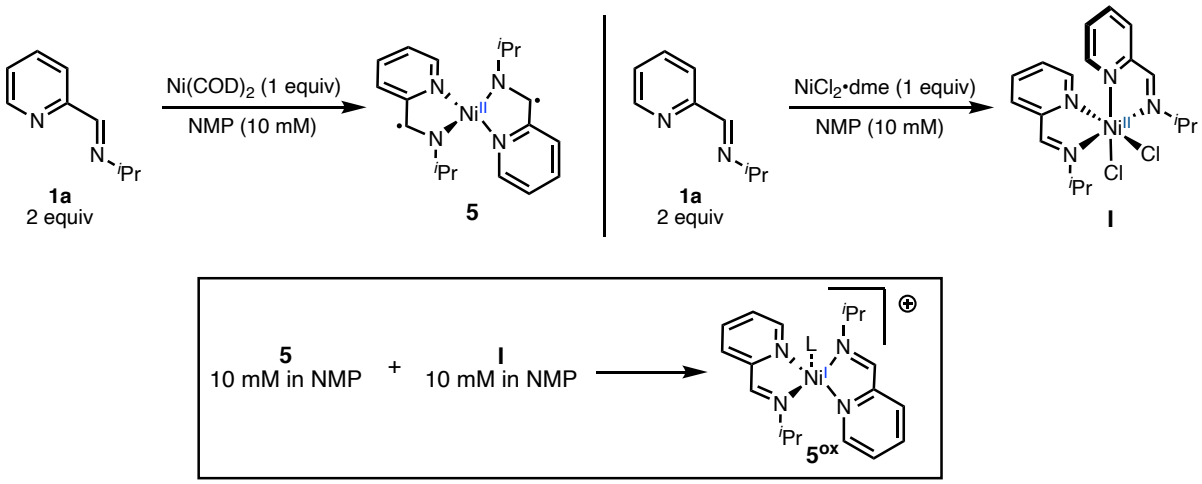
To an oven-dried 1-dram vial equipped with a stir bar was charged with 2-imino pyridine **1a** (29.6 mg, 0.20 mmol) in a nitrogen-filled glovebox. To the vial was then added $Ni(COD)_2$ (27.5 mg, 0.10 mmol) which immediately turned dark violet as it made contact with the **1a** in the vial. The residue was then dissolved in NMP (250 µL, 0.4 M) to give an opaque, royal purple solution. This was then stirred for 30 minutes to ensure complete complexation followed by addition of benzyl bromide (20.5 mg, 0.12 mmol) and TMSCl (25.4 µL, 0.20 mmol). The vials were sealed with a Teflon cap, removed from the glovebox, and stirred for 18 hours at 600 rpm. The resulting suspension was diluted with CH_2Cl_2 (0.5 ml) and extracted 3x with 1N HCl (0.5 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased. The resulting aqueous solution was extracted 3x with EtOAc and the combined organic phases were concentrated under reduced pressure and analyzed by ^1H NMR to obtain the reaction yield. Average yield of **3a** over 2 runs: 51 % yield (0.051 mmol).

7. Electron Paramagnetic Resonance (EPR) Studies

7.1. General EPR Details

X-Band EPR spectra (9.4 Hz, continuous wave) using a Bruker EMX spectrometer with Bruker Win-EPR software. Samples were collected at 77 K using a vacuum-insulated quartz liquid N_2 dewar. For maximum sensitivity, several microwave frequencies were scanned between 20 mW to 20 µW where 2 mW was found to be optimal. EPR data was simulated in MATLAB with Easyspin.

7.2. EPR Sample Preparation



In a N_2-filled glovebox, an oven-dried 20 mL scintillation vial with a stir bar was charged with $Ni(COD)_2$ (13.7 mg, 50 μmol, 1 equiv) and 1 mL of NMP. To the stirring suspension was added **1a** (14.8 mg, 100 μmol, 2 equiv) causing the solution to turn a deep royal purple and was allowed to stir for 15 minutes to form **5**. Concurrently, an oven-dried 1 dram vial with a stir bar was charged with $NiCl_2$•dme (11.0 mg, 50 μmol, 1 equiv). To the vial was added 1 mL of NMP to give a blue solution followed by **1a** (14.8 mg, 100 μmol, 2 equiv) causing the solution to turn light green to form **I**. After 15 minutes the NMP solution of **I** was transferred to the solution of **5** in NMP. The 1 dram vial was then rinsed with 3 mL of NMP (final concentration 10 mM) to ensure quantitative transfer. This solution was then stirred for 15 minutes and turned from dark purple to black. An aliquot of this solution was then transferred to an EPR tube which was then rapidly frozen at 77 K in a liquid N_2 dewar and was analyzed by EPR.

7.3. EPR Data

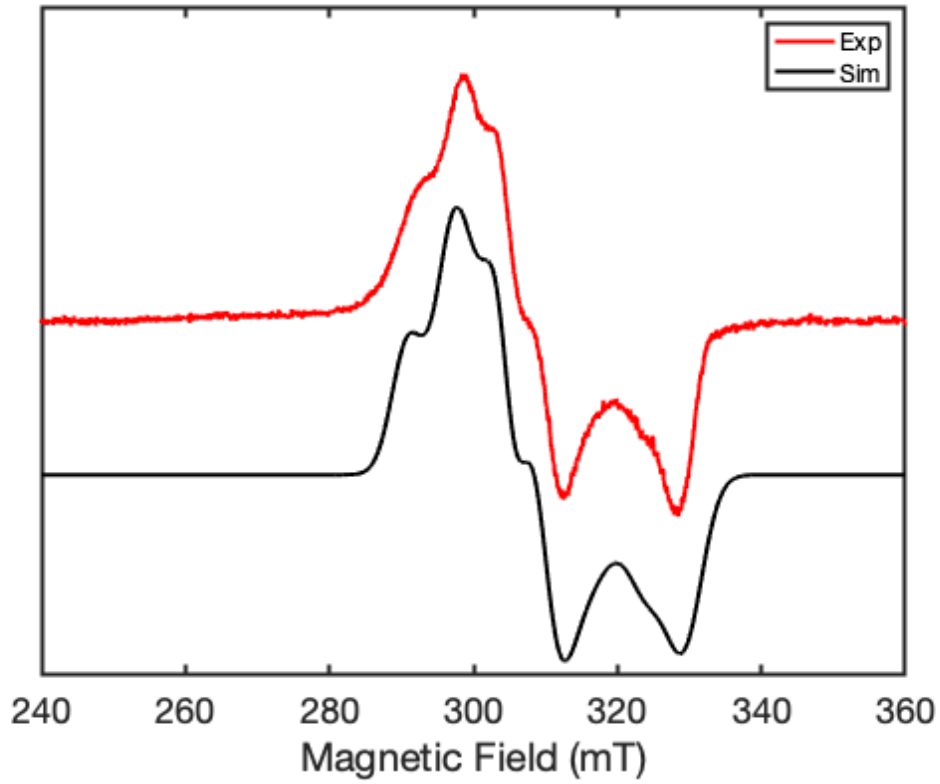


Figure S9. X-band EPR spectrum (red) of the comproportionation reaction between **5** and **I** in (10 mM) NMP with the following parameters: Temperature = 77 K, solvent = NMP, microwave frequency = 9.36 GHz, power = 2.181 mW, modulation amplitude = 1200.00 G. Simulated signal is shown (black). See Figure **S10** for simulation details and g values.

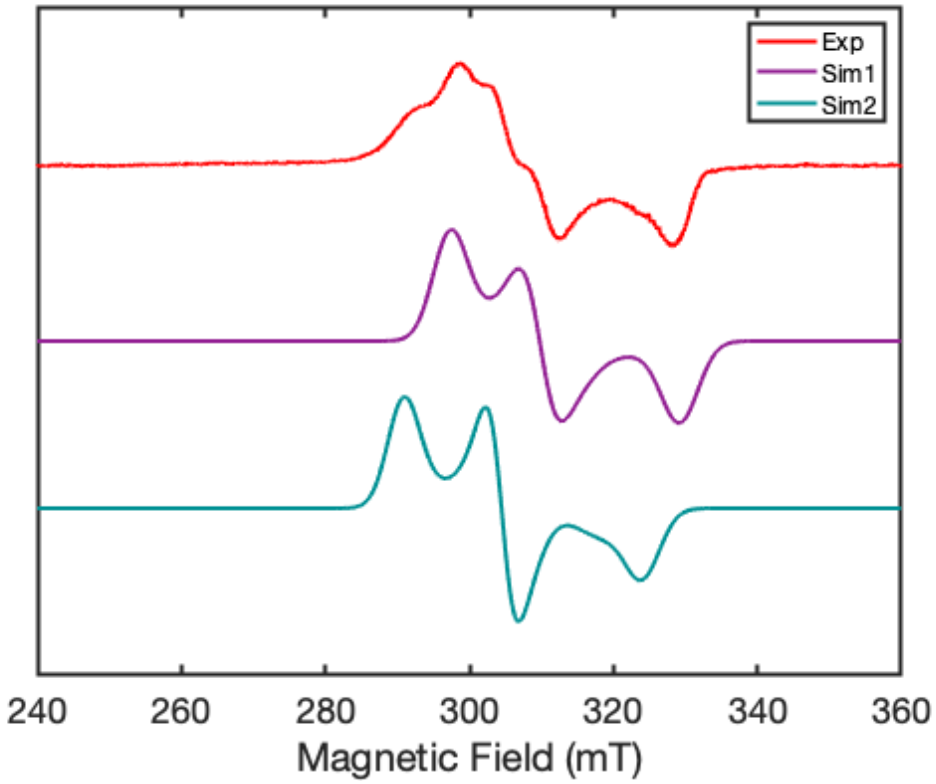


Figure S10. EPR was simulated as two S=1/2 Ni^{I} isomeric species (based on optimal fitting parameters and related work from Wieghardt.[15] Fitting parameters for species 1 (plum): g_1 = 2.25, g_2 = 2.16, g_3 = 2.03, linewidth = 4.4 mT, Γ_1 = 70, Γ_2 = 47, Γ_3 = 85 MHz, weighting factor = 1.0. Fitting parameters for species 2 (teal): g_1 = 2.30, g_2 = 2.20, g_3 = 2.07, linewidth = 3.5 mT, Γ_1 = 106, Γ_2 = 2, Γ_3 = 123 MHz, weighting factor = 0.56. Calculated g tensor values for: $\mathbf{5^{ox}}$ g_1 = 2.21, g_2 = 2.11, g_3 = 2.05, g_{iso} =2.12; $\mathbf{5^{ox}–Cl}$: g_1 = 2.25, g_2 = 2.23, g_3 = 2.19, g_{iso} =2.22.

8. Computational Details

All density functional theory (DFT) calculations were carried out using the ORCA 4.2 software package.[7] Geometry optimizations and numerical frequency calculations were carried out using the B3LYP hybrid functional,[Error! Bookmark not defined.] which was known to accurately describe transition metal complexes with high levels of covalency.[Error! Bookmark not defined.] All atoms were described with the def2-TZVP basis set.[Error! Bookmark not defined.] For all calculations, the resolution of identity (RI) approximation was used to calculate the coulomb integrals and the chain-of-spheres[8] approximation was used for the exchange integrals (RIJCOSX). Weigend's coulomb fitting auxiliary basis set[9] (Def2/J) was also employed for all calculations.

Calculations were converged to tight SCF criteria ($\Delta E <= 1*10^{-8}$ Eh). All stationary points were confirmed as local minima by the absence of imaginary vibrational modes. Fine integration grids were used with the GRID7 and NOFINALGRID settings. Broken symmetry calculations were performed using the method described by Ginsberg[10] and Noodleman *et al*[11]. The broken symmetry notation (*m,n*)[12] is employed where the m (n) is the number of spin up (or spin-down) electrons on each fragment. All graphical representations shown were rendered with the program CYLview[13] and orbital/density surfaces with the program *ChemCraft*.[14]

8.1. DFT Input Files and Coordinates

Input File – $(1a)_2Ni$ BS(0,0) (Low Spin)

```
! UKS B3LYP def2-TZVP def2/J RIJCOSX Grid7 TightSCF NoFinalGrid LargePrint
! Opt NumFreq

% pal nprocs 16 # num of processors
end
%maxcore 9000
%method
Z_solver DIIS
end

*xyz 0 1
C       -0.08651      -3.70002       2.07639
N        0.69789      -2.47950       1.83316
C        0.45604      -1.41247       2.58729
C        1.15663      -0.22934       2.24501
N        2.09886      -0.42527       1.24915
Ni       2.04979      -2.19969       0.50253
N        2.45194      -1.83399      -1.34168
C        3.13733      -2.86225      -1.96491
C        3.33308      -3.98983      -1.12655
N        2.93217      -3.86804       0.13320
C        3.19296      -4.96161       1.07941
C        3.57466      -2.73898      -3.30672
C        3.30958      -1.58023      -4.01101
C        2.59063      -0.54055      -3.36863
C        2.19485      -0.71236      -2.05385
C        2.81676       0.64458       0.83213
C        2.64151       1.92122       1.33545
C        1.66315       2.13562       2.34167
C        0.93376       1.05530       2.79805
H       -0.27266      -1.41630       3.40535
H        3.81281      -4.89507      -1.51148
H        4.12399      -3.56650      -3.76334
```

H	3.64903	-1.46440	-5.04343
H	2.32663	0.37753	-3.89757
H	1.63104	0.06630	-1.53457
H	3.57044	0.44479	0.06589
H	3.26672	2.73740	0.96648
H	1.48984	3.13524	2.74925
H	0.16921	1.17461	3.57027
C	-0.03364	-4.19572	3.53004
H	1.00544	-4.33915	3.86696
H	-0.56364	-5.15742	3.62494
H	-0.51769	-3.48699	4.22121
C	-1.53722	-3.50164	1.60390
H	0.36420	-4.47372	1.43644
H	-2.05826	-2.75609	2.22660
H	-2.10053	-4.44694	1.66624
H	-1.56038	-3.14500	0.56234
C	4.60357	-4.81493	1.67543
H	5.37225	-5.00132	0.90649
H	4.75967	-5.53717	2.49305
H	4.75317	-3.80003	2.07403
C	2.97945	-6.37338	0.51074
H	2.47651	-4.81532	1.90217
H	3.74189	-6.64022	-0.23805
H	1.98994	-6.47302	0.03599
H	3.05516	-7.11503	1.32198

*

Optimized coordinates – $(1a)_2Ni$ (5) (Low Spin)

C	-0.07139688048135	-3.68994745690584	2.12487431847914
N	0.69457607470368	-2.46847311460371	1.82154805145691
C	0.46230487368270	-1.40579204444689	2.56862153431397
C	1.14434009100596	-0.22144322634441	2.22294863299765
N	2.08908020452348	-0.39907719496350	1.23289295160638
Ni	2.05405208904355	-2.18531967202371	0.47923647332427
N	2.49643854225418	-1.81468121815090	-1.36865285410353
C	3.16446186466836	-2.85339073012088	-1.97920690295865
C	3.31760272384933	-3.98920040401533	-1.15196806361930
N	2.91187147934083	-3.87930406652301	0.09674659500334
C	3.11663739078330	-5.01105774748437	1.01483205871569
C	3.63666674260574	-2.74228514674203	-3.29998010570616
C	3.42987520482683	-1.58194872471534	-4.00569252858579
C	2.73521978741020	-0.52733337208899	-3.38020051761558
C	2.30198321662912	-0.68703717184991	-2.08427020650156
C	2.75926602868113	0.69616869616506	0.80989558621606
C	2.53408645796020	1.96185256089880	1.29845706195641
C	1.55641364281730	2.14840111450956	2.29977193544369
C	0.87764936094192	1.04924644715982	2.76459391405816

H	-0.24436539587200	-1.41220981699462	3.39183929255147
H	3.76267991173966	-4.89465032843539	-1.54733269752619
H	4.16585461087004	-3.57878731768715	-3.73981093627253
H	3.79354917566678	-1.47697113063354	-5.01976970038894
H	2.51804955554337	0.39203256272523	-3.90693723882010
H	1.75340643056829	0.10123739387726	-1.58632148319338
H	3.51580560597679	0.52604040965820	0.05503786662332
H	3.11988717088641	2.79058844620730	0.92377829313703
H	1.34556487197089	3.13471108498792	2.69286025990739
H	0.11585794297099	1.14176537769507	3.52896357533661
C	0.11074053819156	-4.19024906155441	3.56442148756822
H	1.16673948233884	-4.32106394706288	3.80795291978854
H	-0.39364895576934	-5.15035231697145	3.69451235474330
H	-0.31777214323576	-3.49409255492280	4.28805617503585
C	-1.55674571487992	-3.48493452800464	1.79467332974312
H	0.31030707160697	-4.45376368456651	1.44663185168743
H	-2.01062574174205	-2.74917438642245	2.46167437112740
H	-2.10423254973763	-4.42282511073171	1.91061235597269
H	-1.67776764610482	-3.13044557318379	0.76984802654670
C	4.47205228314121	-4.86997104291255	1.72112741662872
H	5.29010903289212	-5.05281554296529	1.01952885957022
H	4.55529007731697	-5.59451606866376	2.53456036697896
H	4.58876080603594	-3.86839722947529	2.13538087580025
C	2.97595111228601	-6.40027658488880	0.38279121384763
H	2.34359858105154	-4.91169080470743	1.77668397354347
H	3.79366684408679	-6.62646057336273	-0.30412720758781
H	2.03542278018867	-6.50090537390851	-0.16244896055192
H	3.00275536676520	-7.15809982484962	1.16880542372144

Final Single point energy = -2427.4312451 Eh

Input File – $(1a)_2$Ni BS(0,0) (5) (High Spin)

```
! UKS B3LYP def2-TZVP def2/J RIJCOSX Grid7 TightSCF NoFinalGrid Slowconv
! Opt

%scf
maxiter 1000
end

%output
Print[P_basis] 2
Print[P_MOs] 1
Print[P_ReducedOrbPop_L] 1
Print[P_BondOrder_L] 1
Print[P_FragBondOrder_L] 1
```

```
Print[P_OrbPopMO_L] 1
Print[P_ReducedOrbPopMO_L] 1
end


% pal nprocs 16 # num of processors
end

%maxcore 9000
%method
Z_solver DIIS
end

*xyz 0 5
 C     -0.951965    -2.779945     0.804853
  N     0.259699    -2.102834     1.291891
  C     0.163355    -1.290541     2.329373
  C     1.350443    -0.685445     2.793235
  N     2.463620    -0.955323     2.021895
  Ni    2.053936    -2.206995     0.539021
  N     1.742323    -2.523282    -1.369608
  C     2.678467    -3.365674    -1.930862
  C     3.726973    -3.721126    -1.055626
  N     3.657444    -3.292665     0.193550
  C     4.729961    -3.669707     1.127692
  C     2.550432    -3.801319    -3.265637
  C     1.486983    -3.378194    -4.023452
  C     0.544277    -2.500162    -3.446775
  C     0.714281    -2.114017    -2.137559
  C     3.636564    -0.413382     2.404333
  C     3.780399     0.382584     3.518903
  C     2.647019     0.657126     4.313447
  C     1.438701     0.124188     3.943490
  H    -0.780918    -1.086001     2.824841
  H     4.551035    -4.324971    -1.419412
  H     3.297312    -4.471572    -3.673059
  H     1.371032    -3.710044    -5.047326
  H    -0.291167    -2.118372    -4.016995
  H     0.018994    -1.432443    -1.667480
  H     4.484679    -0.624744     1.764898
  H     4.747774     0.798084     3.765959
  H     2.730258     1.277822     5.196037
  H     0.541774     0.312628     4.521249
  C    -1.455537    -3.820099     1.814489
  H    -0.645229    -4.482391     2.122697
  H    -2.245541    -4.426493     1.365088
  H    -1.863838    -3.341612     2.707932
  C    -2.071478    -1.810464     0.402491
  H    -0.643524    -3.321370    -0.090273
  H    -2.502866    -1.304444     1.269126
```

H	-2.876169	-2.354760	-0.097181
H	-1.703037	-1.044378	-0.280688
C	6.144799	-3.487931	0.559935
H	6.361578	-4.207074	-0.232116
H	6.881618	-3.649528	1.350048
H	6.285166	-2.484870	0.151832
C	4.534816	-5.105218	1.637839
H	4.625304	-3.001741	1.984372
H	4.717330	-5.829427	0.840031
H	3.520480	-5.251628	2.011436
H	5.234461	-5.317148	2.449504

Optimized coordinates – $(1a)_2Ni$ (5) (High Spin)

C	-0.67546185593229	-3.01194225132354	0.92708152761451
N	0.42185027785309	-2.14512275088691	1.35709043685846
C	0.27564528000301	-1.31235792858595	2.38383064783419
C	1.37589458224275	-0.53820945874821	2.80674309984266
N	2.55366162706074	-0.72430748576660	2.09817672072619
Ni	2.20468422617664	-1.90443895458006	0.47692934150778
N	1.77952259766498	-2.29063061590460	-1.46521155960331
C	2.55888972003137	-3.32553819770884	-1.94712921159489
C	3.48133275460832	-3.86633290826890	-1.02959788003236
N	3.54603526470520	-3.37824541431330	0.21011174374495
C	4.54799023363377	-3.91417448488668	1.13750299156853
C	2.40078613021566	-3.75701305275399	-3.28640821131654
C	1.47988829073571	-3.14798893768625	-4.09894613837900
C	0.70545783110605	-2.07659559763725	-3.59339277021777
C	0.89995869127111	-1.69731482795463	-2.28356029587924
C	3.64682896609949	-0.03975167619023	2.47042703095854
C	3.67040603206030	0.84501486773517	3.52626249042815
C	2.47001490049755	1.06401314045836	4.24394358441745
C	1.33796771803904	0.38380815391404	3.88069174346983
H	-0.67015343136389	-1.21172307967440	2.90927433326902
H	4.14020678172387	-4.66434306401669	-1.35901269956403
H	3.01434682121694	-4.57186533811043	-3.65097000188068
H	1.34312538238766	-3.48308378167296	-5.11962790927482
H	-0.02429527181179	-1.56689936367529	-4.20587410603150
H	0.32460334196373	-0.88574080162952	-1.85233421673640
H	4.54182071776966	-0.22705303128079	1.88674700027297
H	4.58570328144591	1.35471913858034	3.79146892748243
H	2.44695341891206	1.76388857215933	5.06956499811675
H	0.40280869534655	0.53895332715564	4.40535018097080
C	-1.12386070295983	-3.98233590569120	2.02889670659211
H	-0.26918651137828	-4.51420948783956	2.45026931425936
H	-1.81982242832530	-4.71758085398521	1.61803551282206
H	-1.63264918222916	-3.45852403537860	2.84184804464185
C	-1.86926459359883	-2.22494633961223	0.36735387872994
H	-0.26656389676660	-3.61097962558761	0.11018584818412

```
H   -2.35533346271860    -1.63177861865786     1.14602425214132
H   -2.61364803209557    -2.90751673609144    -0.04911651188103
H   -1.55088880888699    -1.54730414961070    -0.42498168358554
C   5.98047210835223     -3.76814126952864     0.60074281549449
H   6.14772409012766     -4.40647269955022    -0.26939446276233
H   6.70291629159882     -4.06158047195875     1.36583302140057
H   6.18667568751465     -2.73789488205202     0.30389133657664
C   4.26691101614032     -5.37147314218721     1.53487640008259
H   4.46763781644977     -3.30527628775653     2.04108670449169
H   4.40728607395273     -6.04573261803369     0.68651383314665
H   3.24560313840414     -5.48761539513916     1.90098397237021
H   4.95153639075551     -5.68726367808600     2.32525721872257
```

Final Single point energy = -2427.425281762070 Eh

Input File – $(1a)_2Ni$ (5) BS(2,2)

```
! UKS B3LYP def2-TZVP def2/J RIJCOSX Grid7 TightSCF NoFinalGrid Slowconv
! Opt NumFreq

%scf
maxiter 500
brokensym 2,2
end

%output
Print[P_basis] 2
Print[P_MOs] 1
Print[P_ReducedOrbPop_L] 1
Print[P_BondOrder_L] 1
Print[P_FragBondOrder_L] 1
Print[P_OrbPopMO_L] 1
Print[P_ReducedOrbPopMO_L] 1
end


% pal nprocs 16 # num of processors
end

%maxcore 9000
%method
Z_solver DIIS
 end

 *xyz 0 1
 C  (2) -0.67546185593229    -3.01194225132354     0.92708152761451
 N  (2) 0.42185027785309     -2.14512275088691     1.35709043685846
 C  (2) 0.27564528000301     -1.31235792858595     2.38383064783419
 C  (2) 1.37589458224275     -0.53820945874821     2.80674309984266
 N  (2) 2.55366162706074     -0.72430748576660     2.09817672072619
```

Ni (1)	2.20468422617664	-1.90443895458006	0.47692934150778
N (2)	1.77952259766498	-2.29063061590460	-1.46521155960331
C (2)	2.55888972003137	-3.32553819770884	-1.94712921159489
C (2)	3.48133275460832	-3.86633290826890	-1.02959788003236
N (2)	3.54603526470520	-3.37824541431330	0.21011174374495
C (2)	4.54799023363377	-3.91417448488668	1.13750299156853
C (2)	2.40078613021566	-3.75701305275399	-3.28640821131654
C (2)	1.47988829073571	-3.14798893768625	-4.09894613837900
C (2)	0.70545783110605	-2.07659559763725	-3.59339277021777
C (2)	0.89995869127111	-1.69731482795463	-2.28356029587924
C (2)	3.64682896609949	-0.03975167619023	2.47042703095854
C (2)	3.67040603206030	0.84501486773517	3.52626249042815
C (2)	2.47001490049755	1.06401314045836	4.24394358441745
C (2)	1.33796771803904	0.38380815391404	3.88069174346983
H (2)	-0.67015343136389	-1.21172307967440	2.90927433326902
H (2)	4.14020678172387	-4.66434306401669	-1.35901269956403
H (2)	3.01434682121694	-4.57186533811043	-3.65097000188068
H (2)	1.34312538238766	-3.48308378167296	-5.11962790927482
H (2)	-0.02429527181179	-1.56689936367529	-4.20587410603150
H (2)	0.32460334196373	-0.88574080162952	-1.85233421673640
H (2)	4.54182071776966	-0.22705303128079	1.88674700027297
H (2)	4.58570328144591	1.35471913858034	3.79146892748243
H (2)	2.44695341891206	1.76388857215933	5.06956499811675
H (2)	0.40280869534655	0.53895332715564	4.40535018097080
C (2)	-1.12386070295983	-3.98233590569120	2.02889670659211
H (2)	-0.26918651137828	-4.51420948783956	2.45026931425936
H (2)	-1.81982242832530	-4.71758085398521	1.61803551282206
H (2)	-1.63264918222916	-3.45852403537860	2.84184804464185
C (2)	-1.86926459359883	-2.22494633961223	0.36735387872994
H (2)	-0.26656389676660	-3.61097962558761	0.11018584818412
H (2)	-2.35533346271860	-1.63177861865786	1.14602425214132
H (2)	-2.61364803209557	-2.90751673609144	-0.04911651188103
H (2)	-1.55088880888699	-1.54730414961070	-0.42498168358554
C (2)	5.98047210835223	-3.76814126952864	0.60074281549449
H (2)	6.14772409012766	-4.40647269955022	-0.26939446276233
H (2)	6.70291629159882	-4.06158047195875	1.36583302140057
H (2)	6.18667568751465	-2.73789488205202	0.30389133657664
C (2)	4.26691101614032	-5.37147314218721	1.53487640008259
H (2)	4.46763781644977	-3.30527628775653	2.04108670449169
H (2)	4.40728607395273	-6.04573261803369	0.68651383314665
H (2)	3.24560313840414	-5.48761539513916	1.90098397237021
H (2)	4.95153639075551	-5.68726367808600	2.32525721872257

*Optimized coordinates – $(1a)_2Ni$ BS(2,2)

C	-0.82966725295907	-2.97306713556467	0.98391231232957
N	0.31564234965178	-2.15527474656864	1.40782141871046
C	0.18661233428015	-1.33365819506513	2.42525572669296
C	1.32336723113946	-0.57496948947910	2.81296607198333
N	2.45429284502804	-0.80784045035236	2.06392406346494

Ni	2.11753418788747	-2.18194211647260	0.59157108406639
N	1.80730737748709	-2.38982914395920	-1.40140706855030
C	2.66651854234869	-3.30142609460453	-1.96359592895860
C	3.63871133700863	-3.82578467504436	-1.07114459864131
N	3.63406068386660	-3.40203483160523	0.17808972585921
C	4.65664348682686	-3.93044270469426	1.09807499949608
C	2.56123406887550	-3.65040384601567	-3.32424709364504
C	1.59405290476536	-3.06390578955357	-4.10564791322658
C	0.73247912049560	-2.11135073207650	-3.52593502716818
C	0.88201265069838	-1.81674660505081	-2.18780151942203
C	3.56414020275364	-0.11371601738159	2.37404419350835
C	3.62863002751118	0.80548319982150	3.40042012551173
C	2.47421252842772	1.04528959947848	4.17137853294205
C	1.32541467023087	0.35382753235277	3.87111665751198
H	-0.74588001742733	-1.21556780975476	2.97154102682376
H	4.36121280100347	-4.54818633399696	-1.43956806609851
H	3.24853369356283	-4.37906660171230	-3.73659968489463
H	1.49340461786156	-3.32930051696091	-5.15051795826389
H	-0.03220987487715	-1.61562434895246	-4.10767980364031
H	0.23844146902882	-1.09163645342390	-1.70488962134146
H	4.43422482929762	-0.32033657840444	1.76167551809855
H	4.55448653054053	1.32556247694397	3.60510426880362
H	2.49152854072316	1.76261765538979	4.98170850251515
H	0.41282833897479	0.51533399946811	4.43254171105362
C	-1.29663195204607	-3.94015376684175	2.07947861570671
H	-0.45555934592671	-4.50803479167501	2.48105002423090
H	-2.02357114475044	-4.64470896680287	1.66867936084098
H	-1.77506831063915	-3.40942228204270	2.90613888016039
C	-1.99346728089541	-2.12185590998760	0.46081942566359
H	-0.46036283971450	-3.57423842264255	0.15078687748887
H	-2.46073753745544	-1.54583541991035	1.26324088180872
H	-2.75926448757613	-2.76183013597538	0.01663442695652
H	-1.65056205108871	-1.42191592936799	-0.30126124978734
C	6.08382252180126	-3.78607083923497	0.55105479119808
H	6.26233964219568	-4.45088125340704	-0.29636774561966
H	6.80716089441652	-4.04808921722188	1.32656496589356
H	6.27933532732471	-2.76314241839612	0.22368482975174
C	4.37677434030353	-5.38454233057516	1.50308869809208
H	4.58176804085155	-3.31690715271850	1.99841875882622
H	4.51608674562748	-6.06140174982159	0.65663405032687
H	3.35657157902320	-5.49943129834275	1.87275900108364
H	5.06361363353594	-5.69444336179592	2.29392175185709

Final Single point energy = -2427.44810734845 Eh

Input File – $(1a)_2Ni^{I}$ cation– Structure 5^{ox}-cation

```
! UKS B3LYP def2-TZVP def2/J RIJCOSX Grid7 TightSCF NoFinalGrid
! Opt NumFreq

%scf
maxiter 5000
end

% pal nprocs 16 # num of processors
end

%maxcore 9000
%method
Z_solver DIIS
end

*xyz 1 2
Ni       0.51596       2.09723      -0.02143
N        1.81002       1.51809       1.33417
C        2.35675       2.17322       2.41468
C        3.32582       1.54135       3.24432
C        3.72963       0.22863       2.98842
C        3.21863      -0.41494       1.87415
C        2.31312       0.27836       1.04395
C        1.94083      -0.21588      -0.09597
N        1.18628       0.67240      -0.89632
C        0.38934       0.16841      -1.99026
N       -0.16644       3.48433       0.94890
C       -0.65038       3.32205       2.30746
C       -0.74338       4.51006       0.15069
C       -0.44499       4.48045      -1.09272
N        0.30543       3.41515      -1.45021
C        0.81731       3.41399      -2.71424
C        0.48725       4.41011      -3.65458
C       -0.38946       5.43407      -3.30178
C       -0.85928       5.48487      -1.99617
H        2.10844       3.19485       2.62629
H        3.77585       2.05881       4.08381
H        4.46582      -0.27545       3.61731
H        3.57251      -1.41803       1.63193
H        0.91009       4.37908      -4.65095
H       -0.66834       6.19923      -4.02091
H       -1.50924       6.30673      -1.69242
H        1.50976       2.68711      -2.99876
H       -1.38555       5.28894       0.52767
H        2.24614      -1.20527      -0.42055
C       -0.50344       4.64554       2.99402
H        0.55043       4.91314       2.78345
H       -0.69834       4.60717       4.07343
H       -1.21392       5.37289       2.56605
C       -2.11500       2.87816       2.13570
```

H	-0.18599	2.54663	2.95985
H	-2.63824	3.42984	1.31716
H	-2.70846	3.05330	3.04734
H	-2.09435	1.80994	1.81735
C	-0.34142	-1.12207	-1.60208
H	0.38288	-1.90666	-1.30508
H	-0.88086	-1.52782	-2.48417
H	-1.03995	-0.91156	-0.76664
C	1.27951	-0.13300	-3.12592
H	-0.39797	0.90573	-2.27466
H	2.03737	-0.85363	-2.76667
H	1.77314	0.78459	-3.40276
H	0.66321	-0.51383	-3.95883

*

Optimized coordinates – $(1a)_2Ni^{I}$ cation– Structure 5^{ox}-cation

Ni	0.86668948178079	2.34373126908244	-0.05349092107067
N	2.19137284337807	1.66568639702621	1.25013265054364
C	2.73636546055795	2.28845641823813	2.31284464235365
C	3.70981418252361	1.69773435388661	3.11749493212786
C	4.14110400547722	0.40050451215240	2.82417205572819
C	3.59418559913333	-0.25193996855542	1.72045203604887
C	2.63206477682334	0.40489374023037	0.94691274963695
C	2.02287804079151	-0.15826991062898	-0.24321813339487
N	1.16464547689342	0.58344628819015	-0.87713438438844
C	0.44534573642135	0.07829861155353	-2.06798486041708
N	-0.34710864531494	3.54982224150299	0.91648319139516
C	-0.81863848907384	3.33436847276040	2.30267671266730
C	-0.77156901744477	4.55317275743465	0.20827184668137
C	-0.29453440050272	4.64722568698935	-1.15872117188268
N	0.54509764315184	3.62827973444604	-1.52263035764586
C	1.07737241822241	3.65738327343779	-2.75958614819228
C	0.79561596144076	4.66630212769202	-3.67977989965004
C	-0.08209378272296	5.69277984011979	-3.31808996661902
C	-0.63154644312627	5.68177039813570	-2.03708517801509
H	2.38092178248726	3.30012744195258	2.51337458727689
H	4.11996351047010	2.25292018284593	3.96051766864292
H	4.89436037435653	-0.08901222539984	3.44129931407601
H	3.90802086243901	-1.26031327171365	1.44807310081955
H	1.26172165641352	4.64164633662294	-4.66429719523258
H	-0.32695624593520	6.48949490496955	-4.02033994762582
H	-1.31266810036221	6.46749026369357	-1.70810377509851
H	1.76028207075683	2.84435534872303	-3.00987365934374
H	-1.46265590081787	5.30749391544666	0.59539527448741
H	2.29123696370020	-1.16863531605443	-0.56504844719297
C	-1.59775625724950	4.49488118365771	2.92071254262963
H	-1.03237729909225	5.43736899512491	2.89109457639443
H	-1.80238209158107	4.26522569150410	3.97477770736791
H	-2.56984009927747	4.64871576059044	2.42901203183016

C	-1.61599590885385	2.02187428869902	2.34264378489570
H	0.10109967383892	3.18031017374853	2.89233398380984
H	-2.55357768718930	2.12318831011814	1.77727536048871
H	-1.86464865340668	1.76584733429559	3.38123641876040
H	-1.03626526994738	1.19545976522246	1.90974124195912
C	-1.04971244662453	-0.01154535184039	-1.72582957612469
H	-1.22734897611980	-0.79864017700929	-0.97893119511815
H	-1.62661523941233	-0.25449936899212	-2.62815940684242
H	-1.41911531029175	0.94087900573238	-1.32224721834388
C	0.97711686293287	-1.23001016700869	-2.65214290136927
H	0.56370383748324	0.87104699392680	-2.82610713623952
H	0.81218759623364	-2.08207531289966	-1.97600226461422
H	2.04800665374394	-1.17200576049644	-2.89434691053008
H	0.43875279289497	-1.44892518915429	-3.58375775566983

Final Single Point Energy = –2427.283556656272

EPR g-tensor values

g(tot) = 2.0498914 2.1114845 2.2104202 iso = 2.1239320

Input File – $(1a)_2Ni^{I}Cl$ – Structure 5^{ox}-Cl (not shown in text)

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7       1.422289000     1.090697000     0.764874000
6       0.401372000     0.921321000     1.621705000
6       0.058226000    -0.297284000     2.189291000
6       0.821599000    -1.436538000     1.831022000
6       1.869925000    -1.289572000     0.943384000
6       2.175578000    -0.010785000     0.400603000
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7       0.466660000     4.144535000     0.430781000
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1	2.465272000	-2.155223000	0.648204000
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1	-3.104976000	2.389510000	-3.737219000
1	-2.856508000	4.058659000	-1.900939000
1	0.858411000	0.949393000	-2.766945000
6	0.684235000	4.619732000	2.868991000
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1	1.171787000	5.307345000	3.577609000
1	1.079913000	3.609316000	3.054810000
6	5.538328000	2.563691000	-1.062708000
1	6.004233000	1.836413000	-0.376084000
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1	5.134877000	3.404343000	-0.479095000
1	0.580898000	6.094449000	1.281388000
1	2.053707000	5.129474000	1.255847000
1	4.789275000	1.122418000	-2.513043000
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17	2.720062000	4.694190000	-1.397898000
1	-1.163679128	5.232292730	-0.003459350
1	3.872757602	-0.666009171	-0.718639988

*

Optimized coordinates – $(1a)_2Ni^{I}Cl$ – Structure 5^{ox}-Cl

Ni	1.773684	2.748519	-0.441386
N	1.337728	1.115032	0.794175
C	0.313973	0.926189	1.644589
C	-0.017682	-0.304618	2.192577
C	0.752012	-1.436281	1.819386
C	1.802422	-1.269308	0.937534
C	2.098978	0.021781	0.428770
C	3.166806	0.304448	-0.476342
N	3.287567	1.533500	-0.941481
C	4.443347	1.888833	-1.750263
N	0.375015	4.147715	0.439693
C	0.758428	5.139418	1.431384
C	-0.676130	4.285697	-0.270952
C	-0.911218	3.352378	-1.388620
N	0.100366	2.495808	-1.647986
C	-0.012489	1.622576	-2.650317

C	-1.152679	1.555742	-3.457084
C	-2.202748	2.443014	-3.206670
C	-2.080135	3.360202	-2.159500
H	-0.264999	1.819488	1.902259
H	-0.850959	-0.390422	2.892710
H	0.510469	-2.423155	2.223599
H	2.415849	-2.115864	0.616208
H	-1.206201	0.826591	-4.268152
H	-3.106373	2.419559	-3.820645
H	-2.876379	4.073949	-1.934926
H	0.842679	0.959411	-2.812783
C	1.211784	4.512194	2.748120
H	0.386885	3.996644	3.265927
H	1.602040	5.292785	3.419879
H	2.016377	3.781942	2.571738
C	5.518788	2.581909	-0.908155
H	5.898840	1.914360	-0.116697
H	6.368541	2.889934	-1.540079
H	5.085824	3.481742	-0.446254
H	-0.054651	5.873087	1.594287
H	1.607365	5.669665	0.963652
H	4.865271	0.990035	-2.244192
H	4.109586	2.591413	-2.528759
Cl	2.691700	4.703564	-1.375914
H	-1.394397	5.109548	-0.117481
H	3.875094	-0.489246	-0.758889

EPR g-tensor values

g(tot) =2.1899638 2.2366671 2.2529868 iso = 2.2262059

8.2. Calculated Geometries of 5 and 5^{ox}

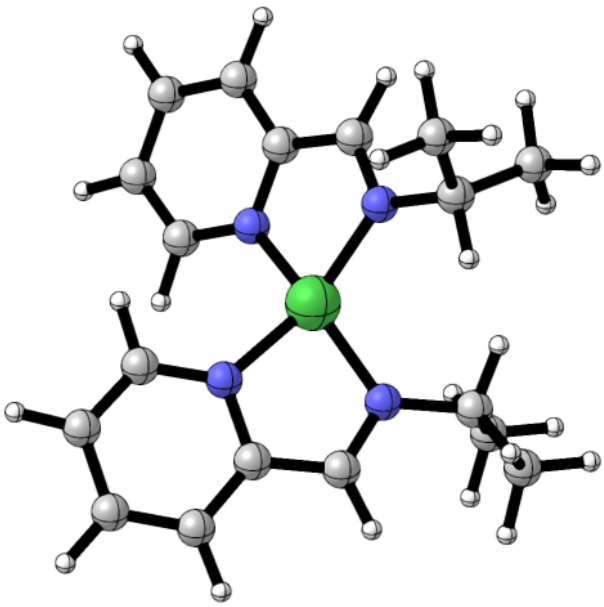

Figure S11: "BS(0,0)" low spin optimized geometry of **5**.

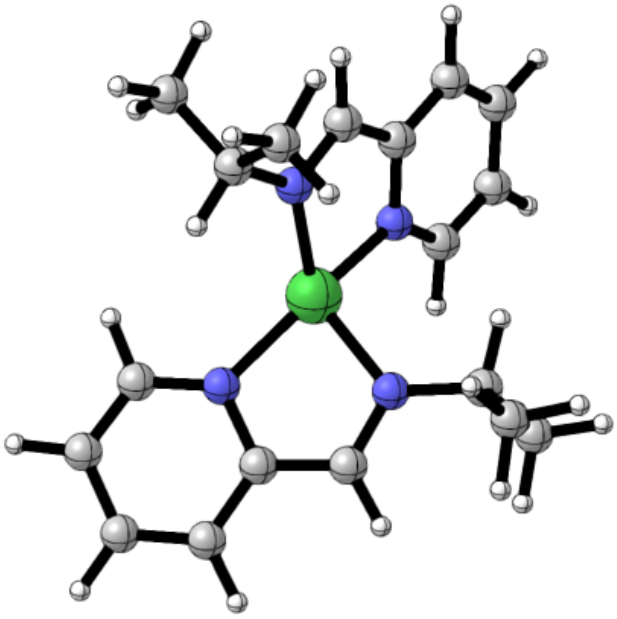

Figure S12: "BS(0,0)" high spin optimized geometry of **5**.

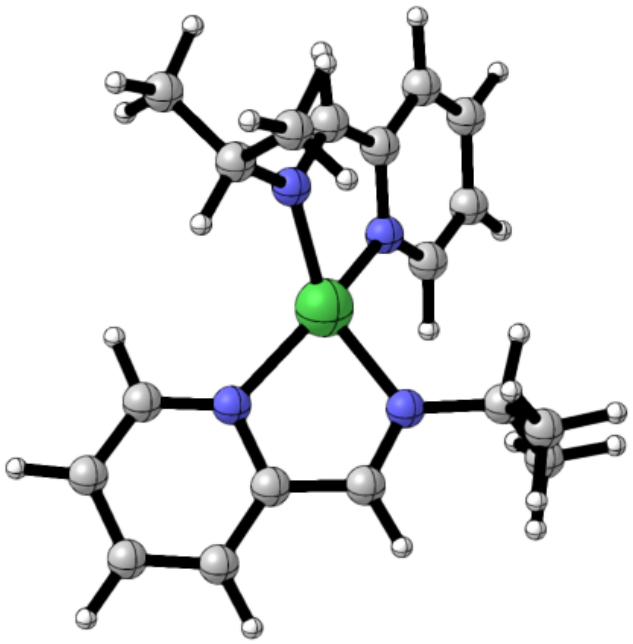

Figure S13: BS(2,2) optimized geometry of **5**.

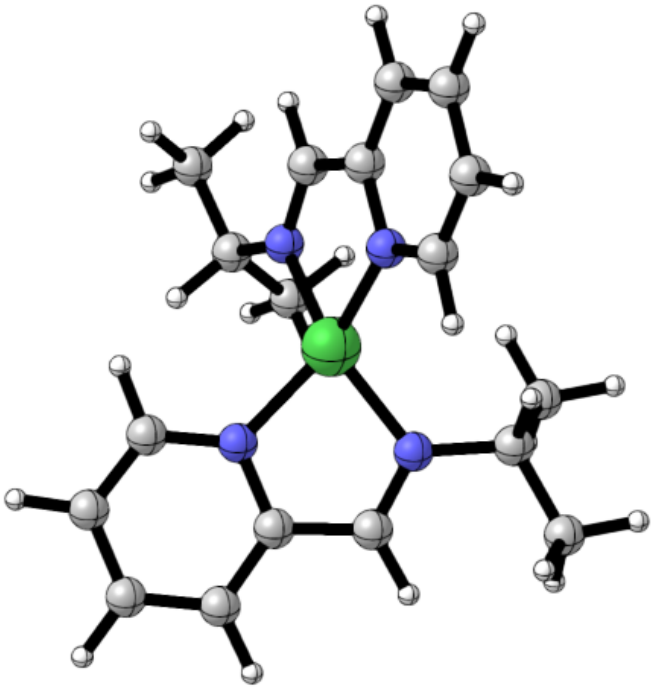

Figure S14: Optimized geometry of $\mathbf{5}^{ox}$ cation.

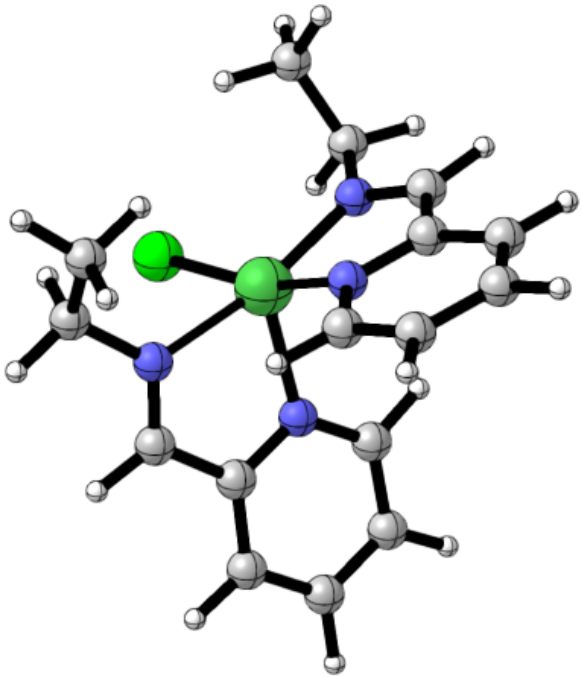

Figure S15: Optimized geometry of neutral **5^{ox}-Cl** complex (not featured in text).

9. Comparison of 5/5^{ox} with redox-active iminopyridine Ni complexes

Calculations on neutral (**1a**)$_2$Ni^0 (**5**) complexes converged to the broken symmetry solution BS(2,2) where two anionic ligand-centered radicals were antiferromagnetically coupled to the high spin nickel center. The ferromagnetically coupled alternative and the non-BS solutions were found to be higher in energy. Broken Symmetry calculations on the oxidized, formally Ni^I complex **5^{ox}** and **5^{ox}-Cl,** all converged to the non-BS solution over the BS(2,1) or high spin solutions. Localization of spin density on the Ni^I center is consistent with our EPR data (Figure **S9-S10**). Our spectroscopic and computational data are in agreement with the studies on related complexes published by Wieghardt.[15] Notably the redox noninnocence of *N*-aryl imines **S-I** and **S-II** (Figure **S16**) studied by Wieghardt and coworkers were not electronically distinct from the *N*-alkyl imines studied herein (Figure **S17**). It is our belief that redox non-innocence of **5** as well as the covalency and stability of **5^{ox}** enables the generation and capture of alkyl radicals in the reaction.

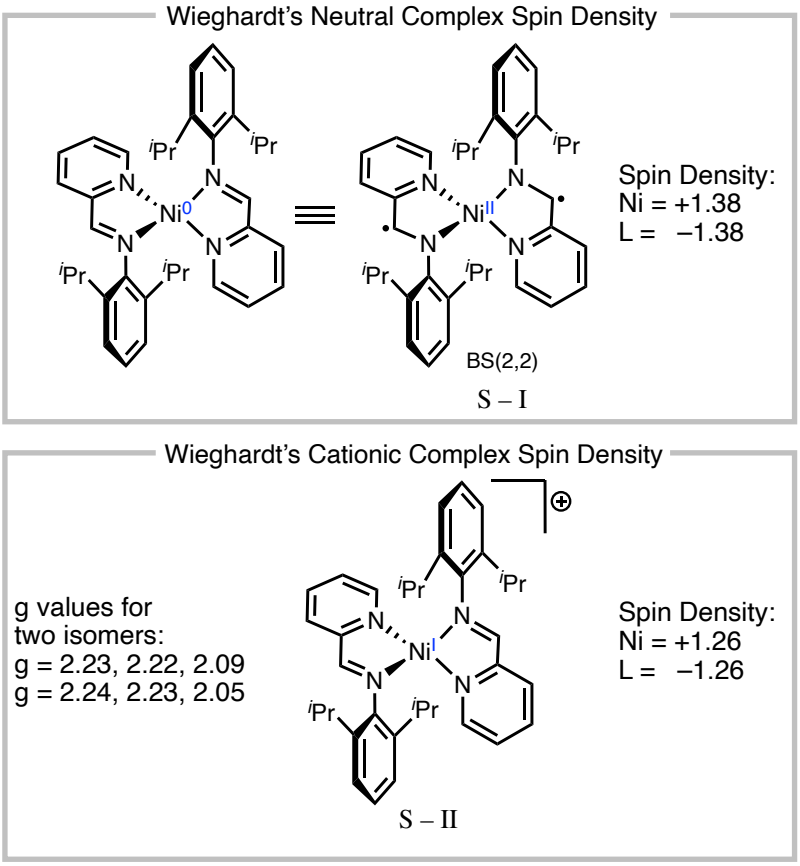

Figure S16: Spin density and EPR results obtained by Wieghardt[18] on redox active imine Ni complexes.

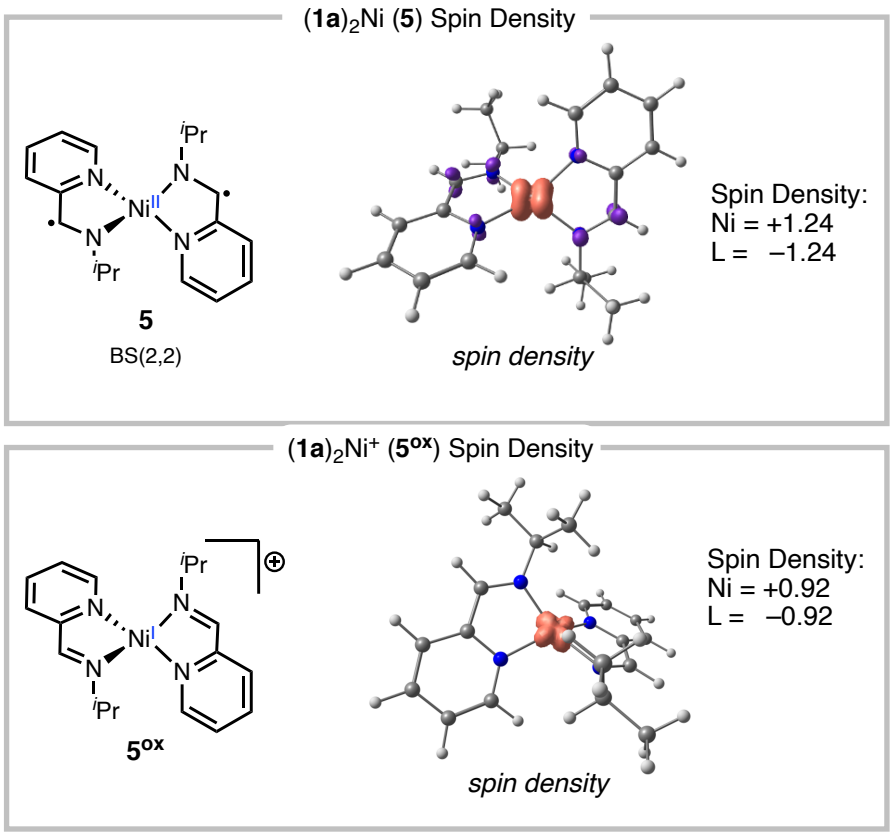

Figure S17. Computational results on **5** and **5^{ox}** showing similar electronic structures as **S–I** and **S-II**. A spin density shown in orange and β spin density shown in purple.

10. X-Ray Diffraction Data for 1a'

Low-temperature diffraction data (φ- and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON II CPAD detector with Mo-Kα radiation (λ = 0.71073 Å) from a IμS HB micro-focus sealed X-ray tube. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEXII software.[16] Absorption corrections were applied using SADABS.[17] The structure was solved by intrinsic phasing using SHELXT[18] and refined against F2 on all data by full-matrix least squares with SHELXL-2014[18] using established refinement techniques.[19] All non-hydrogen atoms were refined anisotropically. Unless otherwise noted, all hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). Crystallographic data for **1a'** can be obtained free of charge from The Cambridge Crystallographic Data Centre (CCDC) via www.ccdc.cam.ac.uk/data_request/cif under CCDC

deposition numbers CCDC 2079525. Graphical representation of the structures with 50% probability thermal ellipsoids was generated using Mercury visualization software.[20]

Table S1: Crystal and Refinement Data for 1a'

CCDC Number	2079525
Formula	$C_{18}H_{26}N_4$
Formula Weight	298.43
Crystal System	Triclinic
Space Group	P–1
a, Å	5.859(3)
b, Å	8.709(6)
c, Å	8.720(5)
α, °	95.09(2)
β, °	103.38(3)
γ, °	100.86(4)
Volume, Å	421.0(4)
T (K)	100
d_{calc}, g/cm ^{3}	1.082
Z	1
R_1,[a] wR_2,[b] [I>2σ(I)]	0.0506, 0.1679
GOF	1.05

[a] $R_1 = \Sigma||Fo|-|Fc||/\Sigma|Fo|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(Fo^2)^2]]^{1/2}$.

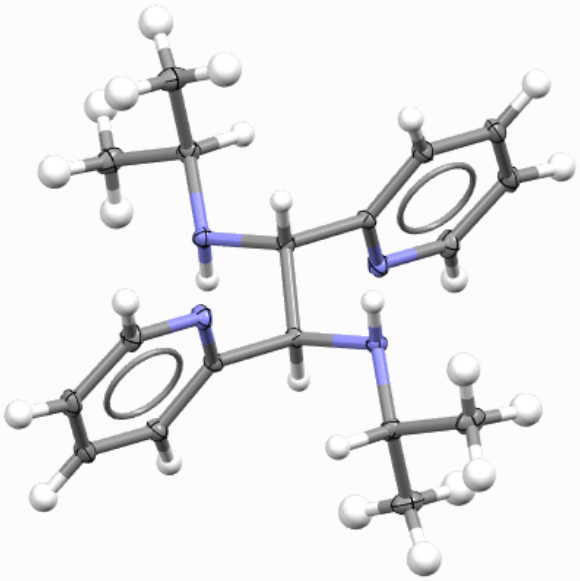

Figure S18: Structure of **1a'**with 50% probability anisotropic displacement ellipsoids.

11. Elemental Analysis of Commercial Mn^0

Samples were measured on an Agilent 8800 ICP-MS instrument. ICP-MS was used to quantify trace Ni impurities in the commercial Mn^0 metal powder sample that was used throughout this publication. Three samples were prepared where sample A is the commercial metal, sample B is a procedural digestion blank to establish a background response, and sample C which is the commercial sample that was spiked with a transition metal analytical standard containing 500 ppb Ni. Sample data was quantified against a calibration curve (Figure **S19**) and amount of trace Ni in sample A was corrected for matrix/digestion effects determined by samples B and C.

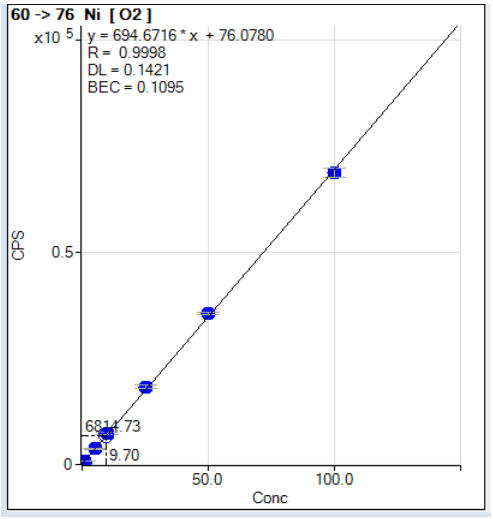

Figure S19: Ni calibration curve of measured counts/s against concentration in ppb.

Sample preparation: To a 50 mL PTFE digestion tube was added Mn^0 metal powder (108.2 mg) followed by 2 mL of conc. HNO_3 (sample A). To the procedural blank tube (sample B) was also added 2 mL of conc. HNO_3, then all samples were refluxed under a watch glass for 2h at 80 ºC. The homogenous solutions were then diluted to 50 mL with conc. HNO_3. These solutions were then diluted again by diluting 1 mL to 50 mL in conc. HNO_3 to make the instrument ready samples. Another Mn-containing sample (sample C) was prepared the same as sample A except 1 mL of a transition metal standard containing 500 ppb Ni was added. The standard adds a net 10 ppb Ni to the sample C over the unspiked sample A in the instrument ready samples.

Average Concentrations:

Sample Name	Avg Conc. (ppb)	Conc. RSD (%)
Sample **A**	2.3	18.6
Sample **B**	0.6	46.5
Sample **C** (**A** +10ppb Ni)	9.6	6.4

Table S2: Average concentration of Ni measured in each sample with relative standard deviations (RSD).

Calculation of Trace Ni in Mn sample:

$$\frac{[Ni]_C - [Ni]_A}{[Ni]_{Std}} \times 100\% = \frac{9.6\,ppb - 2.3\,ppb}{10\,ppb} \times 100\% = 73\%$$

Equation S1: Digestion recovery of Ni calculated from measured [Ni] in samples A and C ($[Ni]_A$ and $[Ni]_C$) and the amount added from the standard ($[Ni]_{std}$).

From the digestion recovery (equation **S1**) and procedural blank (sample B) the measured concentration of Ni can be corrected by taking the difference of the concentration in sample A (2.3 ppb) and the background from sample B (0.6 ppb) giving 1.7 ppb Ni. This value is then further corrected by dividing by the recovery, 73% (equation **S1**) to give a final corrected concentration of 2.3 ppb Ni. A 2.3 ppb concentration from the 108.2 mg sample corresponds to a final concentration of **54.1 ppm**. This corresponds to 54.1 μg of total Ni per gram of Mn metal added. As a consequence In each reaction on a 0.3 mmol scale used in this chemistry, ~900 ng of nickel species (0.005 mol%) are added through the addition of our Mn^0 reductant.

12. References

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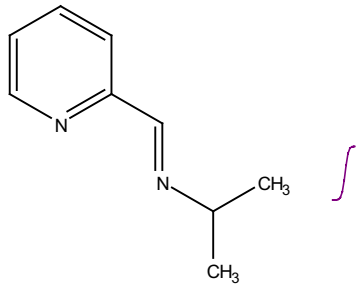
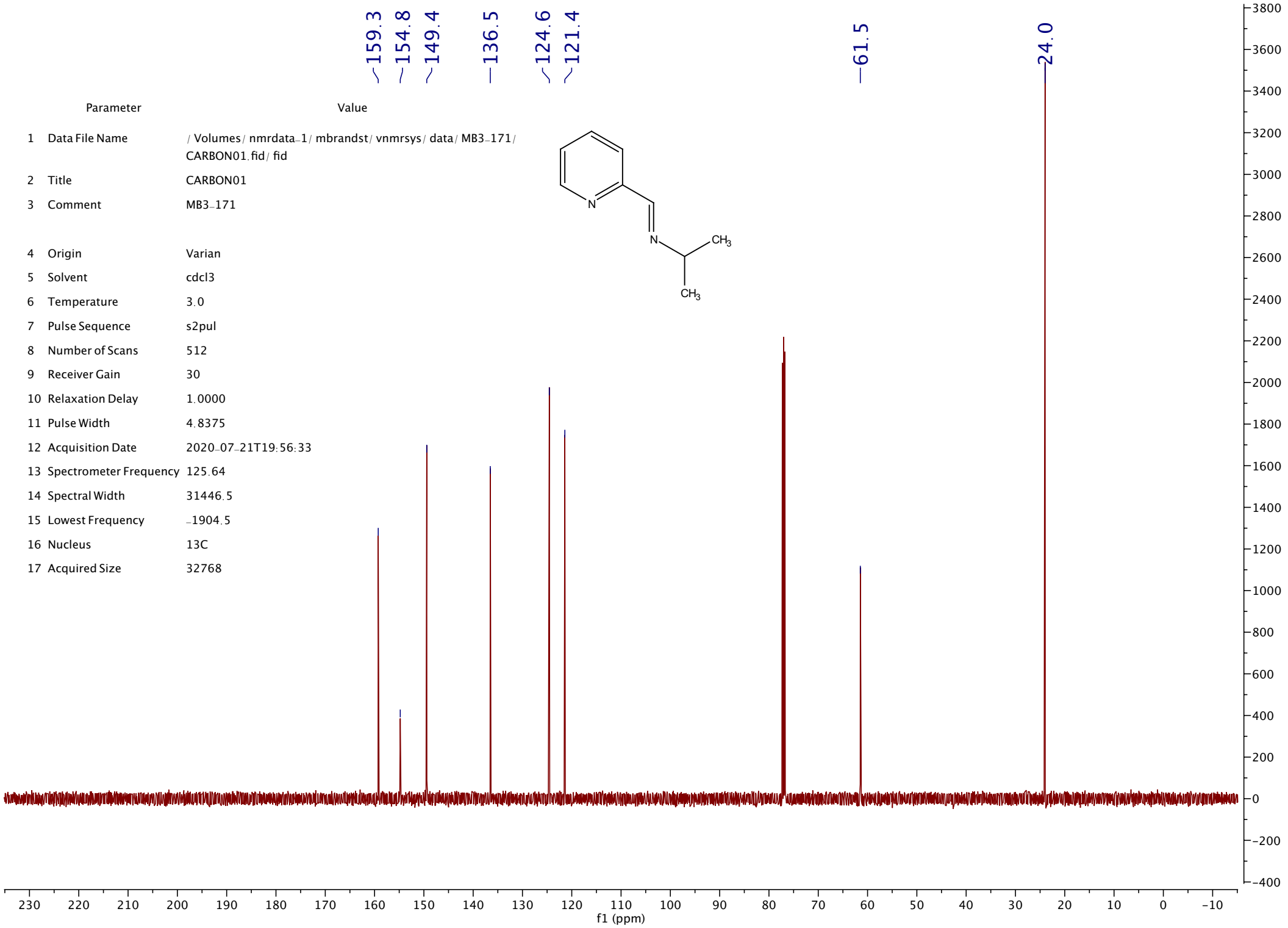
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000





	Parameter	Value
1	Data File Name	/Volumes/nmrdata-1/mbrandst/vnmrsys/data/MB3-171/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3-171
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020-07-21T19:56:33
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

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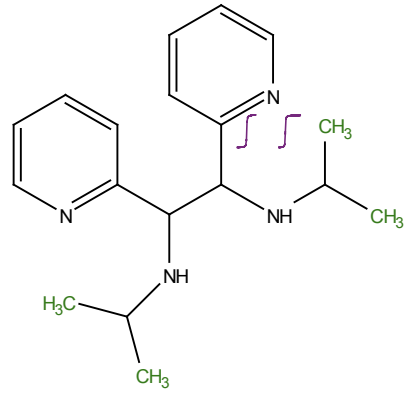
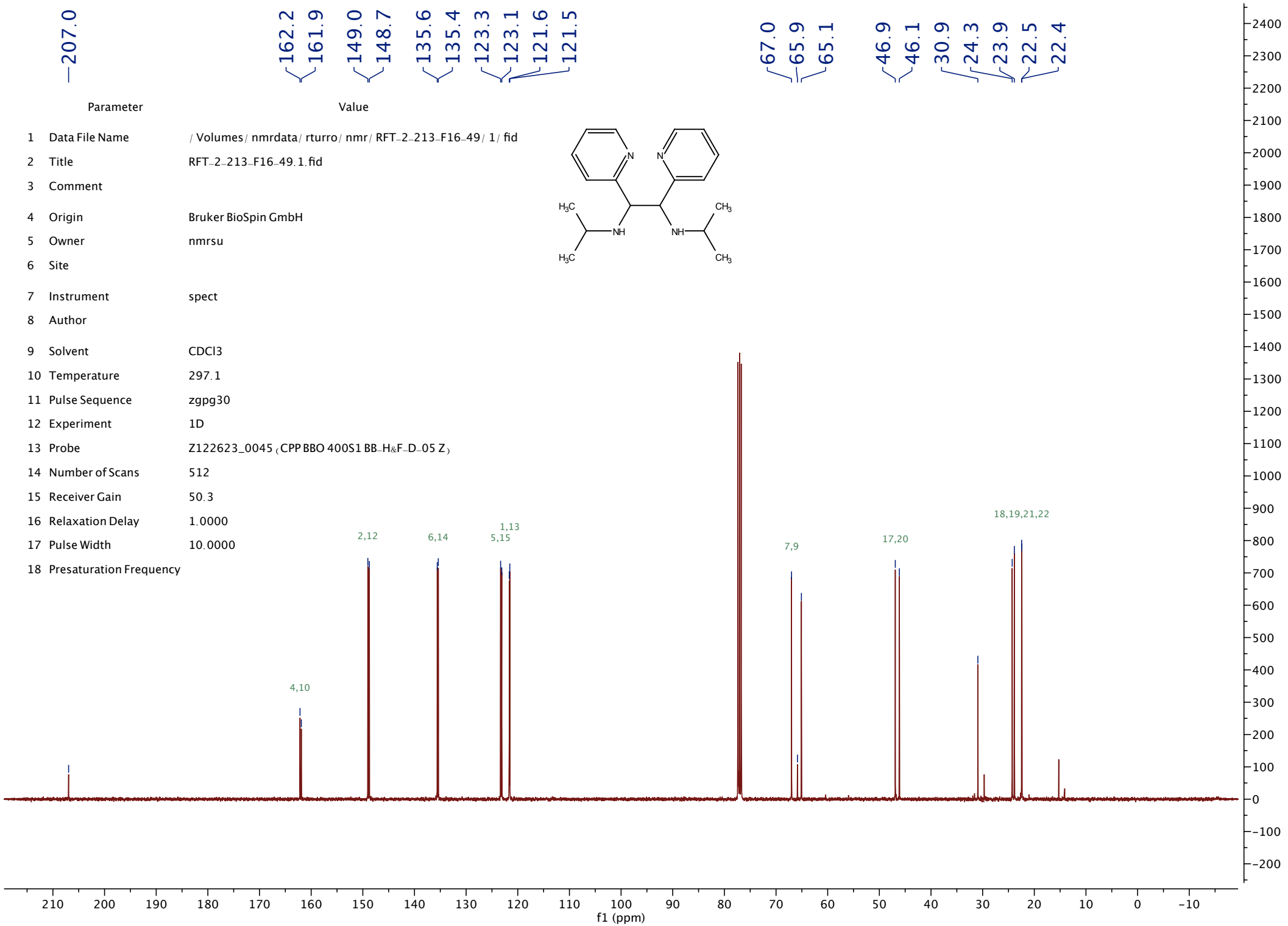
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_2_213_F16_49/2/fid
2	Title	RFT_2_213_F16_49.2.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
14	Number of Scans	16
15	Receiver Gain	30.3
16	Relaxation Delay	1.0000
17	Pulse Width	12.5000




207.0
162.2
161.9
149.0
148.7
135.6
135.4
123.3
123.1
121.6
121.5
67.0
65.9
65.1
46.9
46.1
30.9
24.3
23.9
22.5
22.4
Parameter
Value
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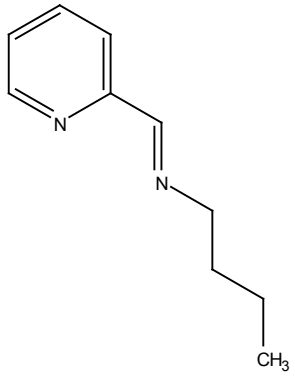
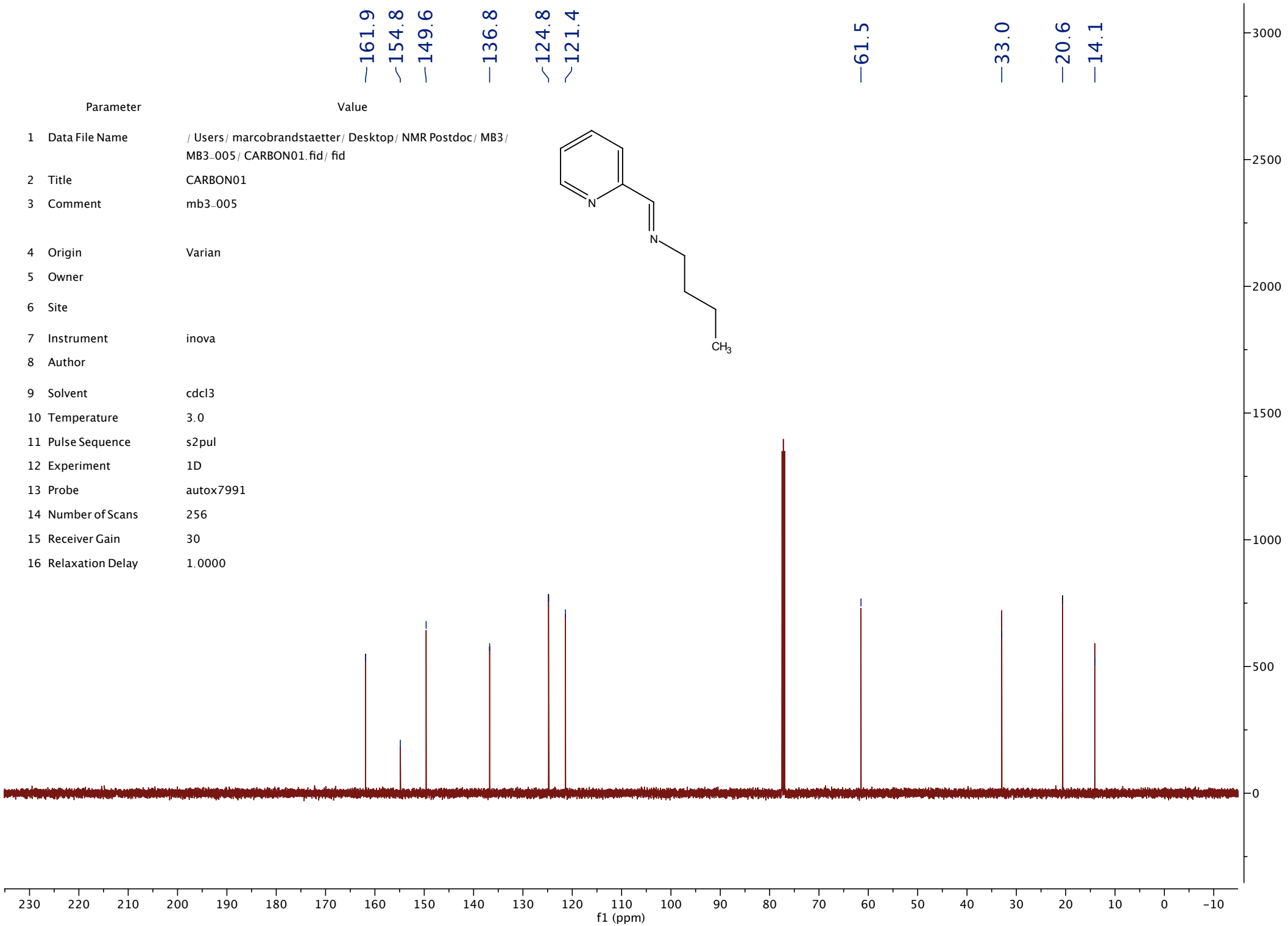
2 Title RFT_2_213_F16_49.1.fid
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Instrument spect
8 Author
9 Solvent CDCl3
10 Temperature 297.1
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Probe Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
14 Number of Scans 512
15 Receiver Gain 50.3
16 Relaxation Delay 1.0000
17 Pulse Width 10.0000
18 Presaturation Frequency
N
N
H3C
NH
NH
CH3
H3C
CH3
4,10
2,12
6,14
1,13
5,15
7,9
17,20
18,19,21,22
f1 (ppm)

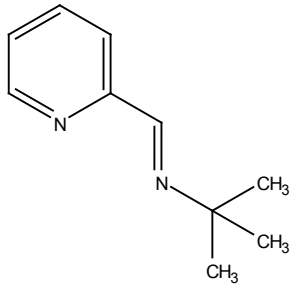
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_005 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb3_005
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	52
16	Relaxation Delay	1.0000





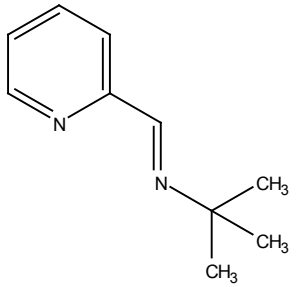
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_005 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	mb3_005
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	256
15	Receiver Gain	30
16	Relaxation Delay	1.0000

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_046 / 1 / fid
2	Title	mb3_046.1.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
14	Number of Scans	16
15	Receiver Gain	64.2
16	Relaxation Delay	1.0000
17	Pulse Width	12.5000

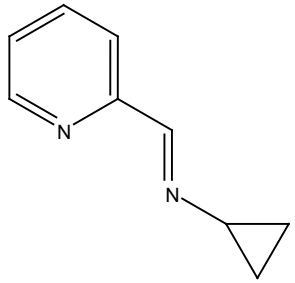


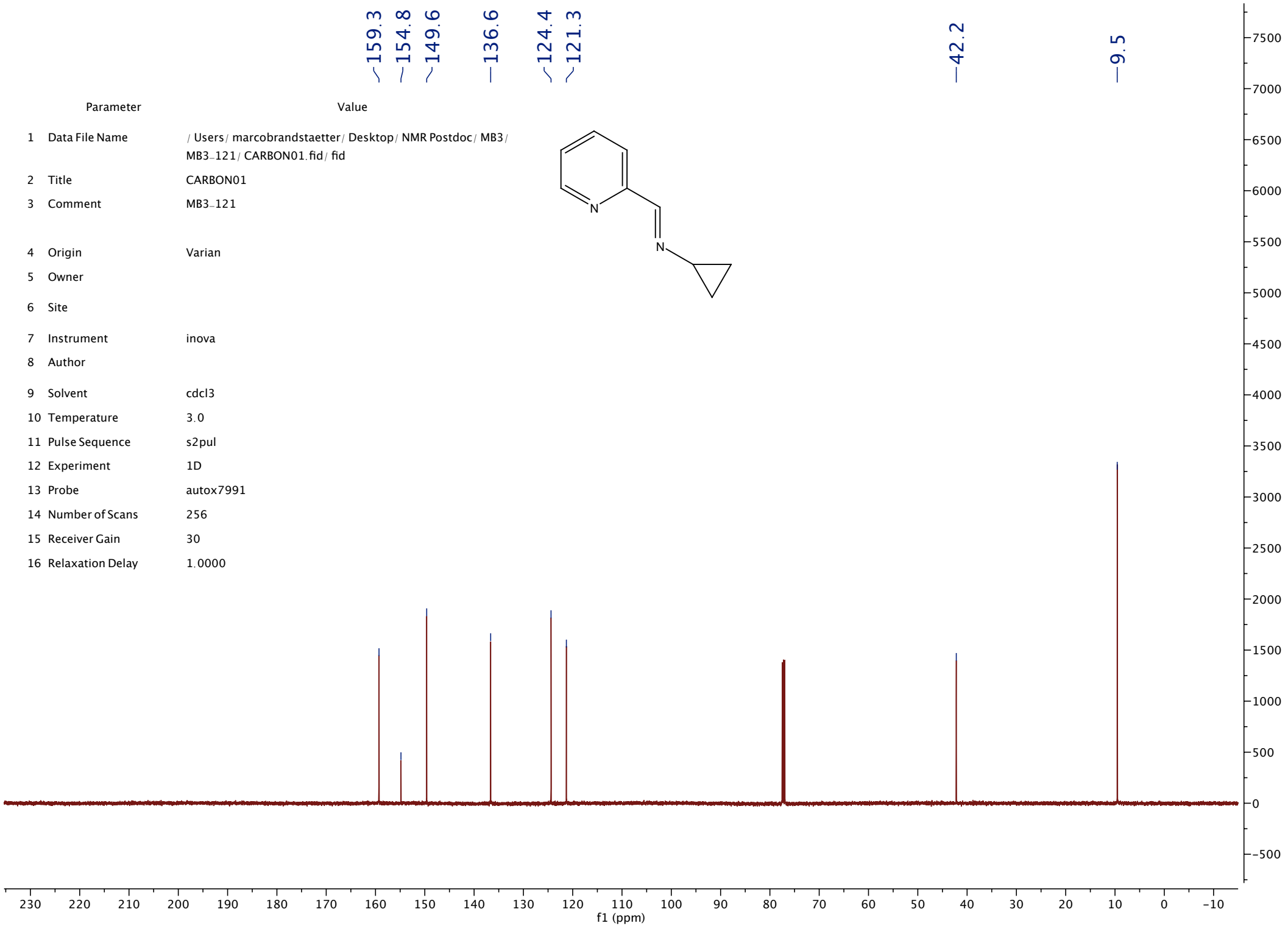
156.6
155.7
149.5
136.7
124.6
121.2
58.0
29.8

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_046 / 2 / fid
2	Title	mb3_046.2.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
14	Number of Scans	512
15	Receiver Gain	55.5
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000



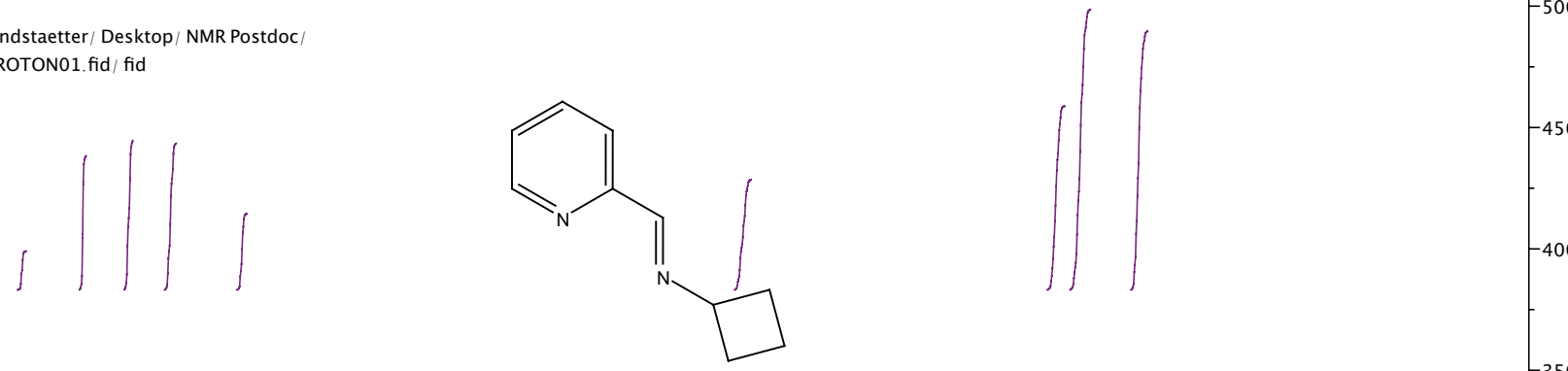
Parameter	Value
1 Data File Name	/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB3/ MB3_121/ PROTON01.fid/ fid
2 Title	PROTON01
3 Comment	MB3_121
4 Origin	Varian
5 Owner	
6 Site	
7 Instrument	inova
8 Author	
9 Solvent	cdcl3
10 Temperature	3.0
11 Pulse Sequence	s2pul
12 Experiment	1D
13 Probe	autox7991
14 Number of Scans	16
15 Receiver Gain	32
16 Relaxation Delay	1.0000

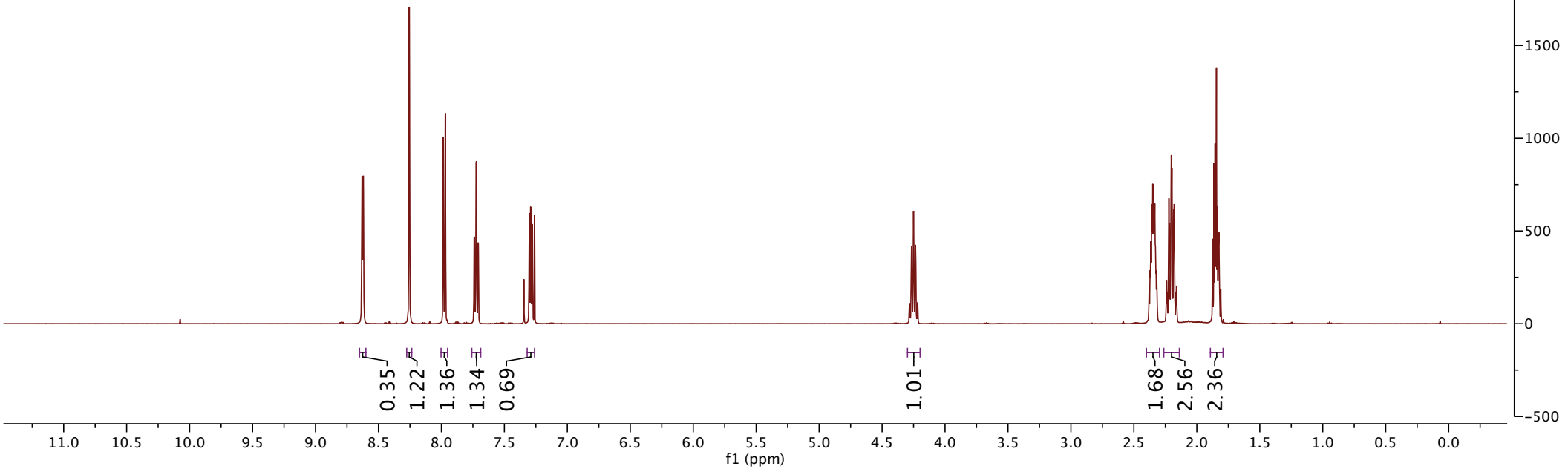


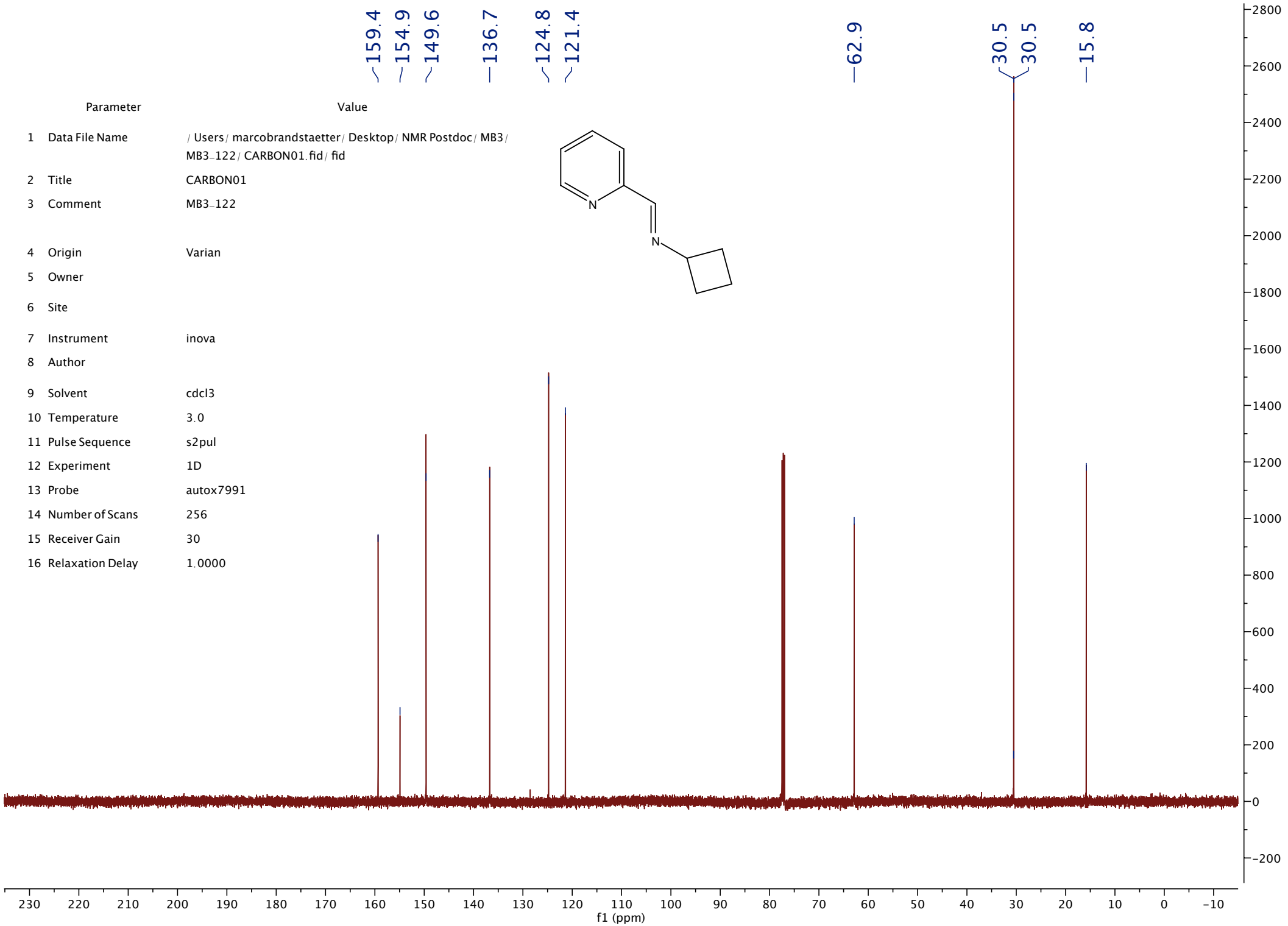


	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_121 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB3_121
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	256
15	Receiver Gain	30
16	Relaxation Delay	1.0000

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_122 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB3_122
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	16
15	Receiver Gain	34
16	Relaxation Delay	1.0000

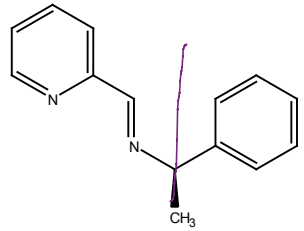






	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_122 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB3_122
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	256
15	Receiver Gain	30
16	Relaxation Delay	1.0000

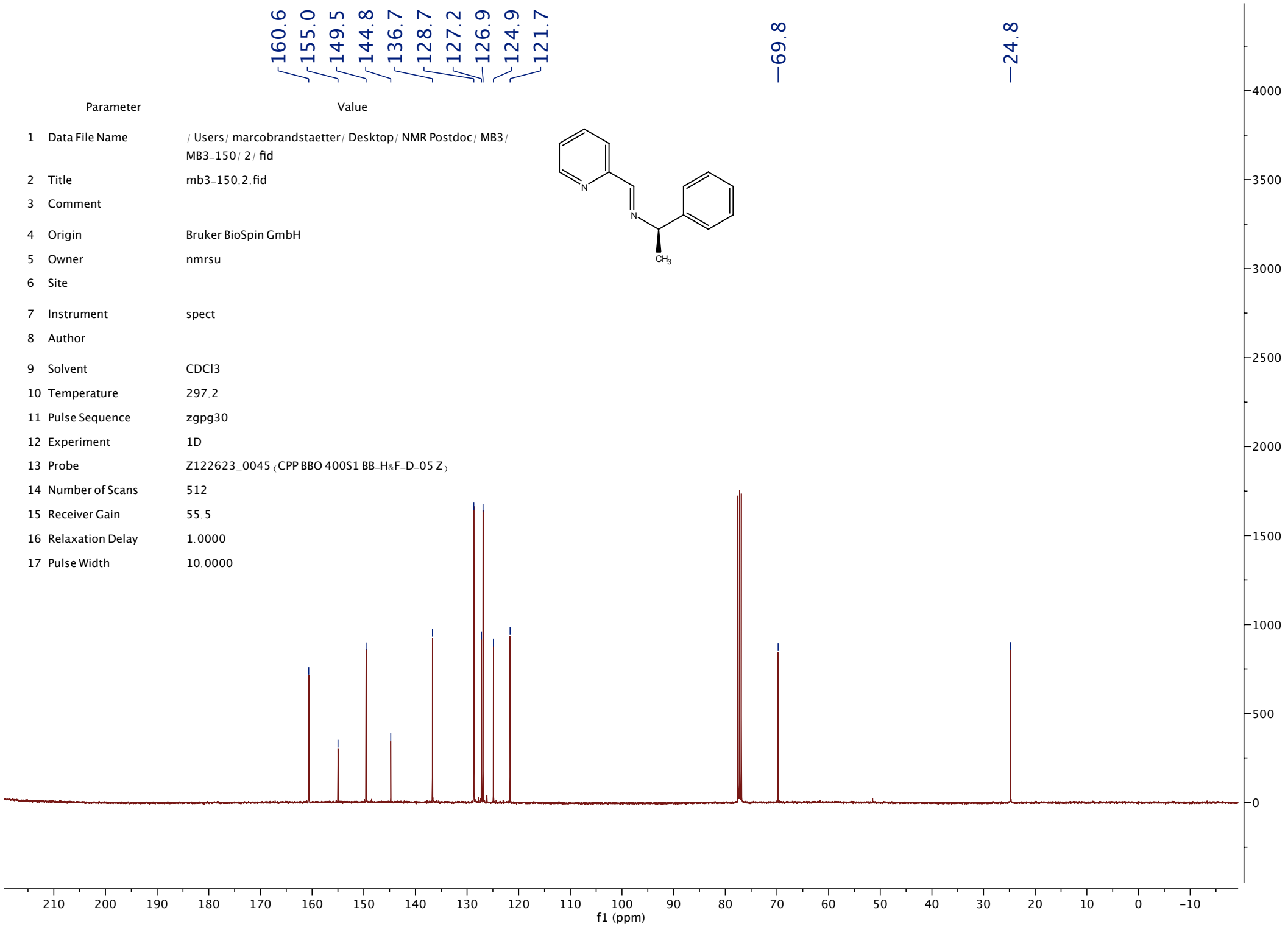
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_150 / 1 / fid
2	Title	mb3_150.1.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
14	Number of Scans	16
15	Receiver Gain	98.9
16	Relaxation Delay	1.0000
17	Pulse Width	12.5000



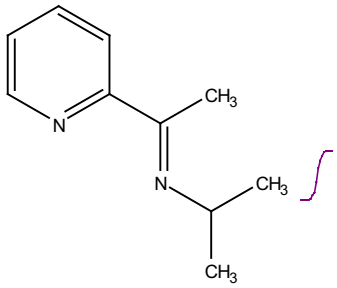
G (ddd) 7.30
C (dt) 8.10
B (m) 7.44
D (ddd) 8.64
A (m) 7.74
H (m) 7.26
J (q) 4.65
I (d) 1.61
E (s) 8.47
F (m) 7.35

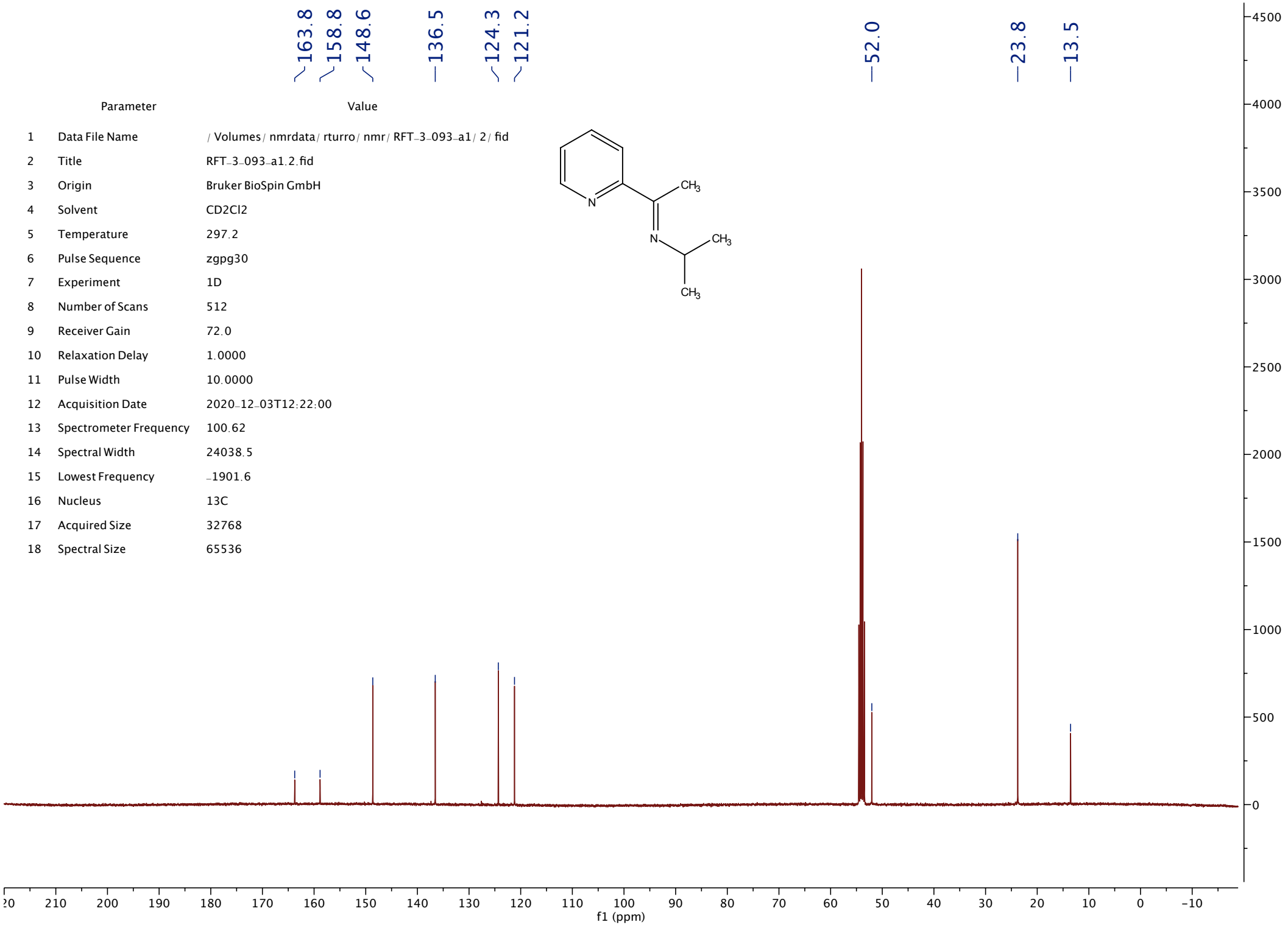
1.19 0.82 1.29 1.00 1.87 2.12 1.31 1.68 1.15 0.04

f1 (ppm)


160.6
155.0
149.5
144.8
136.7
128.7
127.2
126.9
124.9
121.7
69.8
24.8
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_150 / 2 / fid
2 Title mb3_150.2.fid
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Instrument spect
8 Author
9 Solvent CDCl3
10 Temperature 297.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Probe Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
14 Number of Scans 512
15 Receiver Gain 55.5
16 Relaxation Delay 1.0000
17 Pulse Width 10.0000
N
N
CH3
4000
3500
3000
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ RFT-3-093-a1/ 1/ fid
2	Title	RFT-3-093-a1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CD2Cl2
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	127.1
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020-12-03T12:00:47
13	Spectrometer Frequency	400.13
14	Spectral Width	8012.8
15	Lowest Frequency	-1585.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536





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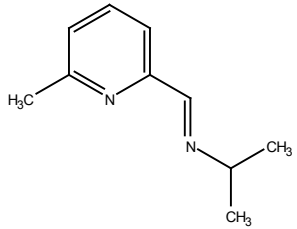
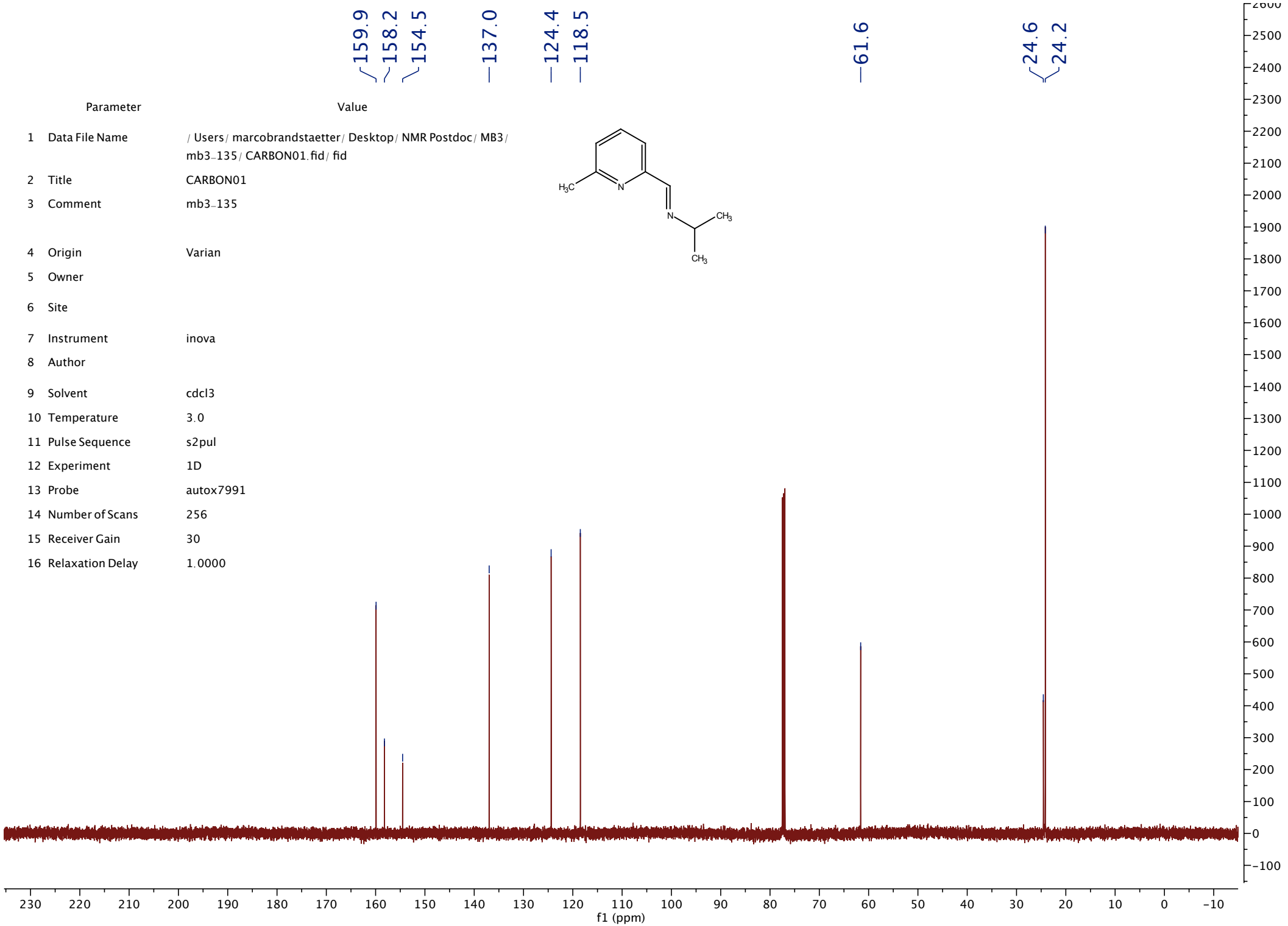
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_093_a1/2/fid
2	Title	RFT_3_093_a1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CD2Cl2
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	72.0
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_12_03T12:22:00
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1901.6
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_135 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb3_135
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	48
16	Relaxation Delay	1.0000




159.9
158.2
154.5
137.0
124.4
118.5
61.6
24.6
24.2
Parameter
Value
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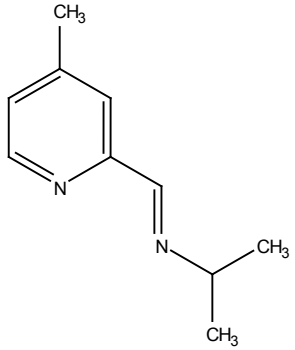
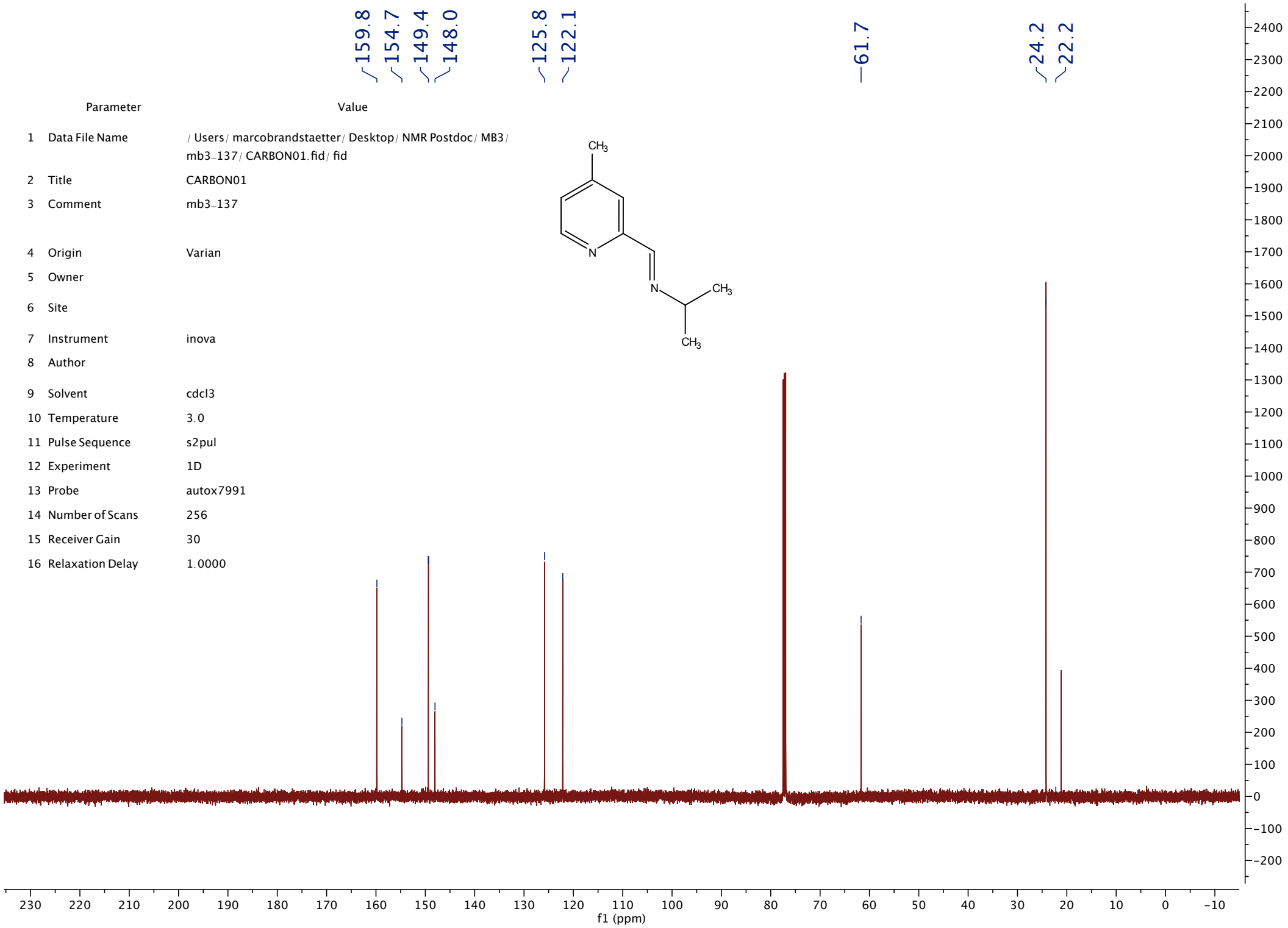
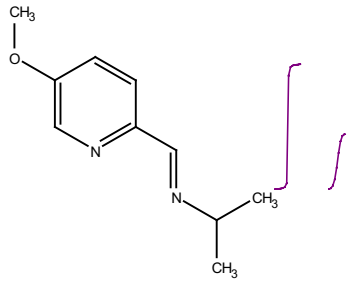
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_135 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
mb3_135
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
H3C
N
N
CH3
CH3
f1 (ppm)

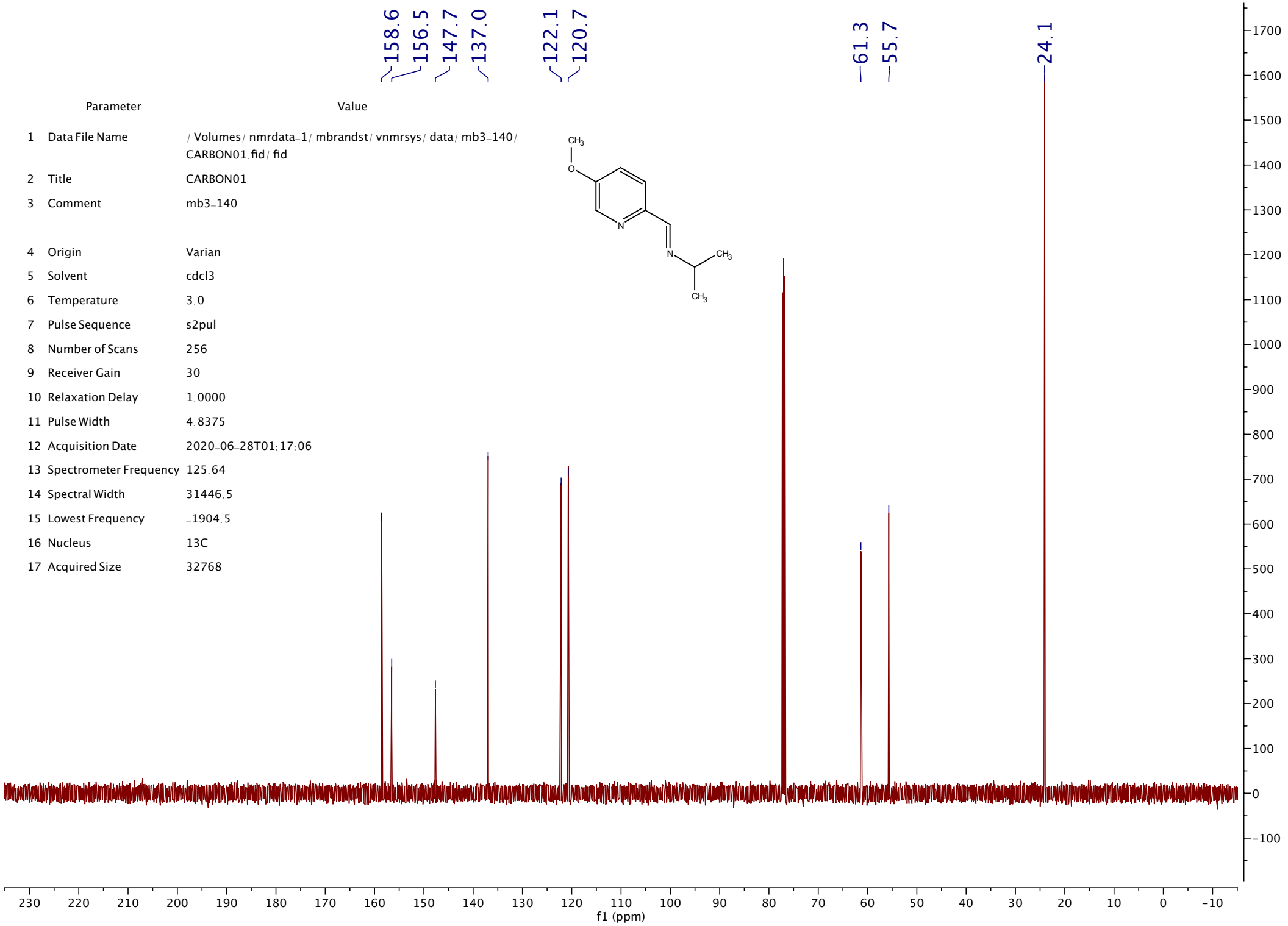
	Parameter	Value
1	Data File Name	/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB3/ mb3_137/ PROTON01.fid/ fid
2	Title	PROTON01
3	Comment	mb3_137
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	50
16	Relaxation Delay	1.0000



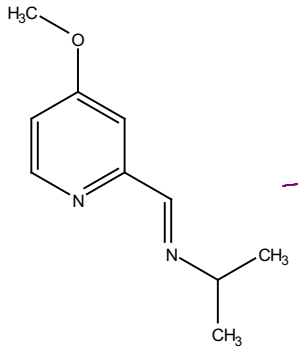

159.8
154.7
149.4
148.0
125.8
122.1
61.7
24.2
22.2
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_137 / CARBON01.fid / fid
2 Title CARBON01
3 Comment mb3_137
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
10 Temperature 3.0
11 Pulse Sequence s2pul
12 Experiment 1D
13 Probe autox7991
14 Number of Scans 256
15 Receiver Gain 30
16 Relaxation Delay 1.0000
CH3
N
N
CH3
CH3
f1 (ppm)

	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb3_140/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb3_140
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_06_28T01:16:18
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000




158.6
156.5
147.7
137.0
122.1
120.7
61.3
55.7
24.1
Parameter
Value
1 Data File Name / Volumes / nmrdata_1 / mbrandst / vnmrsys / data / mb3_140 / CARBON01.fid / fid
2 Title CARBON01
3 Comment mb3_140
4 Origin Varian
5 Solvent cdcl3
6 Temperature 3.0
7 Pulse Sequence s2pul
8 Number of Scans 256
9 Receiver Gain 30
10 Relaxation Delay 1.0000
11 Pulse Width 4.8375
12 Acquisition Date 2020_06_28T01:17:06
13 Spectrometer Frequency 125.64
14 Spectral Width 31446.5
15 Lowest Frequency -1904.5
16 Nucleus 13C
17 Acquired Size 32768
CH3
O
N
N
CH3
CH3
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

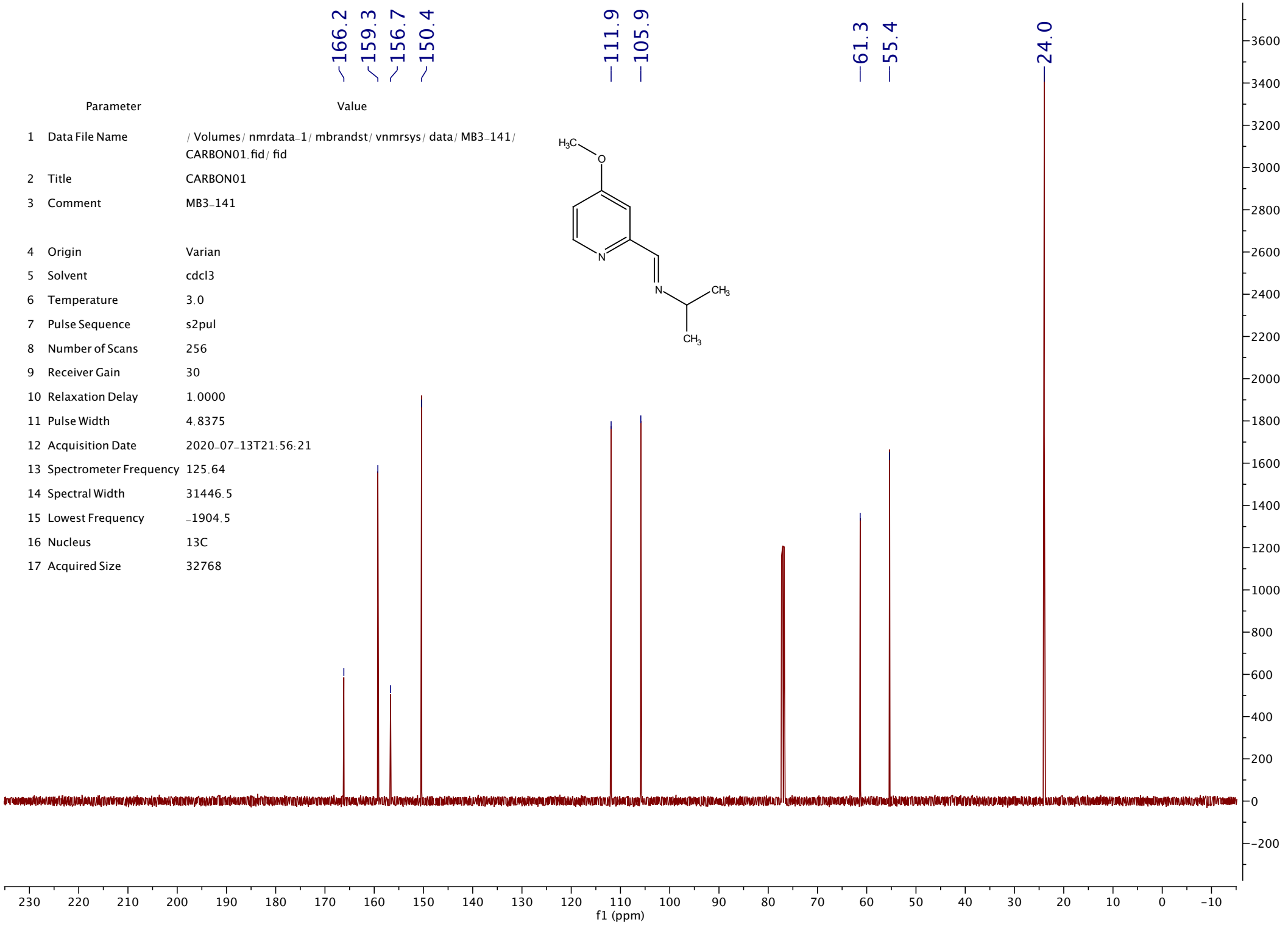
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_141/PROTON02.fid/fid
2	Title	PROTON02
3	Comment	MB3_141
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	42
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T21:55:32
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000



D (dd) 8.41
C (d) 8.33
B (t) 7.49
A (dt) 6.81
F (d) 3.89
E (m) 3.62
G (dd) 1.27

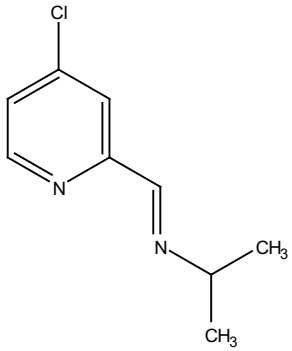
1.02
1.08
0.99
1.00
3.35
1.10
6.38

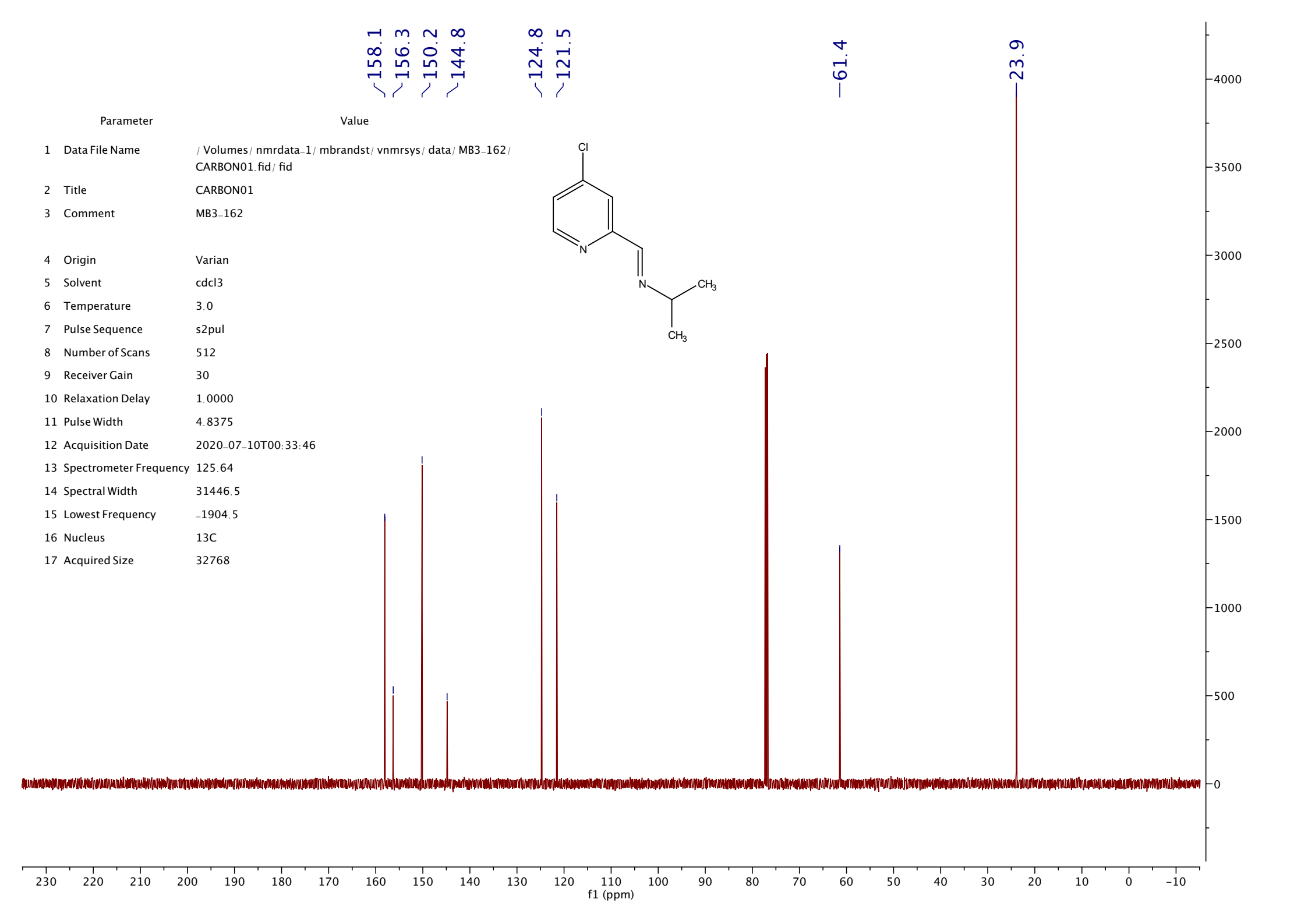
f1 (ppm)



	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_141/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3_141
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T21:56:21
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	_1904.5
16	Nucleus	13C
17	Acquired Size	32768

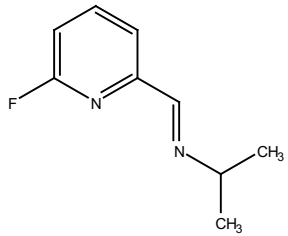
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_162/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB3_162
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_10T00:32:25
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

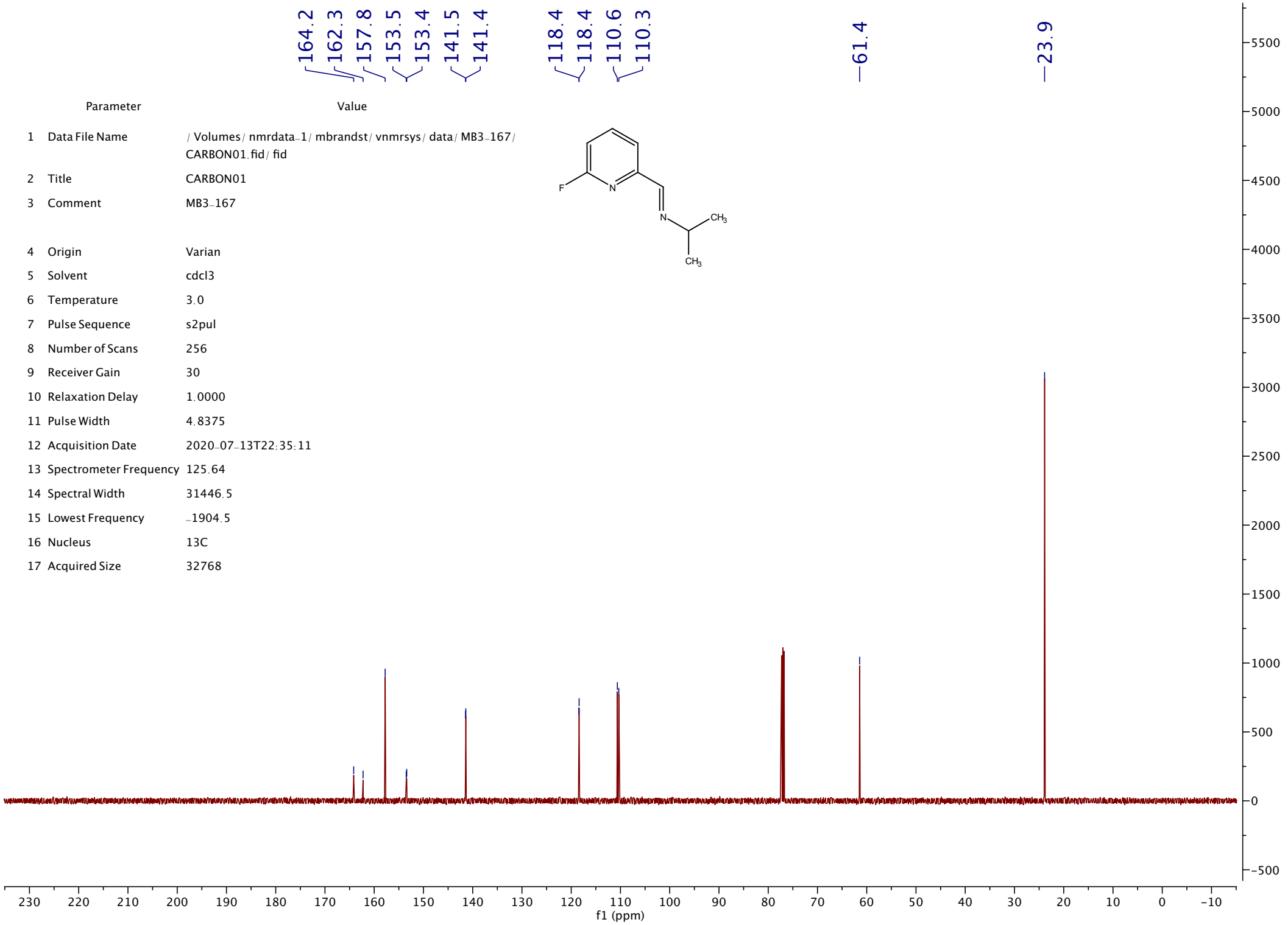




	Parameter	Value
1	Data File Name	/Volumes/nmrdata-1/mbrandst/vnmrsys/data/MB3-162/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3-162
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020-07-10T00:33:46
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

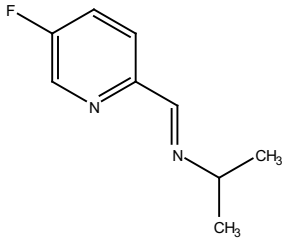
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_167/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB3_167
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T22:34:22
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000





	Parameter	Value
1	Data File Name	/Volumes/nmrdata-1/mbrandst/vnmrsys/data/MB3-167/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3-167
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020-07-13T22:35:11
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

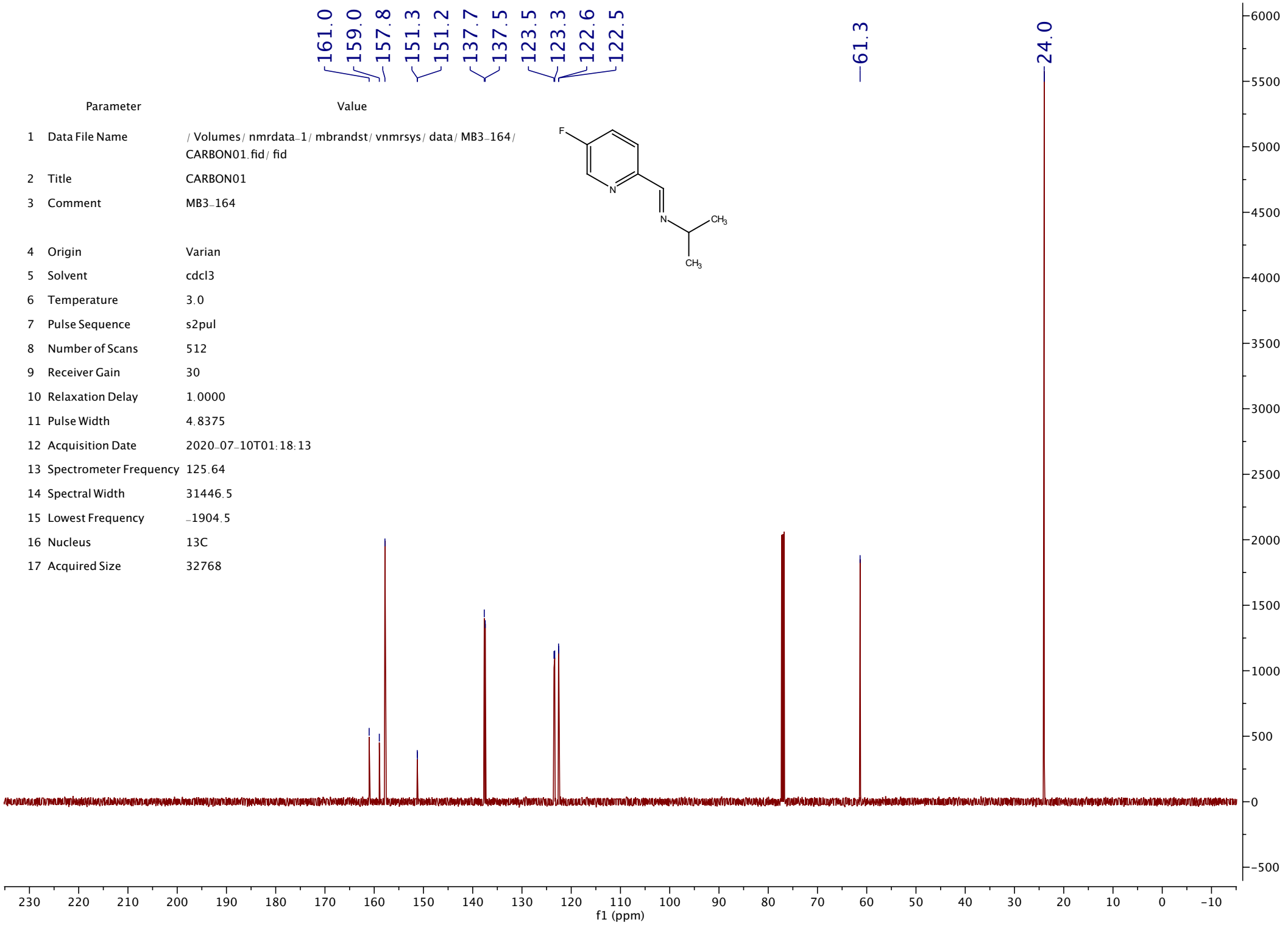
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_164/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB3_164
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_10T01:16:52
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000



C (s) 8.35
D (t) 8.46
B (m) 8.02
A (tt) 7.43
E (pd) 3.62
F (dd) 1.27

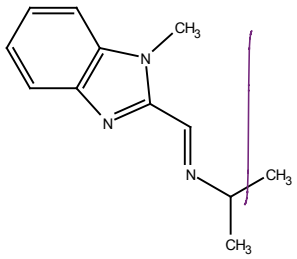
0.84 0.82 0.93 1.00 1.08 5.99

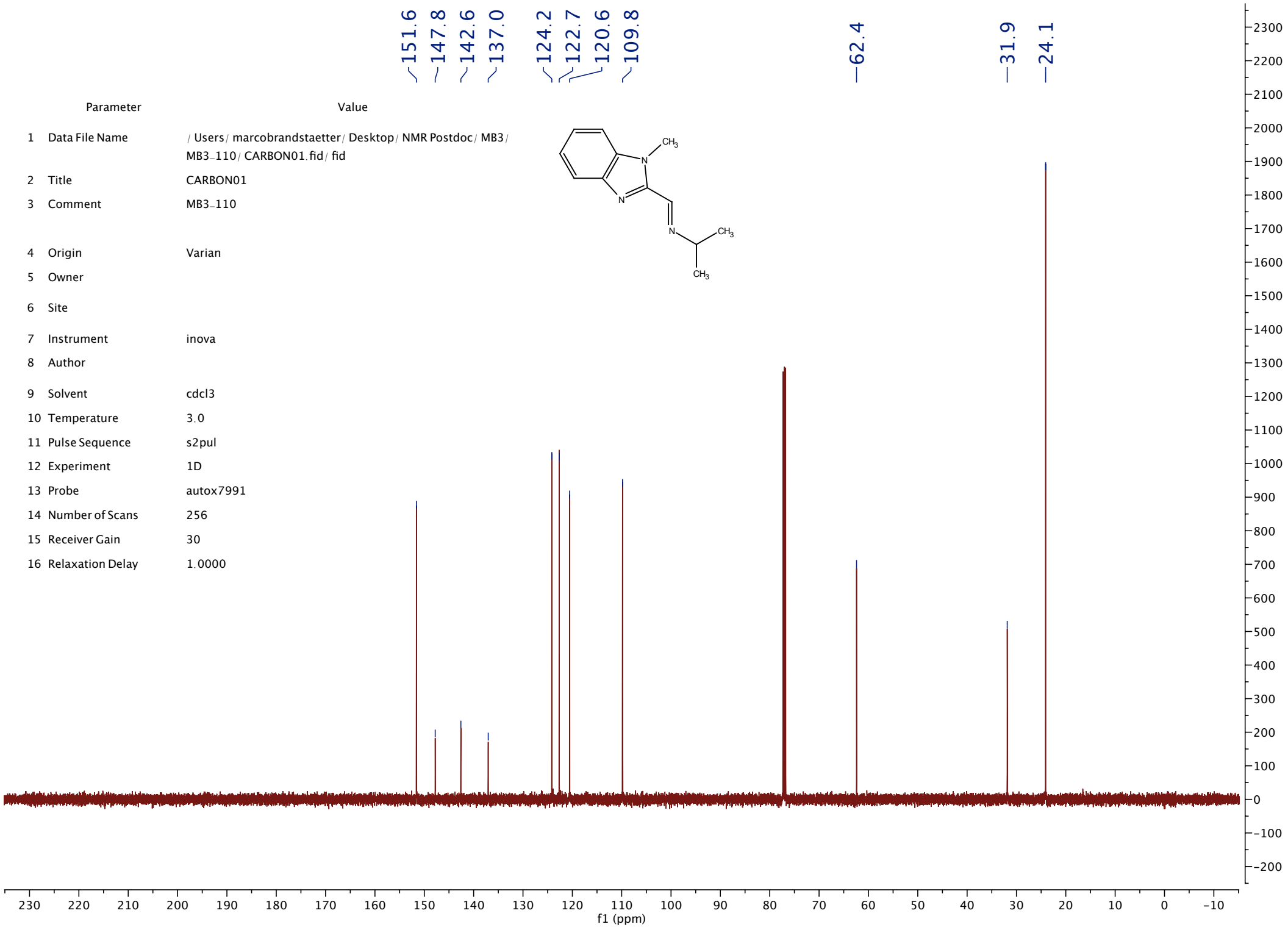
f1 (ppm)



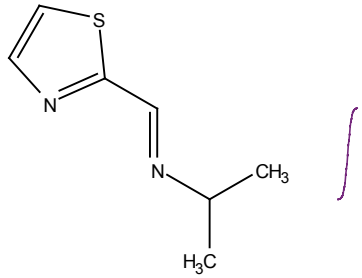
	Parameter	Value
1	Data File Name	/Volumes/nmrdata-1/mbrandst/vnmrsys/data/MB3-164/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3-164
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020-07-10T01:18:13
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

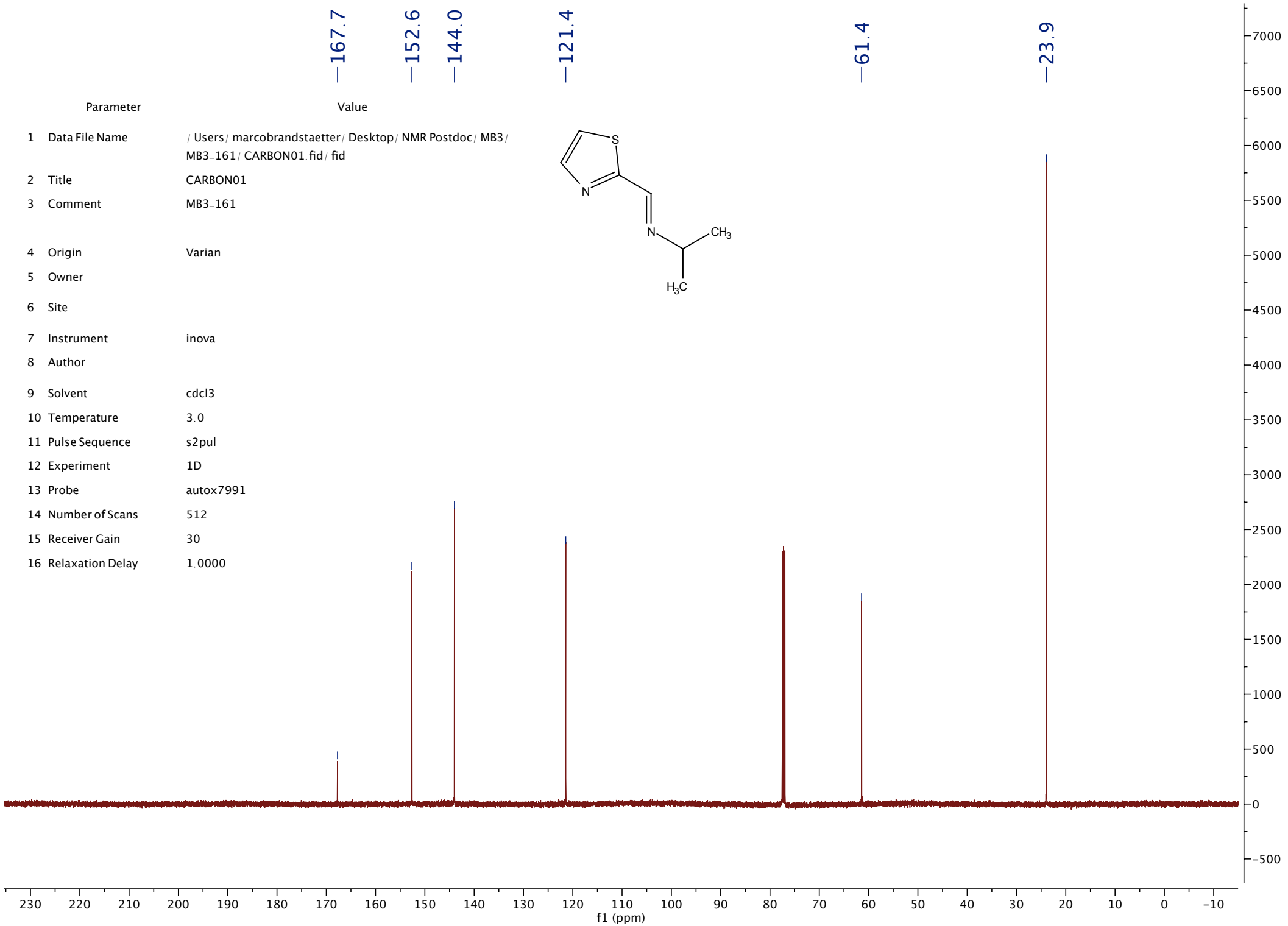
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_110 / PROTON03.fid / fid
2	Title	PROTON03
3	Comment	MB3_110
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	46
16	Relaxation Delay	1.0000




151.6
147.8
142.6
137.0
124.2
122.7
120.6
109.8
62.4
31.9
24.1
Parameter
Value
1 Data File Name
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_110 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
MB3_110
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
CH3
N
N
N
CH3
CH3
f1 (ppm)

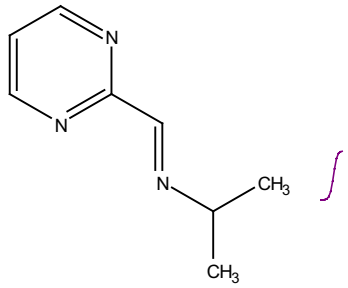
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_161 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB3_161
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	16
15	Receiver Gain	46
16	Relaxation Delay	1.0000

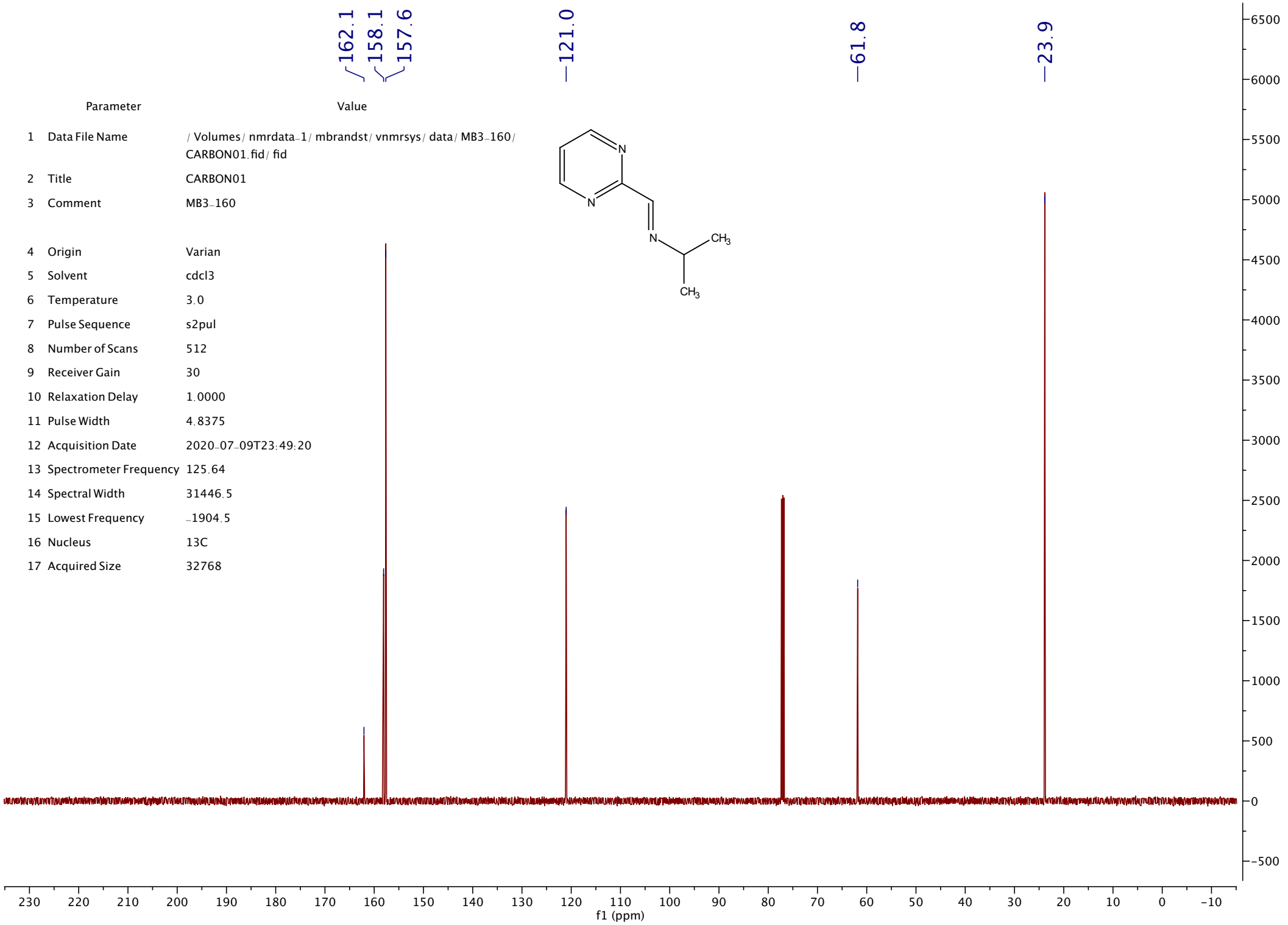




	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_161 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB3_161
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	512
15	Receiver Gain	30
16	Relaxation Delay	1.0000

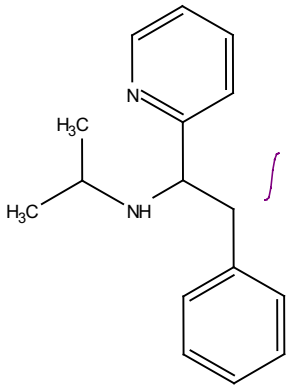
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata_1/ mbrandst/ vnmrsys/ data/ MB3_160/ PROTON01.fid/ fid
2	Title	PROTON01
3	Comment	MB3_160
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_09T23:47:59
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

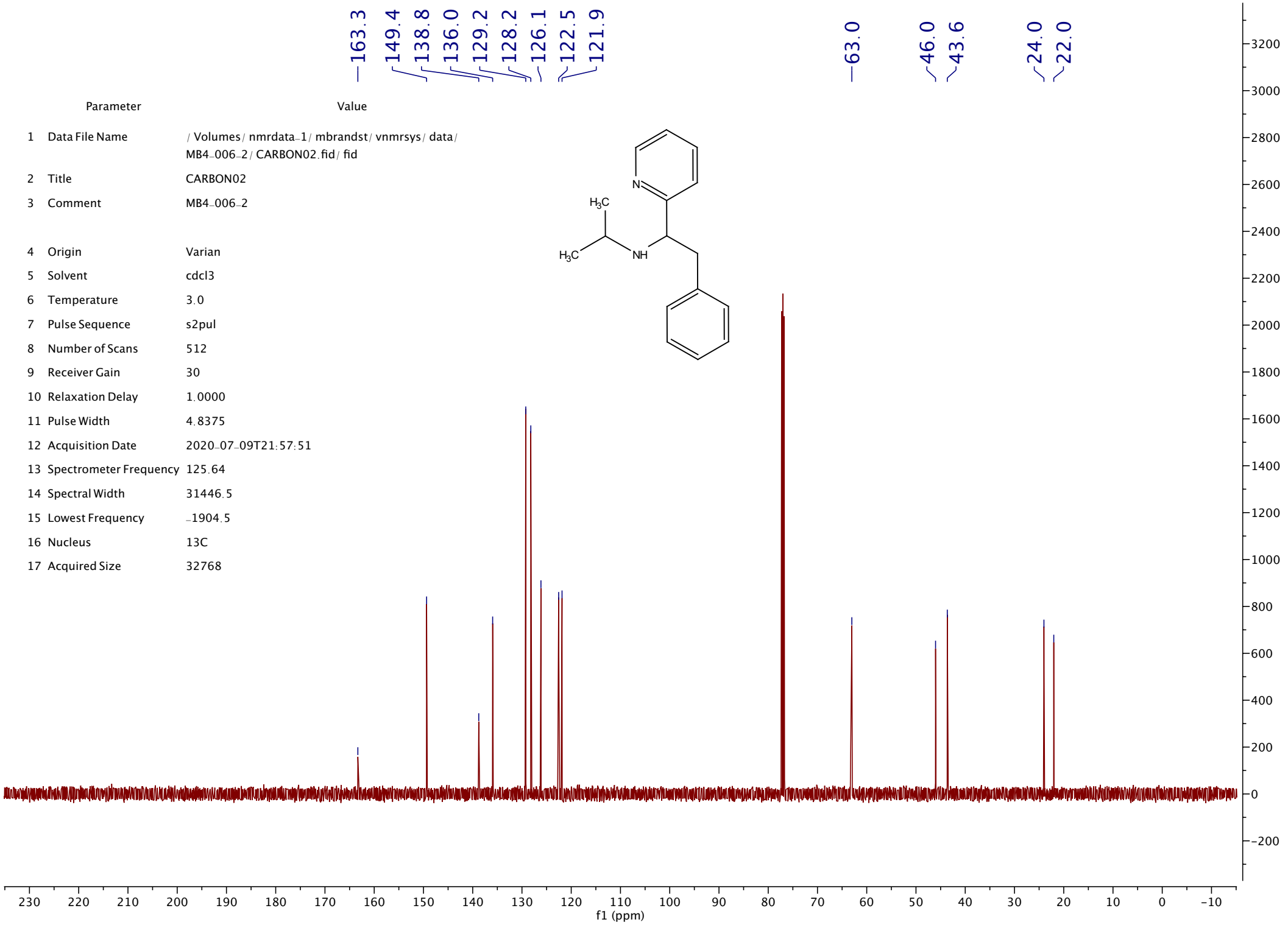




	Parameter	Value
1	Data File Name	/Volumes/nmrdata-1/mbrandst/vnmrsys/data/MB3-160/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3-160
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020-07-09T23:49:20
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

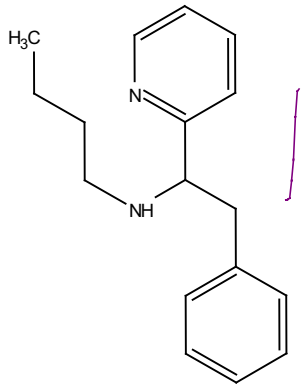
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_006_2/PROTON02.fid/fid
2	Title	PROTON02
3	Comment	MB4_006_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	34
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_09T21:56:30
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

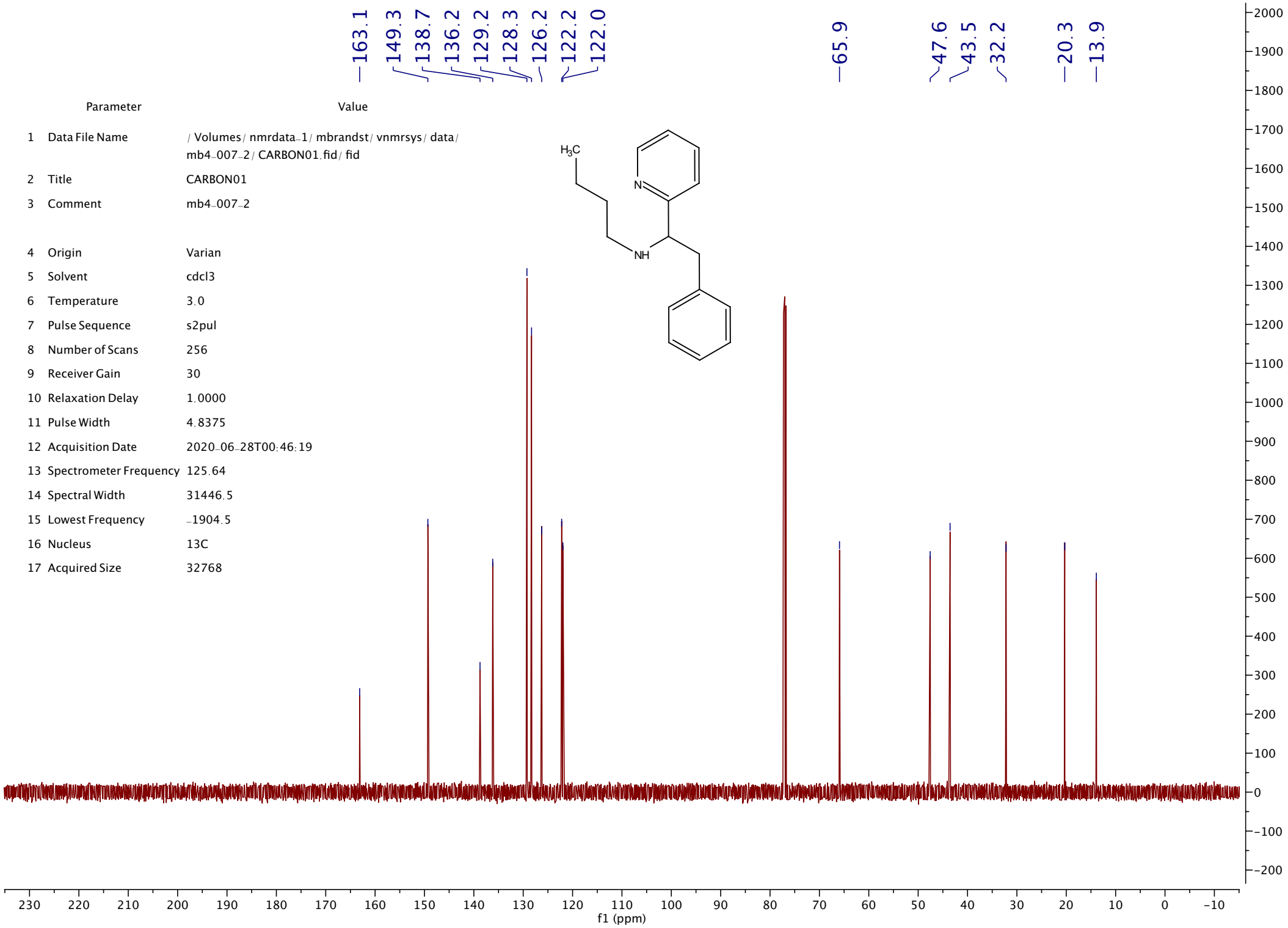




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_006_2 / CARBON02.fid / fid
2	Title	CARBON02
3	Comment	MB4_006_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_09T21:57:51
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

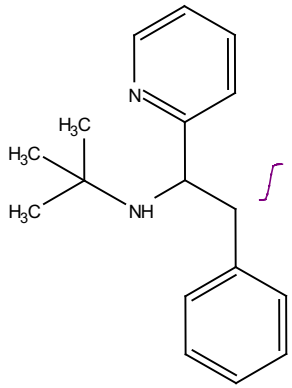
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_007_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb4_007_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_06_28T00:45:30
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

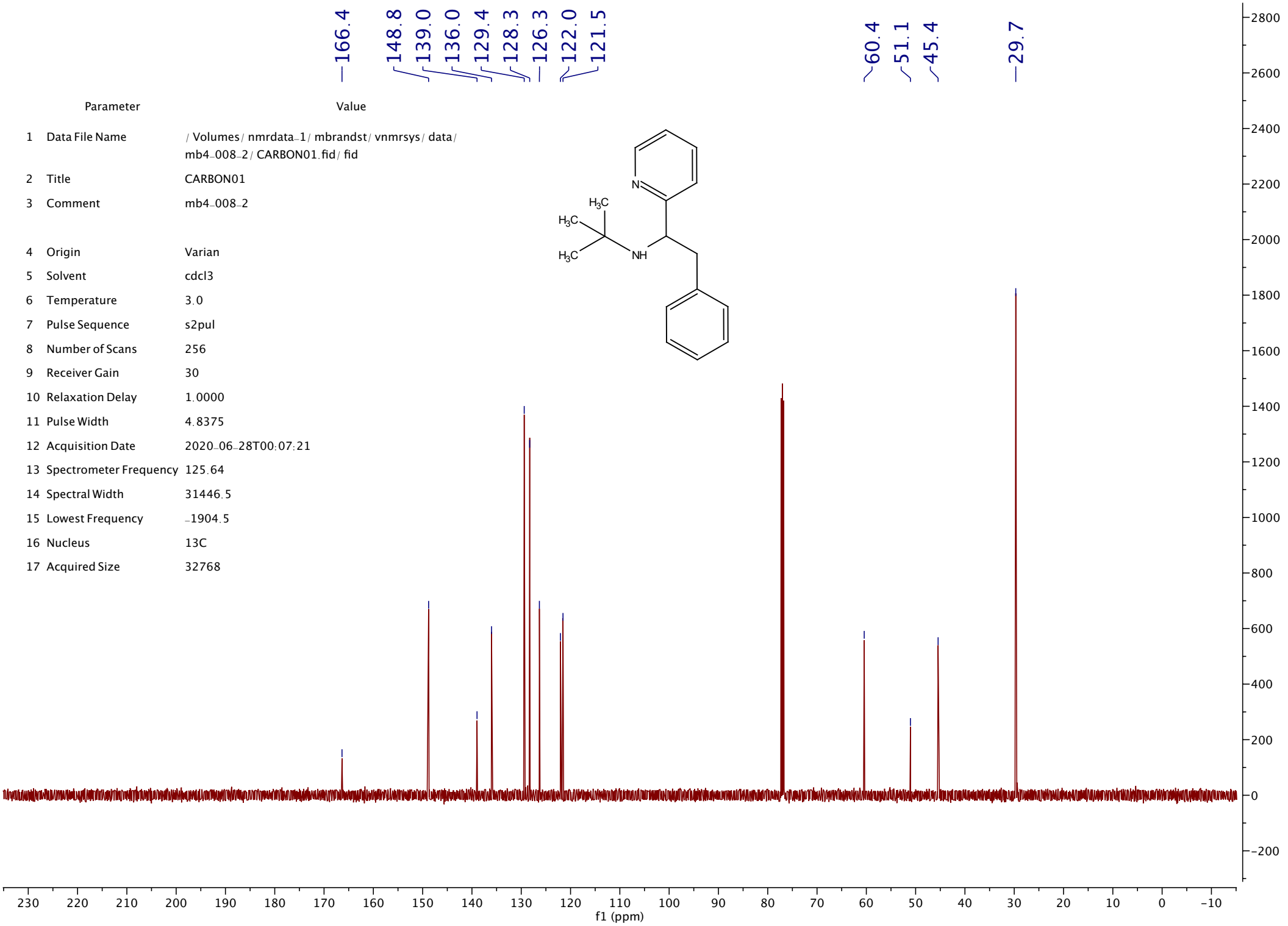




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_007_2/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	mb4_007_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_06_28T00:46:19
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

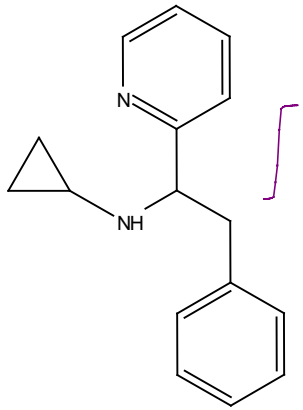
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_008_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb4_008_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_06_28T00:06:32
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

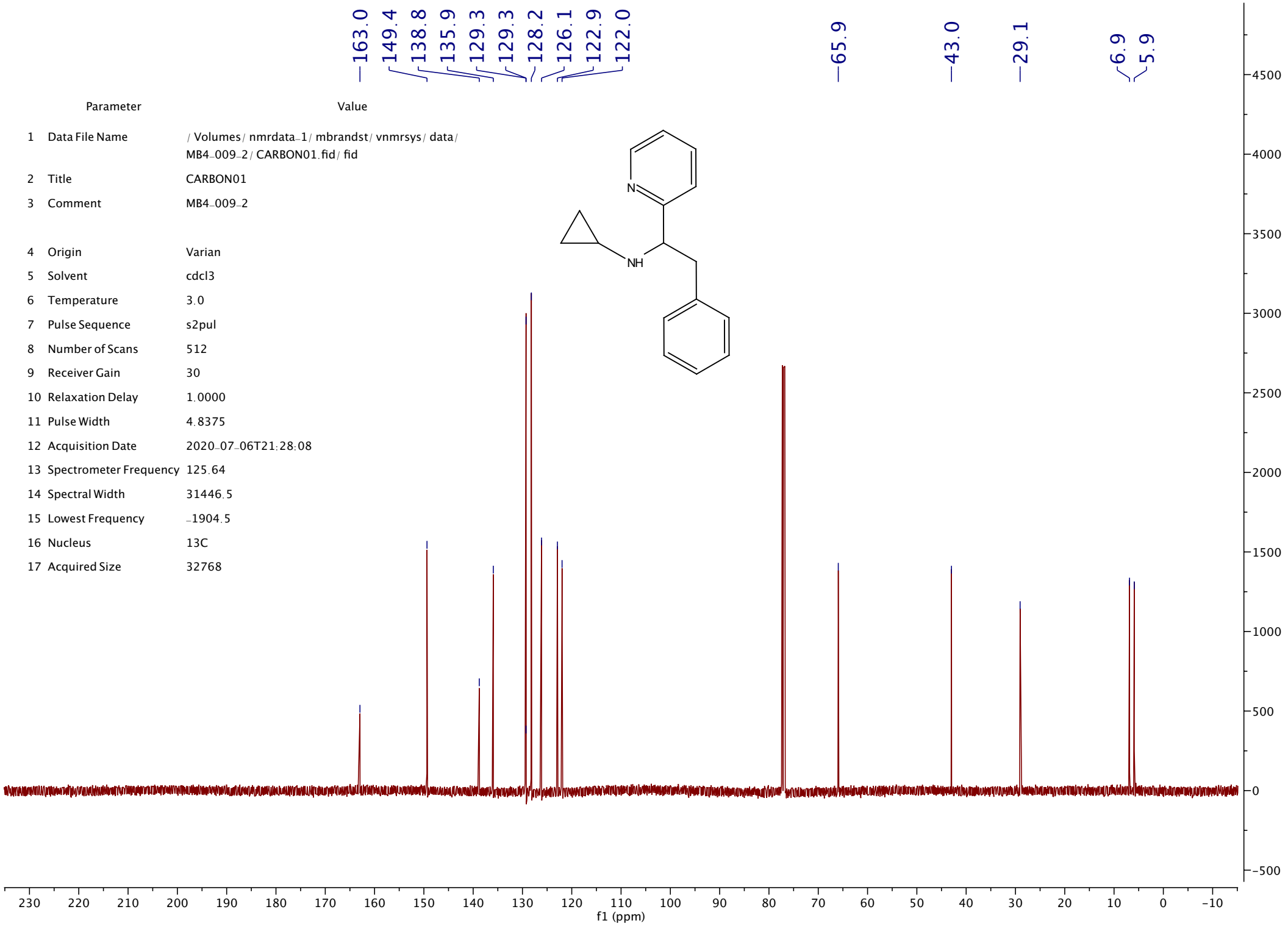




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / mb4_008_2 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	mb4_008_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_06_28T00:07:21
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

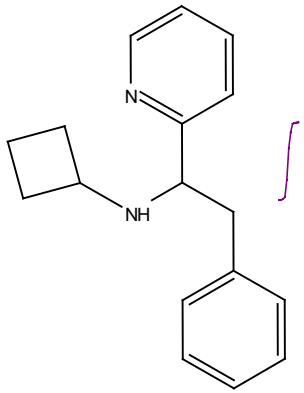
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_009_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_009_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_06T21:26:45
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

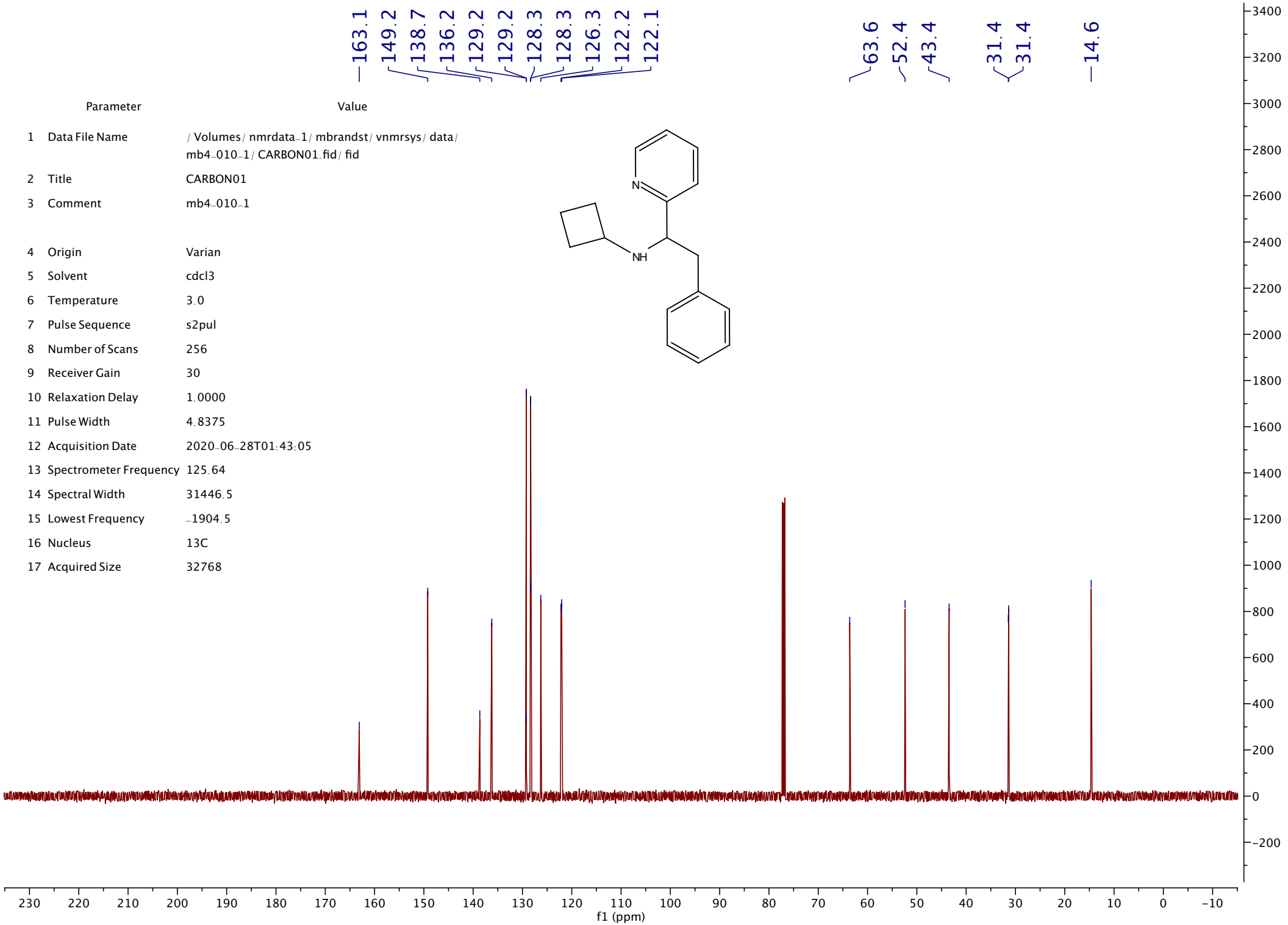




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_009_2 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB4_009_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_06T21:28:08
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

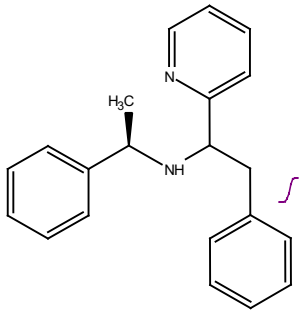
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_010_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb4_010_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_06_28T01:42:16
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

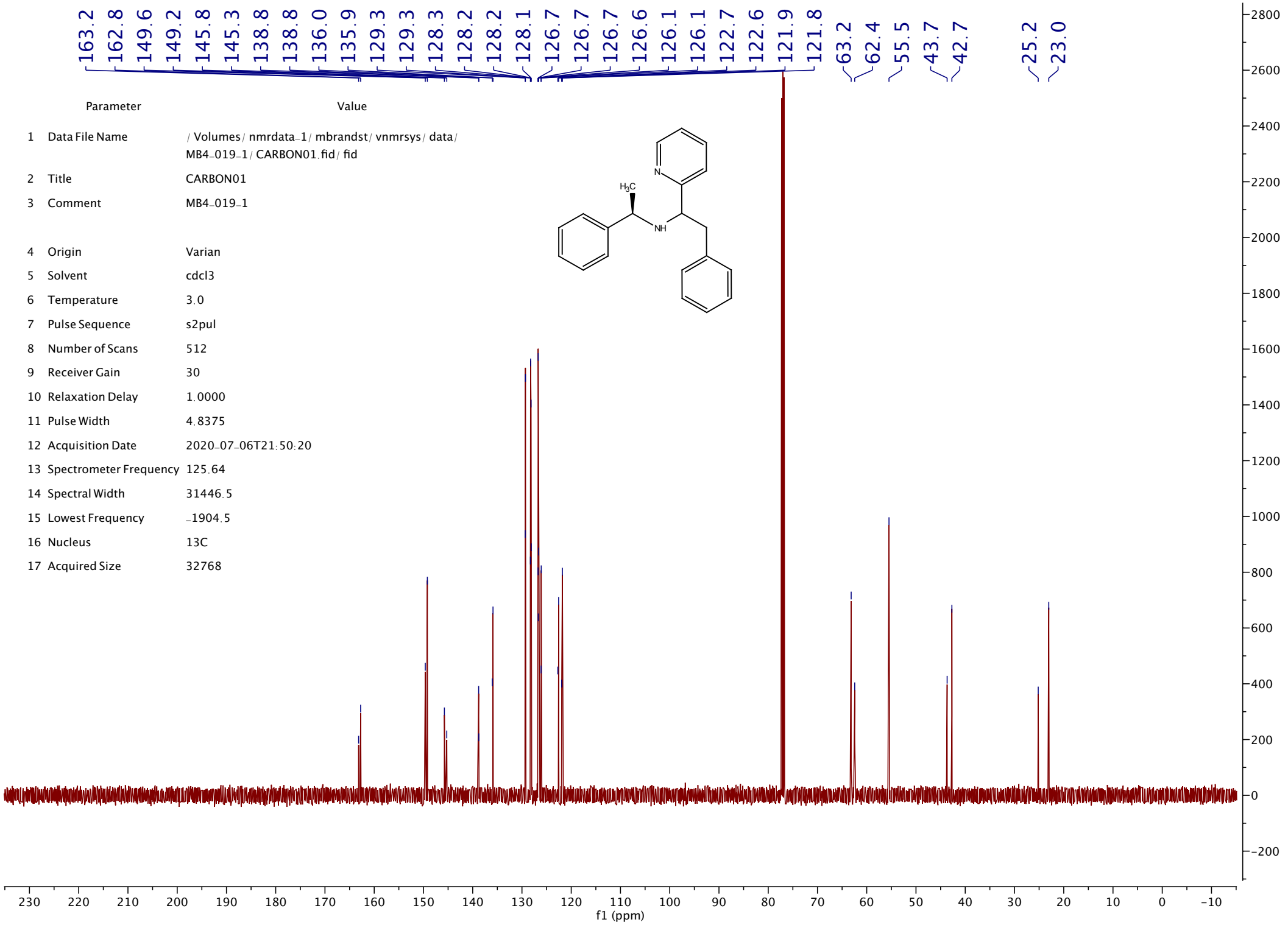




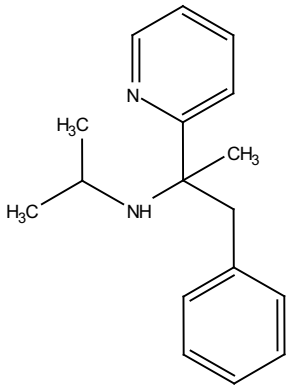
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_010_1/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	mb4_010_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_06_28T01:43:05
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_019_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_019_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_06T21:48:58
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000




163.2
162.8
149.6
149.2
145.8
145.3
138.8
138.8
136.0
135.9
129.3
129.3
128.3
128.2
128.2
128.1
126.7
126.7
126.7
126.6
126.1
126.1
122.7
122.6
121.9
121.8
63.2
62.4
55.5
43.7
42.7
25.2
23.0
Parameter
Value
1 Data File Name / Volumes/ nmrdata_1/ mbrandst/ vnmrsys/ data/ MB4_019_1/ CARBON01.fid/ fid
2 Title CARBON01
3 Comment MB4_019_1
4 Origin Varian
5 Solvent cdcl3
6 Temperature 3.0
7 Pulse Sequence s2pul
8 Number of Scans 512
9 Receiver Gain 30
10 Relaxation Delay 1.0000
11 Pulse Width 4.8375
12 Acquisition Date 2020_07_06T21:50:20
13 Spectrometer Frequency 125.64
14 Spectral Width 31446.5
15 Lowest Frequency _1904.5
16 Nucleus 13C
17 Acquired Size 32768
N
H3C
NH
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

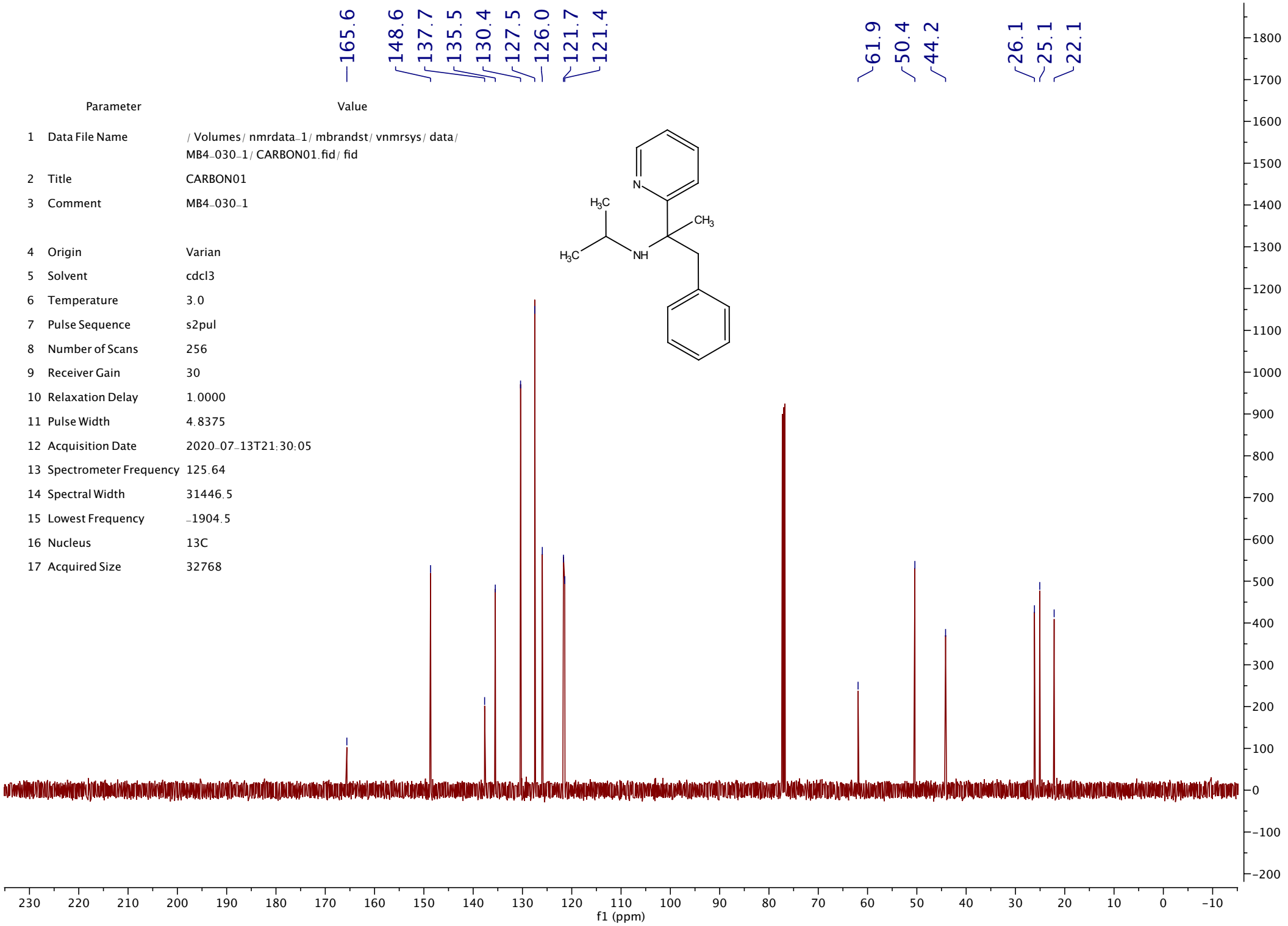
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_030_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_030_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T21:29:16
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000



H (d) 8.65 | J (dd) 7.12 | I (t) 7.48 | K (dd) 7.05 | L (d) 6.65 | B (d) 2.95 | D (m) 2.36 | G (d) 0.84 | A (d) 3.17 | C (p) 2.66 | E (s) 1.51 | F (d) 1.08

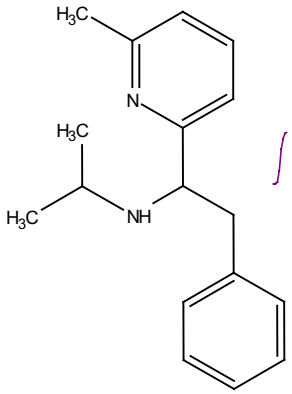
0.89 | 0.95 | 1.14 | 3.68 | 1.94 | 1.00 | 1.00 | 0.94 | 1.62 | 2.67 | 2.69 | 2.70

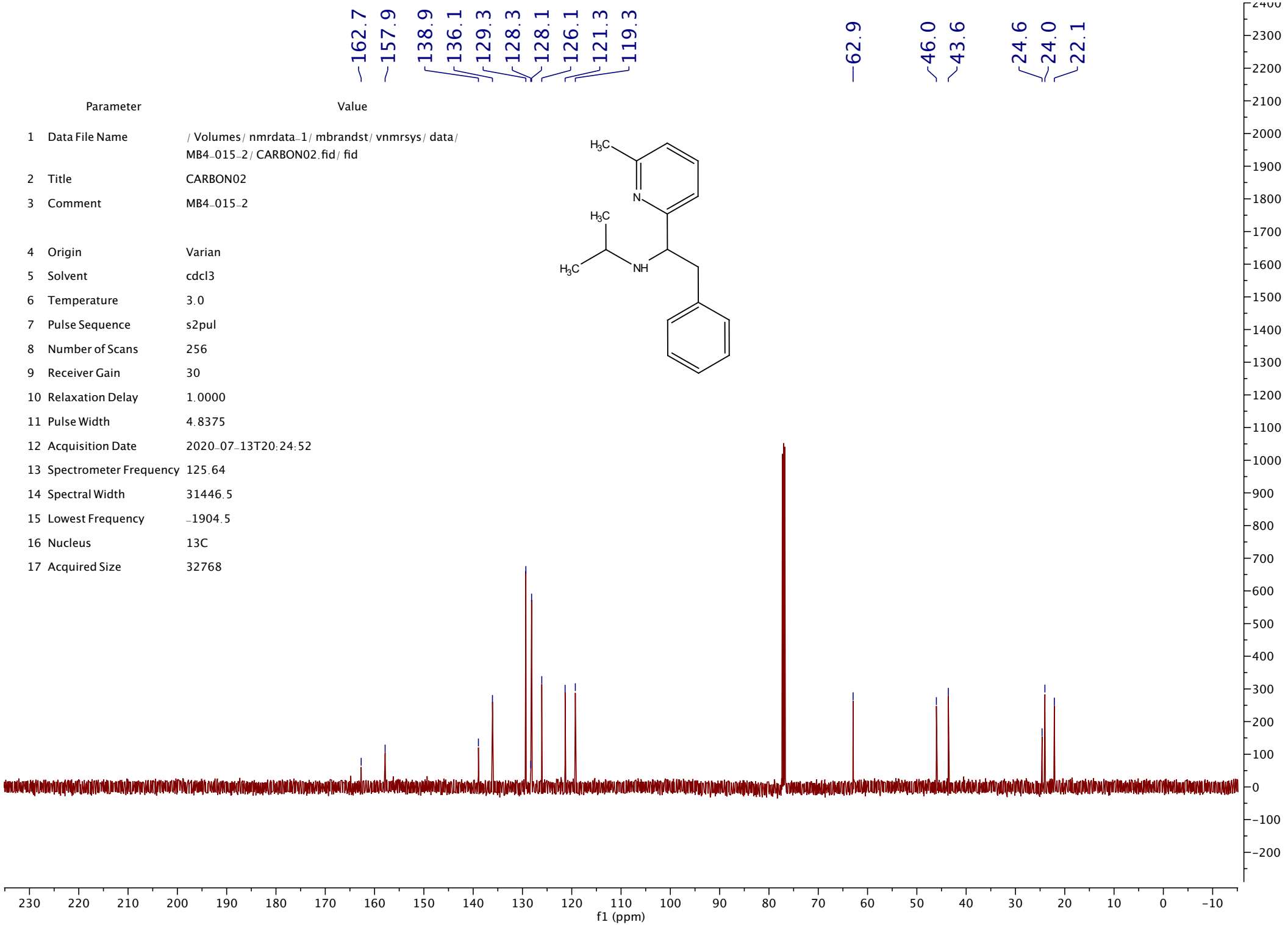
f1 (ppm)



	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_030_1/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_030_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T21:30:05
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

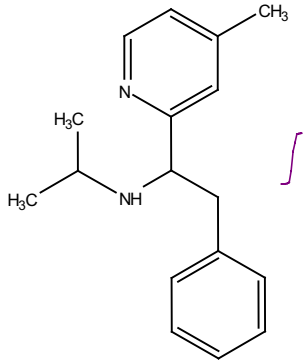
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_015_2/PROTON03.fid/fid
2	Title	PROTON03
3	Comment	MB4_015_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	54
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_24T15:06:27
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

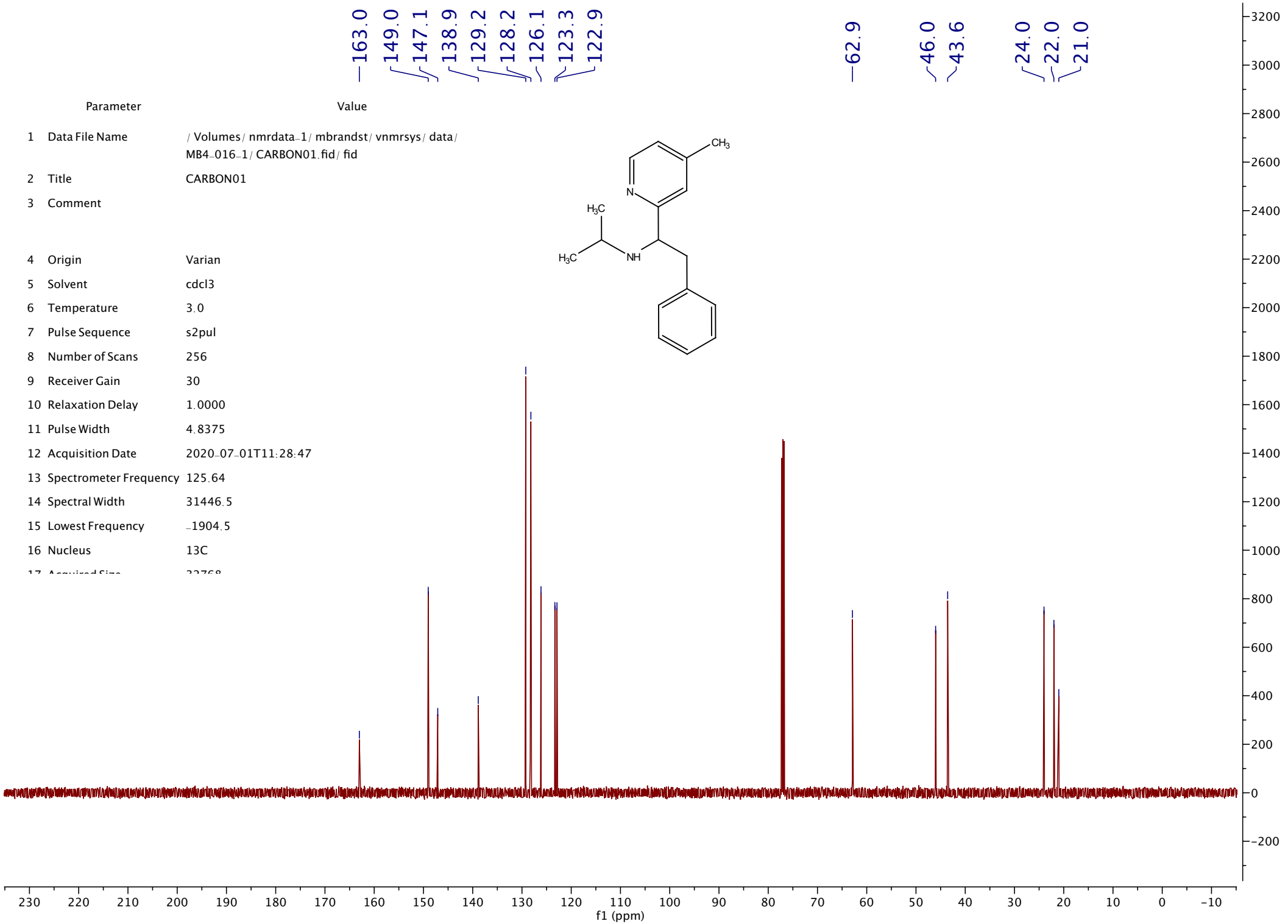




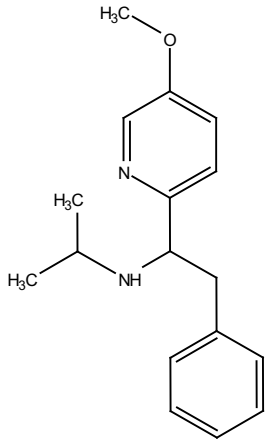
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_015_2 / CARBON02.fid / fid
2	Title	CARBON02
3	Comment	MB4_015_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T20:24:52
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_016_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_01T11:27:58
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000




163.0
149.0
147.1
138.9
129.2
128.2
126.1
123.3
122.9
62.9
46.0
43.6
24.0
22.0
21.0
Parameter
Value
1 Data File Name / Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_016_1 / CARBON01.fid / fid
2 Title CARBON01
3 Comment
4 Origin Varian
5 Solvent cdcl3
6 Temperature 3.0
7 Pulse Sequence s2pul
8 Number of Scans 256
9 Receiver Gain 30
10 Relaxation Delay 1.0000
11 Pulse Width 4.8375
12 Acquisition Date 2020_07_01T11:28:47
13 Spectrometer Frequency 125.64
14 Spectral Width 31446.5
15 Lowest Frequency -1904.5
16 Nucleus 13C
N
H3C
H3C
NH
CH3
f1 (ppm)

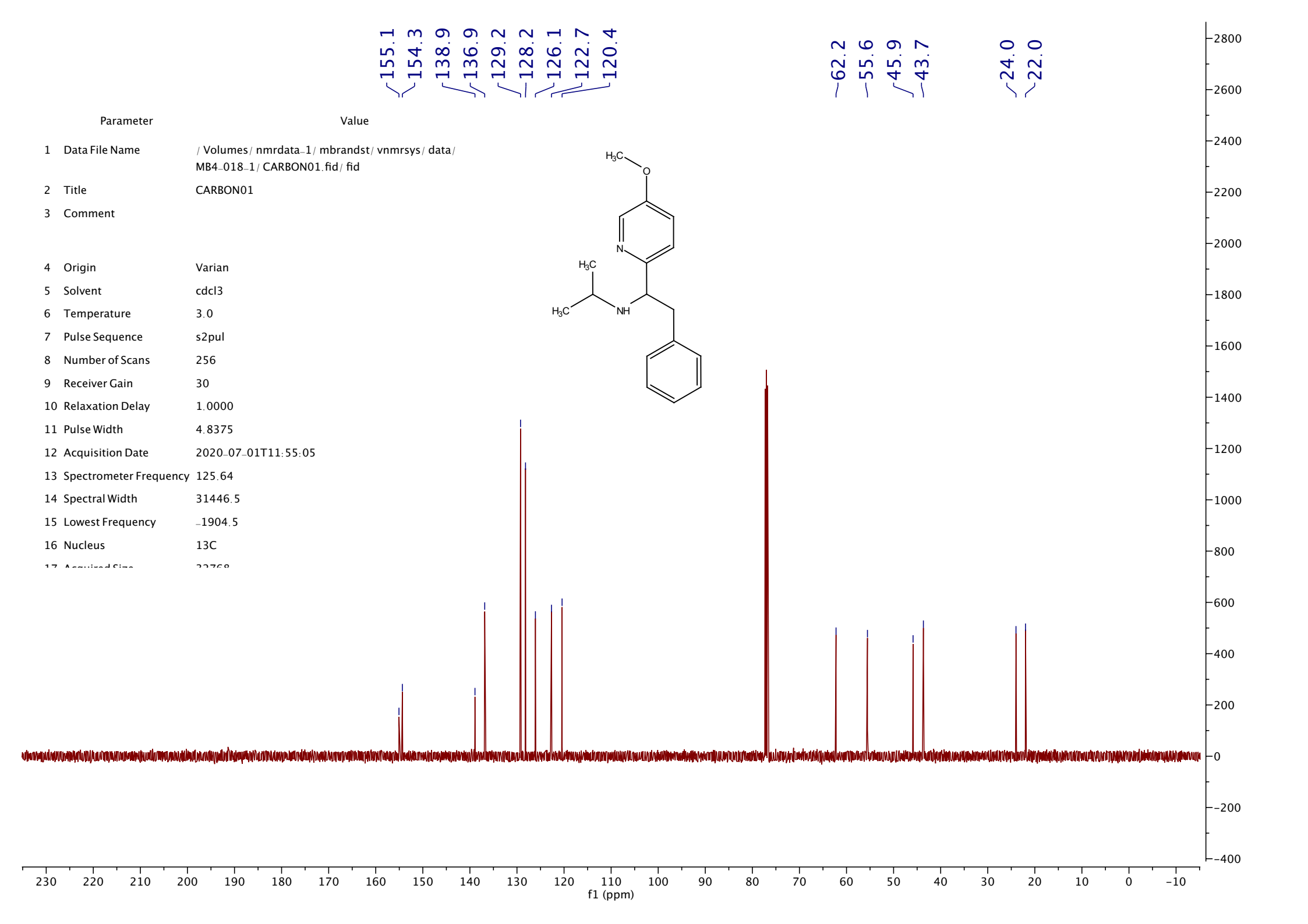
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_018_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_01T11:54:17
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000



A (d) 8.28
B (dd) 7.19
C (m) 7.14
D (m) 7.03
E (d) 6.97
J (t) 4.02
K (s) 3.84
H (hept) 2.55
I (m) 2.98
G (s) 1.83
F (dd) 0.95

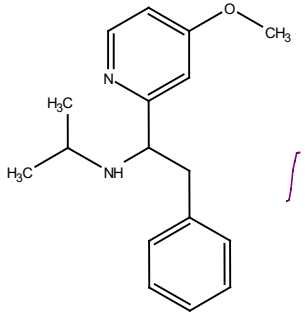
1.00 2.39 1.13 3.59 1.14 1.18 2.92 2.47 1.12 2.93 6.69

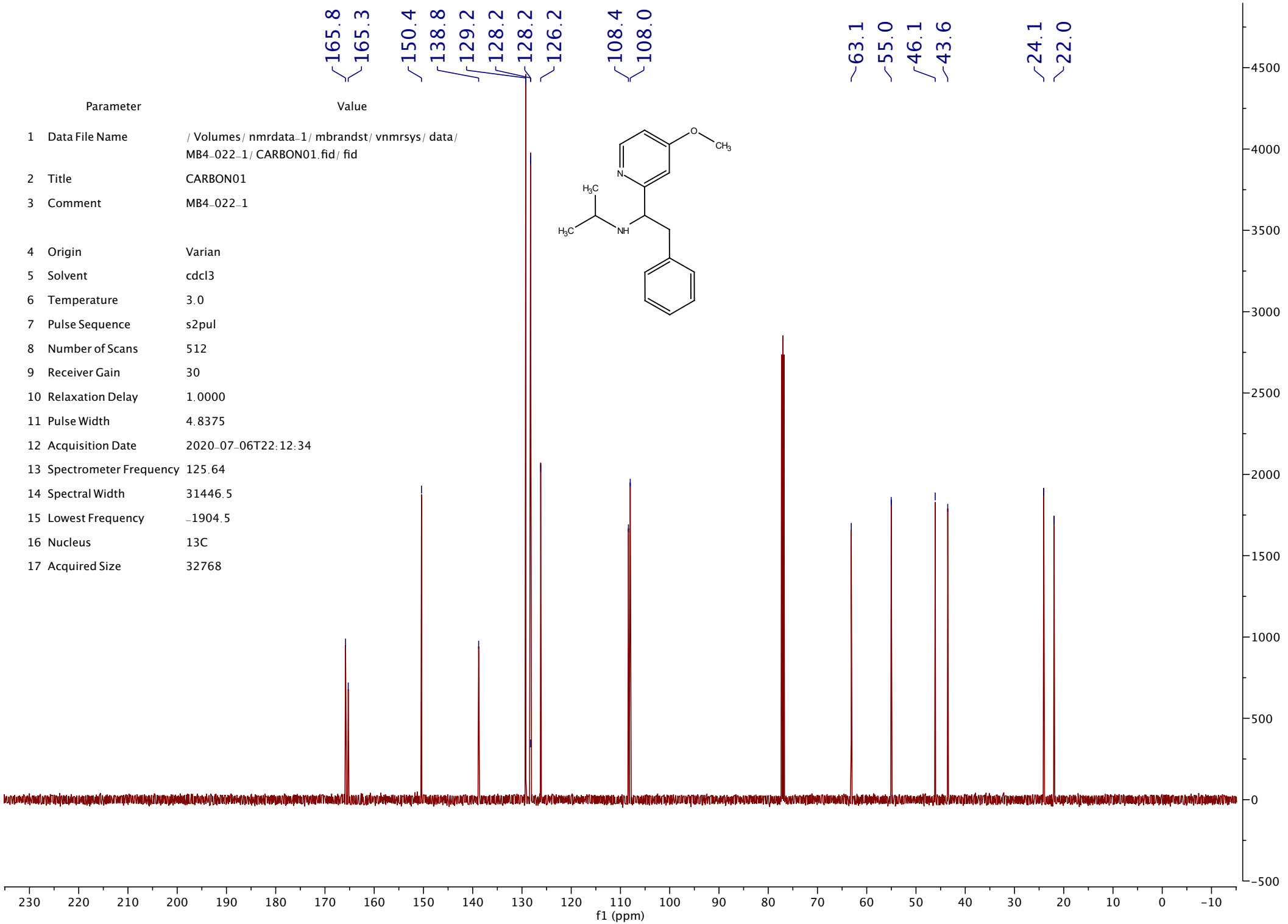
f1 (ppm)



	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_018_1/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_01T11:55:05
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

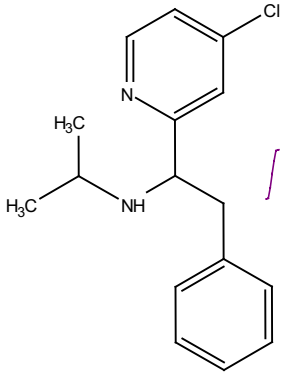
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_022_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_022_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	36
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_06T22:11:13
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

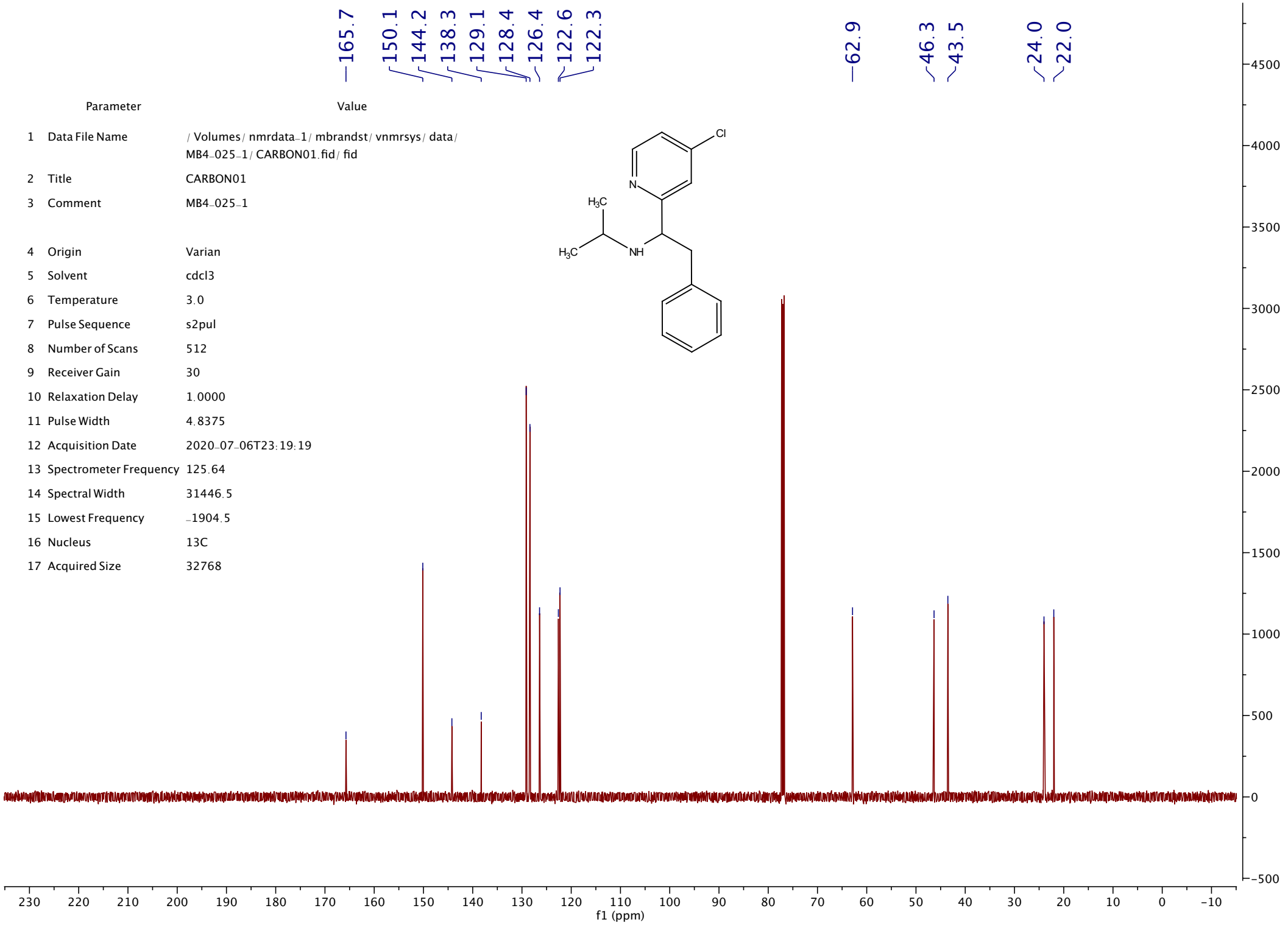




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_022_1/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_022_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_06T22:12:34
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

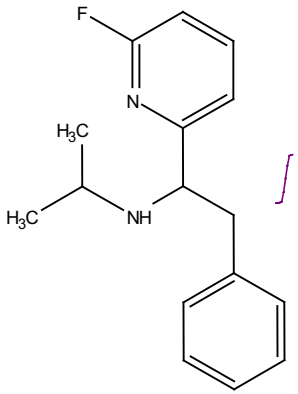
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_025_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_025_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_06T23:17:58
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

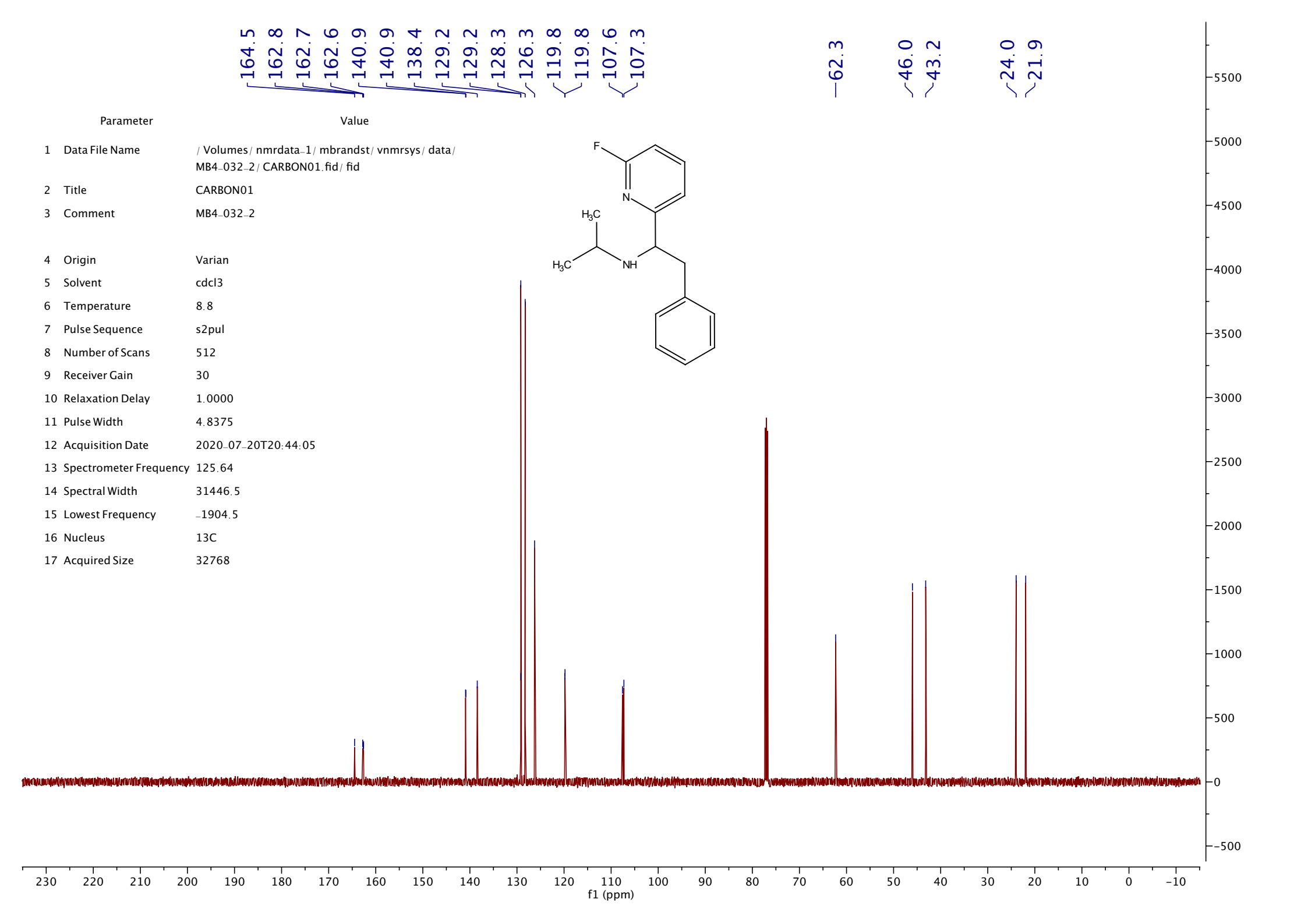




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_025_1 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB4_025_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_06T23:19:19
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

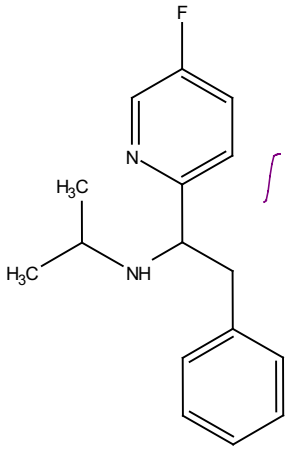
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_032_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_032_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	8.8
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_20T20:42:44
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

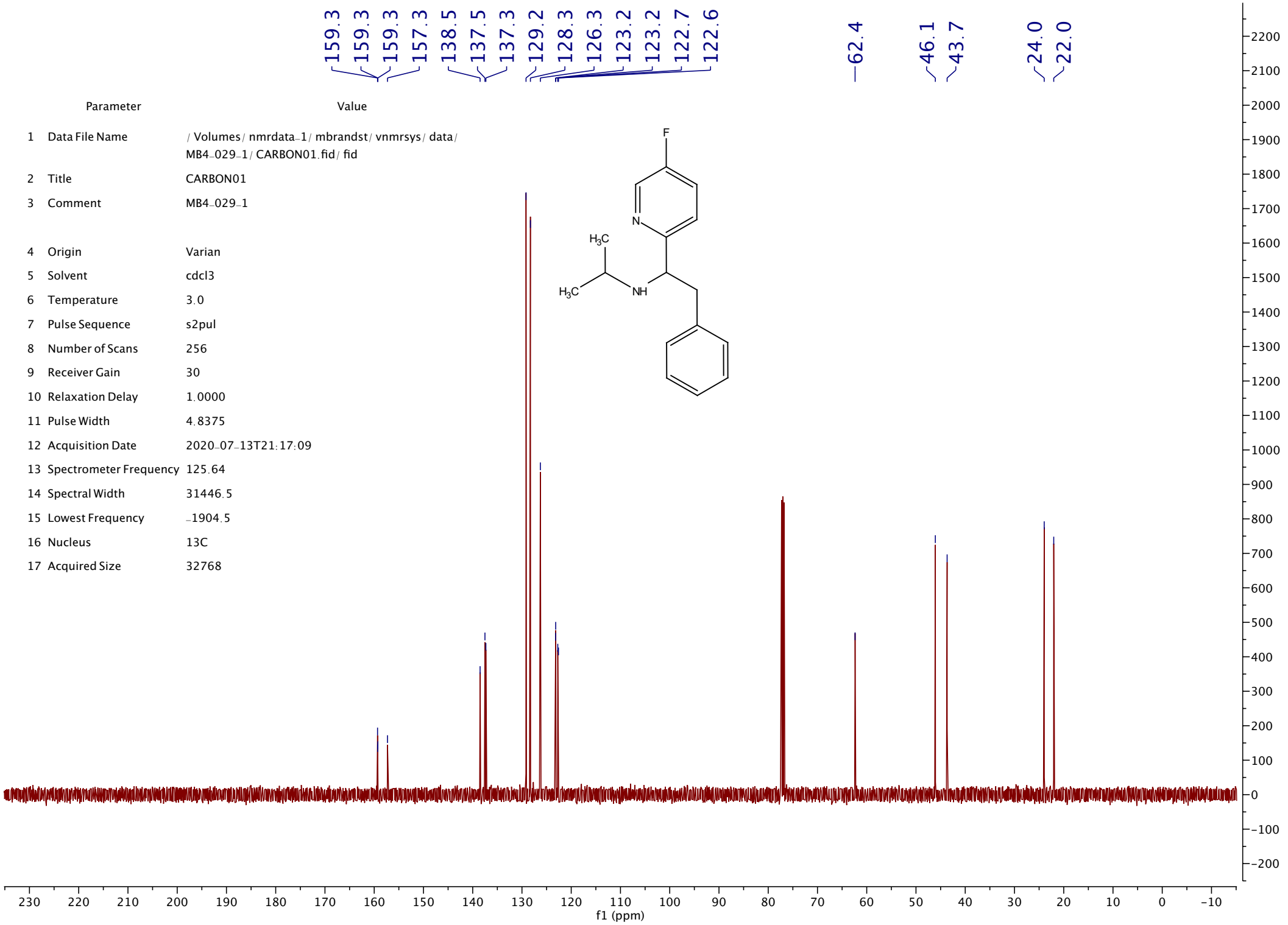




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_032_2/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_032_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	8.8
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_20T20:44:05
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

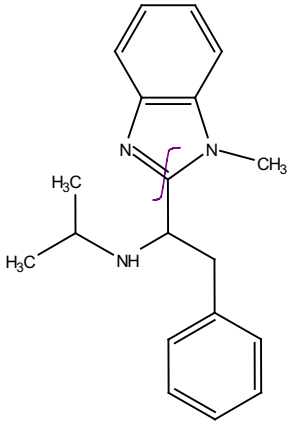
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_029_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_029_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T21:16:19
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

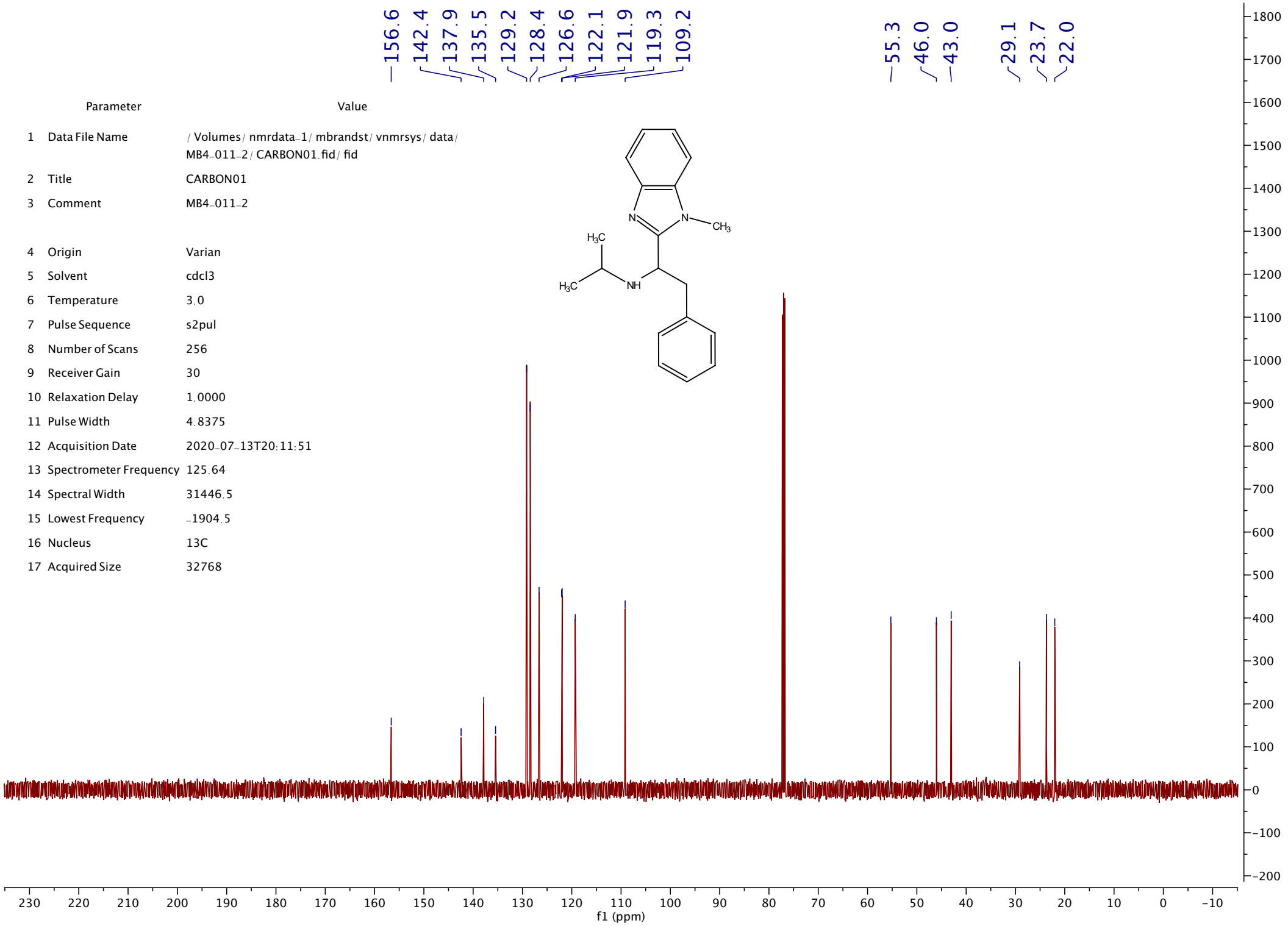




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_029_1/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_029_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T21:17:09
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

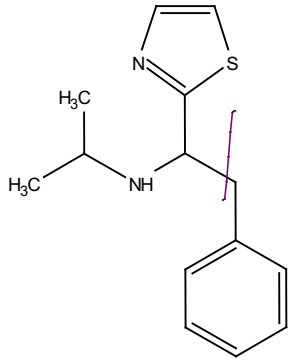
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_011_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_011_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	36
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T20:11:02
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

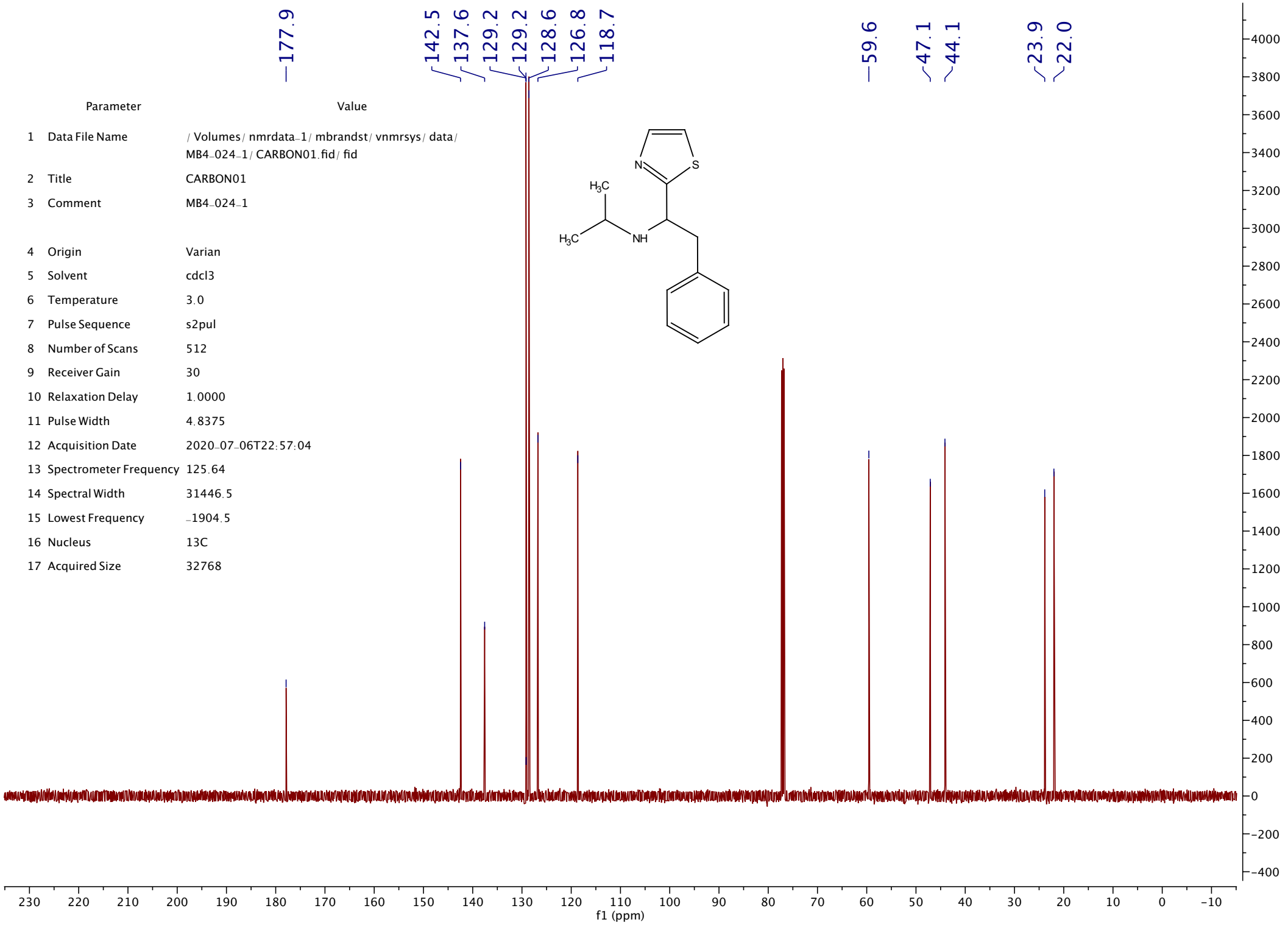




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_011_2/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_011_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T20:11:51
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

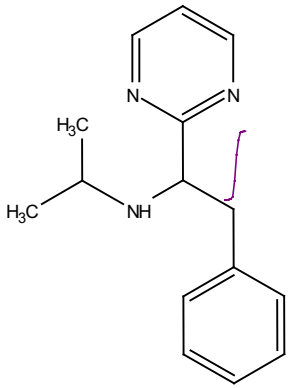
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_024_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_024_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_06T22:55:43
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000

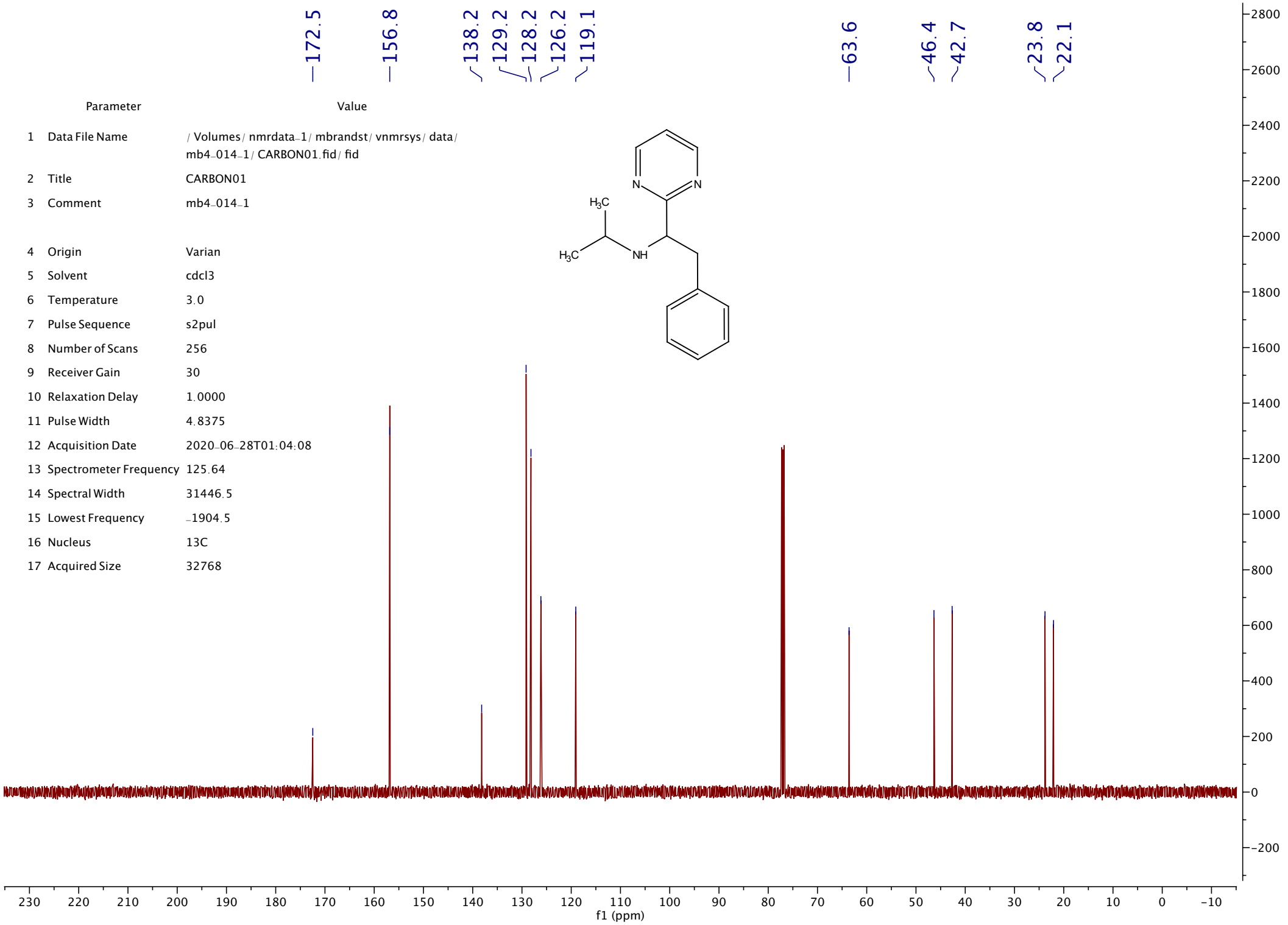




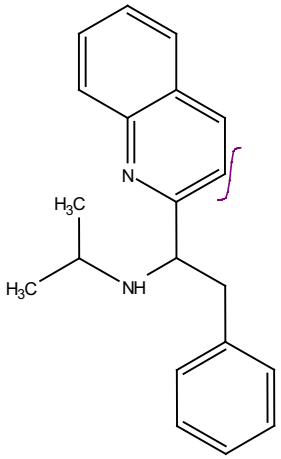
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_024_1 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB4_024_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_06T22:57:04
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

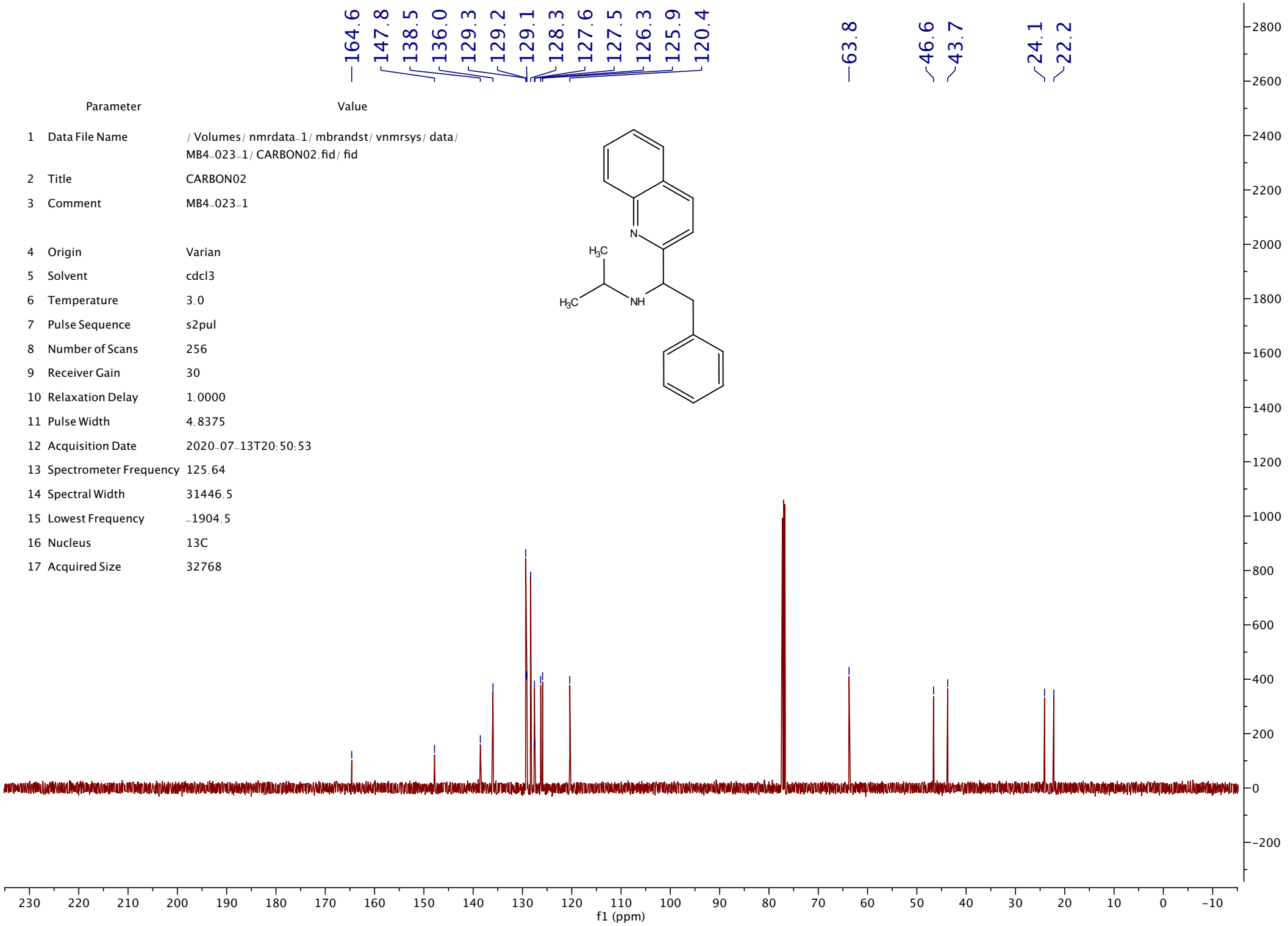
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_014_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb4_014_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_06_28T01:03:19
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000




172.5
156.8
138.2
129.2
128.2
126.2
119.1
63.6
46.4
42.7
23.8
22.1
Parameter
Value
1 Data File Name / Volumes/ nmrdata_1/ mbrandst/ vnmrsys/ data/ mb4_014_1/ CARBON01.fid/ fid
2 Title CARBON01
3 Comment mb4_014_1
4 Origin Varian
5 Solvent cdcl3
6 Temperature 3.0
7 Pulse Sequence s2pul
8 Number of Scans 256
9 Receiver Gain 30
10 Relaxation Delay 1.0000
11 Pulse Width 4.8375
12 Acquisition Date 2020_06_28T01:04:08
13 Spectrometer Frequency 125.64
14 Spectral Width 31446.5
15 Lowest Frequency -1904.5
16 Nucleus 13C
17 Acquired Size 32768
N
N
H3C
H3C
NH
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

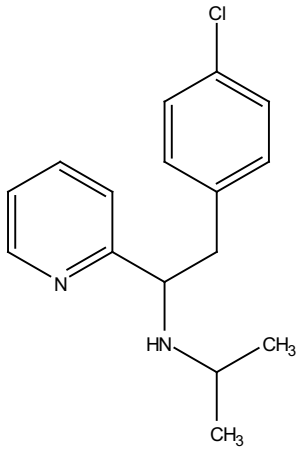
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_023_1/PROTON02.fid/fid
2	Title	PROTON02
3	Comment	MB4_023_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T20:50:04
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

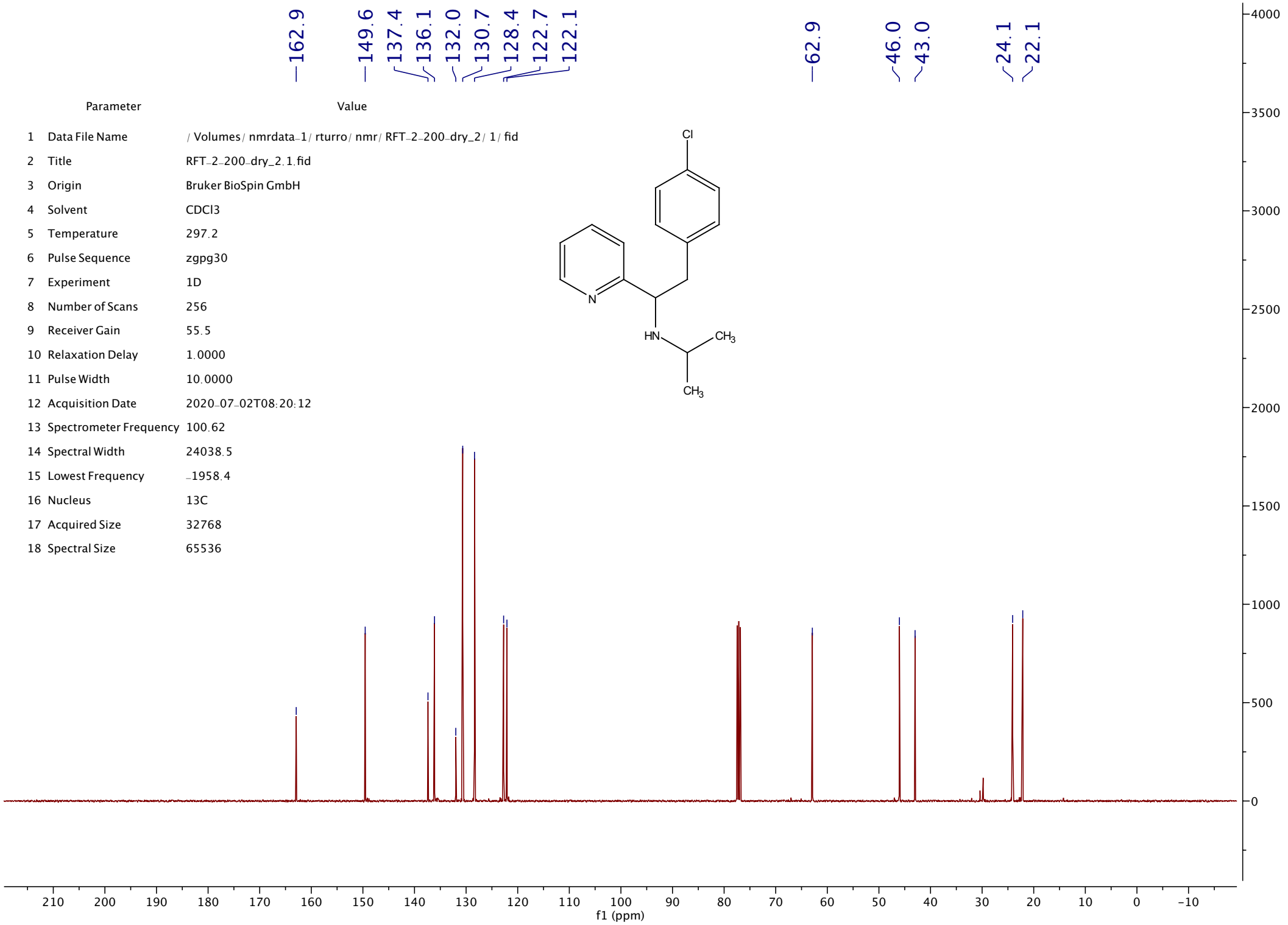




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_023_1/CARBON02.fid/fid
2	Title	CARBON02
3	Comment	MB4_023_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T20:50:53
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

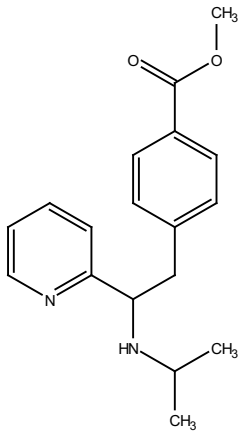
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata_1/ rturro/ nmr/ RFT_2_228_F2/ 1/ fid
2	Title	RFT_2_228_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	32
9	Receiver Gain	21.4
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_19T07:05:03
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1613.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

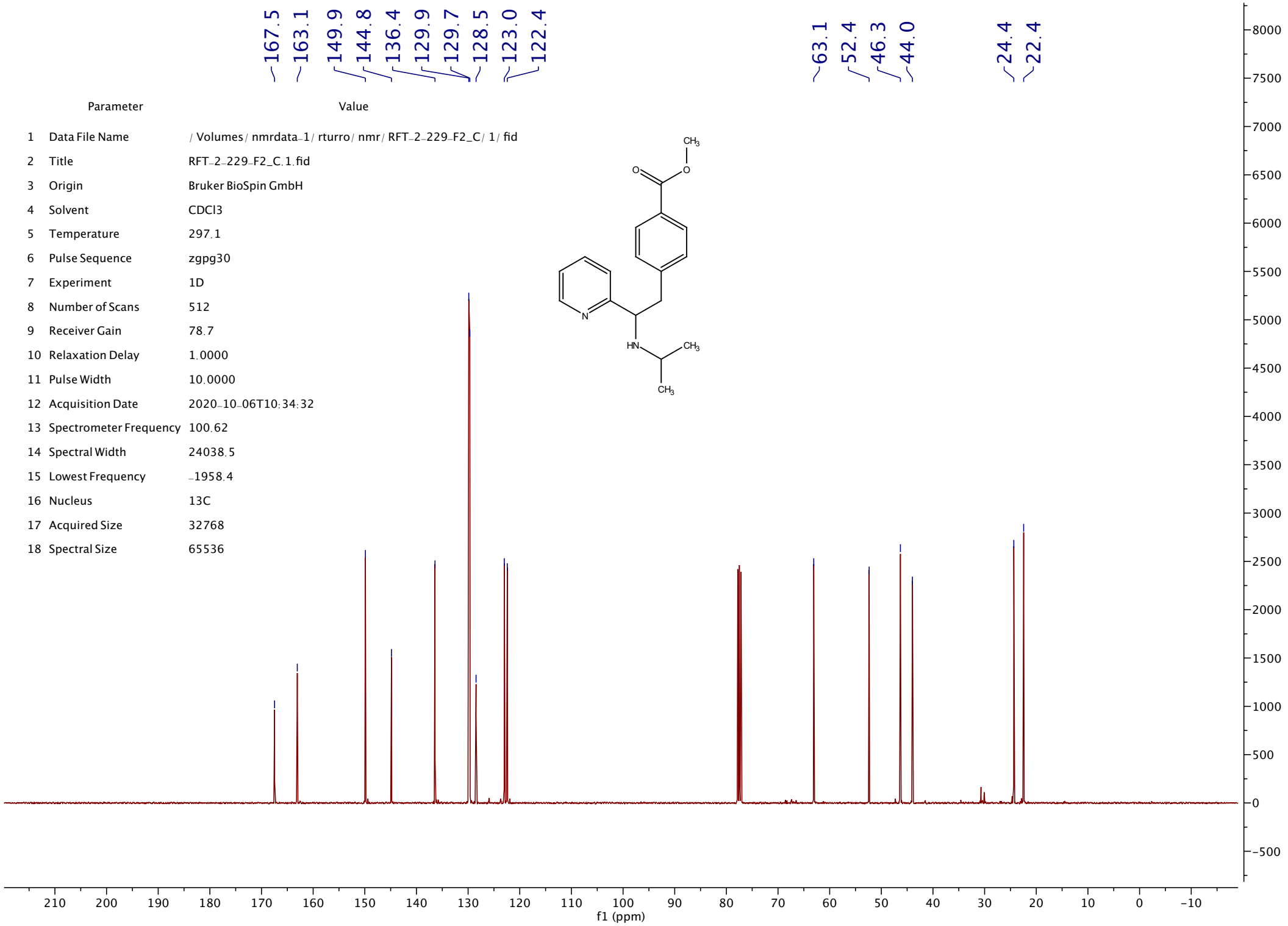




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_200_dry_2 / 1 / fid
2	Title	RFT_2_200_dry_2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	256
9	Receiver Gain	55.5
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_07_02T08:20:12
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	−1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

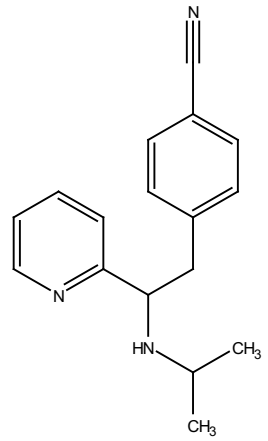
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/RFT_2_229_F2/1/fid
2	Title	RFT_2_229_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	21.4
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_06T07:38:30
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1644.0
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

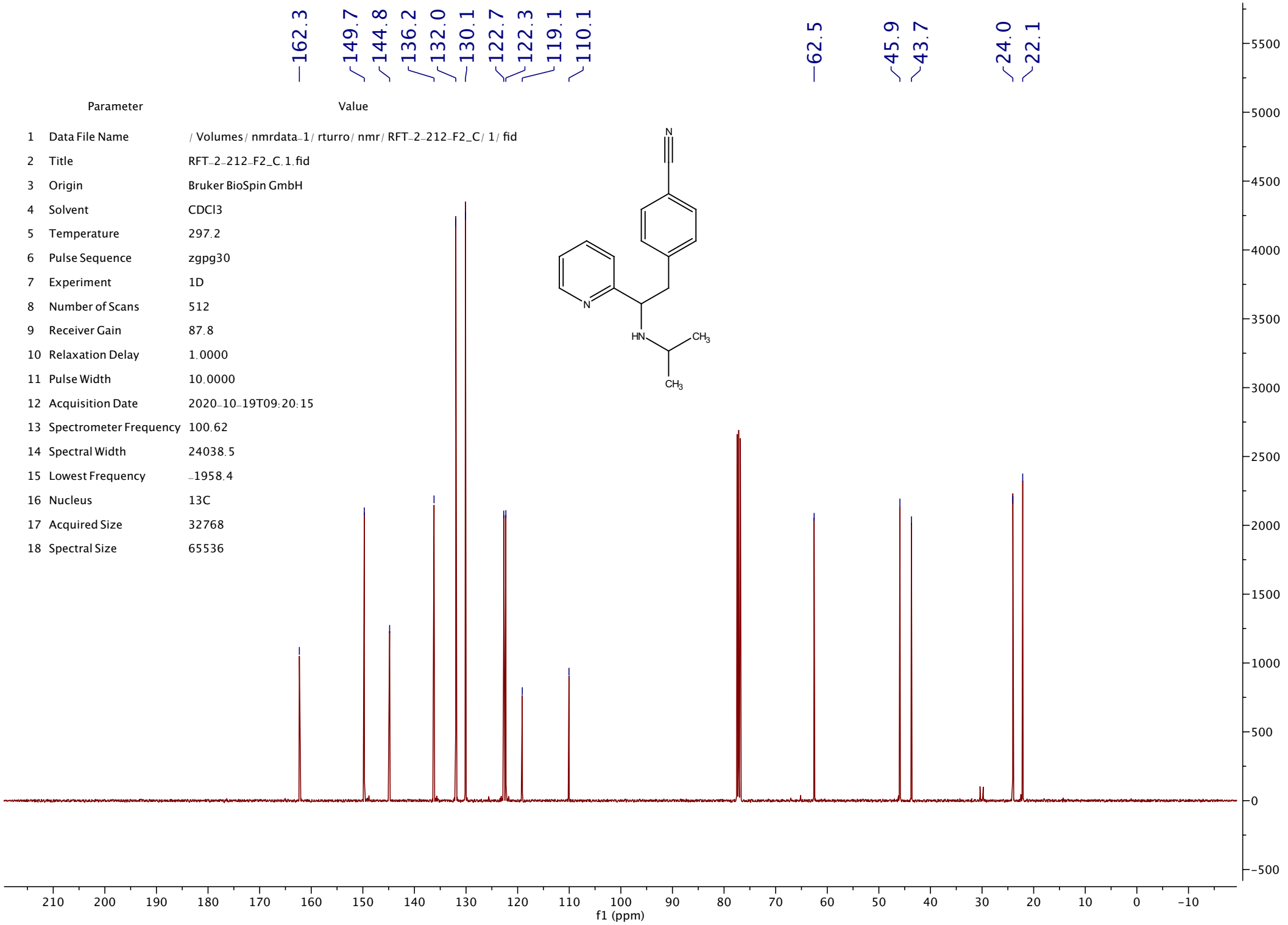




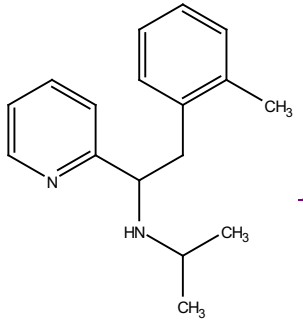
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/RFT_2_229_F2_C/1/fid
2	Title	RFT_2_229_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	78.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_06T10:34:32
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

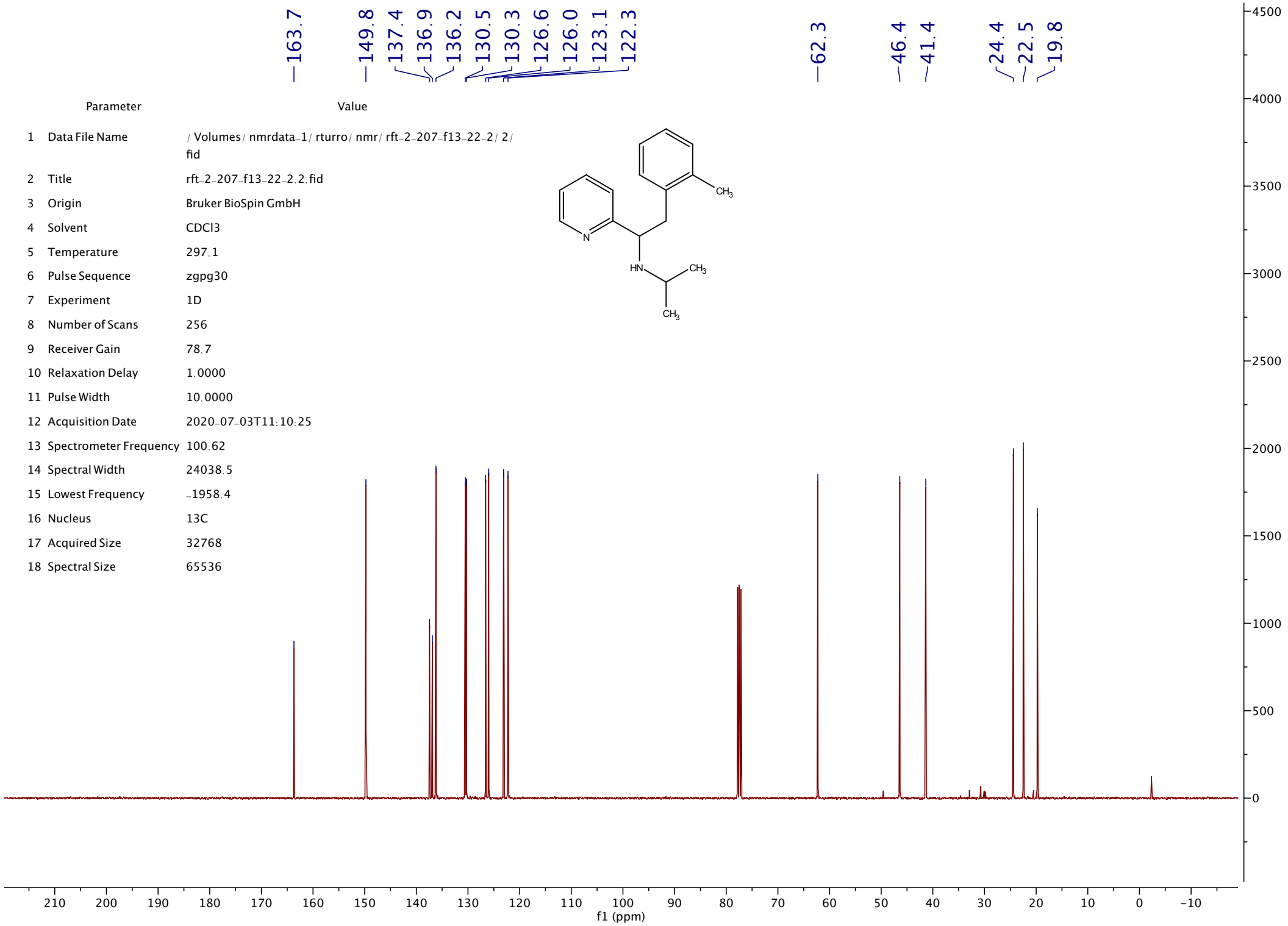
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/RFT_2_212_F2/1/fid
2	Title	RFT_2_212_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_19T06:59:32
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1633.3
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072




162.3
149.7
144.8
136.2
132.0
130.1
122.7
122.3
119.1
110.1
62.5
45.9
43.7
24.0
22.1
Parameter
Value
1 Data File Name / Volumes / nmrdata_1 / rturro / nmr / RFT_2_212_F2_C / 1 / fid
2 Title RFT_2_212_F2_C.1.fid
3 Origin Bruker BioSpin GmbH
4 Solvent CDCl3
5 Temperature 297.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 512
9 Receiver Gain 87.8
10 Relaxation Delay 1.0000
11 Pulse Width 10.0000
12 Acquisition Date 2020_10_19T09:20:15
13 Spectrometer Frequency 100.62
14 Spectral Width 24038.5
15 Lowest Frequency _1958.4
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
N
N
HN
CH3
CH3
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

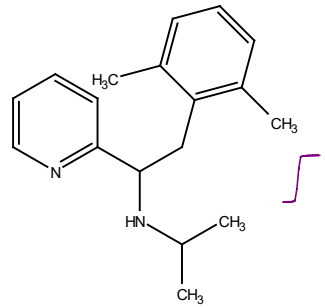
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata_1/ rturro/ nmr/ RFT_2_207_C2_F13_32/ 1/ fid
2	Title	RFT_2_207_C2_F13_32.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	17.5
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_07_02T15:00:58
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1652.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

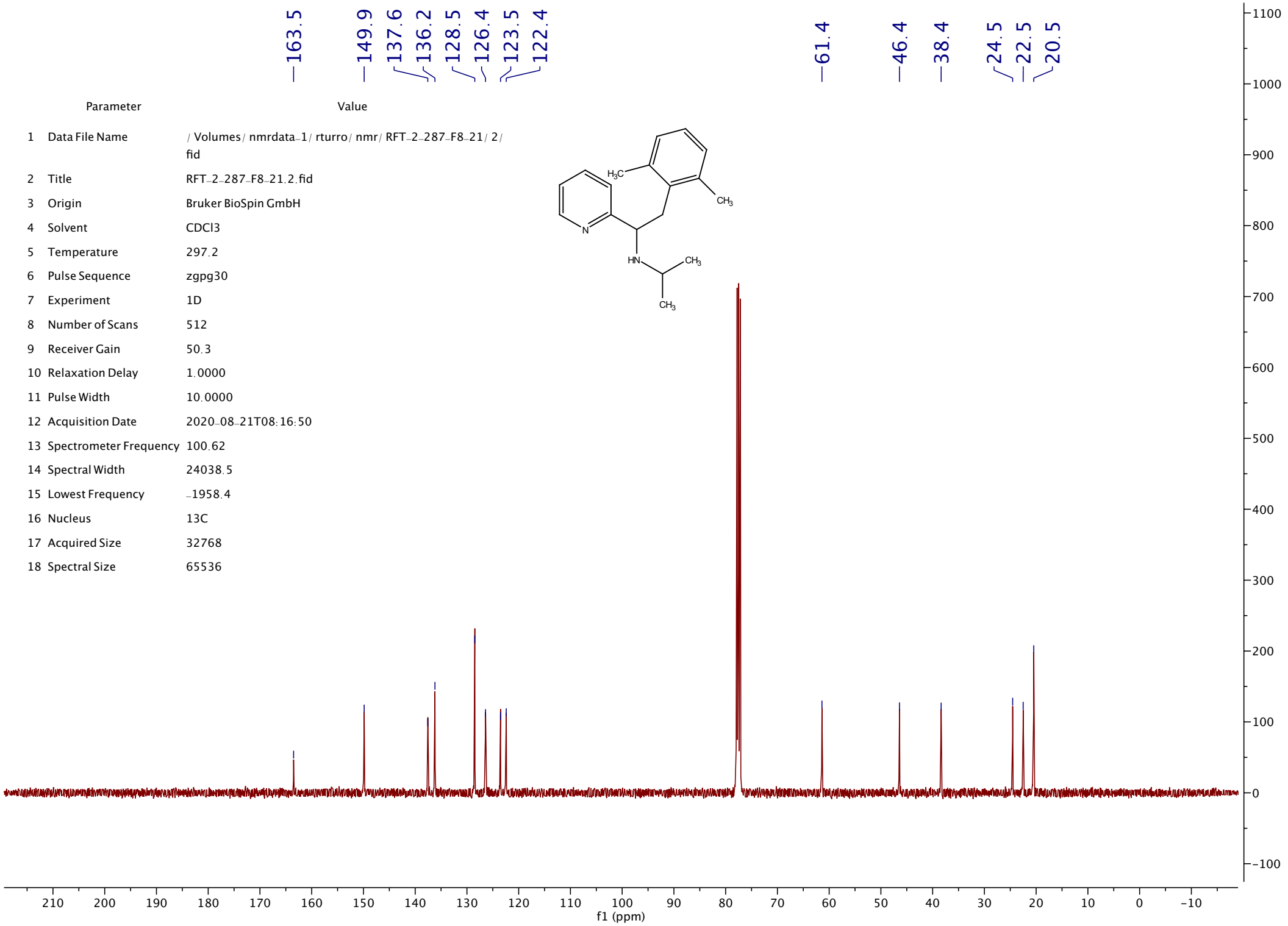




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/rft_2_207_f13_22_2/2/fid
2	Title	rft_2_207_f13_22_2.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	256
9	Receiver Gain	78.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_07_03T11:10:25
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

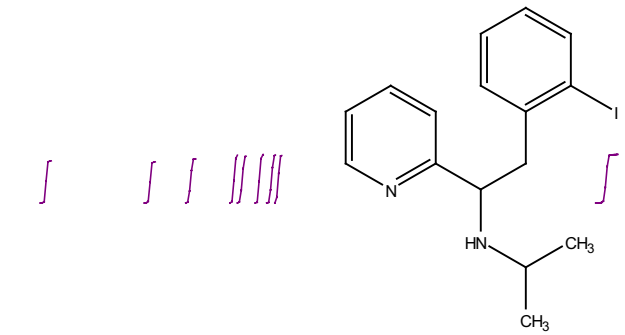
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/RFT_2_287_F8_21/1/fid
2	Title	RFT_2_287_F8_21.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	98.9
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_08_21T07:54:38
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1652.3
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

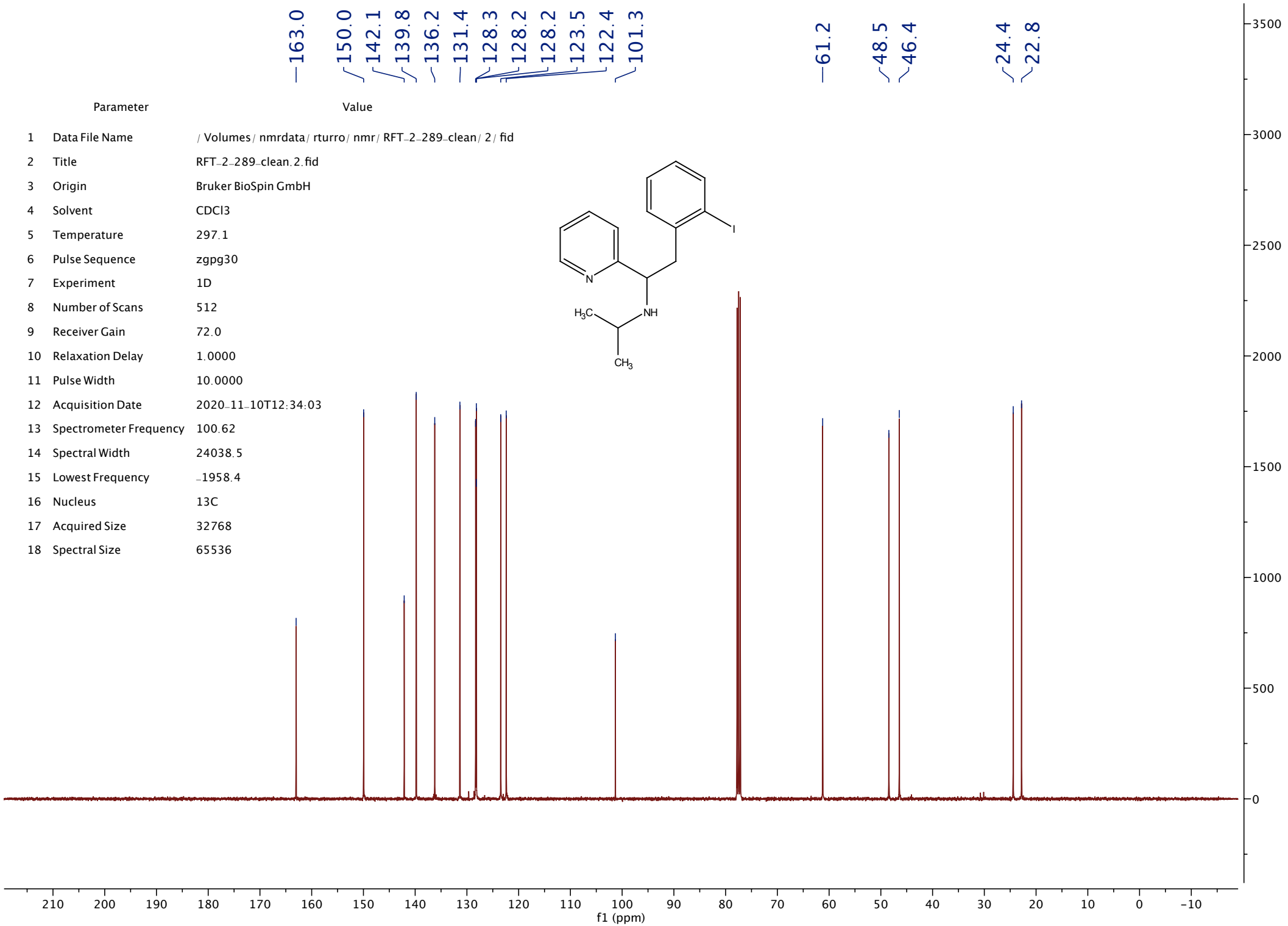




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/RFT_2_287_F8_21/2/fid
2	Title	RFT_2_287_F8_21.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_08_21T08:16:50
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

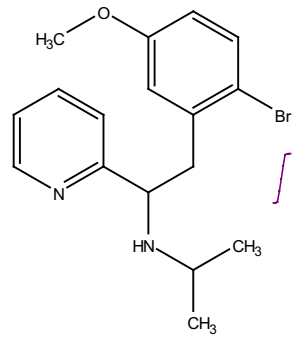
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/vnmrsys/data/RFT_2_289_F8_21/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	RFT_2_289_F8_21
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	23.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	56
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_08_19T09:57:46
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000
18	Spectral Size	65536





	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_2_289_clean / 2 / fid
2	Title	RFT_2_289_clean.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	72.0
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_11_10T12:34:03
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

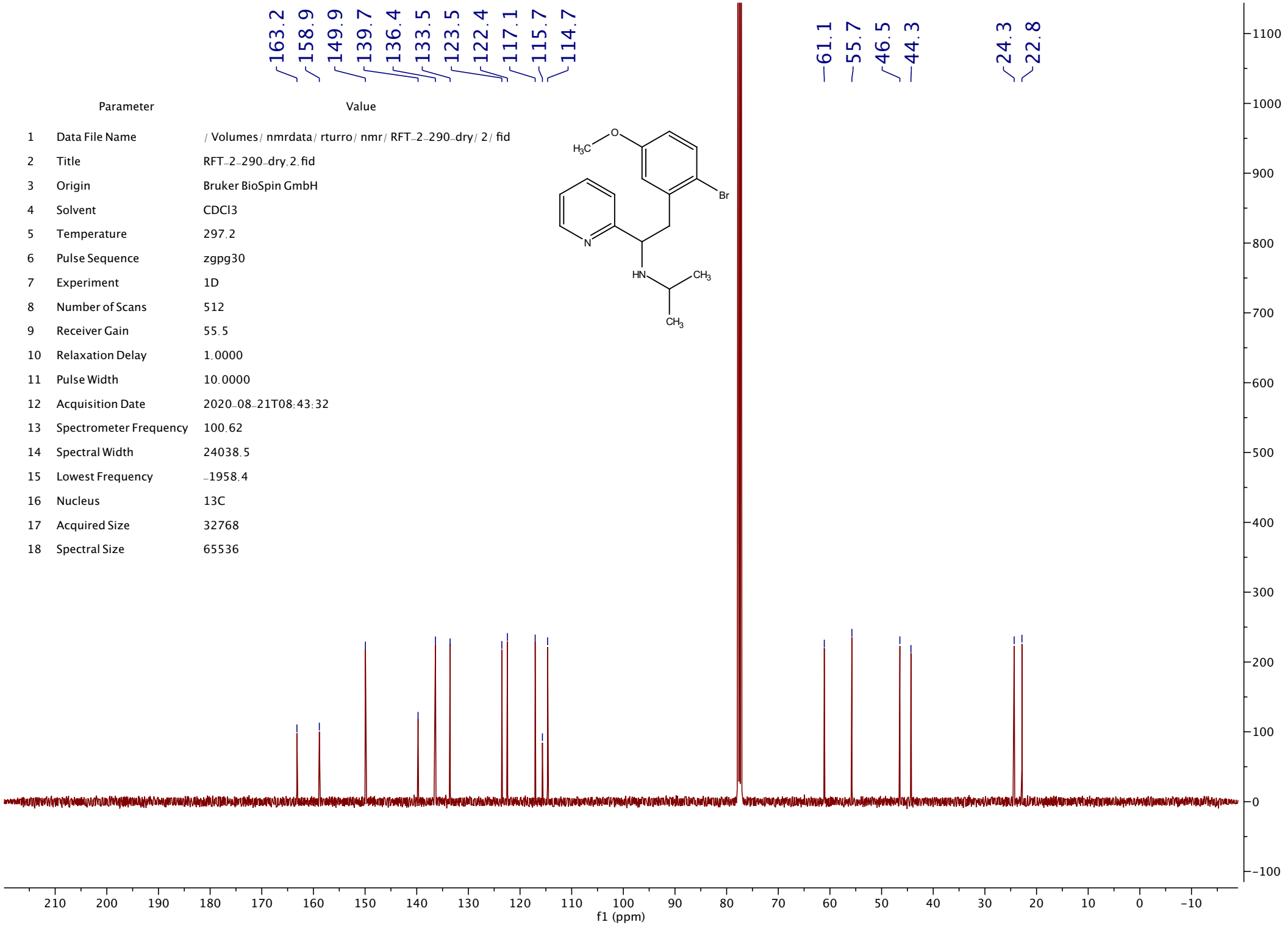
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ RFT-2-290-dry/ 1/ fid
2	Title	RFT-2-290-dry.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020-08-21T08:22:21
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1639.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072



H (ddd) 8.60
J (d) 7.36
I (td) 7.48
K (ddd) 7.11
L (dt) 6.95
M (dd) 6.56
N (d) 6.34
A (dd) 4.16
B (s) 3.58
C (dd) 3.25
D (dd) 2.98
E (p) 2.63
F (s) 1.76
G (t) 1.00

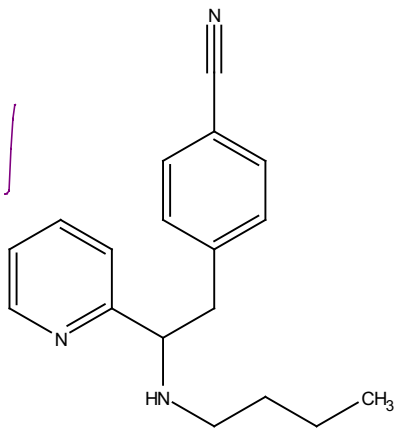
0.95 0.92 0.90 0.94 0.99 0.95 0.99 1.00 2.99 0.93 0.98 0.92 4.57 5.83

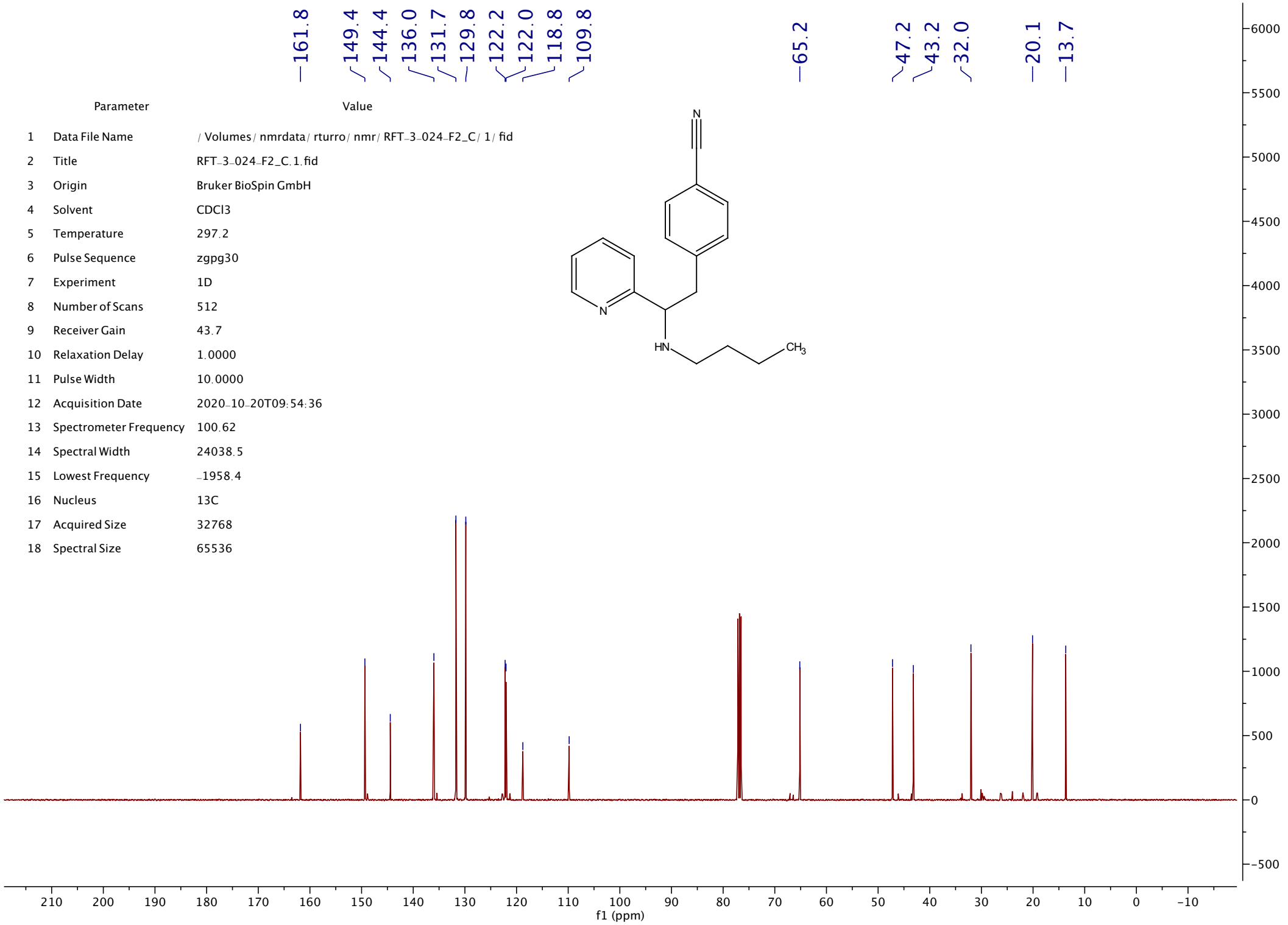
f1 (ppm)



	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_2_290_dry/2/fid
2	Title	RFT_2_290_dry.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	55.5
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_08_21T08:43:32
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

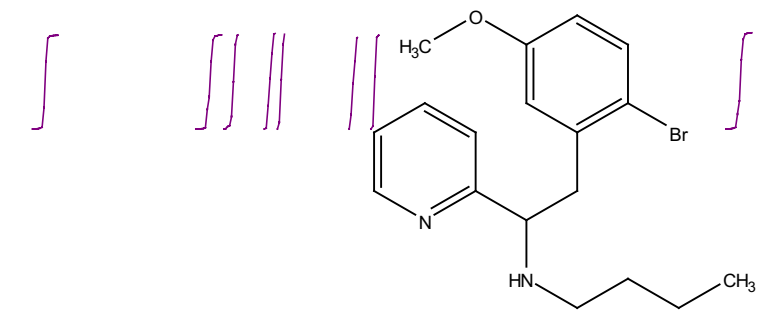
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_024_F2/1/fid
2	Title	RFT_3_024_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_20T08:43:34
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1634.3
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072





	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_024_F2_C/1/fid
2	Title	RFT_3_024_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_20T09:54:36
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

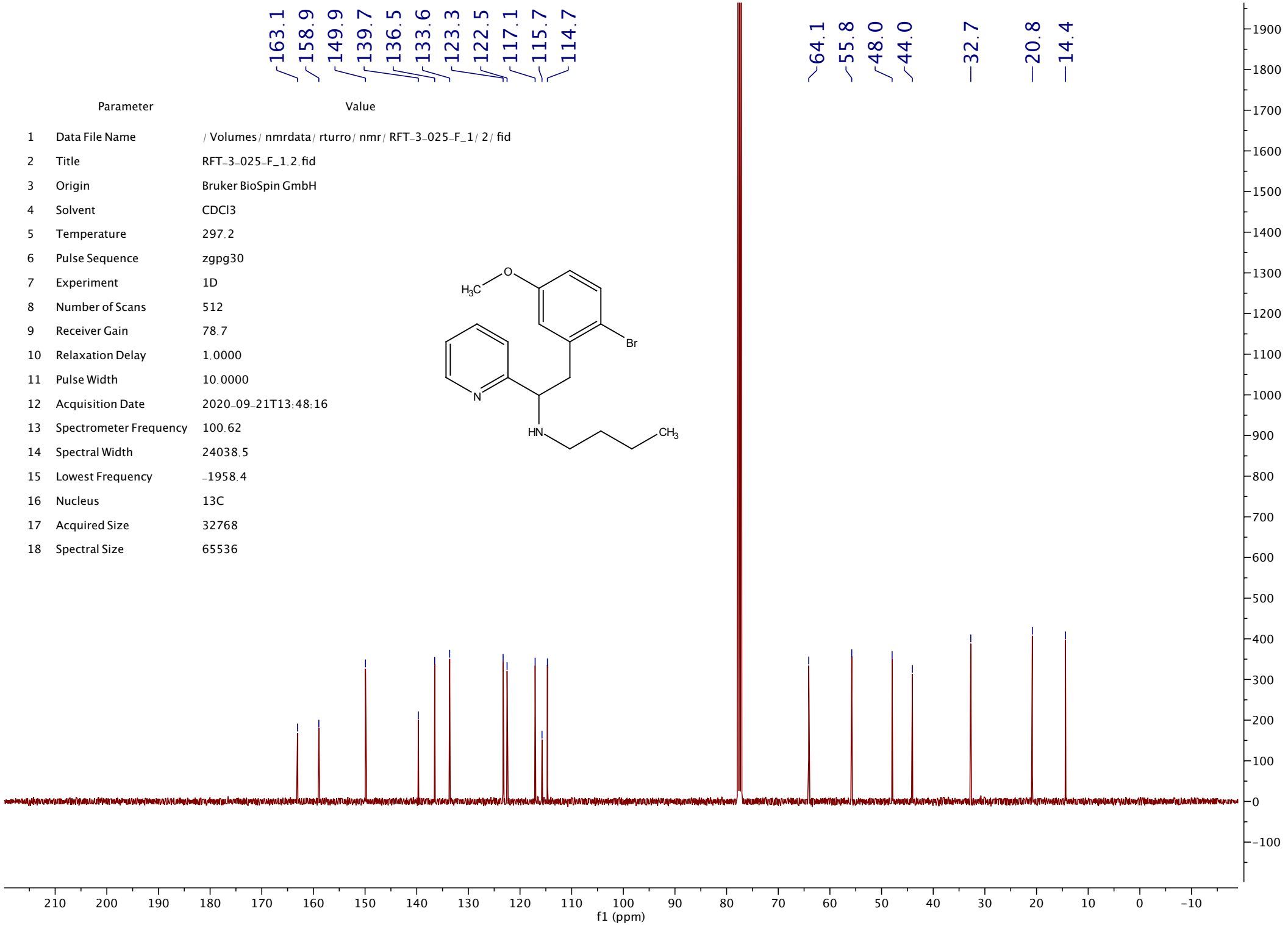
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_025_F_1/1/fid
2	Title	RFT_3_025_F_1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_09_21T13:27:02
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1630.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072



B (ddd) 8.60
C (td) 7.52
D (d) 7.37
E (ddd) 7.13
F (dt) 7.05
G (dd) 6.58
H (d) 6.45
A (t) 4.05
I (s) 3.62
J (dd) 3.21
K (dd) 3.03
L (m) 2.44
M (m) 1.41
N (m) 1.25
O (t) 0.83

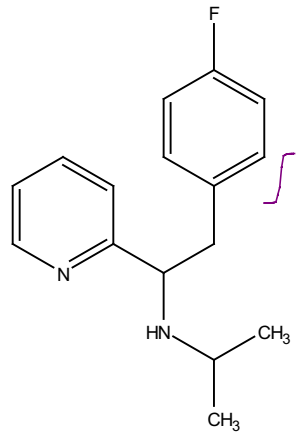
0.97 0.98 0.98 0.99 0.98 0.95 0.97 1.00 2.99 1.04 0.99 2.00 2.22 2.19 3.00

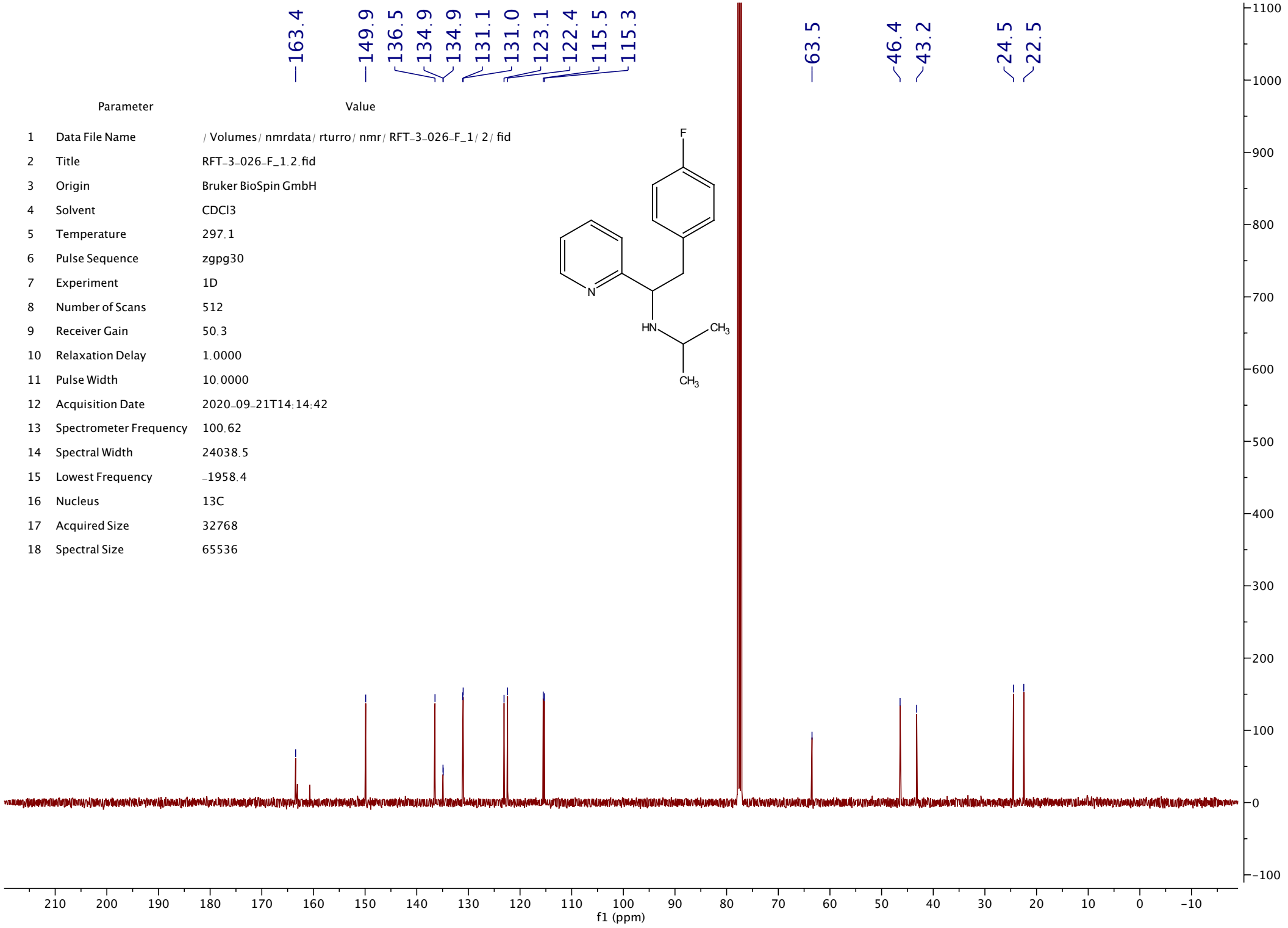
f1 (ppm)



	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_025_F_1/2/fid
2	Title	RFT_3_025_F_1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	78.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_09_21T13:48:16
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

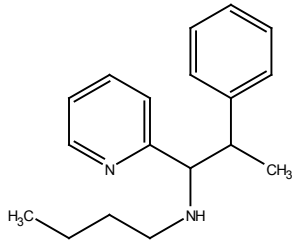
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_026_F_1/1/fid
2	Title	RFT_3_026_F_1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	197.4
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_09_21T13:53:32
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1654.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

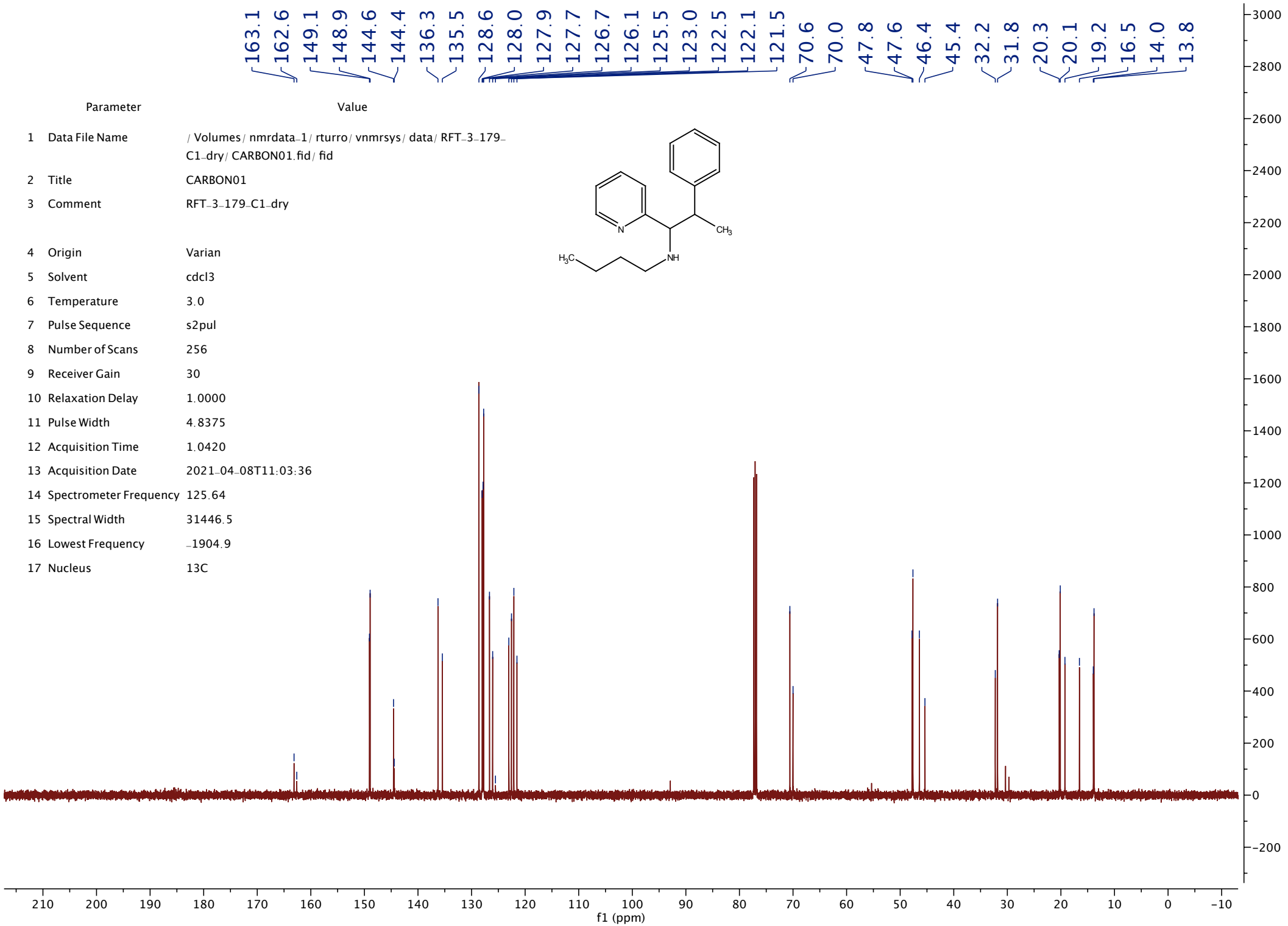




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT-3-026-F_1/2/fid
2	Title	RFT-3-026-F_1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020-09-21T14:14:42
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

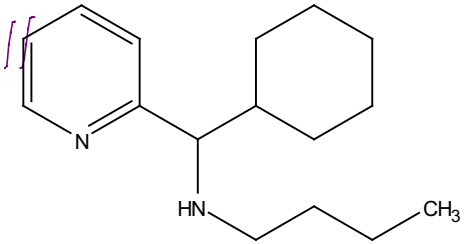
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/vnmrsys/data/RFT_3_179_C1_dry/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	RFT_3_179_C1_dry
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	1
9	Receiver Gain	42
10	Relaxation Delay	10.0000
11	Pulse Width	5.6500
12	Acquisition Time	10.0000
13	Acquisition Date	2021_04_08T11:02:57
14	Spectrometer Frequency	499.59
15	Spectral Width	8000.0
16	Lowest Frequency	-1002.5
17	Nucleus	1H

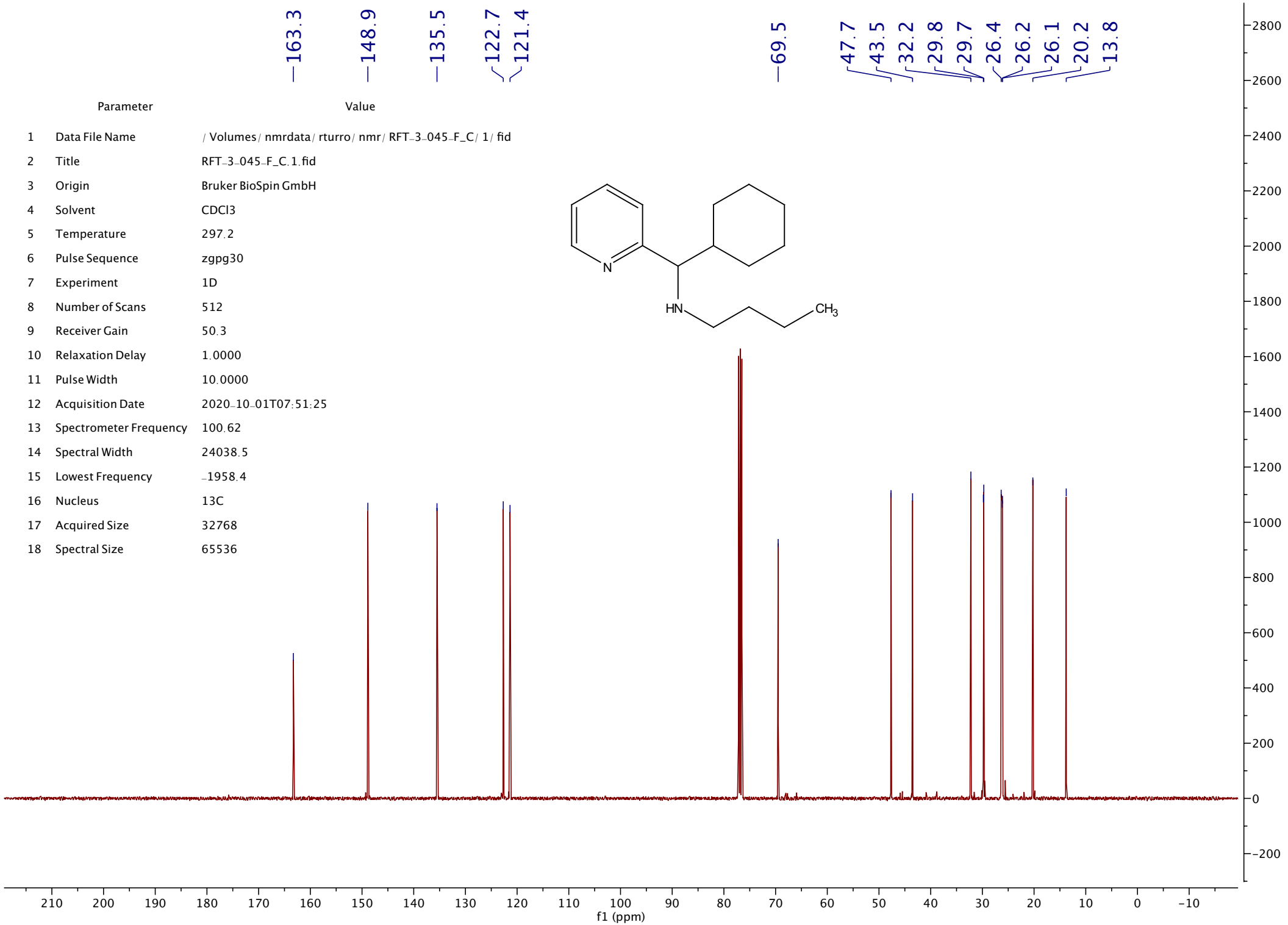




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/vnmrsys/data/RFT_3_179_C1_dry/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	RFT_3_179_C1_dry
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Time	1.0420
13	Acquisition Date	2021_04_08T11:03:36
14	Spectrometer Frequency	125.64
15	Spectral Width	31446.5
16	Lowest Frequency	_1904.9
17	Nucleus	13C

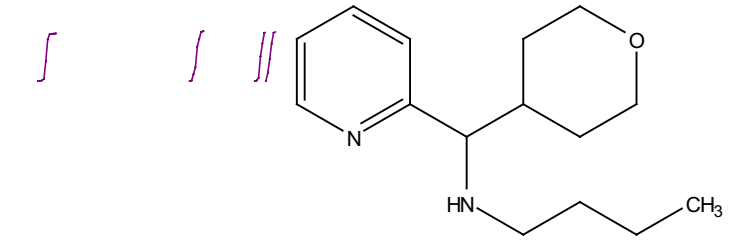
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_045_F/1/fid
2	Title	RFT_3_045_F.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	24.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_01T06:58:10
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1551.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

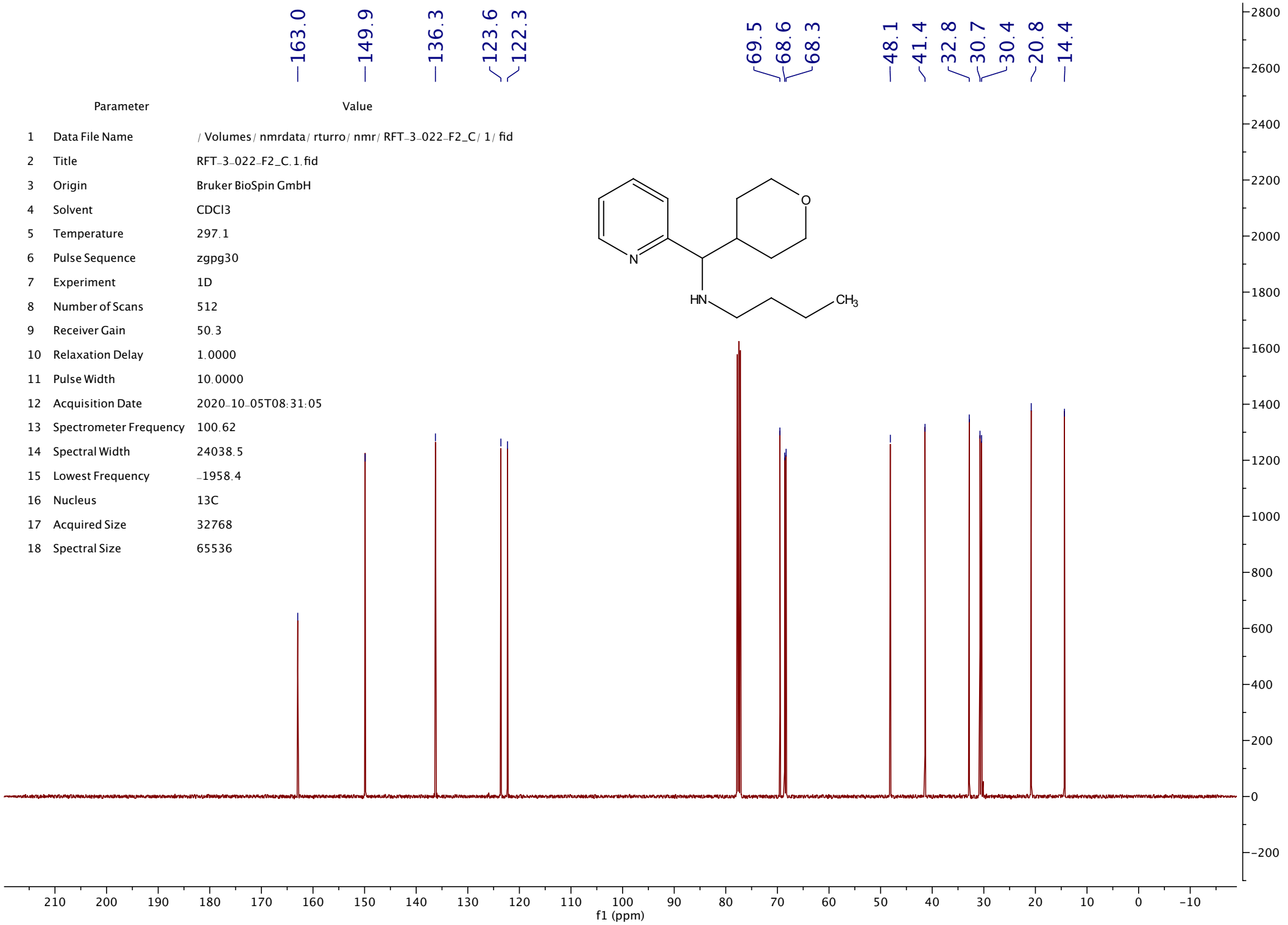




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT-3-045-F_C/1/fid
2	Title	RFT-3-045-F_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020-10-01T07:51:25
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

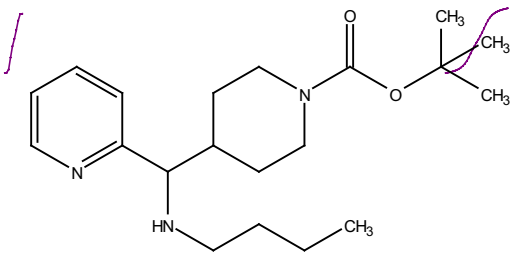
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_022_F2 / 1 / fid
2	Title	RFT_3_022_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	21.4
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_05T07:43:02
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1632.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072





	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_022_F2_C/1/fid
2	Title	RFT_3_022_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_05T08:31:05
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

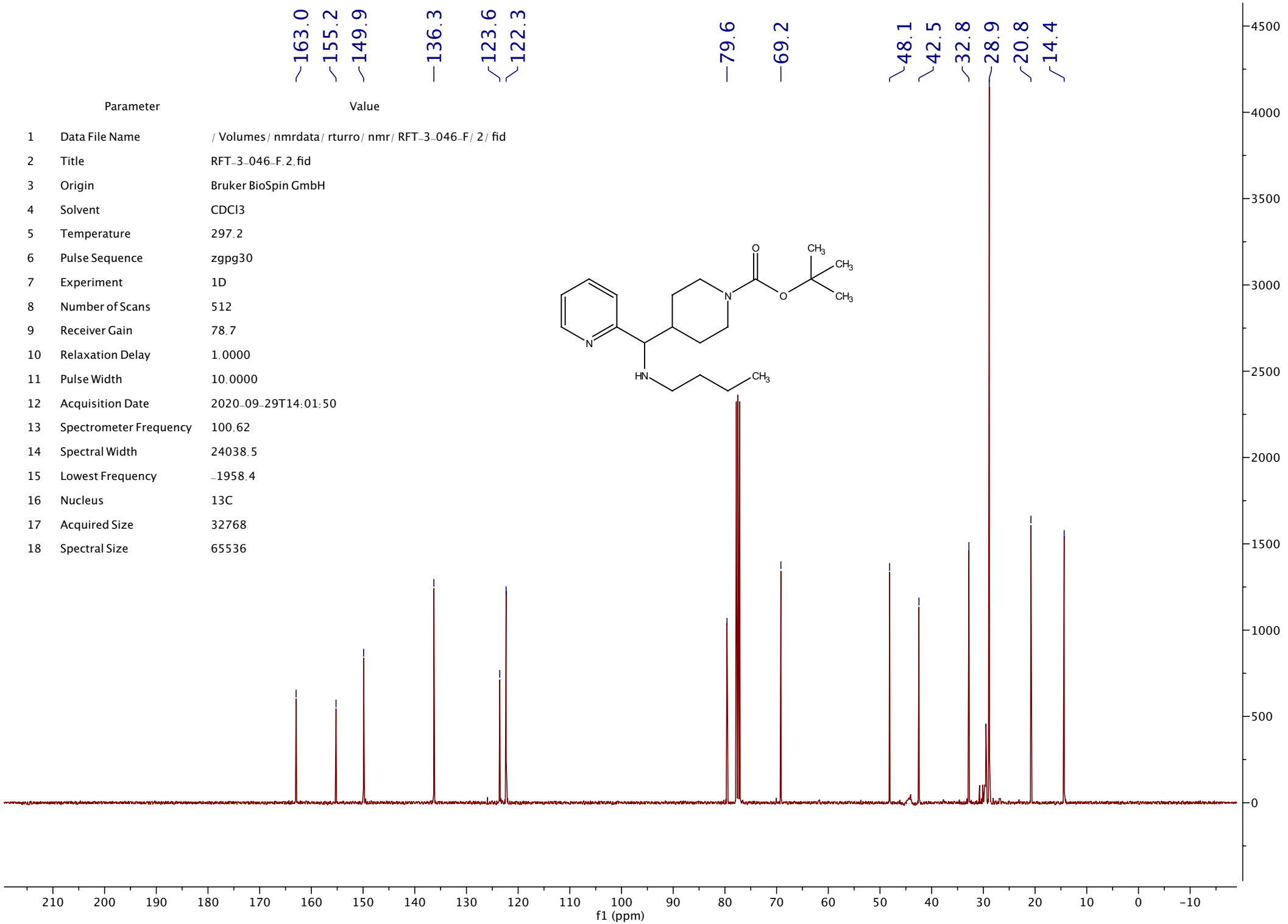
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_047_F / 1 / fid
2	Title	RFT_3_047_F.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	38.0
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_02T10:51:56
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	_1649.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072



J (ddd) 8.56 | K (td) 7.60 | L (m) 7.15 | B (d) 4.04 | A (d) 3.39 | C (dt) 2.59 | D (m) 2.32 | E (m) 1.94 | F (ddt) 1.77 | G (s) 1.41 | H (m) 1.36 | I (t) 0.82

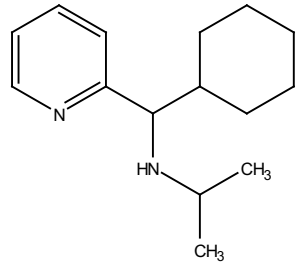
0.89 | 0.92 | 1.84 | 2.02 | 1.00 | 2.10 | 1.92 | 1.01 | 2.54 | 8.97 | 1.46 | 2.84

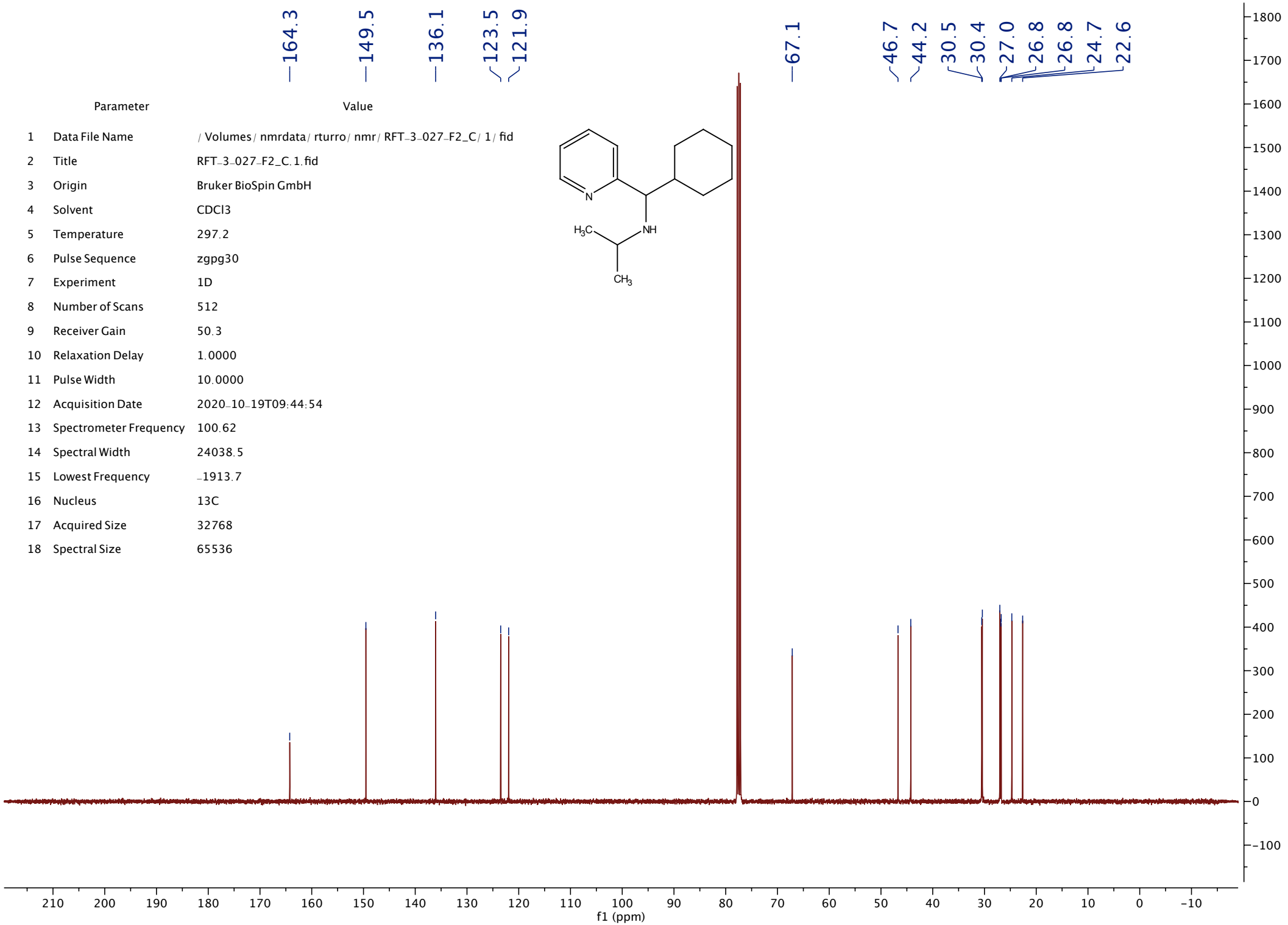
f1 (ppm)



	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_046_F / 2 / fid
2	Title	RFT_3_046_F.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	78.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_09_29T14:01:50
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

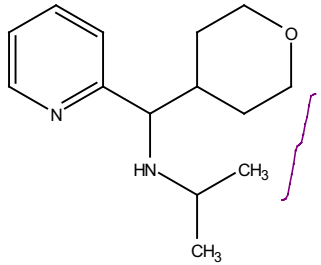
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_027_F2 / 1 / fid
2	Title	RFT_3_027_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	32
9	Receiver Gain	112.8
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_19T07:10:39
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1555.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072





	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_027_F2_C/1/fid
2	Title	RFT_3_027_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_19T09:44:54
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1913.7
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

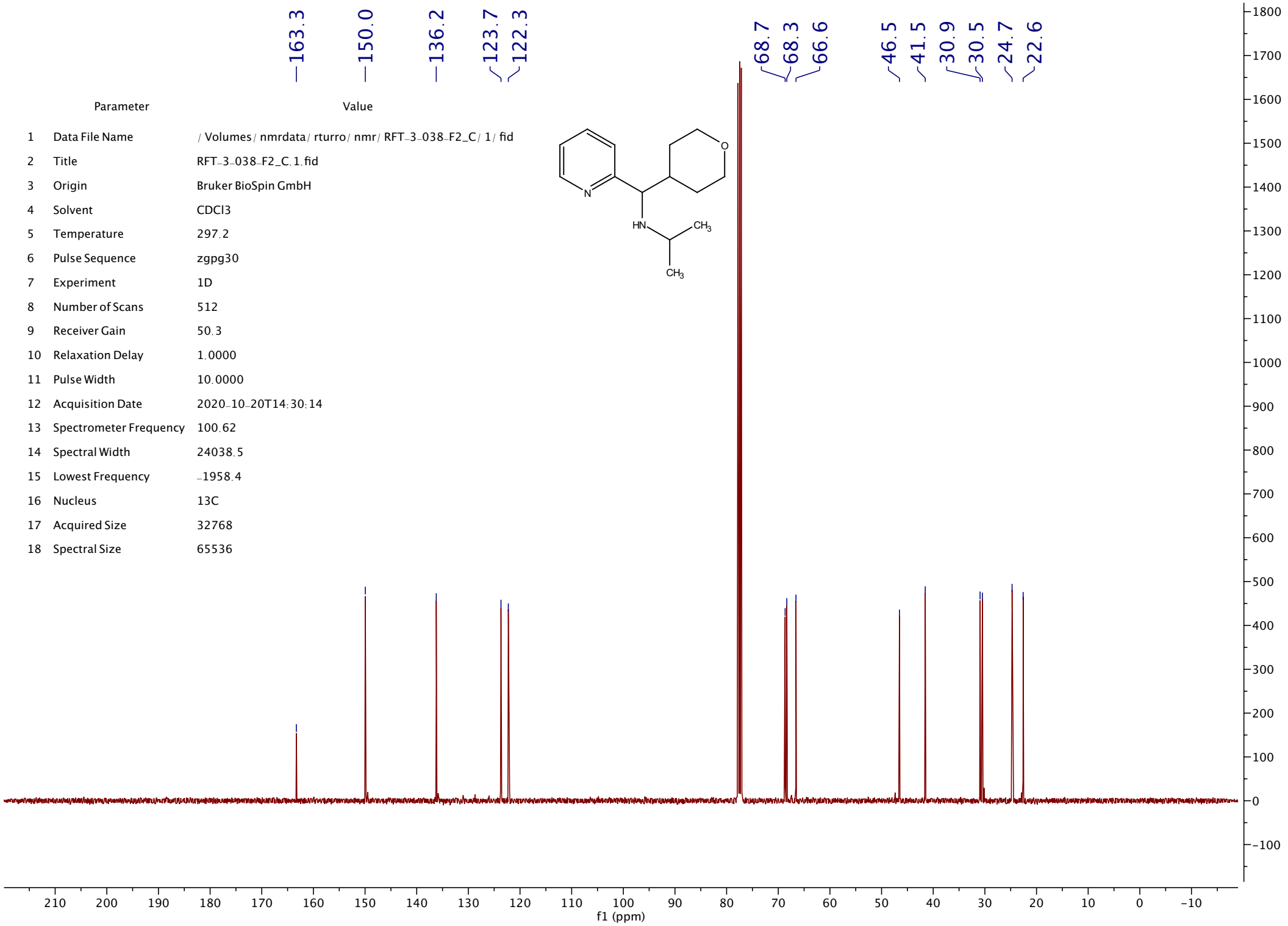
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_2 / rturro / vnmrsys / data / RFT_3_038_F2_DCM / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	RFT_3_038_F2_DCM
4	Origin	Varian
5	Solvent	CDCl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	22
10	Relaxation Delay	1.0000
11	Pulse Width	5.1000
12	Acquisition Date	2020_10_20T10:07:17
13	Spectrometer Frequency	300.09
14	Spectral Width	4796.2
15	Lowest Frequency	-597.5
16	Nucleus	1H
17	Acquired Size	11990



D (dt) 8.58
E (td) 7.60
F (m) 7.15
A (d) 3.48
B (dtd) 3.30
C (m) 3.89
G (p) 2.46
H (m) 1.87
I (m) 1.32
J (m) 1.09
K (dd) 0.96

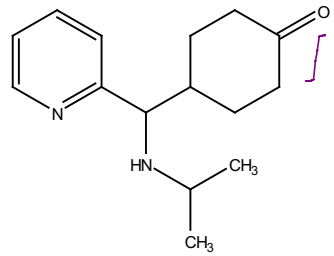
0.89 0.90 2.07 2.25 1.00 2.07 0.92 3.97 2.18 1.03 6.13

f1 (ppm)



	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_038_F2_C/1/fid
2	Title	RFT_3_038_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_20T14:30:14
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

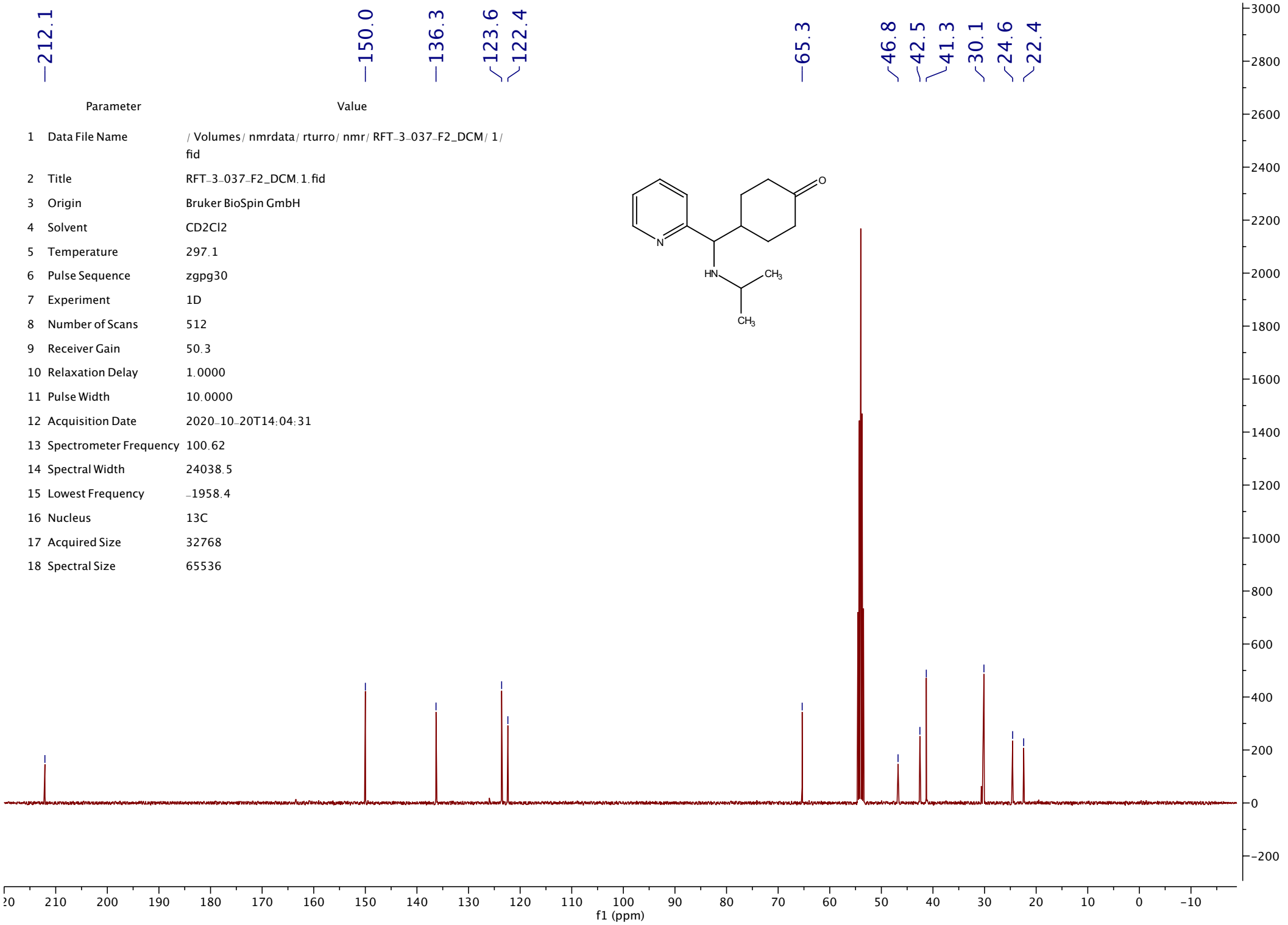
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_038_F2/1/fid
2	Title	RFT_3_038_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_01T06:49:43
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1633.7
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072



B (ddd) 8.57
C (td) 7.60
D (m) 7.15
A (d) 3.55
E (p) 2.45
H (s) 1.95
J (m) 1.42
G (dddd) 2.06
F (m) 2.30
I (ddq) 1.64
K (dd) 0.96

0.97 0.99 2.10 1.00 0.94 4.36 0.90 1.62 1.05 1.98 6.31

f1 (ppm)



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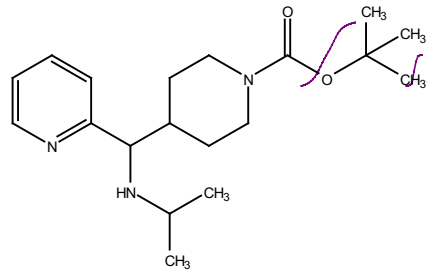
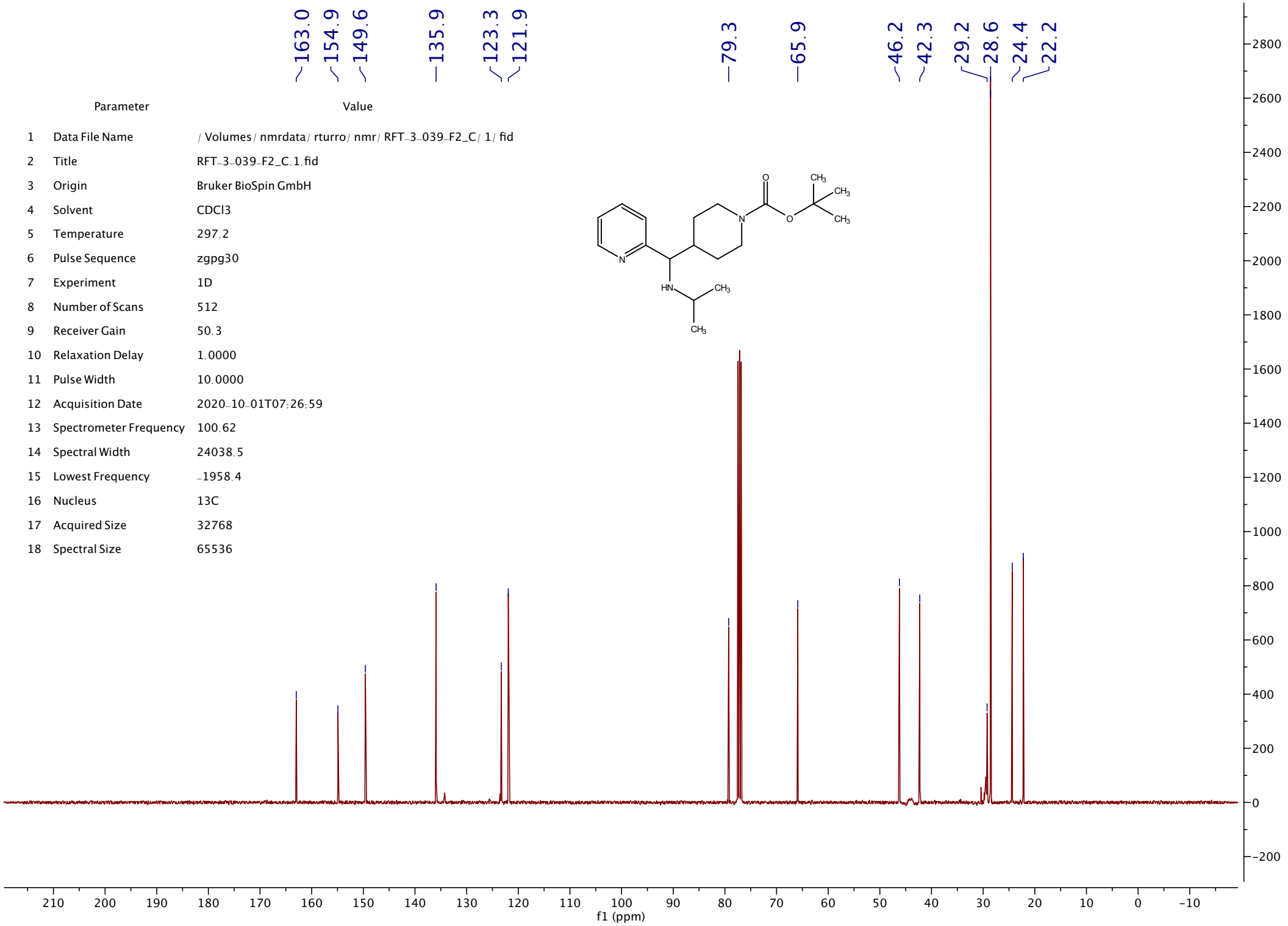
2	Title	RFT-3-037-F2_DCM.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CD2Cl2
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020-10-20T14:04:31
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_039_F2 / 1 / fid
2	Title	RFT_3_039_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	24.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_10_01T06:54:04
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1633.8
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072





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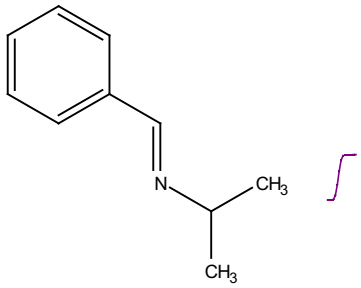
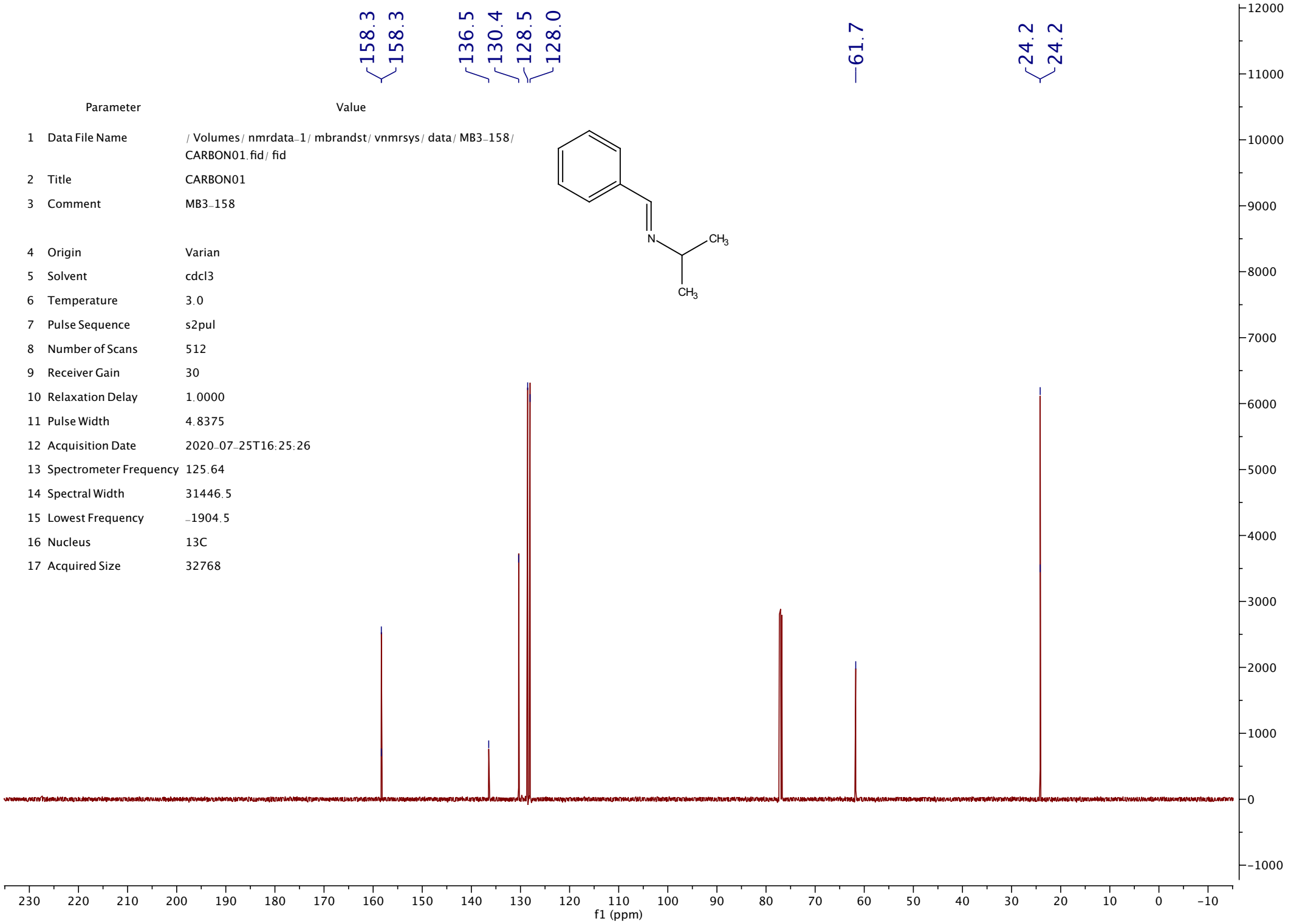
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_01T07:26:59
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB3_158 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB3_158
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_25T16:24:06
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000





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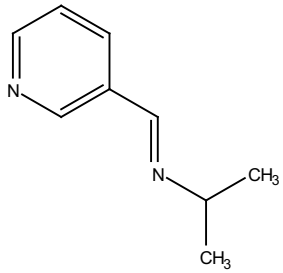
2	Title	CARBON01
3	Comment	MB3-158
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020-07-25T16:25:26
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

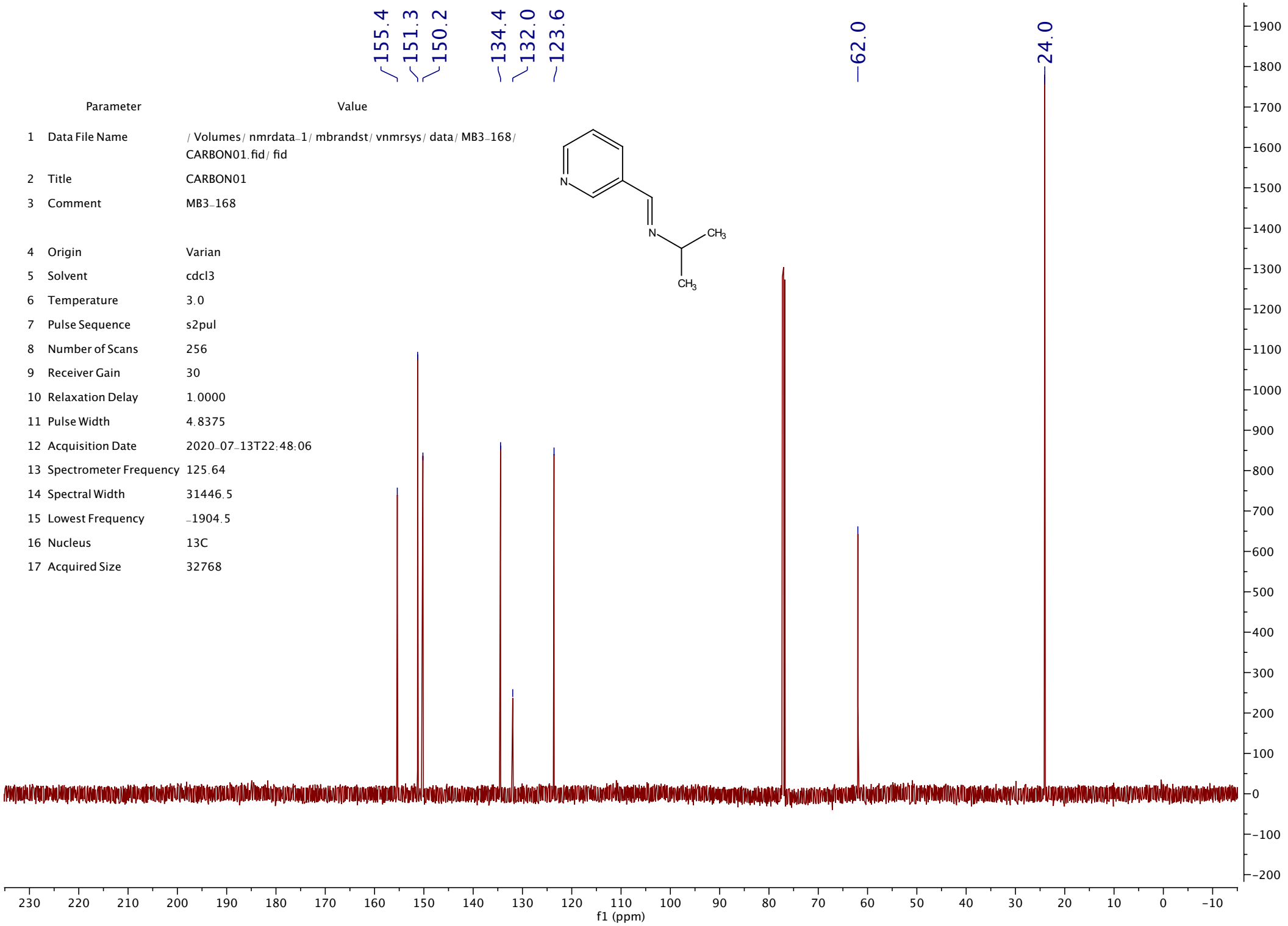
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata_1/ mbrandst/ vnmrsys/ data/ MB3_168/ PROTON01.fid/ fid
2	Title	PROTON01
3	Comment	MB3_168
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_13T22:47:18
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	_1002.4
16	Nucleus	1H
17	Acquired Size	24000



E (d) 8.83
C (s) 8.33
D (dd) 8.62
B (dd) 8.11
A (m) 7.32
F (m) 3.57
G (dt) 1.27

0.90
0.89
1.06
1.08
1.00
1.05
6.19

f1 (ppm)



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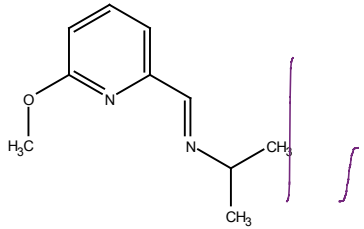
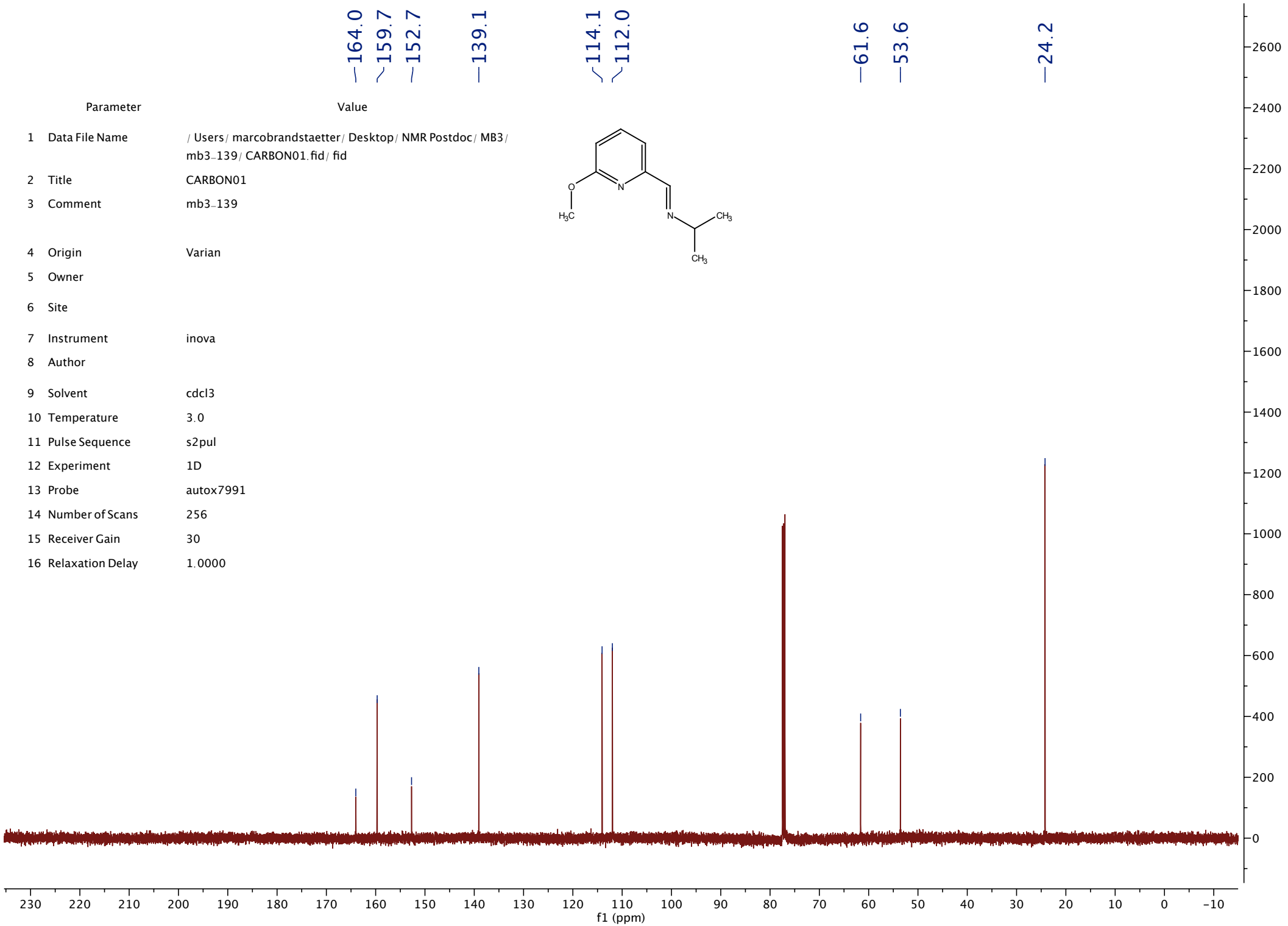
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_168/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3_168
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_13T22:48:06
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	_1904.5
16	Nucleus	13C
17	Acquired Size	32768

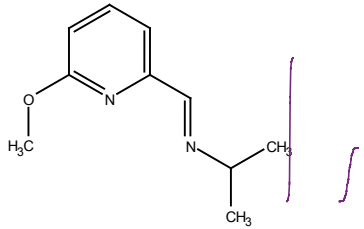
	Parameter	Value
1	Data File Name	/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB3/ mb3_139/ PROTON01.fid/ fid
2	Title	PROTON01
3	Comment	mb3_139
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	52
16	Relaxation Delay	1.0000

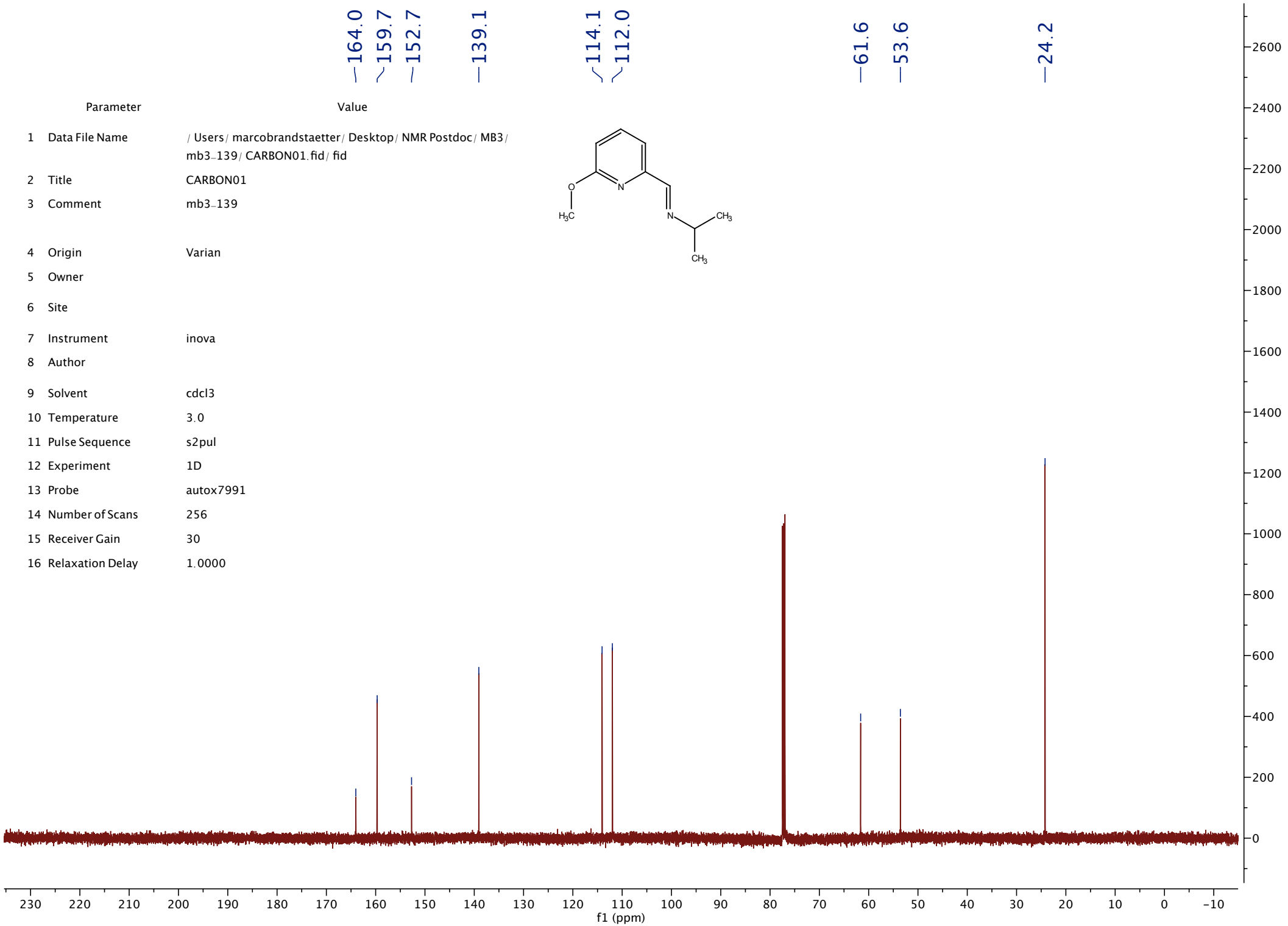




	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_139 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	mb3_139
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	256
15	Receiver Gain	30
16	Relaxation Delay	1.0000

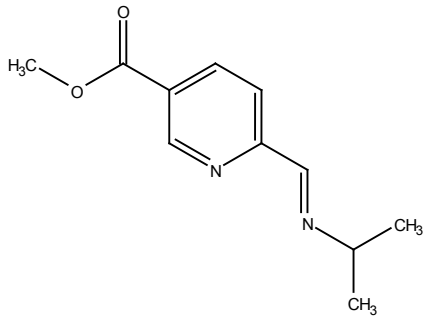
	Parameter	Value
1	Data File Name	/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB3/ mb3_139/ PROTON01.fid/ fid
2	Title	PROTON01
3	Comment	mb3_139
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	52
16	Relaxation Delay	1.0000

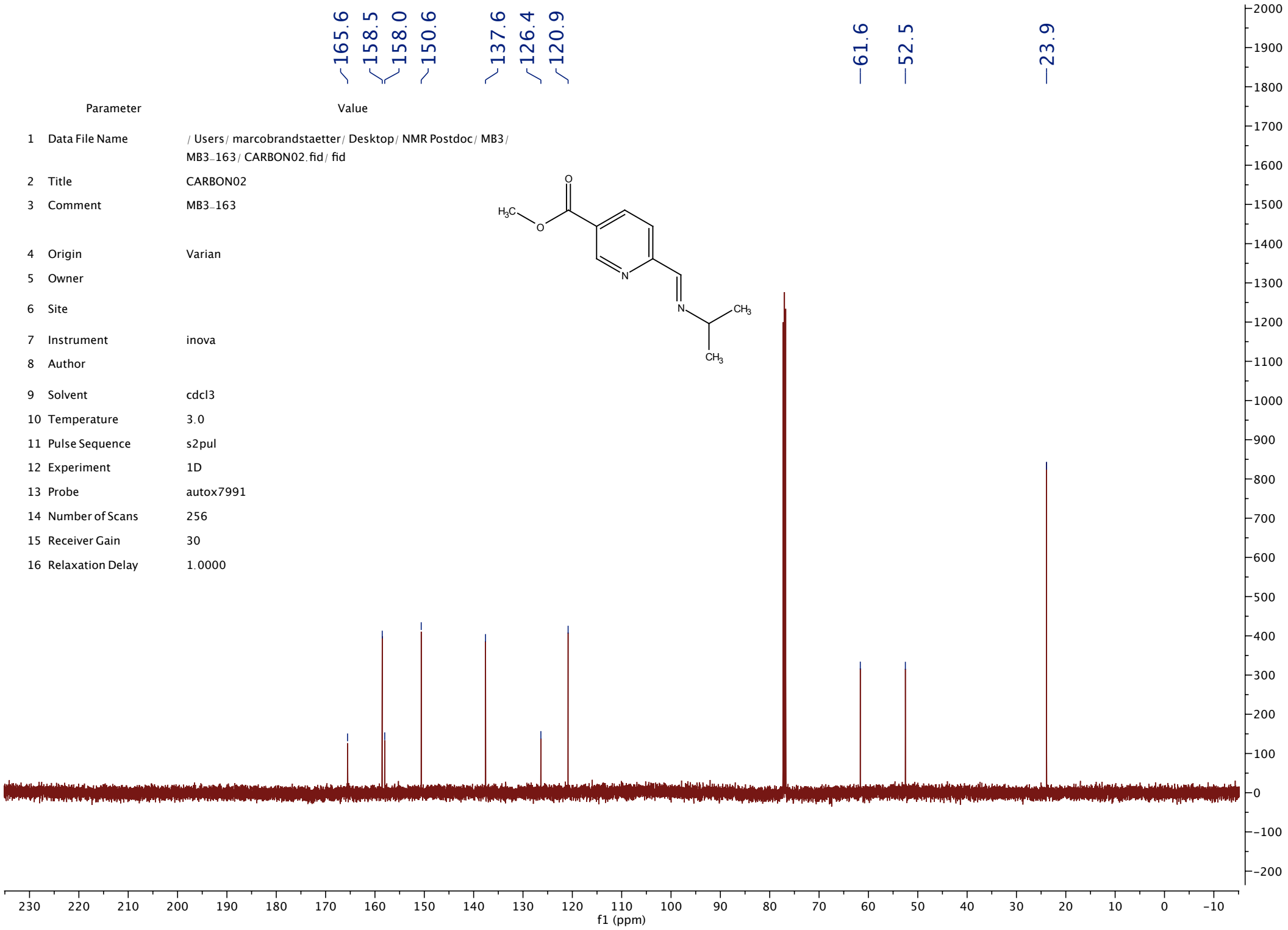




	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_139 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	mb3_139
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	256
15	Receiver Gain	30
16	Relaxation Delay	1.0000

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_163 / PROTON02.fid / fid
2	Title	PROTON02
3	Comment	MB3_163
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	54
16	Relaxation Delay	1.0000




165.6
158.5
158.0
150.6
137.6
126.4
120.9
61.6
52.5
23.9
Parameter
Value
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/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB3/ MB3_163/ CARBON02.fid/ fid
2 Title
CARBON02
3 Comment
MB3_163
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
O
H3C
O
N
N
CH3
CH3
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

	Parameter	Value
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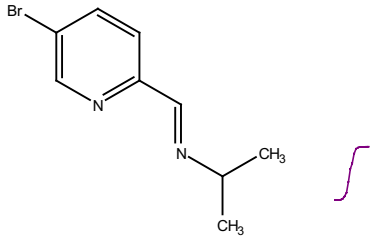
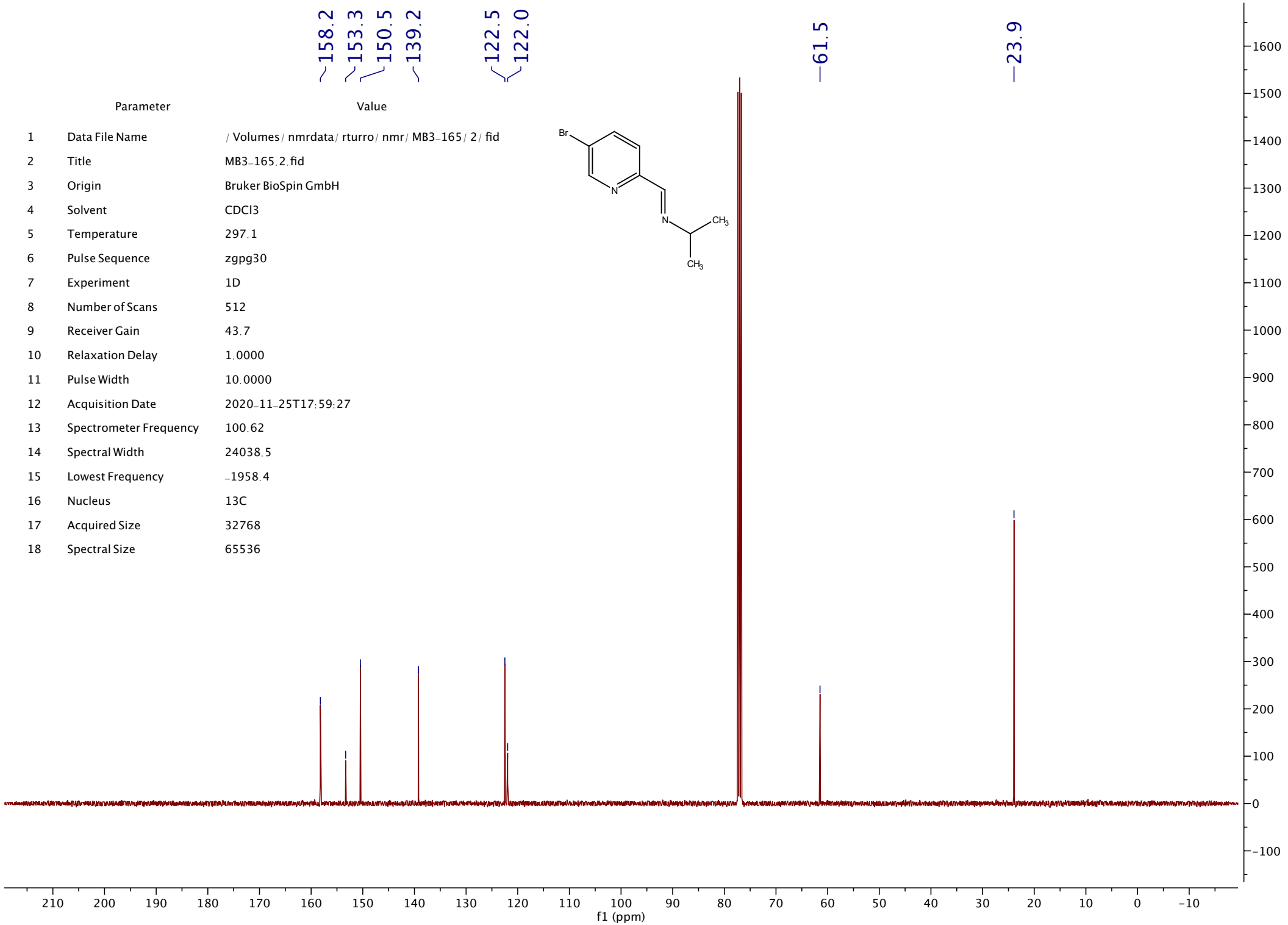
2	Title	MB3_165.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	197.4
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_11_25T17:38:16
13	Spectrometer Frequency	400.13
14	Spectral Width	8012.8
15	Lowest Frequency	_1571.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536





	Parameter	Value
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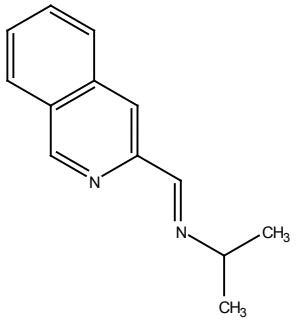
2	Title	MB3_165.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_11_25T17:59:27
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	_1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

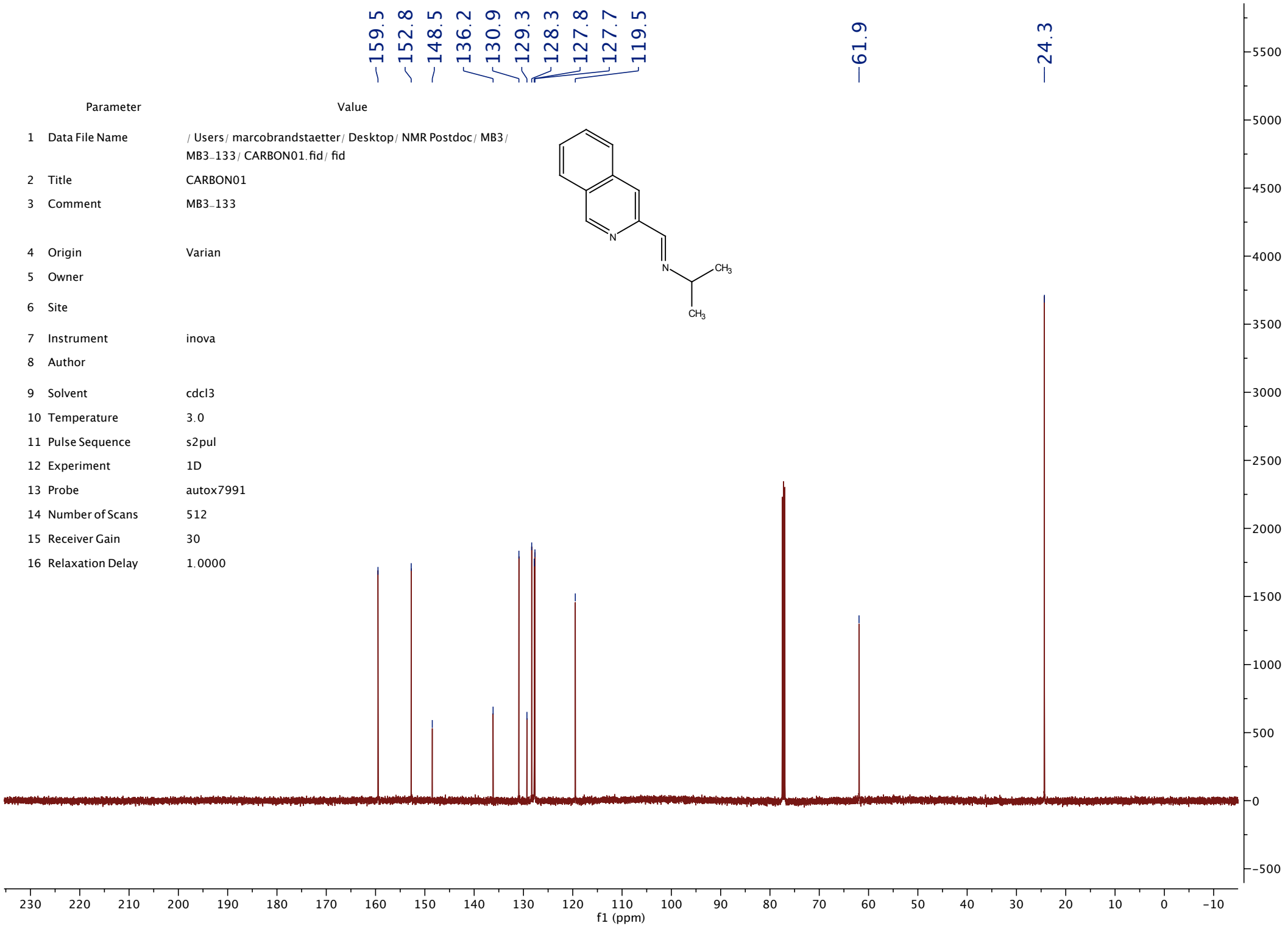
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_133 / PROTON03.fid / fid
2	Title	PROTON03
3	Comment	MB3_133
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	16
15	Receiver Gain	48
16	Relaxation Delay	1.0000

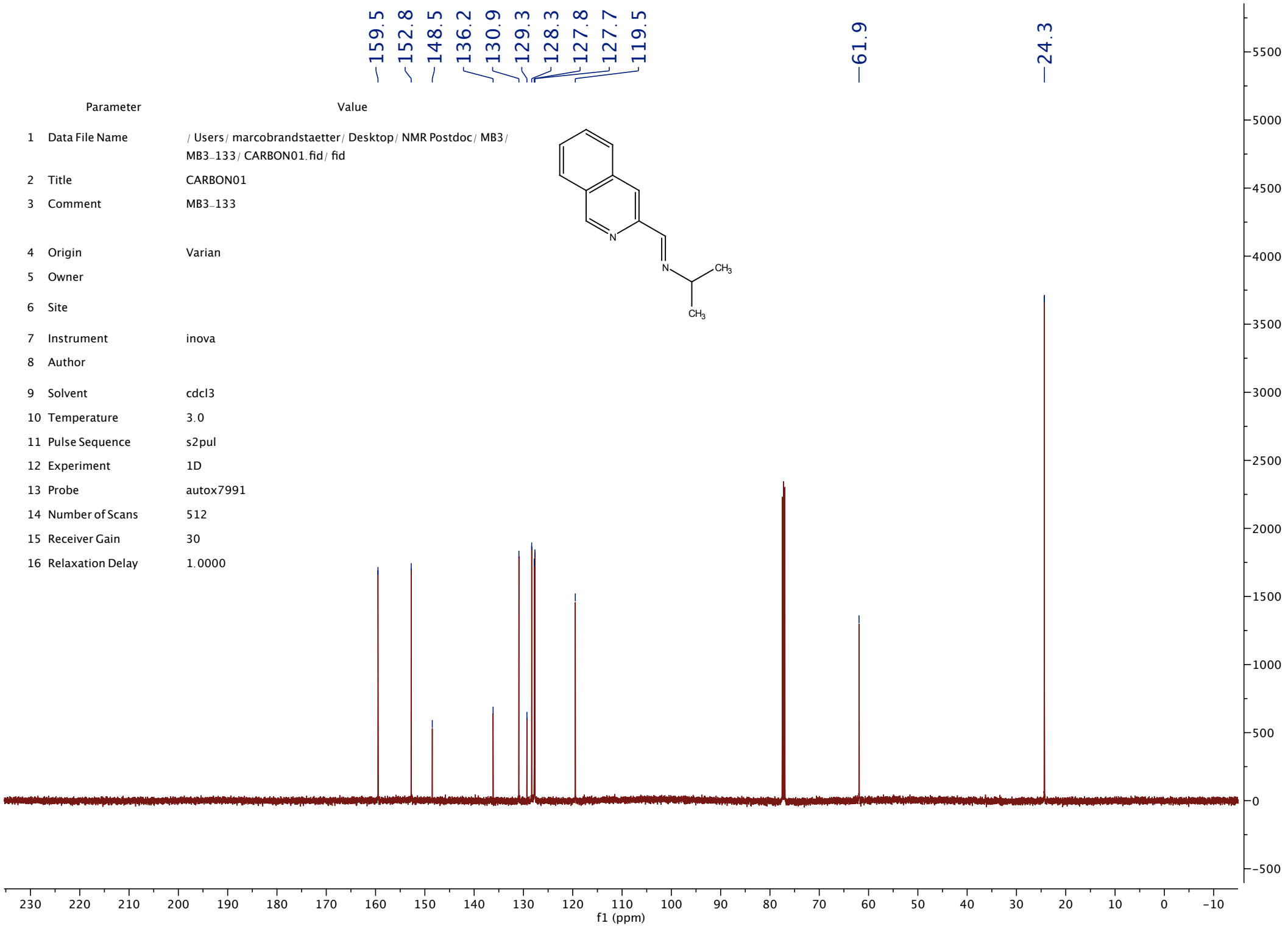


A (s) 9.28
B (s) 8.57
C (s) 8.26
D (d) 7.98
E (d) 7.89
F (t) 7.70
G (t) 7.63
H (hept) 3.69
I (d) 1.34

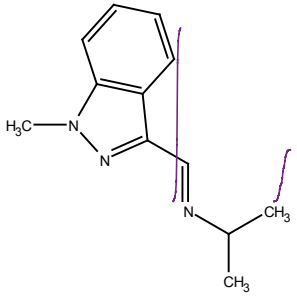
1.00 0.59 1.03 1.17 1.19 0.59 0.67 0.61 3.71

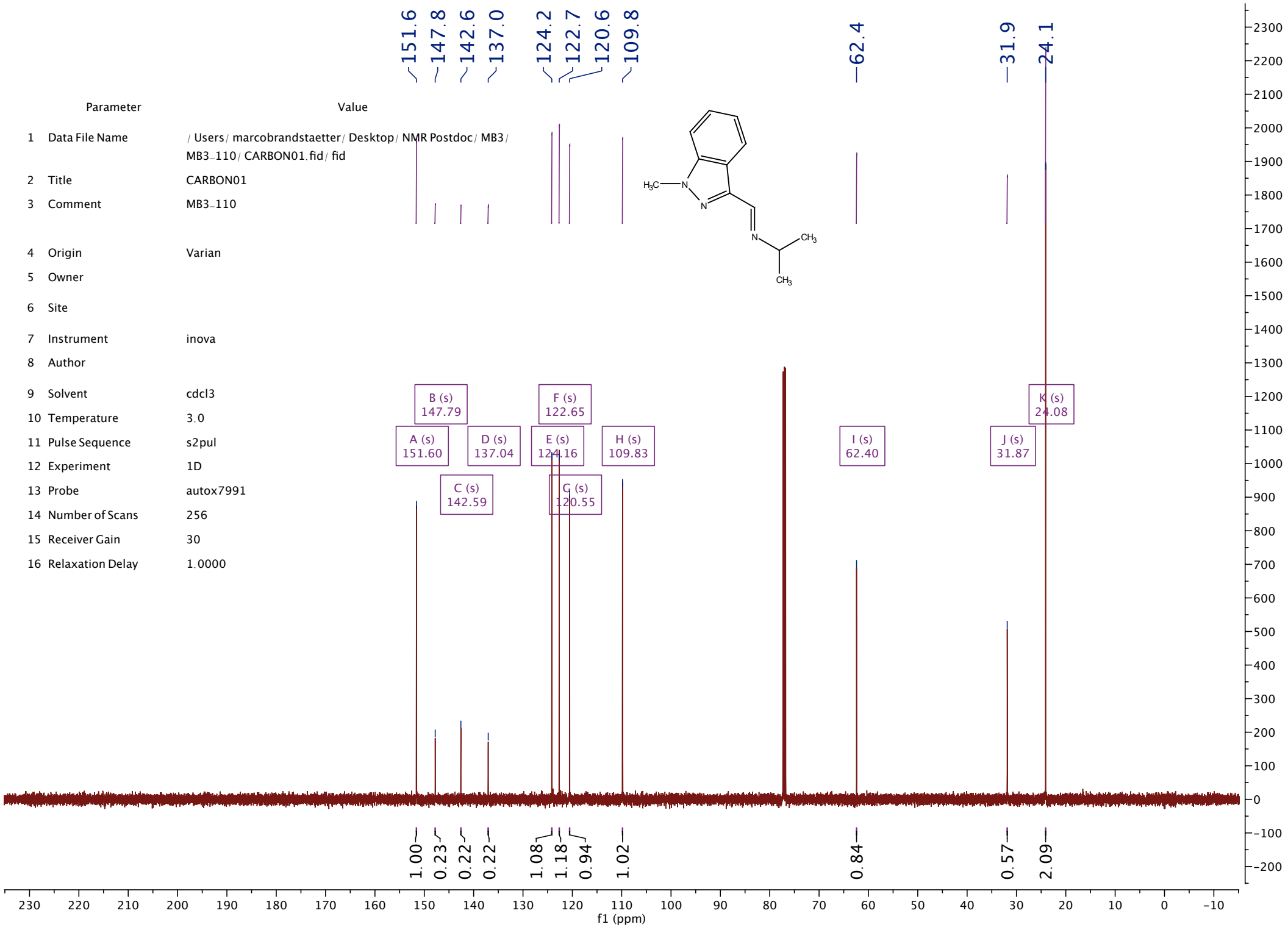
f1 (ppm)


159.5
152.8
148.5
136.2
130.9
129.3
128.3
127.8
127.7
119.5
61.9
24.3
Parameter
Value
1 Data File Name
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_133 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
MB3_133
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
512
15 Receiver Gain
30
16 Relaxation Delay
1.0000
N
N
CH3
CH3
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


159.5
152.8
148.5
136.2
130.9
129.3
128.3
127.8
127.7
119.5
61.9
24.3
Parameter
Value
1 Data File Name
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_133 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
MB3_133
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
512
15 Receiver Gain
30
16 Relaxation Delay
1.0000
N
N
CH3
CH3
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_110 / PROTON03.fid / fid
2	Title	PROTON03
3	Comment	MB3_110
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	46
16	Relaxation Delay	1.0000




151.6
147.8
142.6
137.0
124.2
122.7
120.6
109.8
62.4
31.9
24.1
Parameter
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2 Title
CARBON01
3 Comment
MB3_110
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
B (s) 147.79
F (s) 122.65
K (s) 24.08
A (s) 151.60
D (s) 137.04
E (s) 124.16
H (s) 109.83
I (s) 62.40
J (s) 31.87
C (s) 142.59
G (s) 120.55
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0.22
0.22
1.08
1.18
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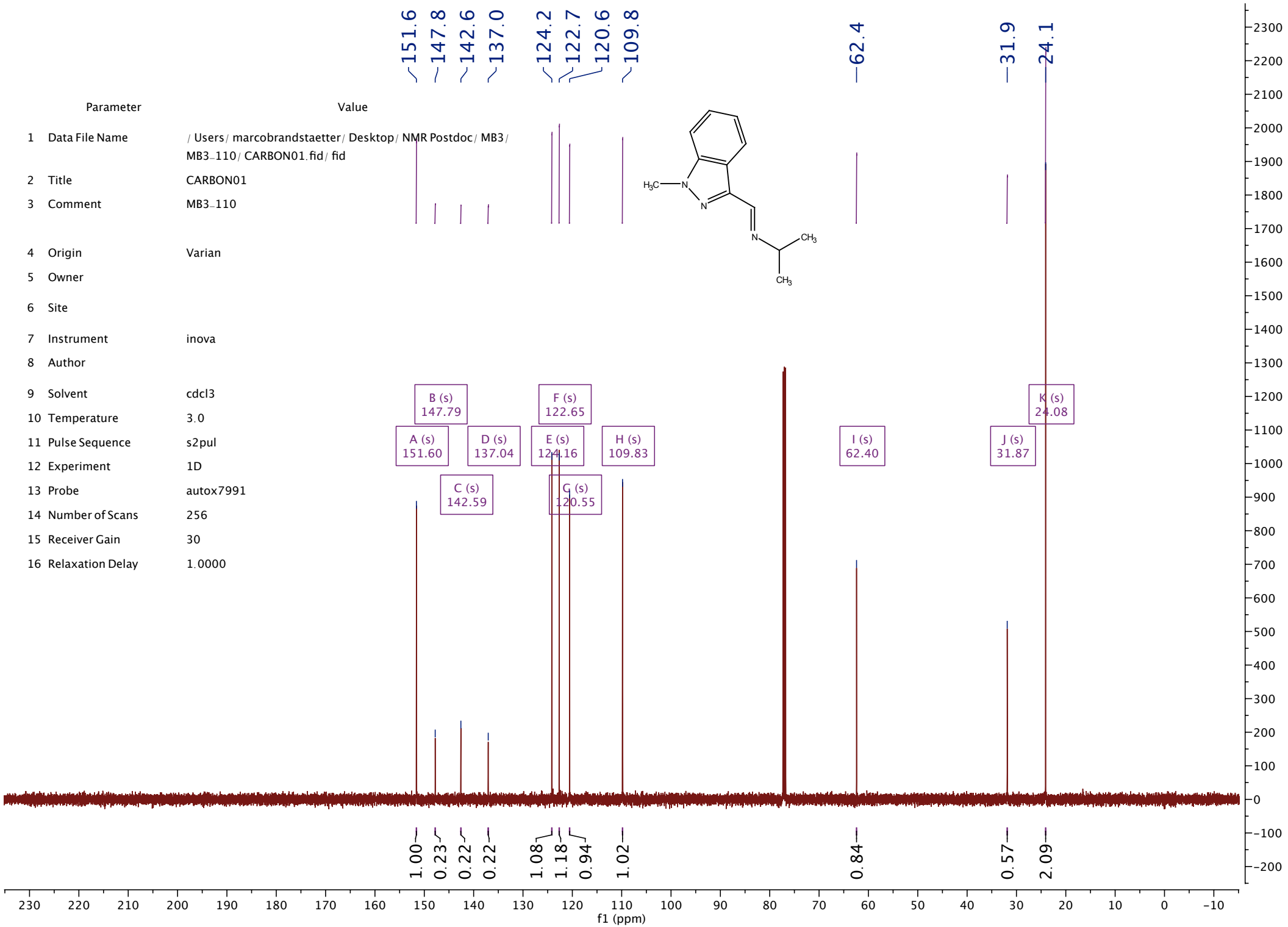
1.02
0.84
0.57
2.09
f1 (ppm)


151.6
147.8
142.6
137.0
124.2
122.7
120.6
109.8
62.4
31.9
24.1
Parameter
Value
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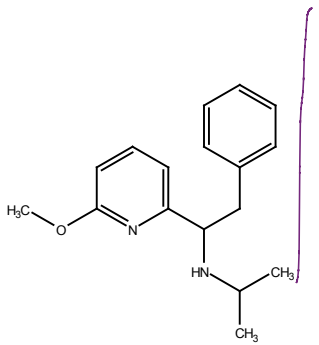
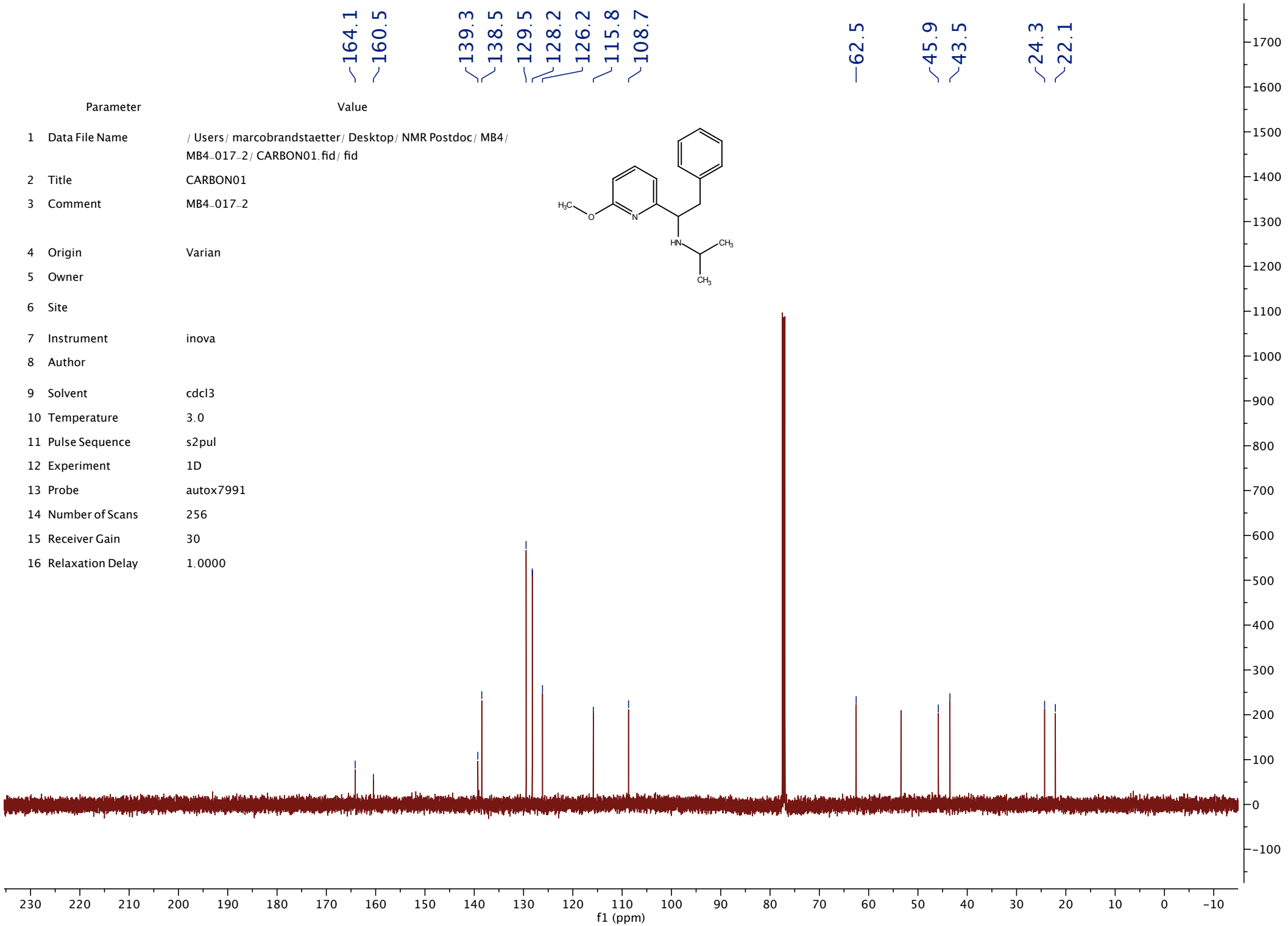
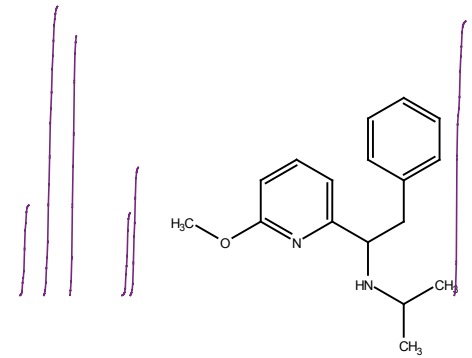
/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB3/ MB3_110/ CARBON01.fid/ fid
2 Title
CARBON01
3 Comment
MB3_110
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
B (s) 147.79
F (s) 122.65
K (s) 24.08
A (s) 151.60
D (s) 137.04
E (s) 124.16
H (s) 109.83
I (s) 62.40
J (s) 31.87
C (s) 142.59
G (s) 120.55
1.00
0.23
0.22
0.22
1.08
1.18
0.94
1.02
0.84
0.57
2.09
f1 (ppm)

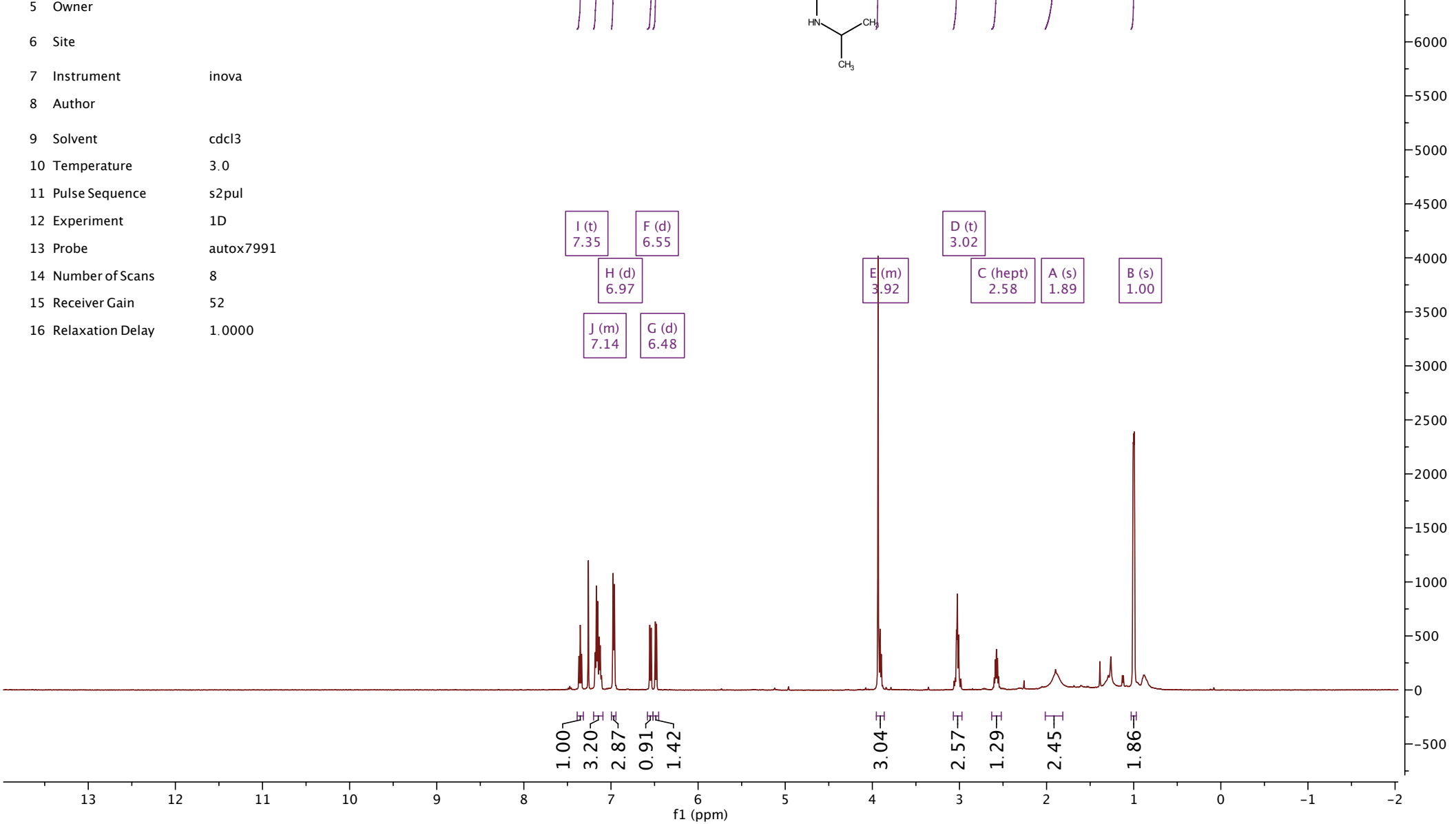
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_017_2 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_017_2
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	52
16	Relaxation Delay	1.0000

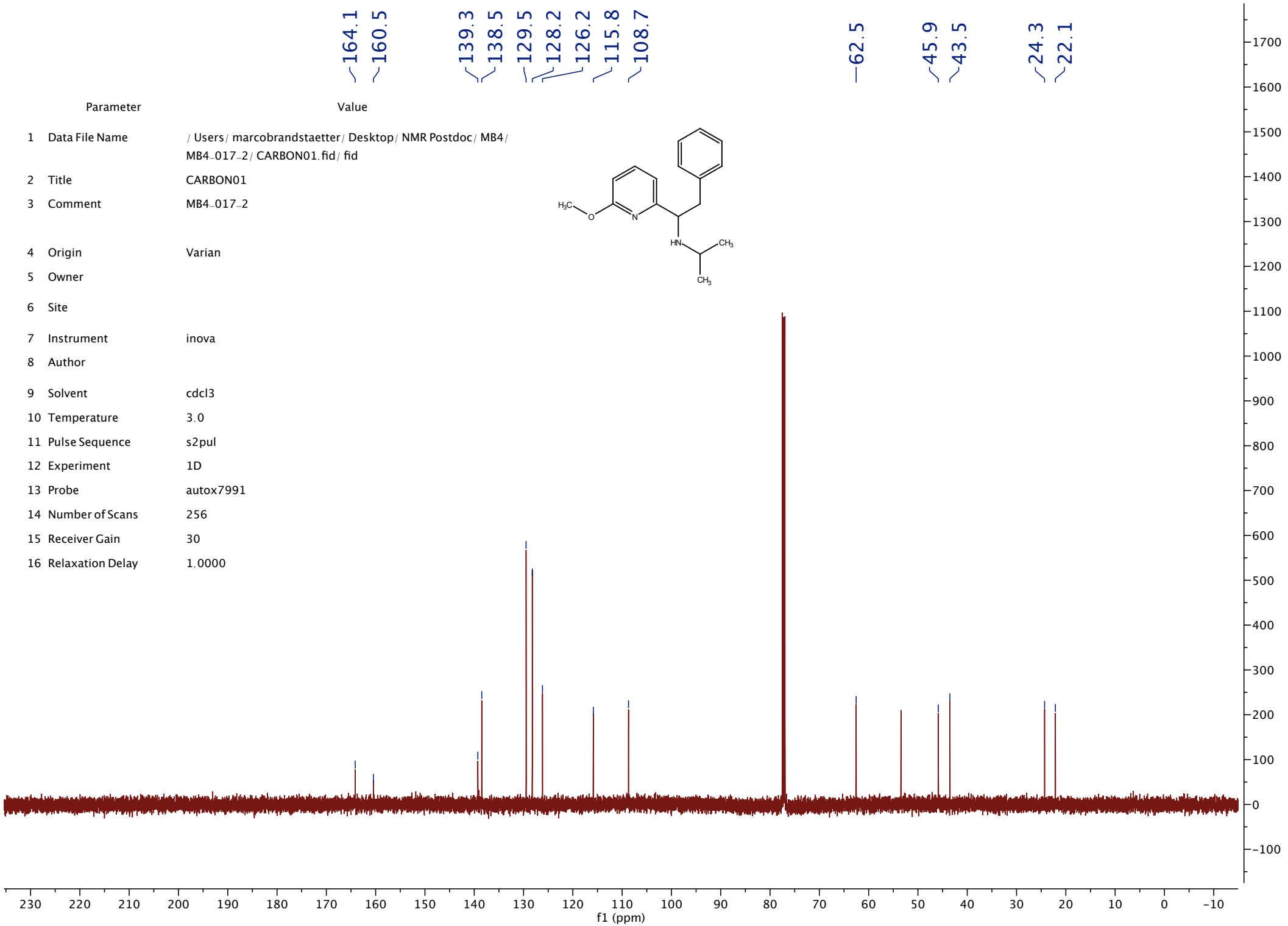



164.1
160.5
139.3
138.5
129.5
128.2
126.2
115.8
108.7
62.5
45.9
43.5
24.3
22.1
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_017_2 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB4_017_2
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
10 Temperature 3.0
11 Pulse Sequence s2pul
12 Experiment 1D
13 Probe autox7991
14 Number of Scans 256
15 Receiver Gain 30
16 Relaxation Delay 1.0000
H3C
O
N
HN
CH3
CH3
f1 (ppm)

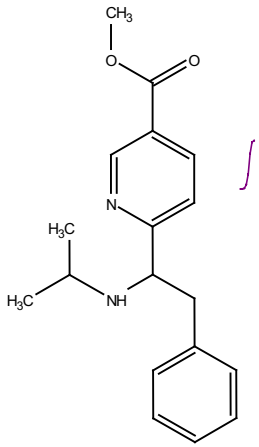
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_017_2 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_017_2
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	52
16	Relaxation Delay	1.0000

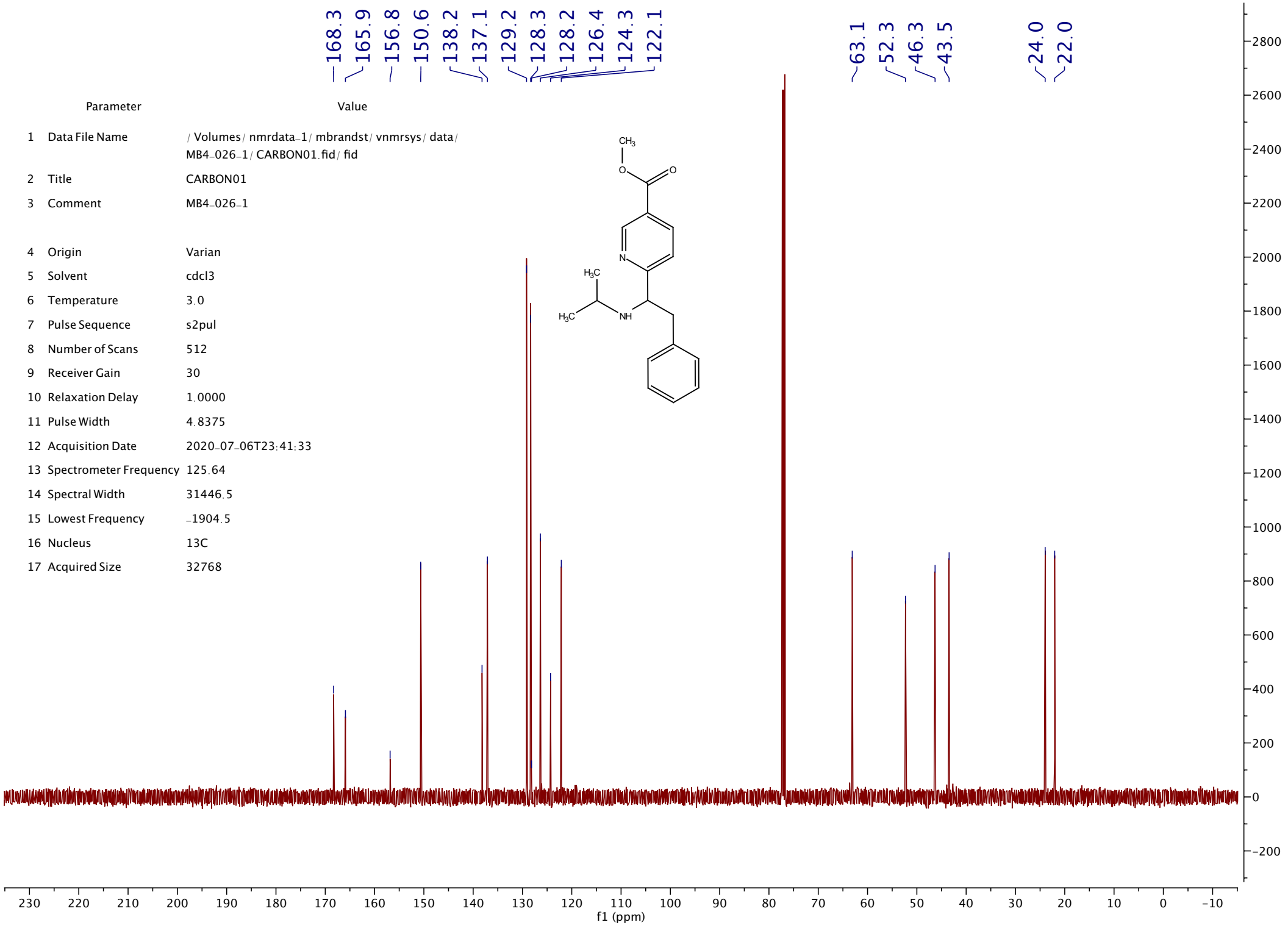





164.1
160.5
139.3
138.5
129.5
128.2
126.2
115.8
108.7
62.5
45.9
43.5
24.3
22.1
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_017_2 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB4_017_2
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
10 Temperature 3.0
11 Pulse Sequence s2pul
12 Experiment 1D
13 Probe autox7991
14 Number of Scans 256
15 Receiver Gain 30
16 Relaxation Delay 1.0000
H3C
O
N
HN
CH3
CH3
f1 (ppm)

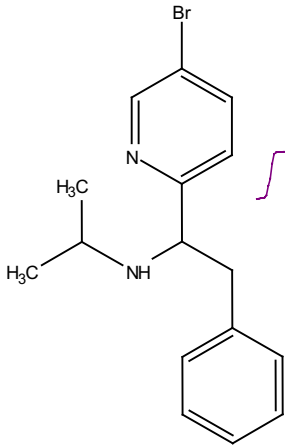
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_026_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_026_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_06T23:40:12
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000

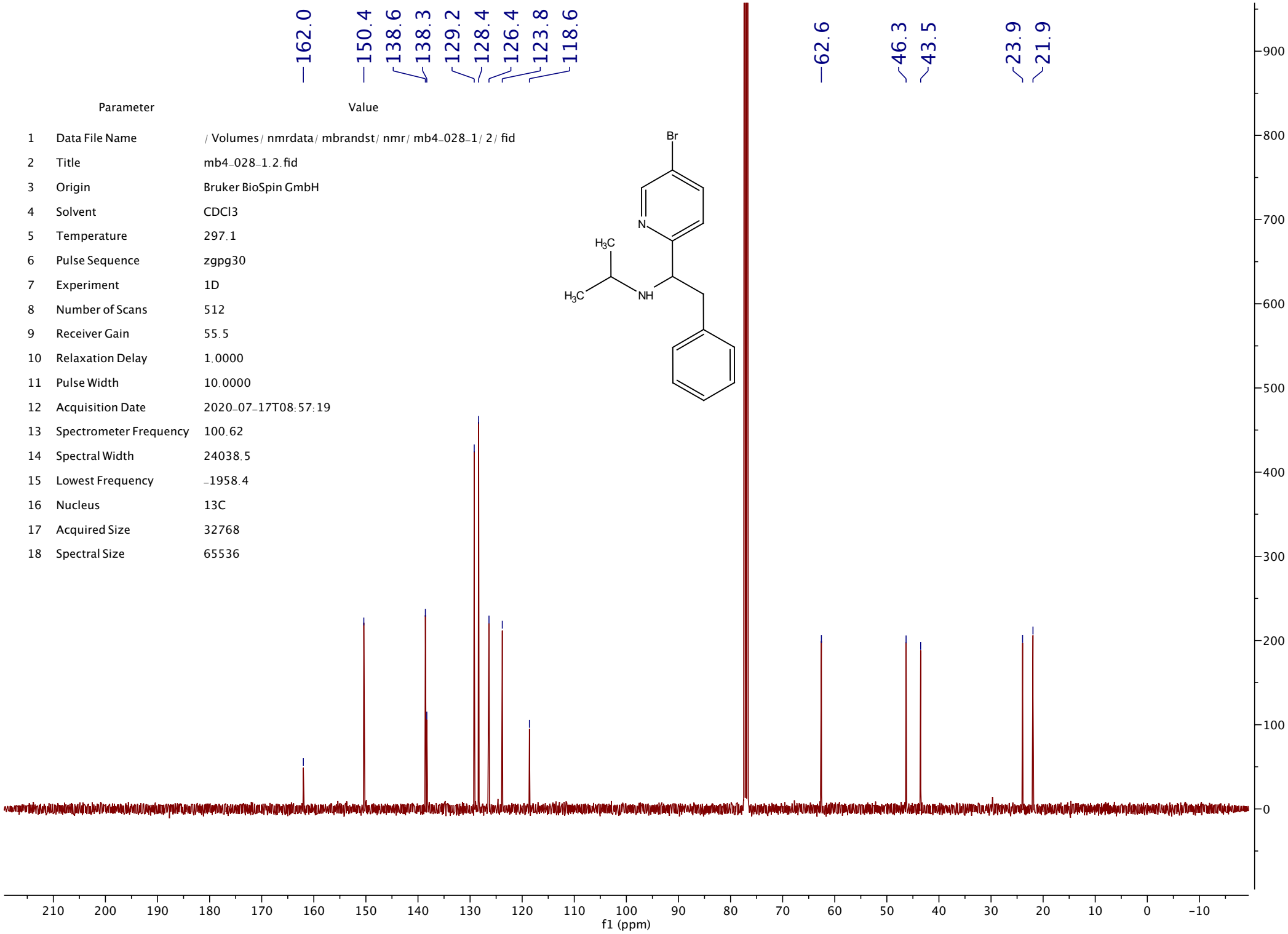




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_026_1 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB4_026_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_06T23:41:33
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

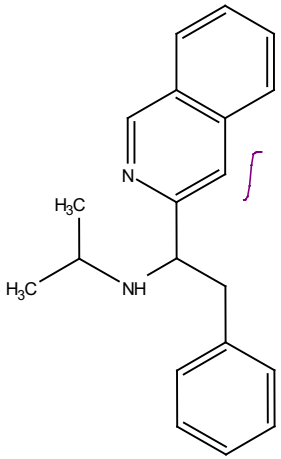
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/mbrandst/nmr/mb4_028_1/1/fid
2	Title	mb4_028_1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2020_07_17T08:36:07
13	Spectrometer Frequency	400.13
14	Spectral Width	11609.9
15	Lowest Frequency	-1640.8
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	131072

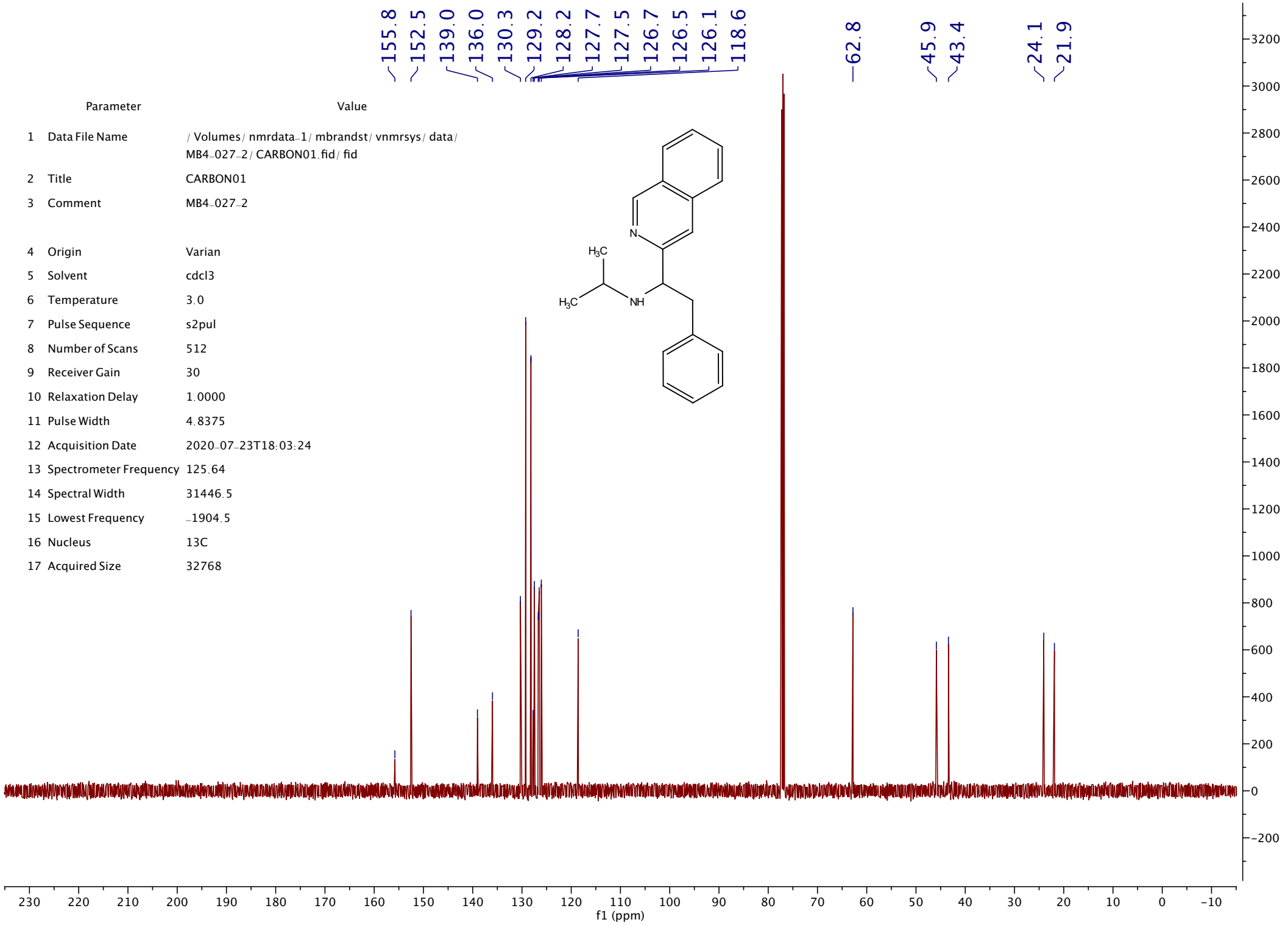




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/mbrandst/nmr/mb4_028_1/2/fid
2	Title	mb4_028_1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	55.5
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_07_17T08:57:19
13	Spectrometer Frequency	100.62
14	Spectral Width	24038.5
15	Lowest Frequency	-1958.4
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_027_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_027_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	54
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_23T18:02:04
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000



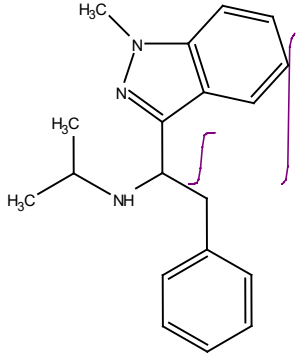


	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_027_2/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_027_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_23T18:03:24
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

PROTON01

MB4_013_1

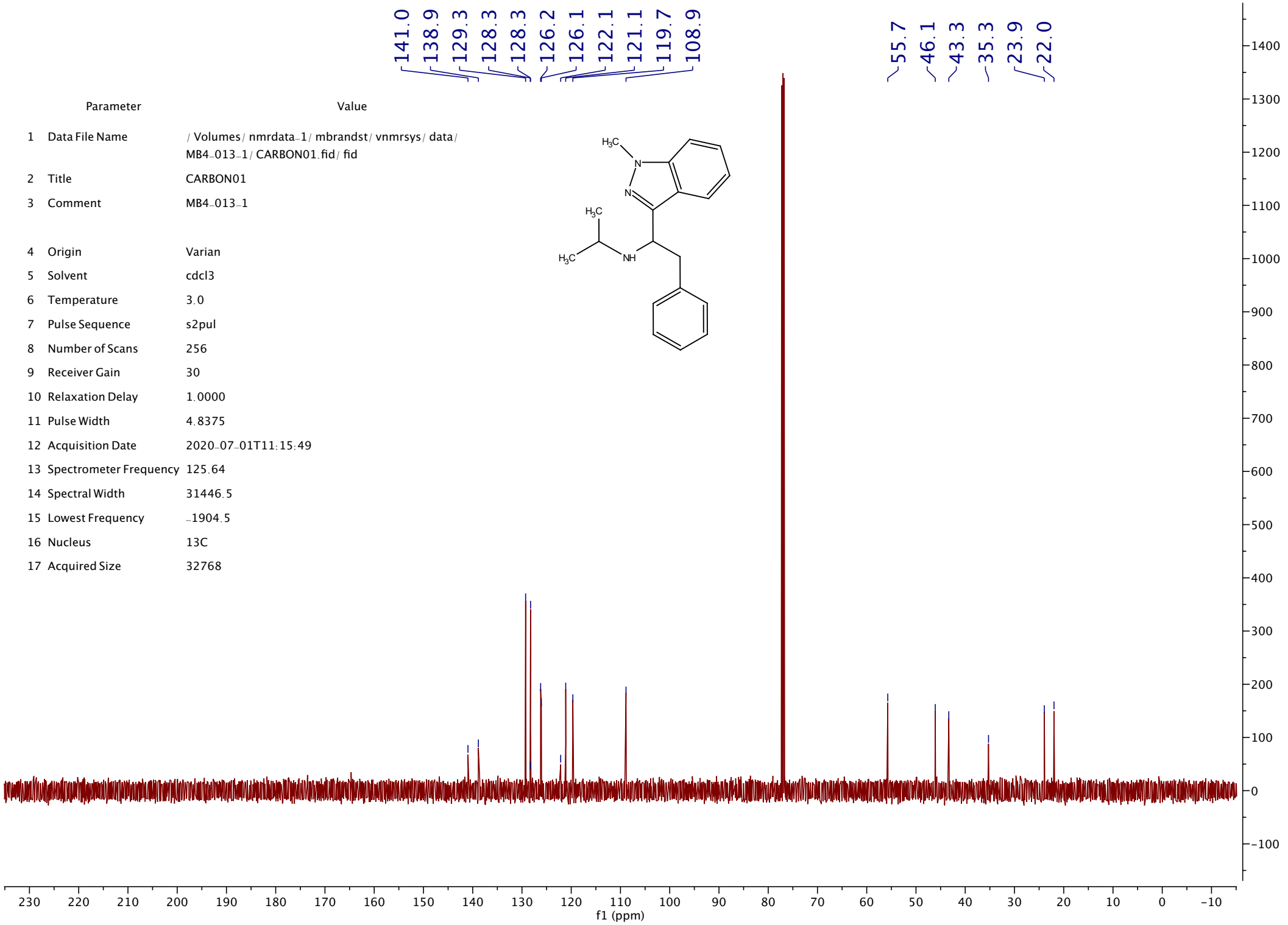
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_013_2 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_013_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	54
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Date	2020_07_23T17:39:44
13	Spectrometer Frequency	499.60
14	Spectral Width	8000.0
15	Lowest Frequency	-1002.4
16	Nucleus	1H
17	Acquired Size	24000



J (ddd) 7.06
H (dd) 7.21
E (d) 7.78
G (m) 7.34
I (m) 7.15
A (t) 4.53
B (s) 4.01
C (m) 3.18
D (hept) 2.68
F (dd) 0.96

0.99 2.09 2.03 3.22 1.22 1.00 2.93 2.00 0.98 5.62

f1 (ppm)



	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_013_1 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB4_013_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_01T11:15:49
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768