Nickel-Catalyzed Reductive Alkylation of Heteroaryl Imines

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Supporting Information

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1. Experimental Details

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 purification unless mentioned otherwise. Tetrahydrofuran (THF) and methylene chloride (CH_2Cl_2) were dried by passing through activated alumina columns. Anhydrous *N*-methylpyrrolidinone (NMP) was purchased from Aldrich and stored in a N_2-filled glovebox. $NiCl_2$·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. 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, $\delta = 7.26$) and $CDCl_3$ (^{13}C, $\delta = 77.0$). $CDCl_3$ for NMR spectra on amine-containing compounds was passed through basic alumina. 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), Field Desorption (FD), or electron impact (EI). Elemental analysis (EA) with ICP-MS on a commercial manganese sample (mentioned above) 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 Resnick High Performance Cluster, a facility supported by the Resnick Sustainability Institute at the California Institute of Technology. Electroanalytical and spectroelectrochemical experiments

were conducted in the Beckman Resource Laser Resource Center at the California Institute of Technology.

2. Optimization of Reaction Parameters (Table 1)

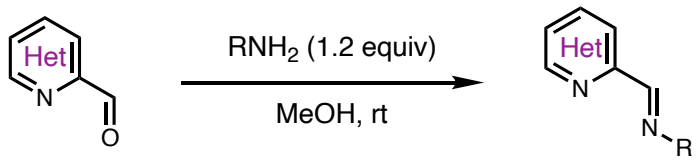
General Procedure: To a 1-dram vial equipped with a stir bar (1.2 cm) was added 2-imino pyridine **1a** (0.3 mmol), benzyl bromide (0.36 mmol, 1.2 equiv), and reductant (Mn^0, 0.3 mmol, 1.0 equiv; Zn^0, 0.6 mmol, 2.0 equiv; TDAE, 0.45 mmol, 1.5 equiv) on the benchtop (or in the glovebox in the case of TDAE following the solvent addition). The vial was brought into a nitrogen-filled glovebox and a stock solution of metal catalyst in NMP (0.75 ml, 0.02 M, 0.05 equiv [M]) and additive (TMSCl, 0.6 mmol, 2.0 equiv; AcOH, 0.3 mmol, 1 equiv; HFIP, 1.5 mmol, 5 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 then further concentrated at 30 °C until most of the NMP was removed and analyzed by ^1H NMR with 1,1,2,2-tetrachloroethane as an internal standard to obtain a quantitative NMR yield.

For electrochemical reaction procedure (Table 1, entry 16-17) see General Procedure 4.

3. Substrate Preparation

3.1. Synthesis of Heteroaryl Imines

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



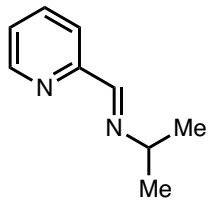
A 1-dram vial equipped with a stir bar was charged with MeOH (0.7 M), heteroaryl aldehyde (1.0 equiv), and primary amine RNH_2 (1.1-1.5 equiv). The resulting solution was stirred at room temperature for 2 hours, followed by concentration in vacuo. The resulting 2-imino-heteroarene was obtained in pure 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.

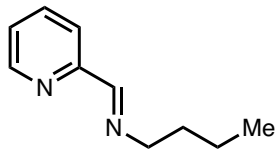
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (d, *J* = 3.1 Hz, 1H), 8.39 (s, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.73 (td, *J* = 7.9, 2.2 Hz, 1H), 7.29 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 3.69 – 3.60 (m, 1H), 1.29 (d, *J* = 6.3 Hz, 6H).

^{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.

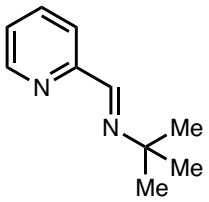
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.64 (d, *J* = 4.8 Hz, 1H), 8.37 (s, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.73 (td, *J* = 7.7, 1.7 Hz, 1H), 7.30 (dd, *J* = 7.5, 4.8 Hz, 1H), 3.68 (t, *J* = 6.8 Hz, 2H), 1.71 (p, *J* = 7.1 Hz, 2H), 1.40 (h, *J* = 7.4 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{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** (326 mg, 2.0 mmol, 95%) was obtained as a yellow oil.

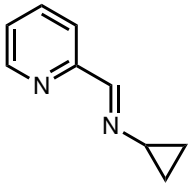
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.66 – 8.58 (m, 1H), 8.35 (s, 1H), 8.01 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.76 – 7.67 (m, 1H), 7.28 (ddd, *J* = 7.5, 4.9, 1.3 Hz, 1H), 1.31 (s, 9H).

^{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.

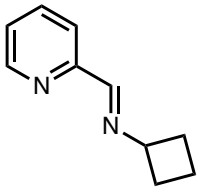
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.88 (d, *J* = 9.0 Hz, 1H), 7.71 (td, *J* = 7.7, 1.7 Hz, 1H), 7.31 – 7.24 (m, 1H), 3.13 (hept, *J* = 6.8, 3.4 Hz, 1H), 1.09 – 1.04 (m, 2H), 1.03 – 0.97 (m, 2H).

^{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.

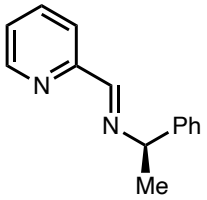
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.6 (d, *J* = 4.8 Hz, 1H), 8.3 (d, *J* = 1.7 Hz, 1H), 8.0 (d, *J* = 7.9 Hz, 1H), 7.7 (td, *J* = 7.7, 1.7 Hz, 1H), 7.3 (dd, *J* = 6.4, 4.8 Hz, 1H), 4.3 – 4.2 (m, 1H), 2.4 – 2.3 (m, 2H), 2.3 – 2.1 (m, 2H), 1.9 – 1.8 (m, 2H).

^{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.

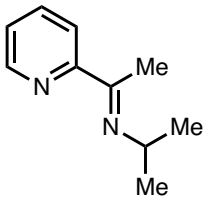
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.64 (ddd, *J* = 4.9, 1.7, 0.9 Hz, 1H), 8.47 (s, 1H), 8.10 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.78 – 7.67 (m, 1H), 7.46 – 7.41 (m, 2H), 7.38 – 7.32 (m, 2H), 7.30 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 7.28 – 7.22 (m, 1H), 4.65 (q, *J* = 6.4 Hz, 1H), 1.61 (d, *J* = 6.7 Hz, 3H).

^{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 with the addition of 3Å molecular sieves (350mg, 2.2 mass equiv) 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.

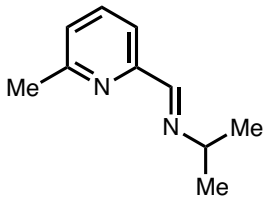
^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.46 (ddd, J = 4.8, 1.8, 1.0 Hz, 1H), 7.98 (dt, J = 8.0, 1.1 Hz, 1H), 7.60 (ddd, J = 8.0, 7.4, 1.8 Hz, 1H), 7.18 (ddd, J = 7.4, 4.8, 1.3 Hz, 1H), 3.83 (hept, J = 6.3 Hz, 1H), 2.25 (s, 3H), 1.11 (d, J = 6.2 Hz, 6H).

^{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.

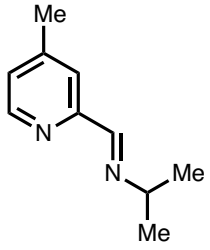
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (s, 1H), 7.81 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 3.62 (hept, *J* = 6.3 Hz, 1H), 2.59 (s, 3H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{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** (224 mg, 1.37 mmol, 83%) was obtained as a yellow oil.

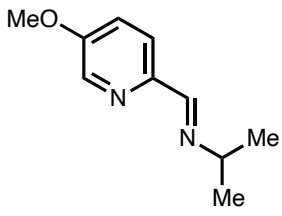
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.48 (d, *J* = 5.0 Hz, 1H), 8.37 (s, 1H), 7.82 (s, 1H), 7.12 (d, *J* = 3.2 Hz, 1H), 3.63 (hept, *J* = 6.3 Hz, 1H), 2.38 (s, 3H), 1.29 (d, *J* = 6.3 Hz, 6H).

^{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.

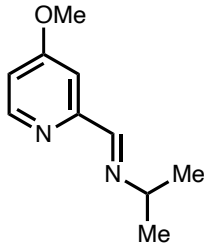
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.34 (s, 1H), 8.30 (d, *J* = 2.9 Hz, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.22 (dd, *J* = 8.7, 2.9 Hz, 1H), 3.89 (s, 3H), 3.60 (hept, *J* = 6.3 Hz, 1H), 1.27 (d, *J* = 6.3 Hz, 6H).

^{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.

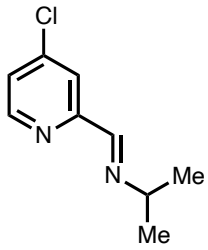
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (d, *J* = 5.8 Hz, 1H), 8.33 (s, 1H), 7.49 (s, 1H), 6.81 (d, *J* = 5.9 Hz, 1H), 3.88 (s, 3H), 3.62 (hept, *J* = 6.5 Hz, 1H), 1.27 (d, *J* = 4.9 Hz, 6H).

^{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 (100.0 mg, 1.70 mmol) following General Procedure 1. After concentration in vacuo, **1l** (224 mg, 1.22 mmol, 87%) was obtained as a yellow oil.

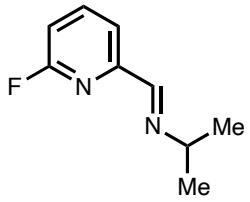
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.51 (d, *J* = 7.0 Hz, 1H), 8.35 (s, 1H), 8.02 (s, 1H), 7.30 (d, *J* = 5.4 Hz, 1H), 3.65 (hept, *J* = 6.2 Hz, 1H), 1.28 (d, *J* = 5.7 Hz, 6H).

^{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 isopropylamine (100.0 mg, 1.70 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).

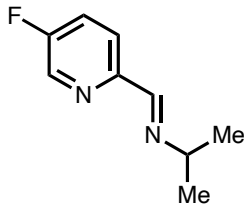
^{13}C NMR (126 MHz, $CDCl_3$): δ 163.4 (d, *J* = 240.1 Hz), 158.0, 153.7 (d, *J* = 12.5 Hz), 141.6 (d, *J* = 7.4 Hz), 118.6 (d, *J* = 4.1 Hz), 110.7 (d, *J* = 36.9 Hz), 61.6, 24.1.

^{19}F NMR (282 MHz, $CDCl_3$) δ -67.84.

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 (100.0 mg, 1.70 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).

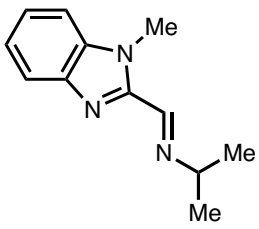
^{13}C NMR (126 MHz, $CDCl_3$): δ 160.2 (d, *J* = 259.2 Hz), 158.0, 151.5 (d, *J* = 3.9 Hz), 137.8 (d, *J* = 24.1 Hz), 123.6 (d, *J* = 18.5 Hz), 122.8 (d, *J* = 5.0 Hz), 61.6, 24.2.

^{19}F NMR (282 MHz, $CDCl_3$) δ -124.70.

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 (88.5 mg, 1.50 mmol) following General Procedure 1. After concentration in vacuo, **1o** (227 mg, 1.13 mmol, 91%) was obtained as a yellow oil.

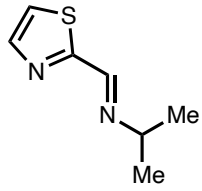
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.53 (s, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.32 (m, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 4.18 (s, 3H), 3.65 – 3.56 (m, 1H), 1.30 (d, *J* = 8.1 Hz, 6H).

^{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.

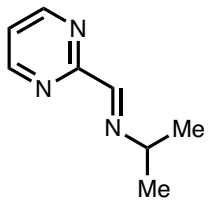
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 (s, 1H), 7.89 (d, *J* = 3.5 Hz, 1H), 7.38 (s, 1H), 3.65 (hept, *J* = 6.4 Hz, 1H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{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.

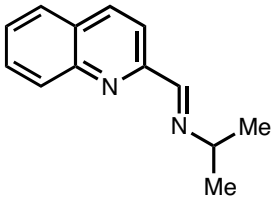
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.84 (d, *J* = 4.9 Hz, 1H), 8.43 (s, 1H), 7.29 (t, *J* = 5.4 Hz, 2H), 3.72 (hept, *J* = 6.4 Hz, 1H), 1.33 (d, *J* = 6.9 Hz, 6H).

^{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.

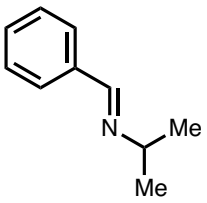
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.17 (s, 2H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.73 (t, *J* = 7.7 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 3.73 (hept, *J* = 6.2 Hz, 1H), 1.33 (d, *J* = 6.4 Hz, 6H).

^{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 $C_{13}H_{15}N_2$ $[M+H]^+$: 199.1235; found 199.1210.

(*E*)-*N*-isopropyl-1-phenylmethanimine (5)



Prepared from benzaldehyde (157 mg, 1.48 mmol) and isopropylamine (105 mg, 1.77 mmol) following General Procedure 1. After concentration in vacuo, **5** (215 mg, 1.46 mmol, 99%) was obtained as a yellow oil.

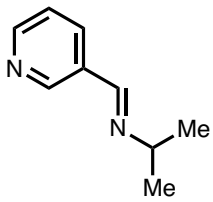
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (s, 1H), 7.77 – 7.69 (m, 2H), 7.40 (t, *J* = 3.9 Hz, 3H), 3.55 (hept, *J* = 6.3 Hz, 1H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{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 $C_{10}H_{14}N$ $[M+H]^+$: 148.1126; found 148.1125

(*E*)-*N*-isopropyl-1-(pyridin-3-yl)methanimine (6)



Prepared from nicotinaldehyde (151 mg, 1.41 mmol) and isopropylamine (91.9 mg, 1.55 mmol) following General Procedure 1. After concentration in vacuo, **6** (199 mg, 1.34 mmol, 95%) was obtained as a yellow oil.

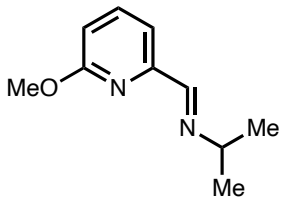
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.62 (d, *J* = 4.7 Hz, 1H), 8.33 (s, 1H), 8.11 (d, *J* = 5.9 Hz, 1H), 7.36 – 7.29 (m, 1H), 3.57 (hept, *J* = 12.6, 6.3 Hz, 1H), 1.27 (d, *J* = 6.4 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 155.6, 151.5, 150.4, 134.6, 132.2, 123.8, 62.0, 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.

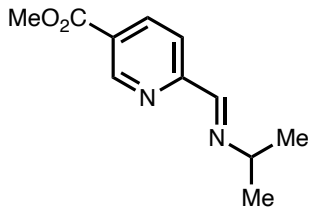
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (s, 1H), 7.64 – 7.56 (m, 2H), 6.75 (dd, *J* = 6.0, 3.0 Hz, 1H), 3.97 (s, 3H), 3.62 (p, *J* = 6.3 Hz, 1H), 1.28 (d, *J* = 6.3 Hz, 6H).

^{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.

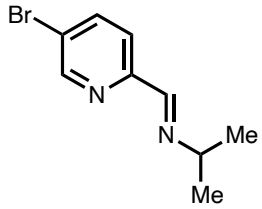
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.22 (s, 1H), 8.43 (s, 1H), 8.32 (d, *J* = 8.2 Hz, 1H), 8.08 (d, *J* = 9.7 Hz, 1H), 3.97 (s, 3H), 3.68 (hept, *J* = 6.4 Hz, 1H), 1.30 (d, *J* = 6.4 Hz, 6H).

^{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.

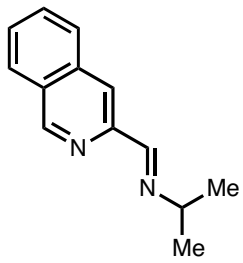
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (dd, J = 2.2, 0.8 Hz, 1H), 8.33 (d, J = 0.7 Hz, 1H), 7.94 – 7.80 (m, 2H), 3.64 (pd, J = 6.3, 0.8 Hz, 1H), 1.27 (d, J = 6.3 Hz, 6H).

^{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.

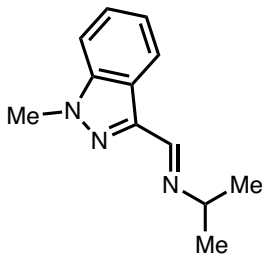
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.28 (s, 1H), 8.57 (s, 1H), 8.26 (s, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 8.3 Hz, 1H), 3.69 (hept, *J* = 5.9 Hz, 1H), 1.34 (d, *J* = 4.8 Hz, 6H).

^{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 $C_{13}H_{15}N_2$ $[M+H]^+$: 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.

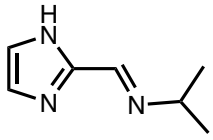
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (d, *J* = 0.8 Hz, 1H), 8.39 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.47 – 7.34 (m, 2H), 7.28 – 7.20 (m, 1H), 4.10 (s, 3H), 3.66 – 3.51 (m, 1H), 1.31 (d, *J* = 6.3 Hz, 6H).

^{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.

(*E*)-1-(1H-imidazol-2-yl)-N-isopropylmethanimine (S1f)



Prepared from 1*H*-imidazole-2-carbaldehyde (1.44 g, 15 mmol) and isopropylamine (1.11 g, 18.8 mmol) following General Procedure 1. After concentration in vacuo, **S1f** (1.87 g, 13.7 mmol, 91%) was obtained as a brown solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (d, *J* = 0.7 Hz, 1H), 7.13 (d, *J* = 1.2 Hz, 1H), 7.06 – 6.98 (m, 1H), 3.52 (pd, *J* = 6.3, 0.8 Hz, 1H), 1.16 (d, *J* = 6.3 Hz, 6H).

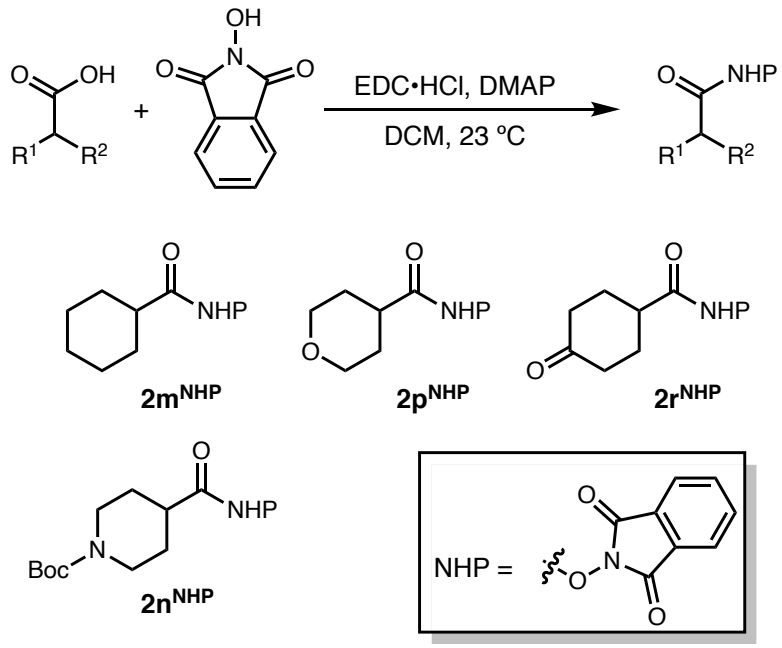
^{13}C NMR (126 MHz, $CDCl_3$): δ 149.15, 145.18, 130.58, 117.59, 60.88, 24.00.

FTIR (NaCl, thin film, cm^{-1}): 2963, 1646, 1558, 1446, 1387, 1108, 998, 755, 683.

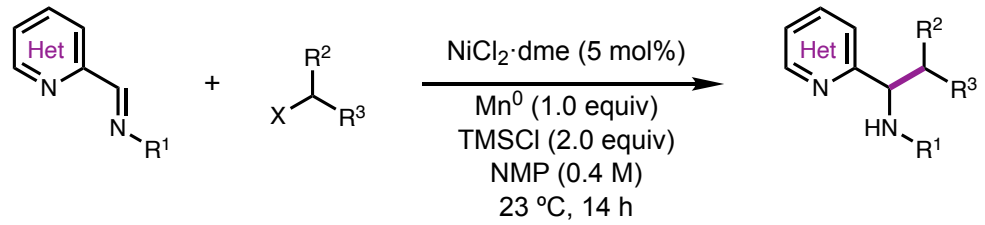
HRMS (ESI, m/z): calc'd for $C_{17}H_{12}N_3$ $[M+H]^+$: 138.1026; found 138.026.

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

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



4. Nickel-Catalyzed Alkylation of Heteroaryl Imines



4.1. 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. The crude material was purified by column chromatography to afford the desired product.

4.2. Challenging Substrates

Substrates here are not featured in the main text and undergo alkylation under the optimized conditions in poor yields. Products **S3a-S3f** were prepared from imines **S1a-S1f** 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.

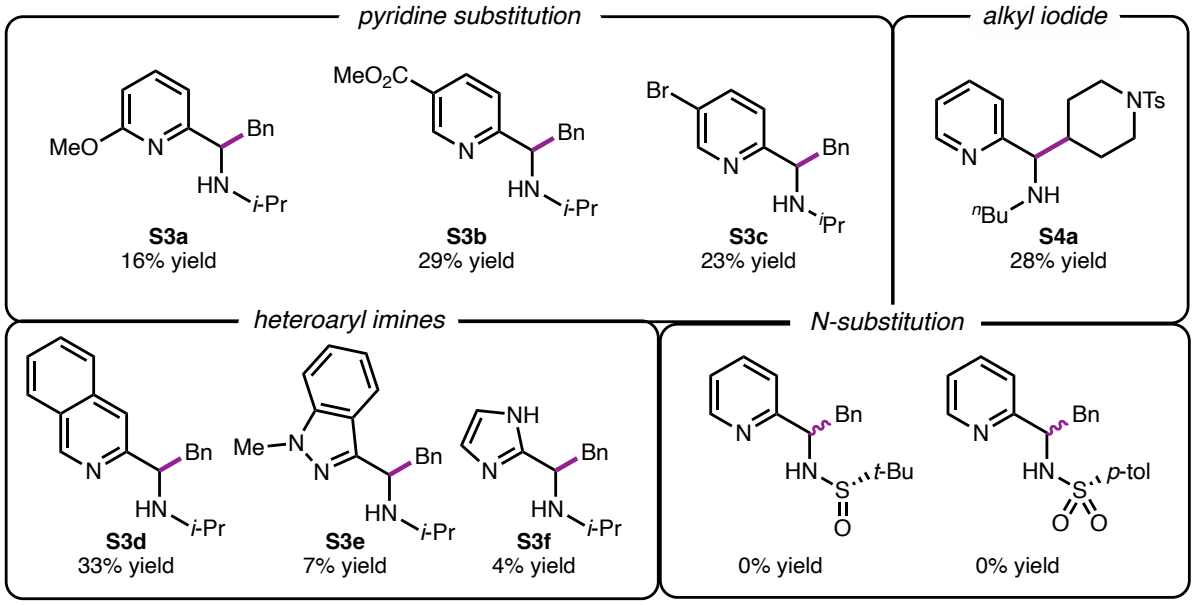


Figure S1: Imine and halide coupling partners that did not perform well in the alkylation reaction.

4.3. Product Distribution for Reactions with 1a and Alkyl Halides

General Details: All reaction were carried out according to General Procedure 3 on a 0.3 mmol scale. Yields determined from quantitative ^{1}H NMR measurements against 1,3,5-trimeoxybenzene or 1,1,2,2-tetrachloroethane. Yields of **1a**' are reported out of 0.15 mmol theoretical yield of **1a'**.

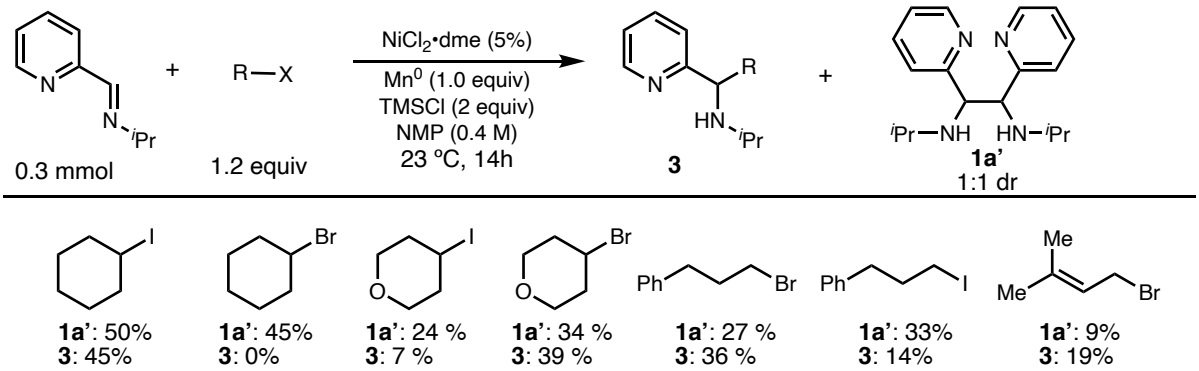
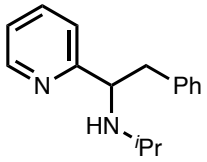


Figure S2: Distribution of desired alkylation versus homocoupling across several alkyl electrophiles. In all cases **1a'** was produced in 1:1 dr determined by ^{1}H NMR. Yields of **1a'** are based on a 0.15 mmol theoretical yield.

4.4. 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).

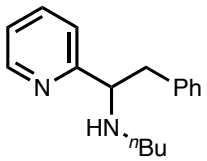
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.58 (d, *J* = 4.7 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 7.3 Hz, 2H), 7.18 – 7.08 (m, 2H), 7.05 (dd, *J* = 17.7, 7.6 Hz, 3H), 4.06 (t, *J* = 7.2 Hz, 1H), 3.04 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.98 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.57 (hept, *J* = 6.3 Hz, 1H), 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, 72%) 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 (d, *J* = 7.4 Hz, 1H), 3.07

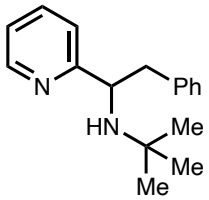
(dd, *J* = 13.3, 6.5 Hz, 1H), 2.95 (dd, *J* = 13.3, 7.8 Hz, 1H), 2.45 – 2.32 (m, 2H), 1.83 (s, 1H), 1.42 – 1.32 (m, 2H), 1.27 – 1.14 (m, 2H), 0.81 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3, 149.5, 139.0, 136.4, 129.5, 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).

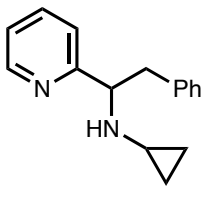
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (d, *J* = 4.8 Hz, 1H), 7.58 (td, *J* = 7.6, 1.8 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.31 – 7.24 (m, 2H), 7.25 – 7.18 (m, 1H), 7.17 (d, *J* = 6.9 Hz, 2H), 7.12 (dd, *J* = 6.3, 4.9 Hz, 1H), 4.13 (dd, *J* = 8.9, 5.7 Hz, 1H), 3.06 (dd, *J* = 13.3, 5.7 Hz, 1H), 2.76 (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).

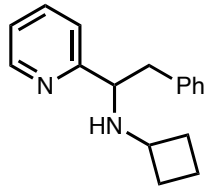
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.60 (d, *J* = 5.0 Hz, 1H), 7.52 (td, *J* = 7.6, 1.8 Hz, 1H), 7.19 (t, *J* = 7.2 Hz, 2H), 7.17 – 7.10 (m, 2H), 7.06 – 7.00 (m, 3H), 4.05 (t, *J* = 7.2 Hz, 1H), 3.10 – 2.97 (m, 2H), 2.20 (s, 1H), 1.96 – 1.88 (m, 1H), 0.35 – 0.25 (m, 3H), 0.25 – 0.19 (m, 1H).

^{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).

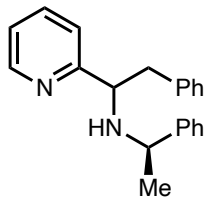
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.57 (d, *J* = 3.4 Hz, 1H), 7.55 (td, *J* = 7.7, 1.8 Hz, 1H), 7.23 (t, *J* = 7.3 Hz, 2H), 7.20 – 7.10 (m, 3H), 7.09 (d, *J* = 7.0 Hz, 2H), 3.95 (dt, *J* = 1627.0, 7.3 Hz, 1H), 3.12 – 3.02 (m, 2H), 2.93 (dd, *J* = 13.3, 8.0 Hz, 1H), 2.15 – 2.07 (m, 1H), 2.02 (s, 1H), 1.91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

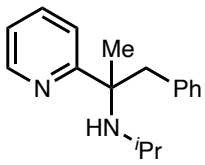
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.66 (d, *J* = 6.5 Hz, 1H, *minor*), 8.59 (d, *J* = 4.9 Hz, 1H, *major*), 7.57 (td, *J* = 7.6, 1.8 Hz, 1H, *minor*), 7.46 (td, *J* = 7.6, 1.8 Hz, 1H, *major*), 7.28 – 7.16 (m, 17H), 7.11 (dd, *J* = 7.6, 4.8 Hz, 1H, *major*), 7.01 (q, *J* = 9.9, 8.7 Hz, 5H, *major*), 6.93 (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).

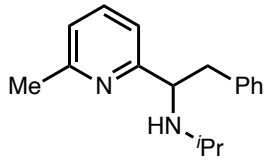
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.65 (d, *J* = 4.7 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.15 – 7.09 (m, 1H), 7.06 (dt, *J* = 14.6, 7.6 Hz, 4H), 6.65 (d, *J* = 6.9 Hz, 2H), 3.17 (d, *J* = 12.7 Hz, 1H), 2.95 (d, *J* = 12.7 Hz, 1H), 2.66 (hept, *J* = 6.4 Hz, 1H), 1.50 (s, 3H), 1.08 (d, *J* = 6.1 Hz, 3H), 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).

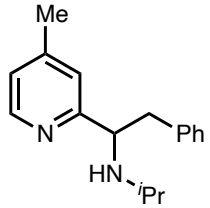
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.18 (m, 2H), 7.17 – 7.13 (m, 1H), 7.08 – 7.02 (m, 2H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 4.05 (t, *J* = 7.1 Hz, 1H), 3.06 (dd, *J* = 13.3, 7.0 Hz, 1H), 2.96 (dd, *J* = 13.6, 7.2 Hz, 1H), 2.63 – 2.57 (m, 1H), 2.56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

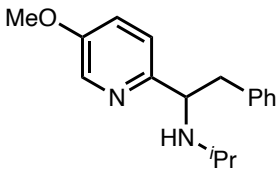
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (d, *J* = 5.0 Hz, 1H), 7.20 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.05 (d, *J* = 7.1 Hz, 2H), 6.94 (d, *J* = 5.1 Hz, 1H), 6.91 (s, 1H), 4.02 (t, *J* = 7.2 Hz, 1H), 3.04 (dd, *J* = 13.3, 7.0 Hz, 1H), 2.94 (dd, *J* = 13.3, 7.4 Hz, 1H), 2.57 (p, *J* = 6.2 Hz, 1H), 2.26 (s, 3H), 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).

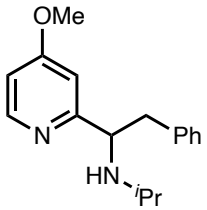
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (d, *J* = 2.9 Hz, 1H), 7.23 – 7.16 (m, 2H), 7.17 – 7.11 (m, 1H), 7.07 – 7.00 (m, 3H), 6.97 (d, *J* = 8.5 Hz, 1H), 4.02 (t, *J* = 7.2 Hz, 1H), 3.84 (s, 3H), 3.05 – 2.93 (m, 2H), 2.55 (hept, *J* = 6.2 Hz, 1H), 1.83 (s, 1H), 0.95 (dd, *J* = 6.2, 2.6 Hz, 6H).

^{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).

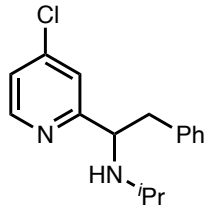
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 – 8.36 (m, 1H), 7.24 – 7.18 (m, 2H), 7.18 – 7.12 (m, 1H), 7.07 (d, *J* = 7.0 Hz, 2H), 6.68 – 6.62 (m, 2H), 4.01 (t, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 3.04 (dd, *J* = 13.3, 6.9 Hz, 1H), 2.92 (dd, *J* = 13.3, 7.5 Hz, 1H), 2.57 (hept, *J* = 6.2 Hz, 1H), 1.92 (s, 1H),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

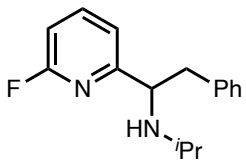
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.46 (d, *J* = 5.3 Hz, 1H), 7.26 – 7.16 (m, 4H), 7.14 (dd, *J* = 5.3, 2.0 Hz, 1H), 7.09 – 7.04 (m, 2H), 4.09 – 4.02 (m, 1H), 3.04 (dd, *J* = 13.4, 6.6 Hz, 1H), 2.90 (dd, *J* = 13.4, 7.7 Hz, 1H), 2.55 (hept, *J* = 6.3 Hz, 1H), 1.71 (s, 1H), 0.94 (dd, *J* = 10.9, 6.2 Hz,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

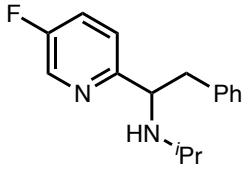
^{13}C NMR (126 MHz, $CDCl_3$): δ 163.8 (d, *J* = 216.9 Hz), 162.8 (d, *J* = 10.6 Hz), 141.1 (d, *J* = 7.7 Hz), 138.6, 129.4, 128.5, 126.5, 120.0 (d, *J* = 3.9 Hz), 107.6 (d, *J* = 37.1 Hz), 62.5, 46.2, 43.4, 24.2, 22.1.

^{19}F NMR (282 MHz, $CDCl_3$): δ -67.71.

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).

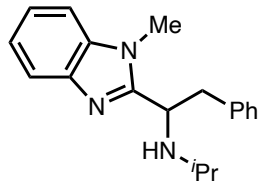
^{13}C NMR (126 MHz, $CDCl_3$): δ 159.48 (d, *J* = 3.7 Hz), 158.5 (d, *J* = 254 Hz), 157.5, 138.7, 137.6 (d, *J* = 23.5 Hz), 129.4, 128.5, 126.5, 123.4 (d, *J* = 3.9 Hz), 122.9 (d, *J* = 17.8 Hz), 62.6, 46.3, 43.9, 24.2, 22.2.

^{19}F NMR (282 MHz, $CDCl_3$): δ -130.02.

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).

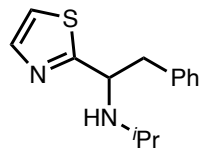
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.5 Hz, 1H), 7.32 – 7.13 (m, 6H), 6.98 (d, *J* = 4.6 Hz, 2H), 4.30 (dd, *J* = 9.1, 5.9 Hz, 1H), 3.33 (dd, *J* = 12.9, 5.7 Hz, 1H), 3.27 (s, 3H), 3.19 – 3.11 (m, 1H), 2.72 (hept, *J* = 6.0 Hz, 1H), 2.20 (s, 1H), 1.04 (dd, *J* = 14.3, 6.2 Hz, 6H).

^{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).

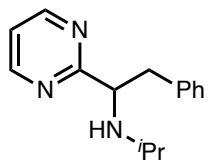
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.76 (d, *J* = 3.3 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.28 – 7.23 (m, 2H), 7.23 – 7.19 (m, 2H), 4.41 (dd, *J* = 9.0, 5.1 Hz, 1H), 3.28 (dd, *J* = 13.6, 5.1 Hz, 1H), 2.91 (dd, *J* = 13.6, 9.0 Hz, 1H), 2.71 (hept, *J* = 6.3 Hz, 1H), 1.64 (s, 1H), 1.01 (d, *J* = 6.4 Hz, 3H),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

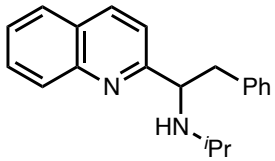
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (d, *J* = 6.7 Hz, 2H), 7.20 – 7.07 (m, 4H), 7.01 (d, *J* = 7.2 Hz, 2H), 4.27 (t, *J* = 7.2 Hz, 2H), 3.15 (dd, *J* = 13.4, 6.6 Hz, 1H), 3.06 (dd, *J* = 13.4, 7.7 Hz, 1H), 2.58 (hept, *J* = 6.1 Hz, 1H), 1.94 (s, 1H), 1.01 (d, *J* = 6.2 Hz, 3H), 0.96 (d, *J* = 6.2 Hz,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

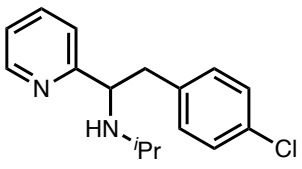
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.25 – 7.11 (m, 5H), 4.31 (t, *J* = 7.2 Hz, 1H), 3.15 (dd, *J* = 13.5, 6.4 Hz, 1H), 3.00 (dd, *J* =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

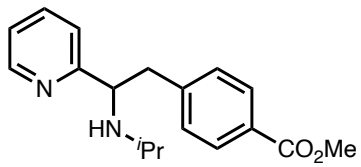
^{1}H NMR (400 MHz, $CDCl_3$): 8.50 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.44 (td, J = 7.6, 1.8 Hz, 1H), 7.11 – 7.01 (m, 3H), 6.95 (dt, J = 7.8, 1.1 Hz, 1H), 6.89 – 6.83 (m, 2H), 3.93 (t, J = 7.2 Hz, 1H), 2.90 (dd, J = 7.2, 1.6 Hz, 2H), 2.48 (p, J = 6.3 Hz, 1H), 1.84 (s, 1H), 0.88 (dd, J = 6.2, 1.3 Hz, 6H).

^{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).

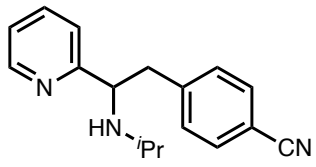
^{1}H NMR (400 MHz, $CDCl_3$): 8.48 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.88 – 7.66 (m, 2H), 7.39 (td, J = 7.6, 1.8 Hz, 1H), 7.09 – 6.93 (m, 3H), 6.89 (dt, J = 7.8, 1.1 Hz, 1H), 3.95 (t, J = 7.2 Hz, 1H), 3.77 (s, 3H), 2.96 (d, J = 7.2 Hz, 2H), 2.46 (p, J = 6.2 Hz, 1H), 1.86 (s, 2H), 0.85 (d, J = 6.3 Hz,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

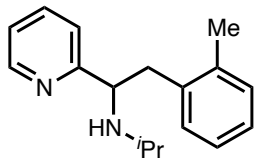
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.67 – 8.51 (m, 1H), 7.52 (td, *J* = 7.6, 1.8 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.14 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 7.7 Hz, 1H), 4.02 (t, *J* = 7.2 Hz, 1H), 3.15 – 2.95 (m, 2H), 2.56 (hept, *J* = 6.1 Hz, 1H), 1.26 (d, *J* = 3.1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

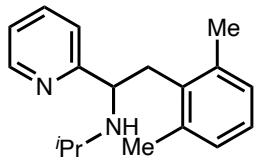
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.35 (td, *J* = 7.6, 1.8 Hz, 1H), 7.02 – 6.92 (m, 3H), 6.92 – 6.86 (m, 1H), 6.83 (dt, *J* = 7.8, 1.1 Hz, 1H), 6.81 – 6.76 (m, 1H), 3.93 (dd, *J* = 8.0, 6.5 Hz, 1H), 3.04 – 2.77 (m, 2H), 2.46 (p, *J* = 6.2 Hz, 1H), 2.08 (s, 3H),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

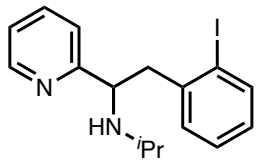
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.40 (td, *J* = 7.6, 1.8 Hz, 1H), 7.09 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 6.94 (dd, *J* = 8.3, 6.5 Hz, 1H), 6.88 (d, *J* = 7.4 Hz, 2H), 6.69 (dt, *J* = 7.7, 1.1 Hz, 1H), 3.95 (dd, *J* = 9.2, 5.3 Hz, 1H), 3.10 (dd, *J* = 13.4, 5.3 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.

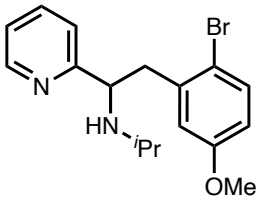
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.62 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.79 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.47 (td, *J* = 7.6, 1.8 Hz, 1H), 7.13 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 7.07 (td, *J* = 7.4, 1.3 Hz, 1H), 6.93 (dt, *J* = 7.7, 1.1 Hz, 1H), 6.83 (td, *J* = 7.6, 1.7 Hz, 1H), 6.78 (dd, *J* = 7.6,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

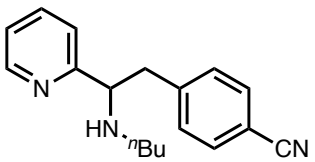
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.41 (td, *J* = 7.6, 1.8 Hz, 1H), 7.29 (d, *J* = 8.7 Hz, 1H), 7.05 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 6.88 (dt, *J* = 7.7, 1.1 Hz, 1H), 6.50 (dd, *J* = 8.8, 3.1 Hz, 1H), 6.27 (d, *J* = 3.1 Hz, 1H), 4.10 (dd, *J* = 8.4, 6.3 Hz, 1H), 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).

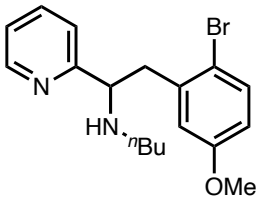
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 – 8.50 (m, 1H), 7.53 (td, J = 7.6, 1.8 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.13 (ddd, J = 7.7, 4.9, 1.2 Hz, 3H), 7.02 (dt, J = 7.8, 1.1 Hz, 1H), 3.90 (t, J = 7.1 Hz, 1H), 3.07 (d, J = 7.1 Hz, 2H), 2.50 – 2.30 (m, 2H), 2.00 – 1.77 (m, 2H), 1.43 – 1.31 (m, 2H), 1.27 – 1.15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

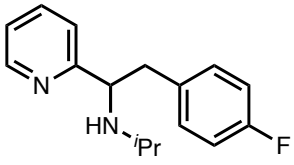
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.52 (td, J = 7.6, 1.8 Hz, 1H), 7.37 (d, J = 8.8 Hz, 1H), 7.13 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 7.05 (dt, J = 7.7, 1.1 Hz, 1H), 6.58 (dd, J = 8.8, 3.1 Hz, 1H), 6.45 (d, J = 3.1 Hz, 1H), 4.05 (t, J = 7.2 Hz, 1H), 3.62 (s, 3H), 3.21 (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).

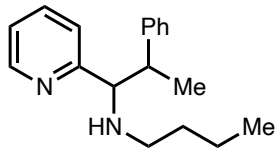
^{13}C NMR (101 MHz, $CDCl_3$): δ 163.00, 160.24, 149.44, 136.02, 134.47, 130.64, 122.65, 121.97, 115.07, 114.86, 63.02, 45.98, 42.76, 24.02, 22.03.

^{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*).

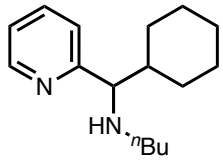
^{13}C NMR (126 MHz, $CDCl_3$): δ 163.22 (*major)*, 162.71 (*minor)*, 149.15 (*minor)*, 149.02 (*major)*, 144.65 (*major)*, 144.52 (*minor)*, 136.35 (*major)*, 135.54 (*minor)*, 128.71 (*major)*, 128.11 (*minor)*, 127.94 (*minor)*, 127.83 (*major)*, 126.74 (*major)*, 126.15 (*minor)*, 123.13 (*minor)*, 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).

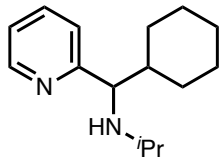
^{1}H NMR (400 MHz, $CDCl_3$):δ 8.54 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.59 (td, J = 7.6, 1.8 Hz, 1H), 7.22 (dt, J = 7.8, 1.1 Hz, 1H), 7.11 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.42 (d, J = 6.9 Hz, 1H), 2.42 – 2.23 (m, 2H), 1.91 (ddq, J = 12.3, 4.0, 2.1 Hz, 2H), 1.83 (d, J = 7.5 Hz, 1H), 1.74 – 1.53 (m, 2H), 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*-(cyclohexyl(pyridin-2-yl)methyl)propan-2-amine (4m)**



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 **4m** (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).

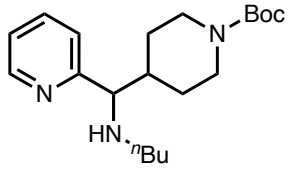
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.73 (td, J = 7.6, 1.8 Hz, 1H), 7.35 (dt, J = 7.8, 1.1 Hz, 1H), 7.25 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.66 (d, J = 6.8 Hz, 1H), 2.60 (hept, J = 6.2 Hz, 1H), 2.08 (dtt, J = 12.1, 3.6, 1.7 Hz, 1H), 1.95 – 1.82 (m, 3H), 1.75 (dddd, J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

***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).

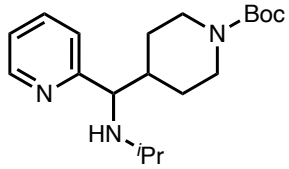
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.60 (td, J = 7.6, 1.8 Hz, 1H), 7.21 – 7.09 (m, 2H), 4.04 (d, J = 38.7 Hz, 2H), 3.39 (d, J = 7.4 Hz, 1H), 2.59 (dt, J = 25.7, 11.8 Hz, 2H), 2.40 – 2.25 (m, 2H), 2.03 – 1.86 (m, 1H), 1.77 (ddt, J = 19.0, 11.3, 3.1 Hz, 3H), 1.41 (s,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

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



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 **4o** (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).

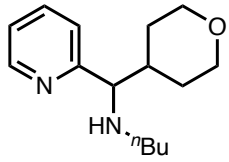
^{1}H NMR (400 MHz, $CDCl_3$): δ δ 8.56 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.59 (td, J = 7.6, 1.8 Hz, 1H), 7.21 – 7.01 (m, 2H), 4.04 (d, J = 37.9 Hz, 2H), 3.46 (d, J = 7.4 Hz, 1H), 2.71 – 2.49 (m, 2H), 2.44 (p, J = 6.2 Hz, 1H), 2.02 – 1.91 (m, 2H), 1.73 (tdt, J = 11.3, 7.4, 3.7 Hz, 1H), 1.40 (s, 9H), 1.22 – 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*-(pyridin-2-yl(tetrahydro-2H-pyran-4-yl)methyl)butan-1-amine (4p)**



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 **4p** (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).

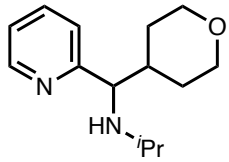
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.60 (td, J = 7.6, 1.9 Hz, 1H), 7.18 (dt, J = 7.8, 1.1 Hz, 1H), 7.12 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.90 (dddd, J = 47.4, 11.5, 4.5, 2.5 Hz, 2H), 3.38 (d, J = 7.4 Hz, 1H), 3.29 (dtd, J = 33.0, 11.9, 2.1 Hz, 2H), 2.43 – 2.23 (m, 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.

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



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 **4q** (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).

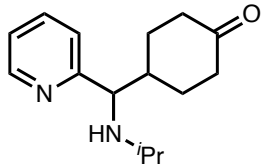
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.58 (dt, J = 4.7, 1.2 Hz, 1H), 7.60 (td, J = 7.6, 1.8 Hz, 1H), 7.23 – 7.08 (m, 2H), 4.04 – 3.78 (m, 2H), 3.48 (d, J = 7.5 Hz, 1H), 3.30 (dtd, J = 25.5, 11.8, 2.1 Hz, 2H), 2.46 (p, J = 6.2 Hz, 1H), 1.98 – 1.75 (m, 4H), 1.41 – 1.22 (m, 2H), 1.15 – 1.03 (m, 1H), 0.96 (dd,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



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 **4r** (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,

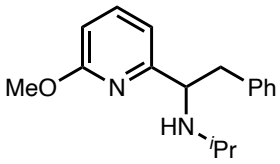
4H), 2.06 (dddd, J = 14.6, 11.5, 6.6, 3.2 Hz, 1H), 1.95 (s, 2H), 1.64 (ddq, J = 12.4, 6.4, 3.2 Hz, 1H), 1.56 – 1.32 (m, 2H), 0.96 (dd, J = 18.3, 6.2 Hz, 6H).

^{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.

***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).

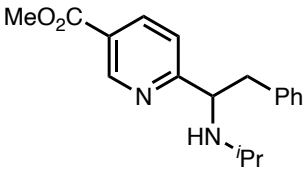
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (t, *J* = 7.7 Hz, 1H), 7.20 – 7.09 (m, 3H), 6.97 (d, *J* = 7.4 Hz, 2H), 6.55 (d, *J* = 7.4 Hz, 1H), 6.48 (d, *J* = 7.1 Hz, 1H), 3.95 – 3.86 (m, 4H), 3.02 (t, *J* = 6.3 Hz, 2H), 2.58 (hept, *J* = 6.3 Hz, 1H), 1.89 (s, 1H), 1.00 (s, 6H).

^{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).

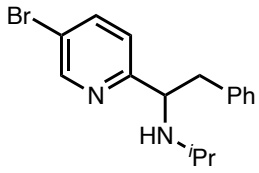
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.17 (d, *J* = 2.1 Hz, 1H), 8.12 (dd, *J* = 8.1, 2.2 Hz, 1H), 7.23 – 7.13 (m, 4H), 7.02 (d, *J* = 6.8 Hz, 2H), 4.13 (t, *J* = 7.2 Hz, 1H), 3.94 (s, 3H), 3.04 (dd, *J* = 13.3, 7.2 Hz, 1H), 2.98 (dd, *J* = 13.3, 7.2 Hz, 1H), 2.58 – 2.49 (m, 1H), 1.78 (s, 1H), 0.95 (d, *J*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

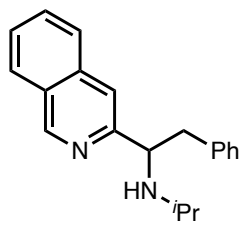
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (dd, *J* = 2.4, 0.7 Hz, 1H), 7.64 (dd, *J* = 8.3, 2.4 Hz, 1H), 7.26 – 7.12 (m, 3H), 7.07 – 6.94 (m, 3H), 4.05 (t, *J* = 7.2 Hz, 1H), 3.05 – 2.90 (m, 2H), 2.54 (hept, *J* = 6.3 Hz, 1H), 2.07 (s, 1H), 0.95 (dd, *J* = 6.3, 2.9 Hz, 6H).

^{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).

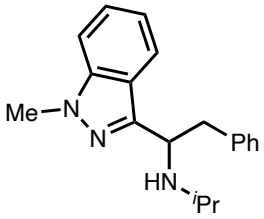
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.27 (s, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.69 (d, *J* = 9.5 Hz, 1H), 7.64 (ddd, *J* = 8.2, 6.7, 1.2 Hz, 1H), 7.55 (ddd, *J* = 8.1, 6.7, 1.3 Hz, 1H), 7.38 (s, 1H), 7.20 – 7.09 (m, 3H), 7.04 (d, *J* = 4.5 Hz, 2H), 4.19 (t, *J* = 7.1 Hz, 1H), 3.20 (dd, *J* = 13.3, 7.5 Hz,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

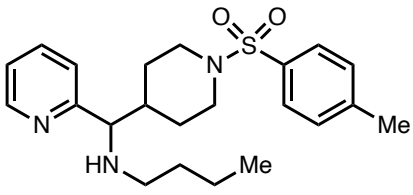
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.2 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.23 – 7.11 (m, 5H), 7.11 – 7.03 (m, 1H), 4.53 (t, *J* = 7.1 Hz, 1H), 4.01 (s, 3H), 3.18 (dd, *J* = 7.1, 2.7 Hz, 2H), 2.68 (hept, *J* = 6.3 Hz, 1H), 1.71 (s, 1H), 0.96 (dd, *J* = 10.7, 6.2 Hz, 6H).

^{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).

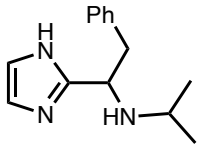
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54 (d, J = 4.8 Hz, 1H), 7.60 (m, 3H), 7.28 (d, J = 7.9 Hz, 2H), 7.14 (m, 2H), 3.81 (d, J = 11.6 Hz, 1H), 3.70 (d, J = 11.4 Hz, 1H), 3.37 (d, J = 14.4 Hz, 1H), 2.42 (s, 3H), 2.40 – 2.25 (m, 1H), 2.18 (td, J = 11.9, 2.6 Hz, 1H), 2.11 (td, J = 11.3, 7.2 Hz, 1H), 2.05 (dd,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

***N*-(1-(1*H*-imidazol-2-yl)-2-phenylethyl)propan-2-amine (S3f)**



Prepared from imine **S1f** (41.2 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** (3.3 mg, 0.014 mmol, 5%) as a yellow oil.

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

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 – 7.18 (m, 5H), 6.94 (d, J = 1.4 Hz, 1H), 6.75 (d, J = 1.4 Hz, 1H), 5.07 (s, 1H), 3.70 (s, 1H), 3.53 (s, 1H), 2.94 (p, J = 6.6 Hz, 1H), 1.69 (d, J = 29.6 Hz, 1H), 1.07 (d, J = 6.6 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 135.71, 129.47, 129.16, 128.63, 128.08, 127.25, 121.25, 53.65, 30.25, 28.60 17.80.

FTIR (NaCl, thin film, cm^{-1}): 3355, 2953, 2914, 1733, 1716, 1558, 1506, 1456, 1167, 910

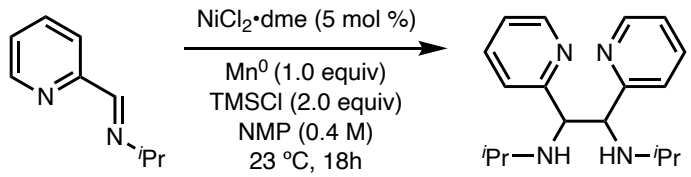
HRMS (ESI, m/z): calc'd for $C_{14}H_{20}N_3$ $[M+H]^+$: 230.1652; found: 230.1648.

5. Mechanistic Experiments

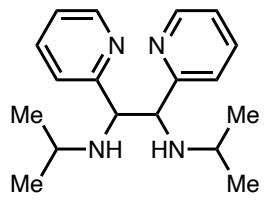
5.1. Imine Homocoupling :

Independent synthesis of 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).

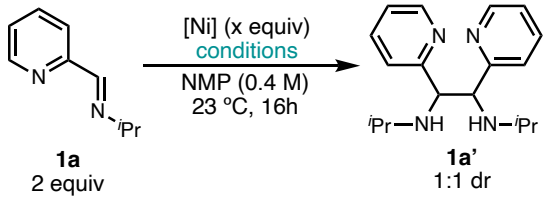
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (dddd, J = 5.0, 3.3, 1.8, 0.9 Hz, 4H), 7.46 (td, J = 7.6, 1.8 Hz, 2H), 7.33 (td, J = 7.6, 1.8 Hz, 2H), 7.05 (ddd, J = 7.5, 4.9, 1.2 Hz, 2H), 7.01 – 6.93 (m, 4H), 6.88 (dt, J = 7.8, 1.1 Hz, 2H), 4.16 (s, 2H), 3.93 (s, 2H), 2.52 (dh, J = 25.0, 6.2 Hz, 4H), 0.97 (d,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

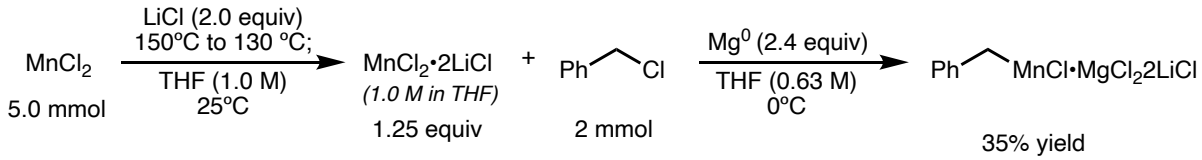
Investigating Conditions that Result in Imine Homocoupling (General Procedure 3)



entry	[Ni] (equiv)	conditions (equiv)	yield **1a'** (%)
1	$Ni(COD)_2$ (1)	–	0
2	$Ni(COD)_2$ (1)	Mn^0 (1)	0
3	$Ni(COD)_2$ (1)	TMSCl (2)	0
4	$Ni(COD)_2$ (1)	Mn^0 (1), TMSCl (2)	0
5	$Ni(COD)_2$ (0.05)	Mn^0 (1)	0
6	$Ni(COD)_2$ (0.05)	TMSCl (2)	trace
7	$Ni(COD)_2$ (0.05)	Mn^0 (1), TMSCl (2)	30
8	$NiCl_2$•dme (0.05)	Mn^0 (1), TMSCl (2)	55
9	–	Mn^0 (1)	0
10	–	TMSCl (2)	0
11	–	Mn^0 (1), TMSCl (2)	74

Table S1. Investigating different parameters that lead to the formation of imine homocoupled product **1a'** in the absence of sp^3 electrophile.

5.2. Probing Intermediacy of Organomanganese Intermediate:

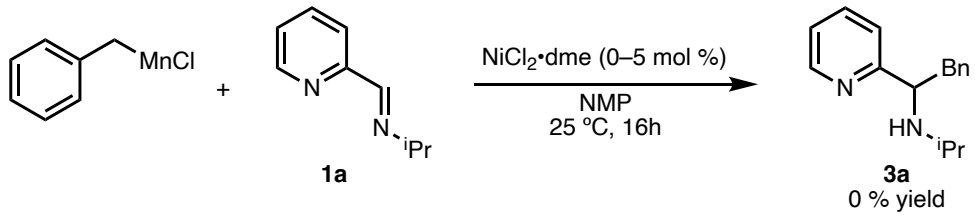


Benzyl organomanganese reagent **6** was prepared according to a procedure from Knochel and coworkers.[6]

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 5 mL 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.

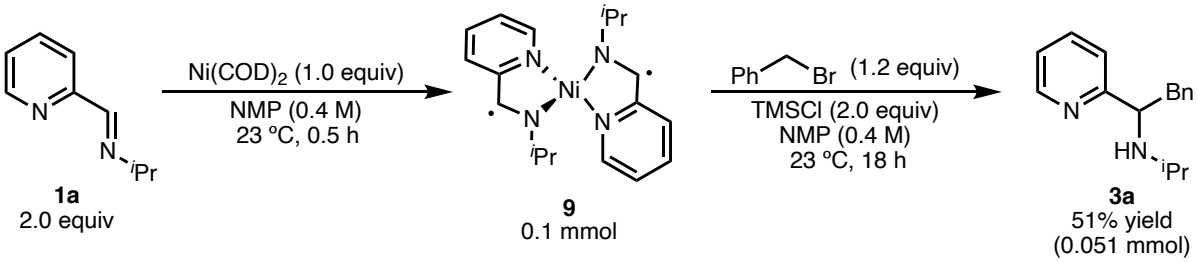
Preparation of Benzylmanganese chloride: A 50 mL round-bottom flask charged with a stir bar was flame-dried under vacuum and allow to cool to 25 ºC under an atmosphere of N_2 then charged with activated Mg^0 turnings (117 mg, 4.80 mmol, 2.4 equiv). The flask was then evacuated and backfilled with N_2 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).



1,2-addition with Organomanganese Reagent: To an oven-dried 1 dram vial with a 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, 5 μmol, 5 mol %) was added and dissolved in 750 μL of NMP. This solution was allowed to stir for 15 min at 27 ºC causing it to turn green (in the presence of Ni). To the solution was then added 545 μL 0.22 M solution of organomanganese reagent 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 ^{1}H 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.

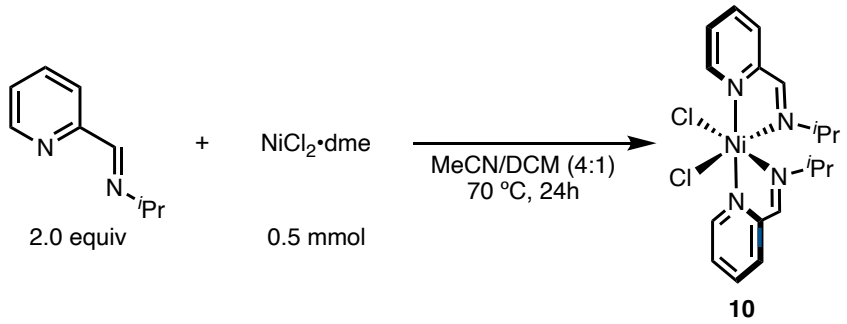
5.3. Stoichiometric Ni^0 Alkylation (Scheme 3b):



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). The vial was then 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 ^{1}H NMR to obtain the reaction yield. Average yield of **3a** over 2 runs: 53 % yield (0.053 mmol).

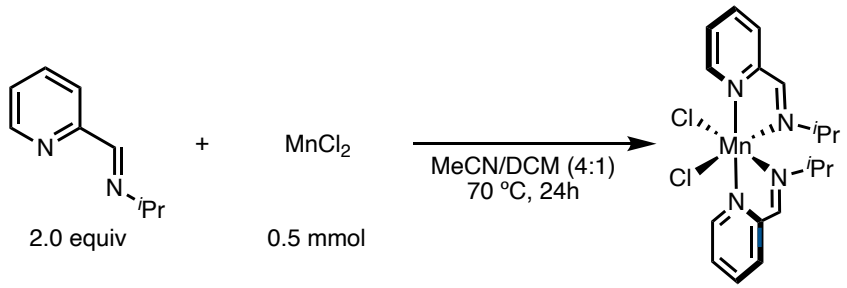
5.4. Synthesis of $1a_2MX_2$ Complexes 10 and 11



Synthesis of 10: Procedure adapted from method described by Andrade-Lopez and coworkers[7]. In a nitrogen-filled glovebox an oven-dried 1 dram vial with a stir bar was charged with $NiCl_2$•dme (110mg, 0.5 mmol, 1 equiv) and suspended in 2mL MeCN then sealed with a septa cap. To a separate 1 dram vial was added 0.5mL DCM and imine **1a** (148mg, 1.0 mmol, 2 equiv) then sealed with a septa cap. The vials were then removed from the glovebox and placed under a flow of N_2. The stirring acetonitrile solution was then heated to 70 ºC where the DCM solution of **1a** was added causing the mixture to become a homogenous green solution. After 5 hours a green precipitate started to form. After 24 hours the solution was cooled to room temperature and filtered. The green powder was washed with cold MeCN two times then dried under high vacuum to give **10** (173 mg, 0.41 mmol, 81% yield) as a green powder. The crude powder could be recrystallized from a minimal amount of 4:1 MeCN:$CHCl_3$ and cooled to –20 ºC to give green rhombic crystals.

FTIR (NaCl, thin film, cm^{-1}): 2969, 1976, 1596, 1442, 1390, 1331, 1300, 1167, 1018, 780, 729, 509.

HRMS (FD, m/z): calc'd for $C_{18}H_{24}N_4ClNi$ $[M\text{-}Cl^-]^+$: 389.10375; found: 389.10334.

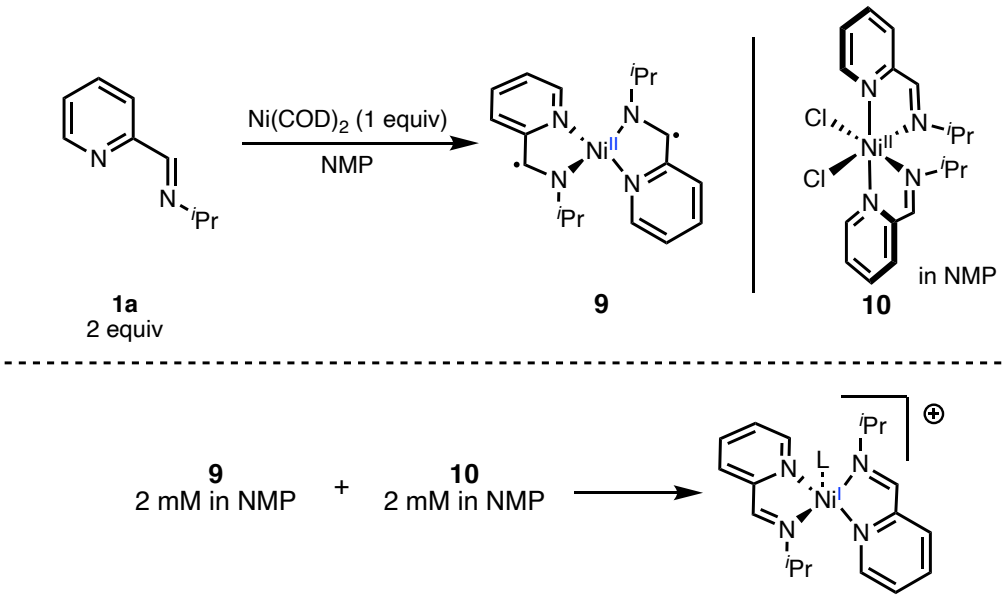


11

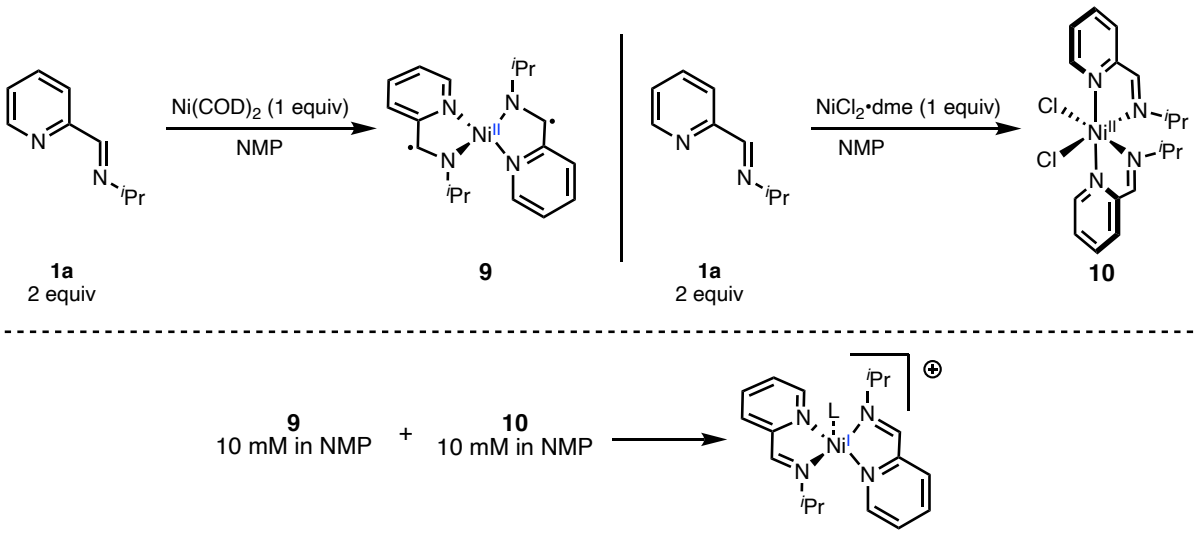
Synthesis of 11: Procedure adapted from method described by Andrade-Lopez and coworkers.[7] In a nitrogen-filled glovebox an oven-dried 1 dram vial with a stir bar was charged with $MnCl_2$ (62.9 mg, 0.5 mmol, 1 equiv) and suspended in 2mL MeCN then sealed with a septa cap. To a separate 1 dram vial was added 0.5 mL DCM and imine **1a** (148 mg, 1.0 mmol, 2 equiv) then sealed with a septa cap. The vials were then removed from the glovebox and placed under a flow of N_2. The stirring acetonitrile solution was then heated to 70 ºC where the DCM solution of **1a** was added causing the mixture to become a cloudy orange solution. After 1 hour an orange precipitate started to form. After 24 hours the solution was cooled to room temperature and filtered. The orange powder was washed with cold MeCN two times then dried under high vacuum to give **11** (194 mg, 0.46 mmol, 92% yield) as a orange solid. The crude powder could be recrystallized from a minimal amount of 4:1 MeCN:$CHCl_3$ and was lightly capped so the solvent can slowly evaporate and allowed to sit for to give orange rhombic crystals.

FTIR (NaCl, thin film, cm^{-1}): 2966, 2929, 1645, 1593, 1461, 1440, 1394, 1363, 1305, 1166, 1012, 874, 784, 749, 637, 506.

5.5. Preparation of $(1a)_2Ni^I$ complex and Spectroscopic Analysis



UV/VIS sample Preparation: In a N_2-filled glovebox, an oven-dried 20 mL scintillation vial with a stir bar was charged with $Ni(COD)_2$ (2.2 mg, 8 μmol, 0.8 equiv) and 2.5 mL of NMP. To the stirring suspension was added **1a** (2.4 mg, 16 μmol, 1.6 equiv) causing the solution to turn a deep royal purple and was allowed to stir for 15 minutes to form **9**. Concurrently, an oven-dried 1 dram vial with a stir bar was charged with **10** (4.3 mg, 10 μmol, 1 equiv). To the vial was added 2.5 mL of NMP to give a green solution. After 15 minutes the NMP solution of **10** was transferred to the solution of **9** in NMP causing the solution to turn black. The solution was stirred for 2 hours then transferred to a quartz cuvette (1 cm pathlength) for UV/VIS analysis.



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 **9**. 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 **10**. After 15 minutes the NMP solution of **10** was transferred to the solution of **9** 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.

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.

EPR Data of $(1a)_2Ni^I$:

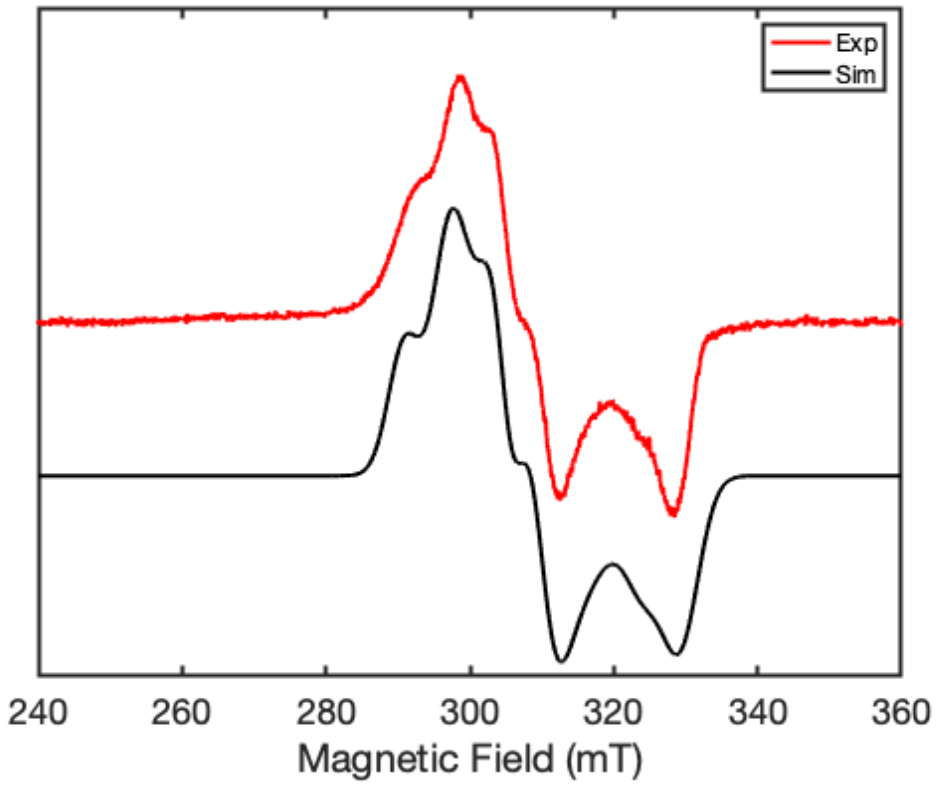


Figure S3. X-band EPR spectrum (red) of the comproportionation reaction between **9** and **10** in (10 mM) NMP with the following parameters: Temperature = 77 K, solvent = NMP, microwave frequency = 9.36 GHz, power = 2.181 mW, modulation amplitude = 1200.00 G. Simulated signal is shown (black). See Figure **S10** for simulation details and g values.

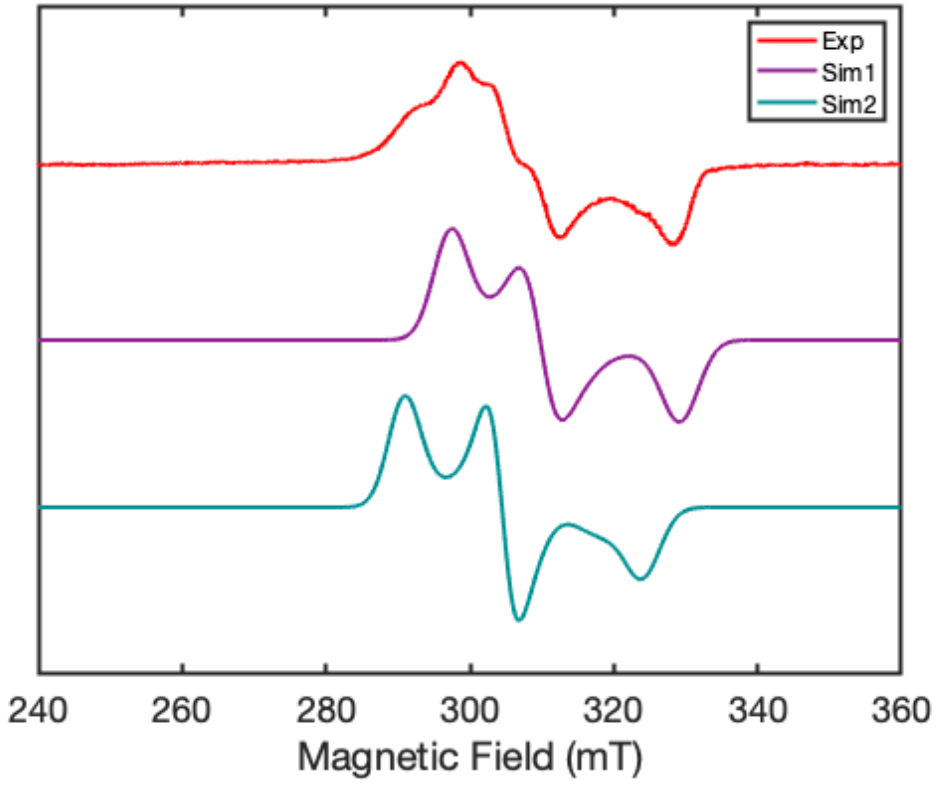
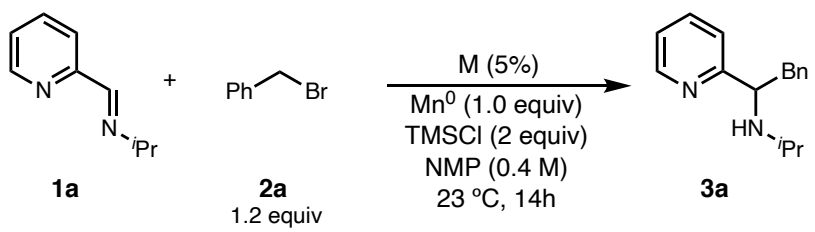


Figure S4. EPR was simulated as two S=1/2 Ni^{I} isomeric species (based on optimal fitting parameters and related work from Wieghardt.[11] Fitting parameters for species 1 (plum): $g_1 = 2.25$, $g_2 = 2.16$, $g_3 = 2.03$, linewidth = 4.4 mT, $\Gamma_1 = 70$, $\Gamma_2 = 47$, $\Gamma_3 = 85$ MHz, weighting 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, $\Gamma_1 = 106$, $\Gamma_2 = 2$, $\Gamma_3 = 123$ MHz, weighting factor = 0.56.

5.6. Alternative Radical Generation Approaches for Alkylation

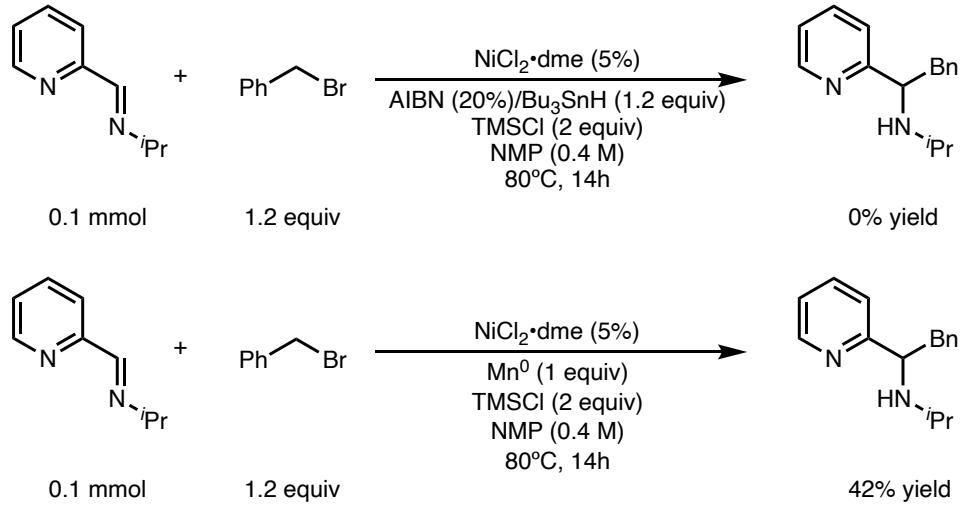
Lewis and Brønsted acids were evaluated as alternative catalysts to facilitate radical addition into heteroaryl imines. Using Lewis acids under otherwise optimized conditions in place of $NiCl_2$•dme did not provide the same yield boost or improve the yield beyond the Mn-mediated background reaction (Scheme S1).



entry	M	yield **3a** (%)
1	–	66
2	$MgBr_2$	58
3	BPh_3	48
4	AcOH	53
5	$AlCl_3$	44

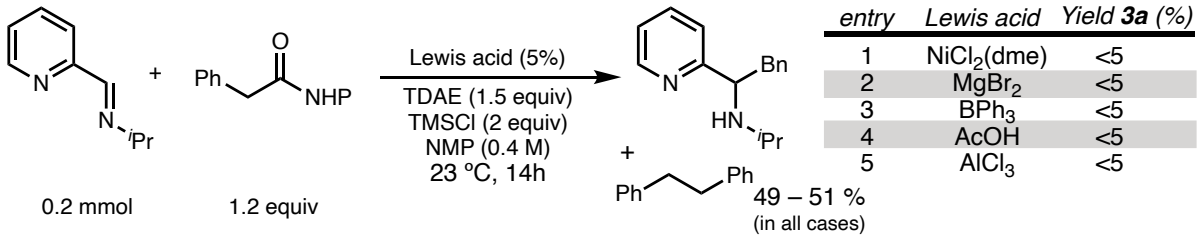
Scheme S1. Alkylation reaction with alternative, non redox-active, metal catalysts. Yields determined by ^{1}HNMR with an internal standard.

Radical generation under thermal AIBN/^{n}Bu$_3$SnH conditions in the absense of Mn^0 did not result in product formation whereas the optimized conditions performed at 80ºC gave alkylated product in 42% yield (Scheme S2).



Scheme S2. Thermal radical generation conditions for a redox-neutral imine alkylation (top) and control experiment of the optimized reaction conditions run at 80ºC (bottom). Yields determined by ^{1}HNMR with an internal standard.

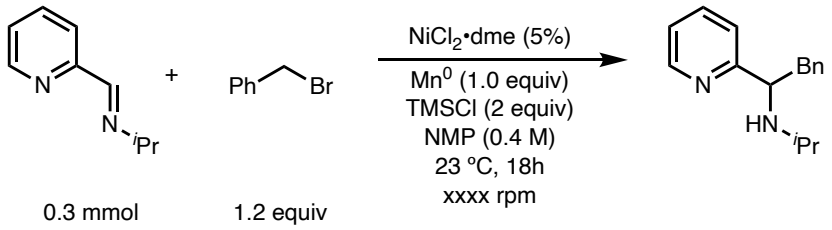
Genration of benzylic radicals through the reduction of NHP esters in the presence of TMSCl and TDAE as a reductant. Across several metal catalysts we observe significant levels of benzyl homocoupled product indicating radical formation and trace levels of alkated products (Scheme S3).



entry	*Lewis acid*	*Yield **3a** (%)*
1	$NiCl_2$(dme)	<5
2	$MgBr_2$	<5
3	BPh_3	<5
4	AcOH	<5
5	$AlCl_3$	<5

Scheme S3. Radical generation under mild reductive conditions employing NHP esters as radical precursors and several metal catalysts. Yields determined by ^{1}HNMR with an internal standard.

5.7. Stir Rate Study

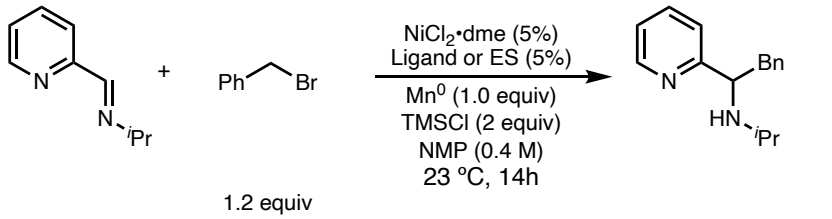


Stir rate (rpm)	*Yield (%)*
300	84
600	88
750	81
1200	81

Scheme S4. Control study showing minimal impact on alkylation yield across several stir rates. Yields determined by ^{1}HNMR with an internal standard.

5.8. Exogenous Ligands and Electron Mediators

The possibility that the role of the nickel catalyst is to act as an electron mediator that accelerates the Mn-mediated reaction was investigated through the addition of exogenous ligands and through the addition of known electron mediatiors (Scheme S5). Exogenous ligands we examed were bidentate nitrogen ligands (dtbbpy), tridentate nitrogen ligands (terpy), and bidentate phosphine ligands (dppe). All ligands or electron shuttles seemed to inhibit the reaction or shut down productive reactivity.



entry	ligand[b]/ES	yield (%)[a]
1	dtbbpy	65
2	terpy	< 5
3	dppe	< 5
4	$Ni(bpy)_3(BF_4)_2$	59
5	CoPc	25

Scheme S5. Using additional ligands and electron shuttles. [a] ^{1}H NMR yield versus standard. [b] Metal and ligand were premixed in NMP for 30 minutes before being added to the reaction.

6. Electroanalytical Experiments

General Details: Cyclic voltammograms were obtained in a N_2-filled glovebox using a standard three electrode cell consisting of a freshly polished (0.3 μm then 0.05 μm alumina) glassy carbon working electrode, platinum counter electrode, and a silver wire non aqueous reference electrode in 10mM $AgNO_3$ (MeCN). Data were collected using a Biologic SP-300 potentiostat and analyzed in EC-Lab. All cyclic voltammograms were measured in NMP with 0.1M $TBAPF_6$ supporting electrolyte and then referenced to freshly sublimed ferrocene (Fc). All voltammagrams were background corrected against blank solvent/electrolyte unless

specified. Peak currents were calculated from linear baseline-corrected "peak analysis" feature in EC-Lab. The reduction potentials are reported versus the reduction potential of the Fc/Fc^{+} peak. Ohmic drop compensation was done with all samples before each scan using positive-feedback iR-compensation at 85% of uncompensated resistance (R_u) measured from potentio electrochemical impedence spectroscopy (PEIS).

6.1. Cyclic Voltammetry of Heteroaryl Imines and Metal Complexes

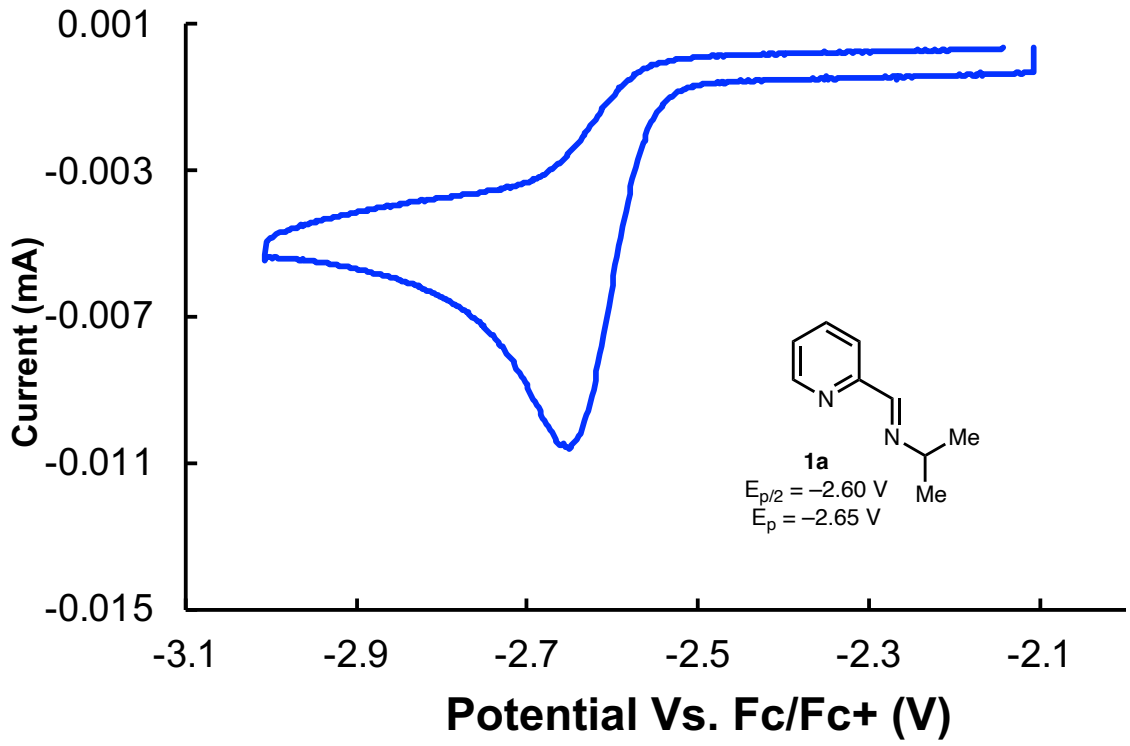


Figure S5. Cyclic voltammogram of 2mM **1a** in 0.1 M $TBAPF_6$ in NMP at 25 ºC ν = 100 mV/s.

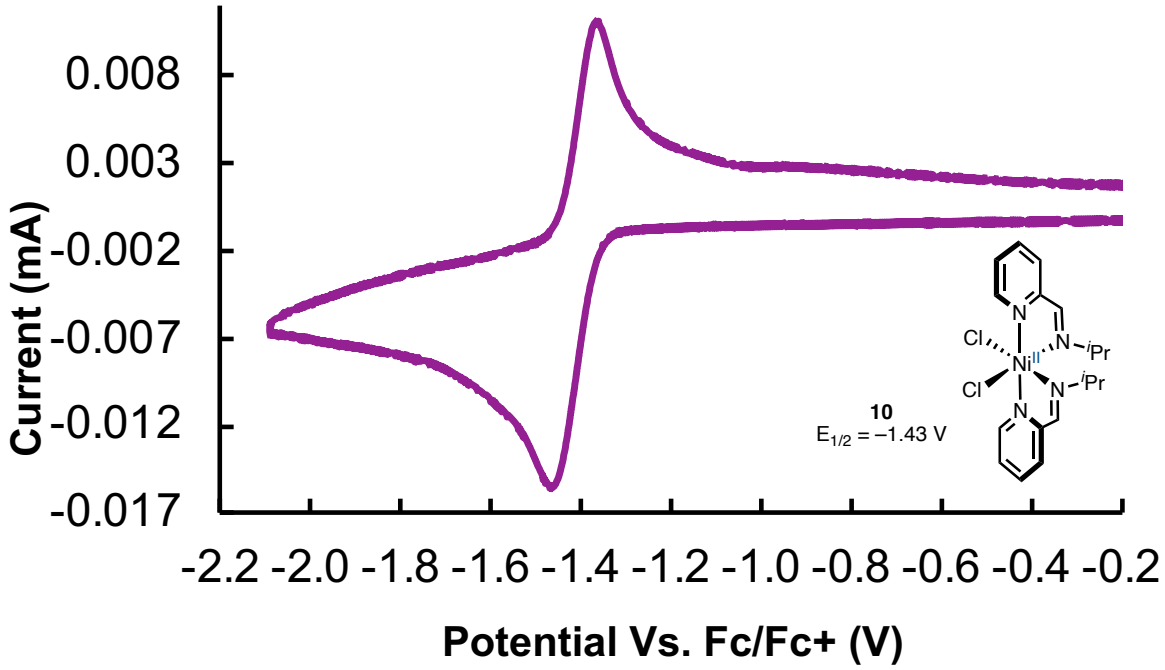


Figure S6. Cyclic voltammogram of independently prepared (1 mM) **10** 0.1 M $TBAPF_6$ in NMP at 25 ºC ν = 100 mV/s.

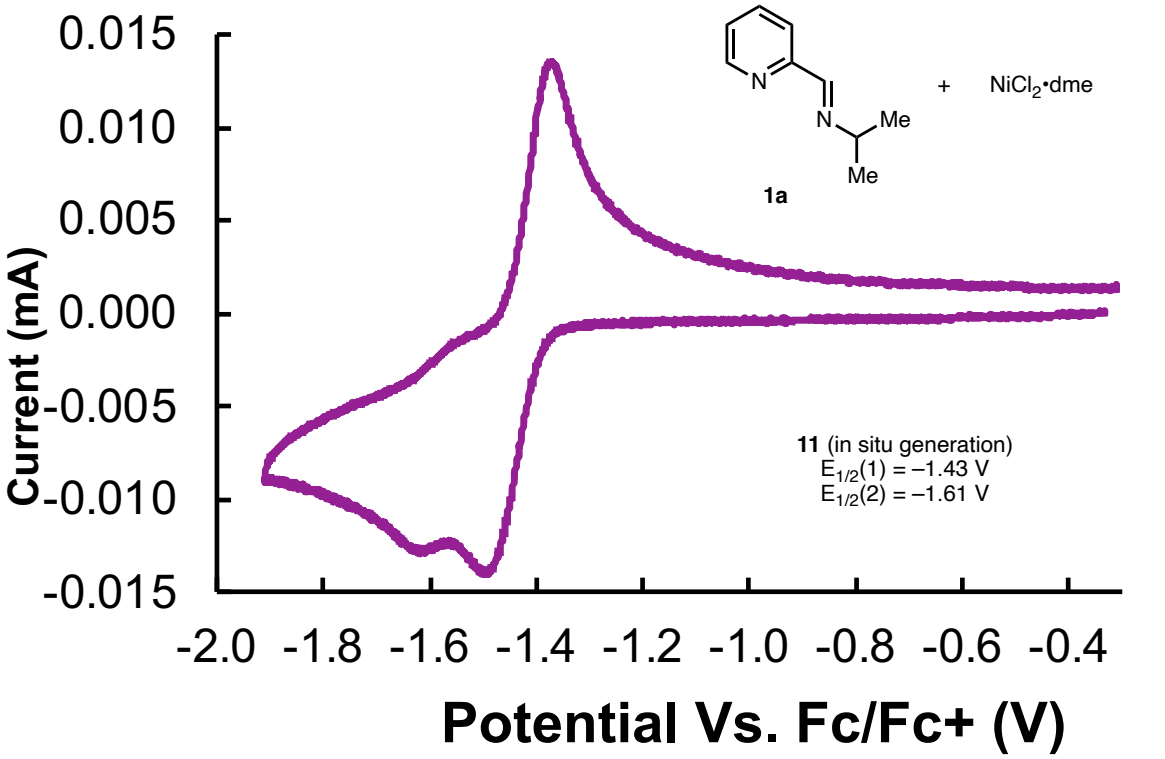


Figure S7. Cyclic voltammogram of *in situ* generated **11** from mixing **1a** (100 mM) and $NiCl_2$•dme (2mM) in the electrochemical cell. 0.1 M $TBAPF_6$ in NMP at 25 ºC ν = 100 mV/s. The second reduction peak is likely small amounts of the Ni complex with three **1a** ligands.[8]

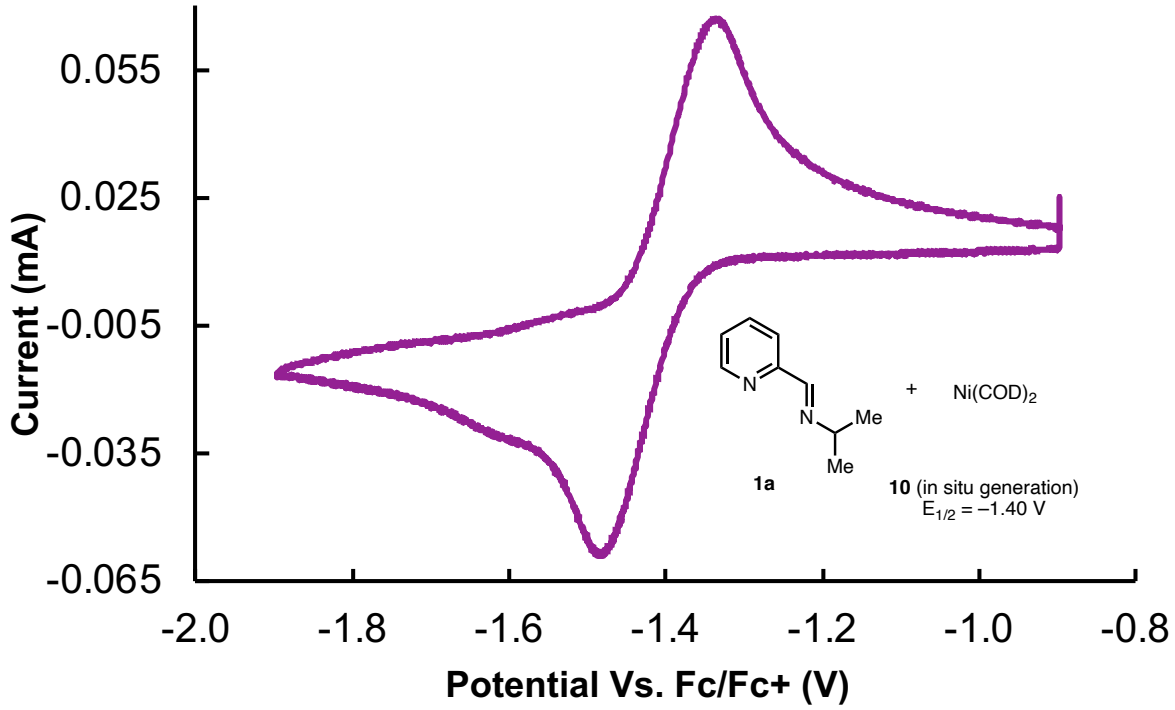


Figure S8. Cyclic voltammogram of *in situ* generated **10** from mixing **1a** (40 mM) and $Ni(COD)_2$ (5 mM) in the electrochemical cell. 0.1 M $TBAPF_6$ in NMP at 25 ºC, ν = 100 mV/s.

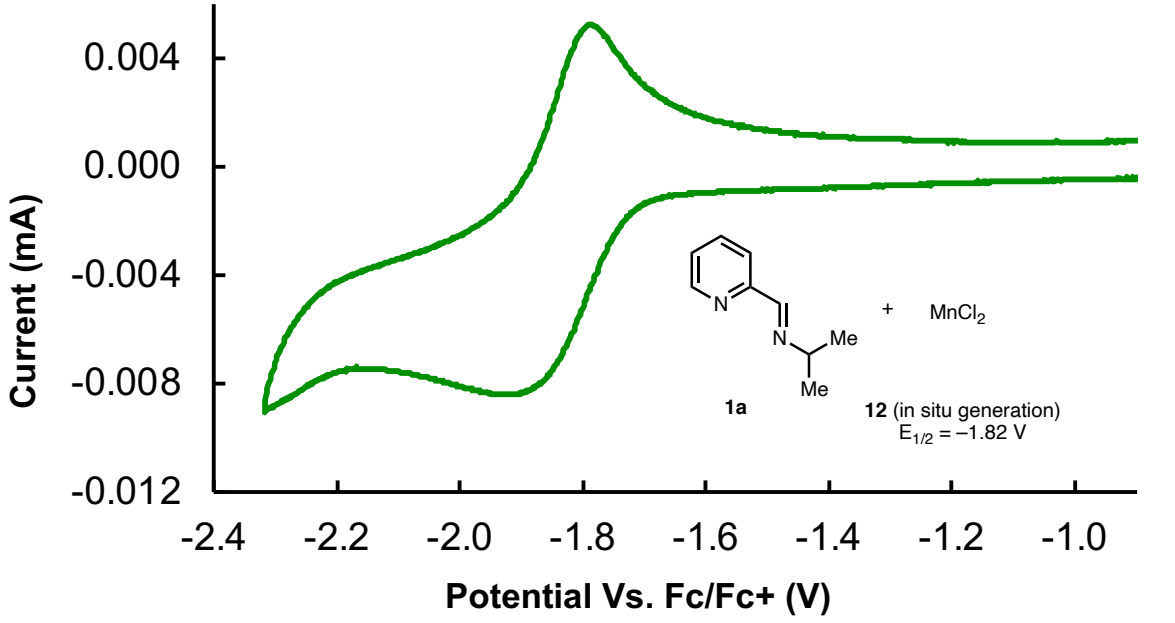


Figure S9. Cyclic voltammogram of *in situ* generated **11** from mixing **1a** (80 mM) and $MnCl_2$ (2 mM) in the electrochemical cell. 0.1 M $TBAPF_6$ in NMP at 25 ºC, ν = 100 mV/s.

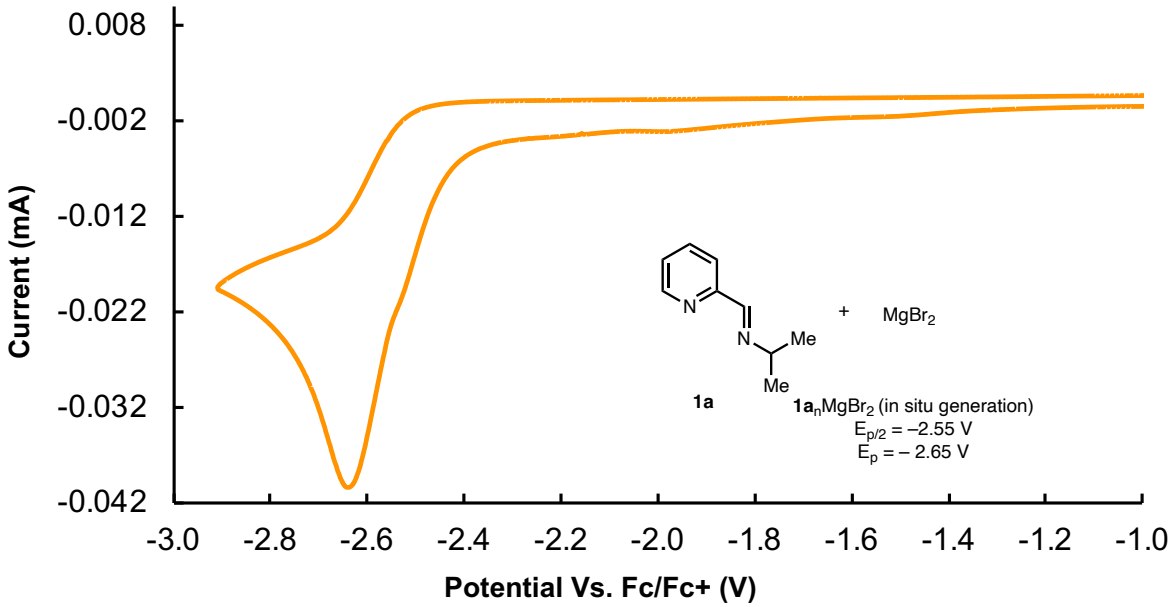


Figure S10. Cyclic voltammogram of *in situ* generated **1a**$_n$MgBr$_2$ complex from mixing **1a** (100 mM) and MgBr$_2$ (2 mM) in the electrochemical cell. 0.1 M TBAPF$_6$ in NMP at 25 ºC, ν = 100 mV/s.

6.2. Effect of Reaction Components on 10

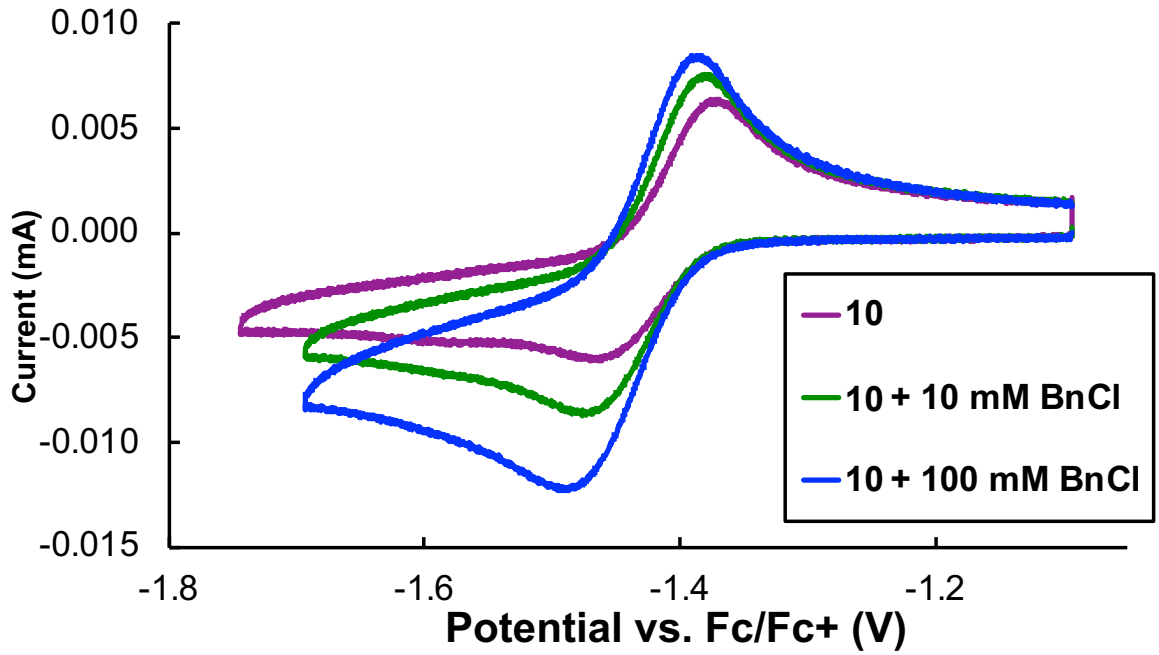


Figure S11. Cyclic voltammograms of **10** (1 mM, purple) followed by the addition of 10 mM BnCl (green) and 90 mM BnCl (100 mM total, blue). All voltammograms taken in 0.1 M TBAPF$_6$ in NMP at 25 ºC, ν = 100 mV/s.

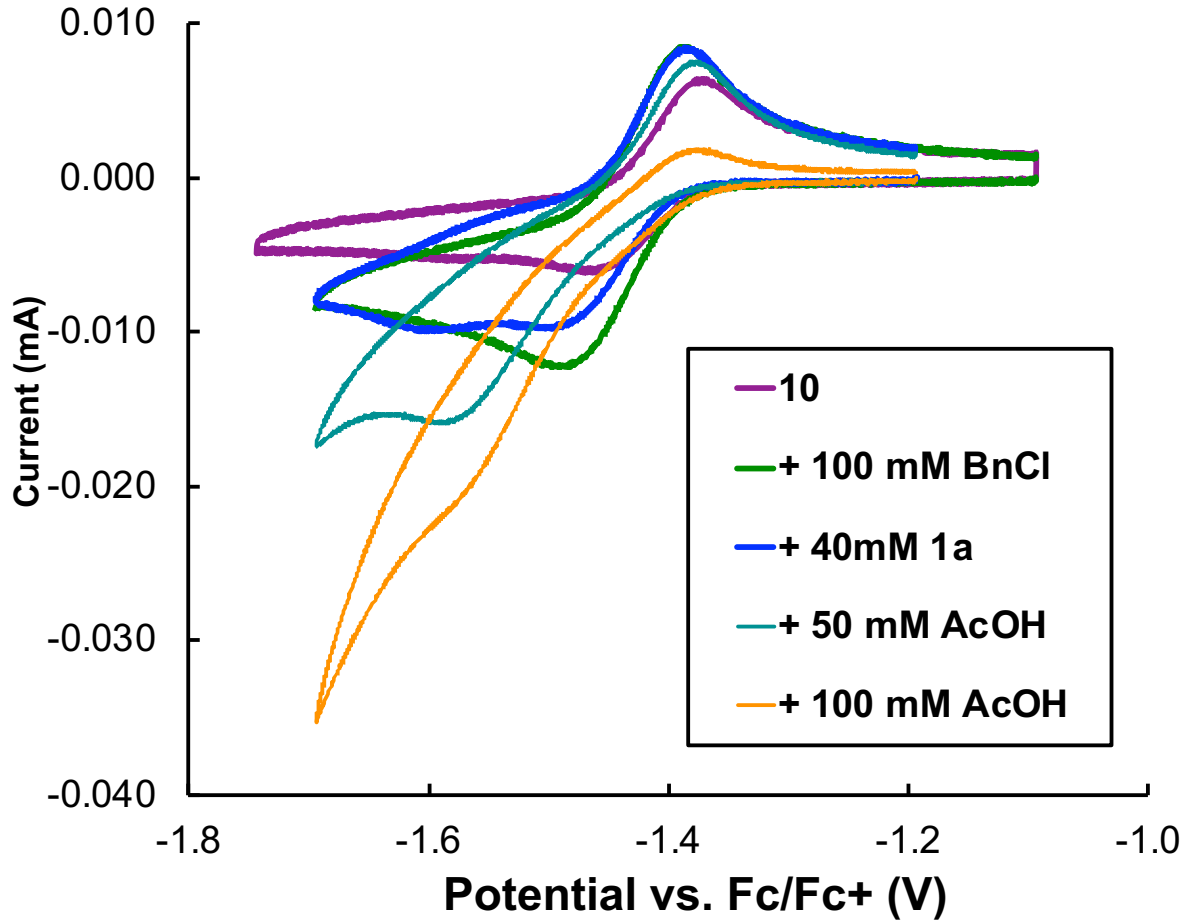


Figure S12. Cyclic voltammograms of **10** (1 mM, purple) followed by the addition of 100 mM BnCl (green). Addition of 40 mM **1a** to allow for turnover for additive studies (blue). Addition of 50 mM AcOH additive (teal) followed by an additional 100 mM AcOH to the same cell (150 mM total, orange). All voltammograms taken in 0.1 M $TBAPF_6$ in NMP at 25 ºC, ν = 100 mV/s.

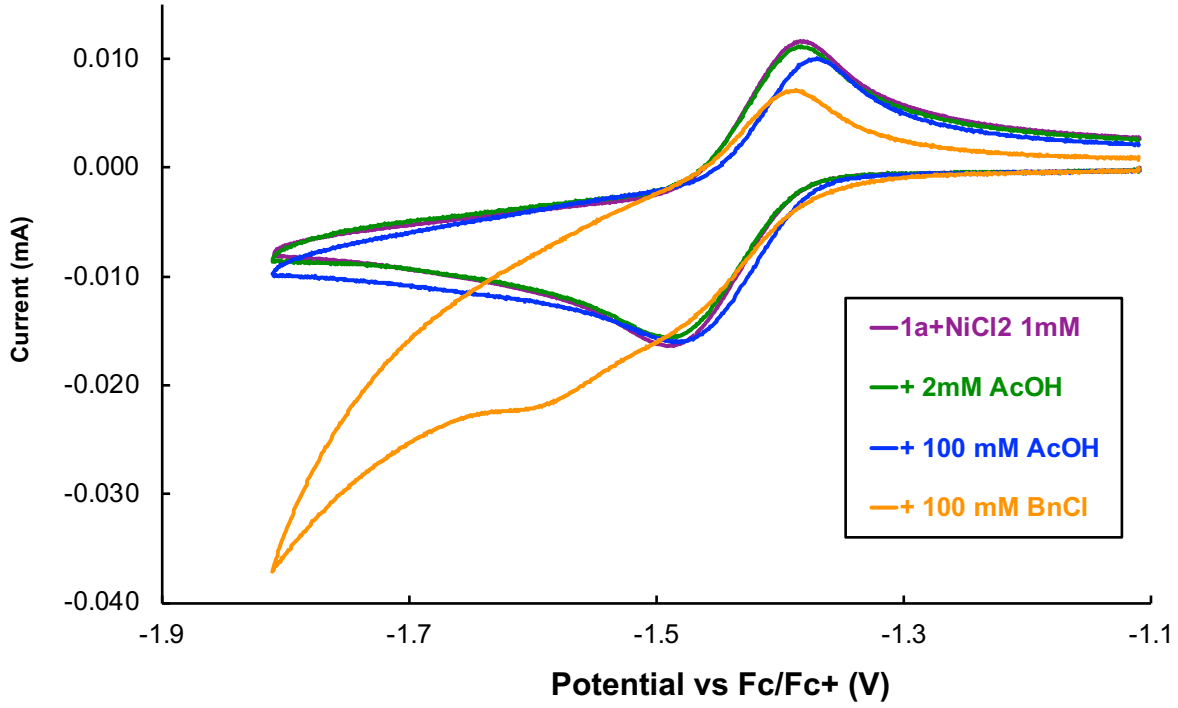
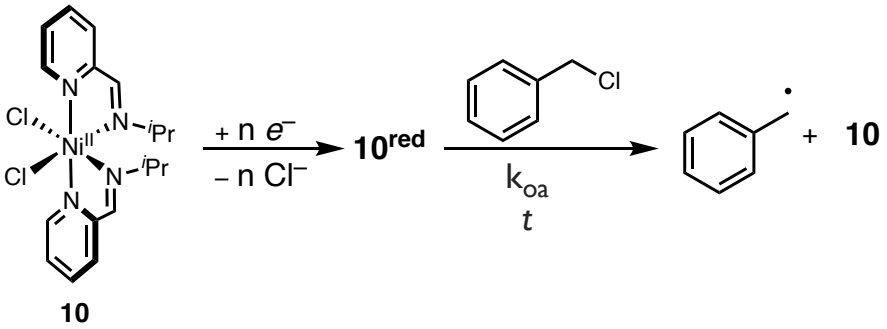


Figure S13. Control experiment for Figure 3c showing voltammetry for different order of addition of reaction components. Cyclic voltammograms of **10** (1 mM, purple) with 20mM excess **1a**. Reaction component addition order: 2 mM AcOH (green), addition of 98 mM AcOH (blue), then 100mM BnCl to the cell. All voltammograms taken in 0.1 M $TBAPF_6$ in NMP at 25 ºC, ν = 100 mV/s.

6.3. Kinetics of Reaction of Reduced 10 (10^{red}) and Benzyl Chloride



Scheme S1. General reaction scheme for reduction of **10** and subsequent oxidative addition with benzyl chloride studied by CV.

To calculate the reaction rate constant between reduced **10** ($\mathbf{10}^{red}$) with benzyl chloride (Scheme S1) a procedure described by Sigman and Minteer was used.[9] This reaction could be studied by mixing **10** with a large excess of benzyl chloride and measuring the cathodic and anodic peak currents (i_{pc} and i_{pa}) of the **10** redox wave at varying scan rates (ν) from 2 V/s to 3 mV/s. Varying the scan rate changes the time it takes to go from E_{pc}, where $\mathbf{10}^{red}$ is generated, to the E_{pa}, where any remaining $\mathbf{10}^{red}$ is reoxidized to **10**, enabling us to calculate the amount

of $\mathbf{10}^{\mathbf{red}}$ remaining after it reacts with benzyl chloride at various time points. In the case of a CV potential window $E_i \rightarrow E_r$ (± 0.25 V to $E_{1/2}$ here) then the reaction time (t) can be calcualted as:

$$t = \frac{\left|E_r - E_{pc}\right| + \left|E_r - E_{pa}\right|}{\nu}$$

where E_{pc} is the potential of the peak cathodic current and E_{pa} is the potential of the peak anodic current. From the Randles-Sevcik equation, the amount of $\mathbf{10}^{\mathbf{red}}$ remaining at time t can be detemined from the baseline-corrected peak height ratios (i_{pa}/i_{pc}):

$$\frac{i_{pa}}{i_{pc}} = \frac{[\mathbf{10}^{red}]_t \sqrt{D_{\mathbf{10}red}}}{[\mathbf{10}^{red}]_0 \sqrt{D_{\mathbf{10}}}}$$

We can simplify this by assuming that the difussion coefficents for the reduced species $\mathbf{11}^{\mathbf{red}}$ and **10** ($D_{\mathbf{10}}^{\mathbf{red}}$ and $D_{\mathbf{10}}$ respectively) are approximately the same:

$$\frac{i_{pa}}{i_{pc}} = \frac{[\mathbf{10}^{red}]_t}{[\mathbf{10}^{red}]_0}$$

Multiplying the fraction by the known initial concetration of **10** (1 mM) will give us the concentration of $\mathbf{10}^{\mathbf{red}}$ at t allowing us to extract a time course. This time course can then be treated as a pseudo-1st order reaction due to large excess of benzyl chloride (100 mM) or be simulated as a second order reaction and analyzed in the COPASI[10] kinetics simulation software.

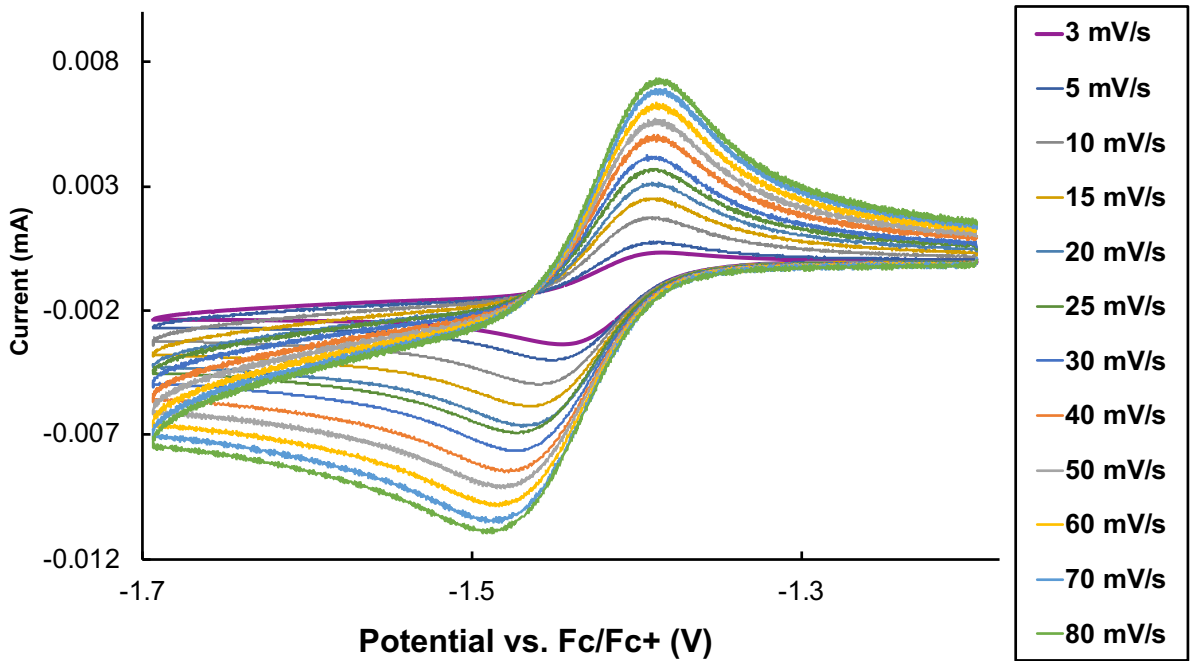


Figure S14: Voltammograms of the reaction of **10** (1 mM) with BnCl (100 mM) in 100 mM $TBAPF_6$ in NMP at 25 ºC with scan rates 3–80 mV/s.

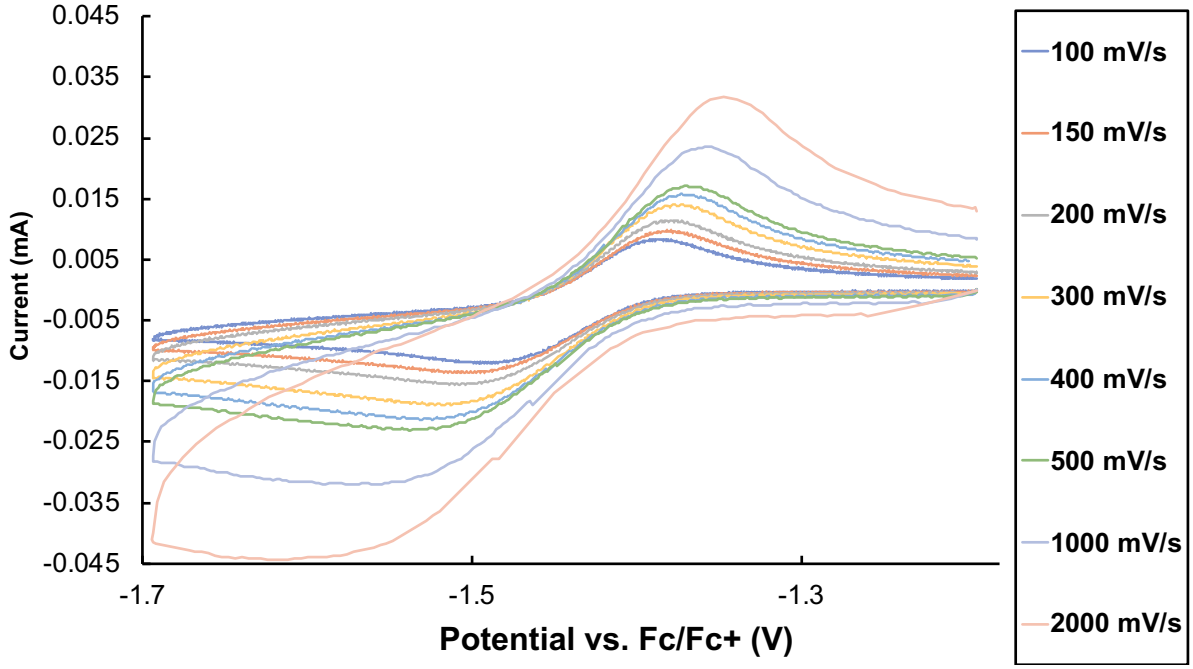


Figure S15: Voltammograms of the reaction of **10** (1 mM) with BnCl (100 mM) in 100 mM $TBAPF_6$ in NMP at 25 ºC with scan rates 100–2000 mV/s.

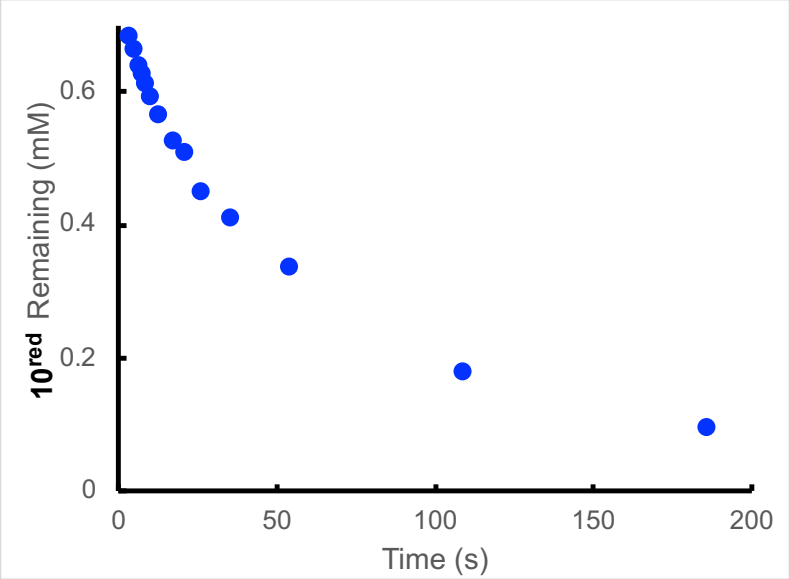


Figure S16. Time course of calculated **10**^{red} remaining over time after reacting with BnCl.

Kinetic Analysis: The net reaction between **10**^{red} and benzyl chloride follows the second order rate equation:

$$rate = k_{oa}[BnCl][10^{red}]$$

Given the large excess of BnCl added, the reaction can be treated as a pseudo-1st order reaction with the rate law:

$$rate = k_{app}[10^{red}]$$

$$k_{app} = k_{oa}[BnCl]$$

For the pseudo-1st order treatment the rate constant k_{app} can be determined from the slope of a plot of ln([**10**^{red}]) vs. time (Figure S17) which can then be used to determine k_{oa} with the known amount of benzyl chloride added ([BnCl]$_0$). From the measured k_{app} = 0.018 s^{-1} we determine the corresponding 2nd order rate constant k_{oa} = 0.18 M^{-1}s^{-1}.

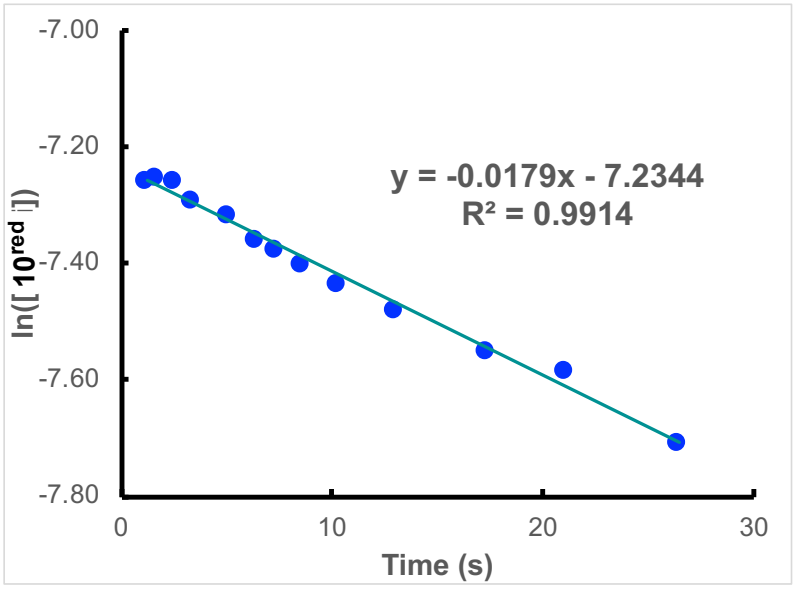


Figure S17. Pseudo-1st order plot with linear regression to determine k_{app} = 0.018 s^{-1}. fit was used for first 26 seconds of the reaction.

A complementary approach utilizing kinetic modeling software was also done with the time course data. The reaction was modeled as a second order process and gave a k_{oa} = 0.17 $M^{-1}s^{-1}$ (Figure S18).

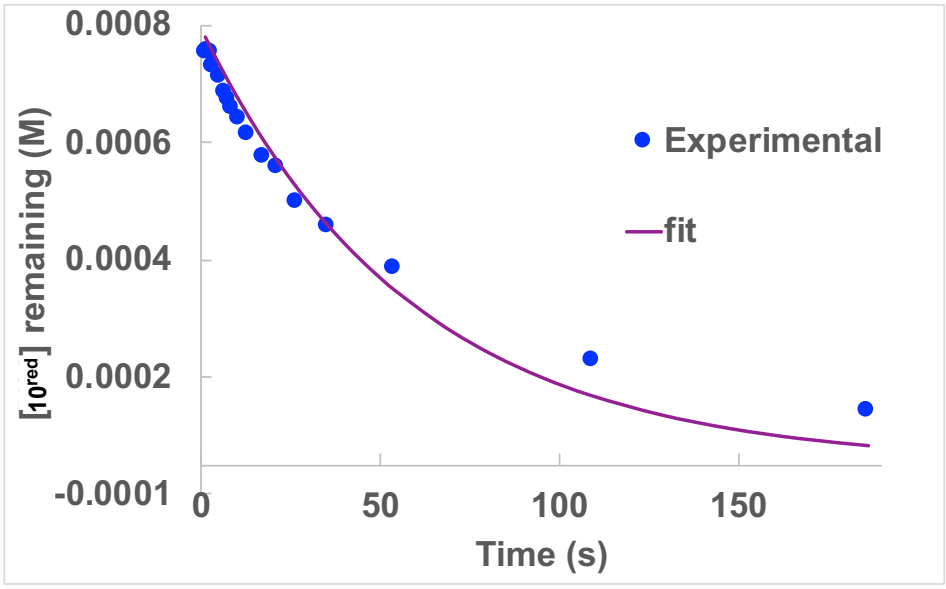


Figure S18. Experimental time course and simulated reaction fit. Fit was used for first entire time course measured.

7. UV/Vis and Spectroelectrochemistry

General Details of UV/Vis studies: All UV/Vis measurements were performed on a Cary 50 spectrophotometer with Cary WinUV software. Samples were prepared in a nitrogen filled glovebox and sealed in a 1 cm quartz cuvette for analysis. Background correction was done against an NMP blank and samples were scanned from 1100 nm to 300 nm. ε values were calculated from the prepared concentration in the case of **9** and **10** and in the case of the Ni^{I} (Figure S21) the reaction (section 5.5) to make the Ni^{I} sample was assumed to be quantitative. This assumption appears to be valid based on the lack of spectral features resembling **9** in the sample and similarities in the known ε values for the analogous Ni^{I} and formally Ni^{0} complexes studied by Wieghardt and Coworkers.[11]

7.1. UV/Vis of Independently Prepared Complexes

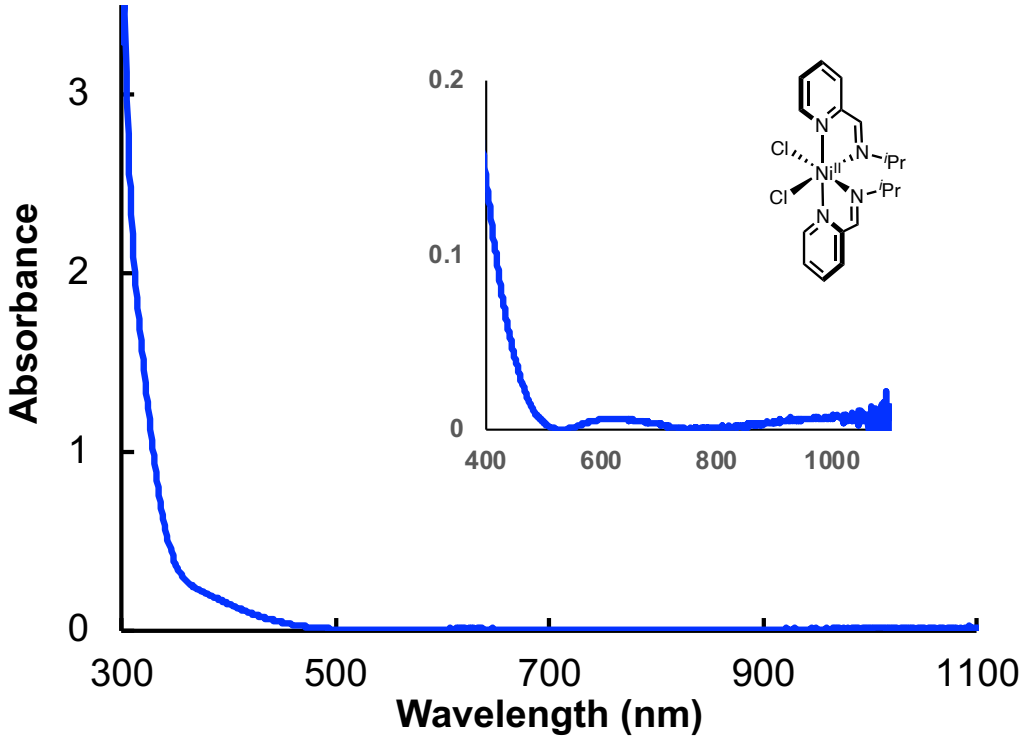


Figure S19. UV/Vis spectrum of **10** (1mM) in NMP. Inset: Close up of 400-1100 nm region to show transitions.

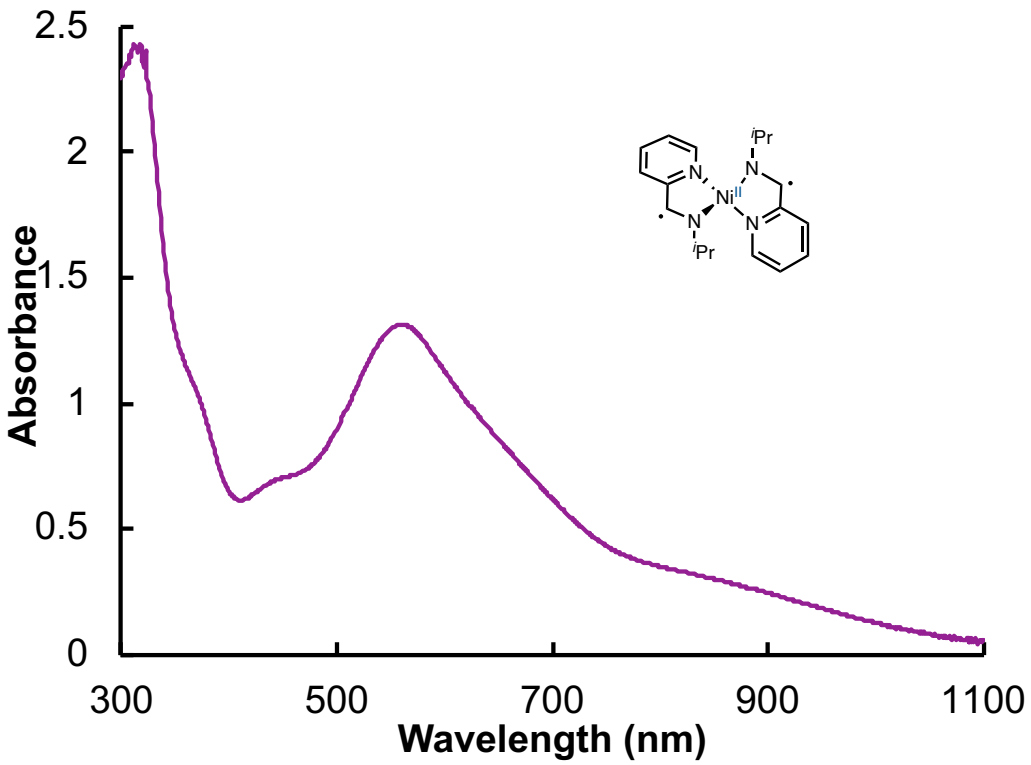


Figure S20. UV/Vis spectrum of **9** (0.26 mM) prepared from **1a** (0.52 mM) and $Ni(COD)_2$ (0.26mM). Inset: Close up of 400-1100 nm region to show smaller transitions.

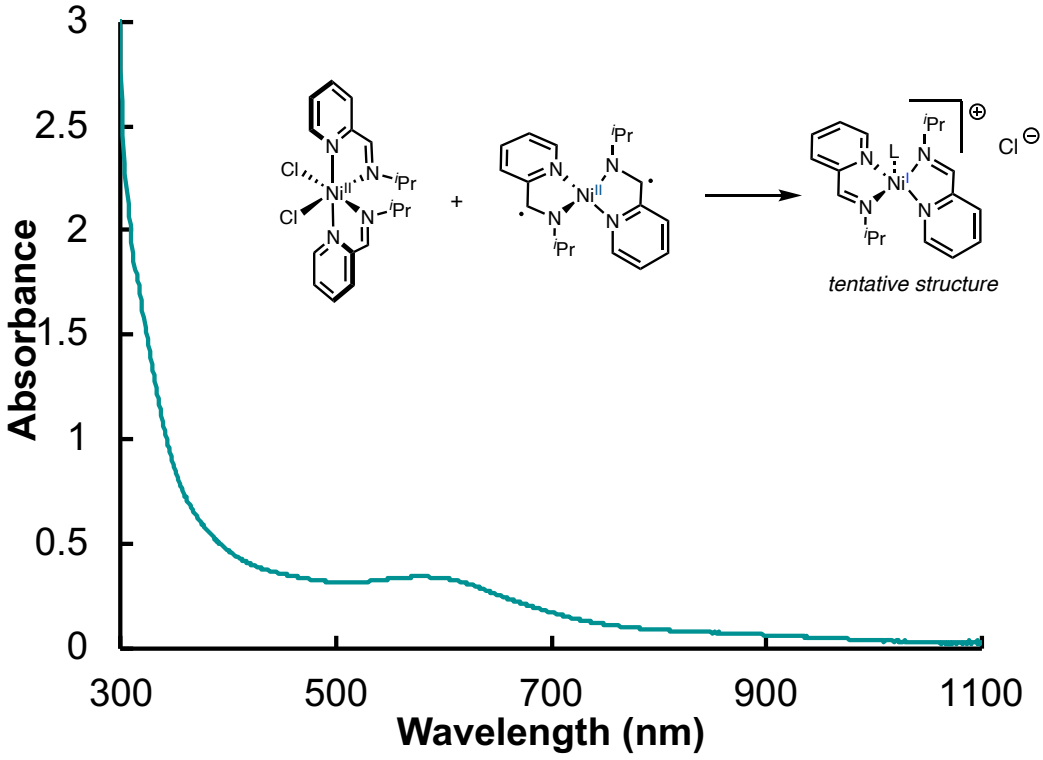


Figure S21. UV/Vis spectrum of $(\mathbf{1a})_2Ni^{I}$ (0.32 mM) prepared from reacting **9** prepared in the same manner as Figure S25 and **10** after 2 hours to ensure complete disproportionation.

7.2. Spectroelectrochemistry of 10

General Details: Spectroelectrochemistry studies were conducted in a nitrogen-filled glovebox. Spectroelectrochemistry kit from Pine Research (AKSTCKIT3) was used with measurements done in a quartz spectroelectrochemical cell with 0.17 cm path length. A three electrode setup composed of a honeycomb electrode containing Pt working and Pt counter electrodes was used along with a silver wire, $Ag/AgNO_3$ (10 mM MeCN), non-aqueous reference electrode. The cell was placed in a Ocean Optics CUV–UV cuvette holder connected to the light source and spectrophotometer with 600 μm core optical fibers. UV/Vis measurements were done with an Hamamatsu L1179 deuterium light source coupled to an Ocean Optics USB4000-UV-Vis-ES detector.

Spectroelectrochemistry Measurement Procedure: An initial cyclic voltammagram was taken of the 1 mM solution of **10** (0.1 M $TBAPF_6$ in NMP to identify redox peaks (Figure S22). For spectroelectrochemistry measurements the cell was held at a constant voltage for 3 minutes where after 2.5 minutes of elecrolysis the spectrum was saved to ensure that the majority of electroactive species were reduced at the electrode despite most of the current passing within the first 5 seconds once sufficiently reducing potentials were reached (Figure S23). Starting at -1.04 V vs. Fc/Fc^+ the potential was then decreased stepwise by 0.1 V increments until significant current started to pass at which point the step sizes decreased to 0.05 V. This was done until the spectrum remained unchanged indicating reduction was complete (–1.94 V vs. Fc/Fc^+). After this the procedure was repeated in the oxidative direction to ensure the reversibility of the process. All spectra were basline corrected at 860 nm and plotted as the 5-point moving average.

Calculating ε in Figure 3b: The UV/Vis spectra remained largely unchanged in intensity and absorbance features at -1.74 V (vs. Fc/Fc^+) suggesting all of **10** at the electrode had been reduced. Assuming this is true the ε was calculated from an assumed concentration of 1 mM of reduced species at each measured wavelength. From these values, the concentration of **9** can be calculated at lower potentials containing <1 mM of **9**. The concentration was calculated by averaging the concentration calculated for each wavelength by A/(ε*0.17 cm) between 320 nm and 630 nm. The average concentration calculated at the $E_{1/2}$ (-1.44 V) was 0.54 ± 0.04 mM.

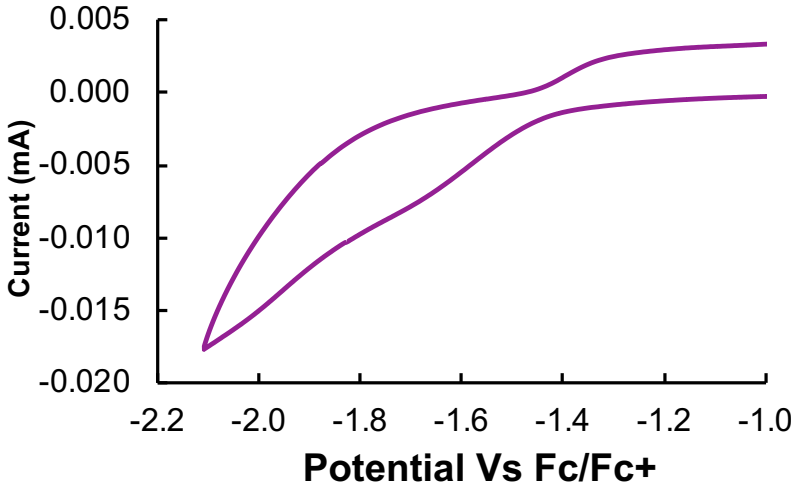


Figure S22. Cyclic voltammogram of **10** (1mM) in 0.1 M $TBAPF_6$ in NMP at 25 ºC in the spectroelectrochemical cell, ν = 50 mV/s.

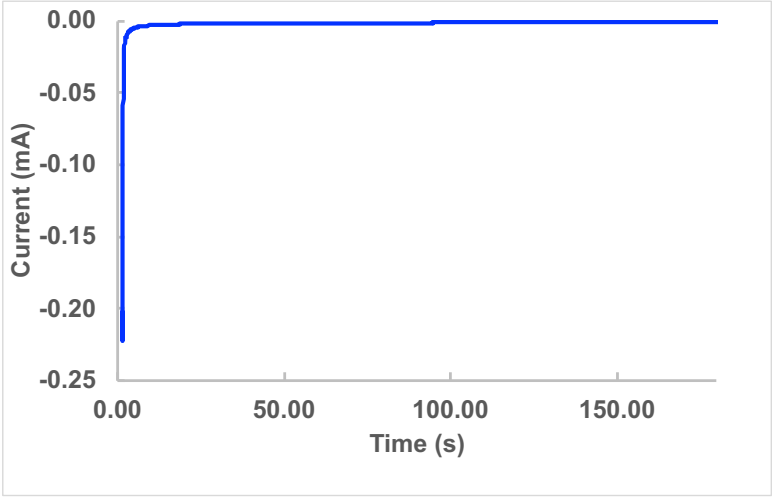


Figure S23. Representative current of electrochemical cell over time under constant potential electrolysis (-1.54 V vs Fc/Fc^+ here). By the time the UV/Vis spectrum was recorded most of the current had passed to generate the reduced species.

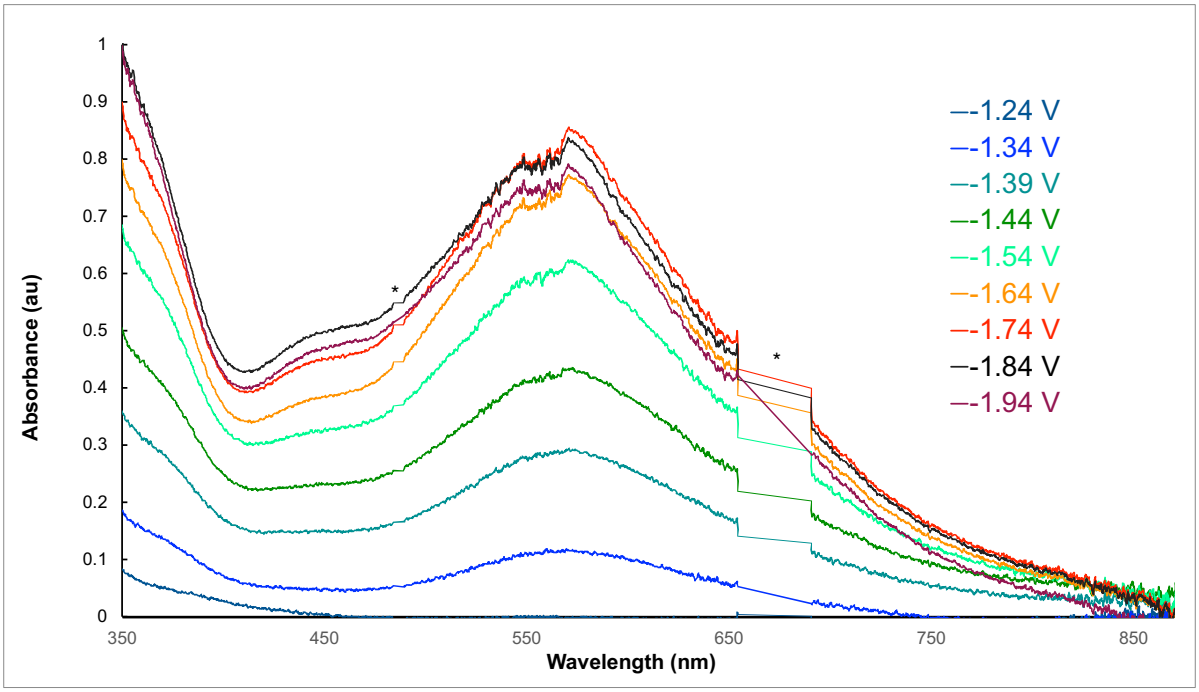


Figure S24. UV/Vis spectroelectrochemical absorbance spectra during stepwise potential scan. Potentials listed are relative to Fc/Fc^{+}. Shown spectra are taken after 2.5 minutes of electrolysis. * Indicates signal saturation inherent to light source and detector used for experiment.

8. Electrocatalytic Imine Alkylation

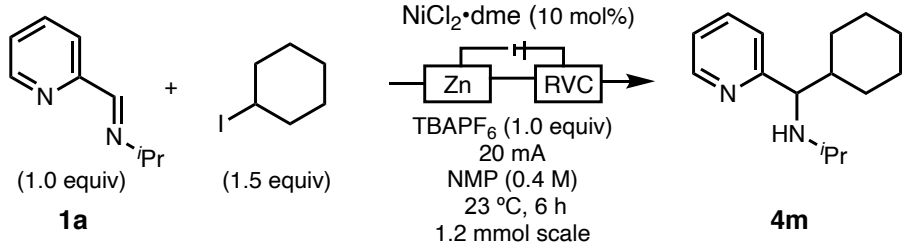
8.1. General Procedure 4: Electrolysis on 1.2 mmol Scale:

In a N_2-filled glovebox, to an oven-dried standard 5 mL ElectraSyn vial charged with a stir bar was added $NiCl_2$·dme (26.4 mg, 0.12 mmol, 0.1 equiv) and $TBAPF_6$ (456 mg, 1.2 mmol, 1 equiv). The solids were then dissolved in 3mL of NMP (0.4 M) and stirred for 10 minutes. To the blue solution was then added heteroaryl imine (1.2 mmol, 1 equiv) causing the solution to turn light green followed by alkyl halide (1.5 equiv, 1.8 mmol). The threading of the vial was then lined with teflon tape and the vial cap fitted with Zn^0 anode (counter electrode) and RVC cathode (working electrode) was attached. The cell was then removed from the glovebox and attached to the Electrasyn 2.0 where the following setup was employed: *New exp. -> Constant current -> -20 mA -> no ref. electrode -> no alternating polarity -> start.* The reaction was stirred at room temperature for 6 hours. The resulting dark solution was diluted with CH_2Cl_2 (30 ml) and extracted 3x with 1N HCl (30 ml). To the combined aqueous phases was added K_2CO_3 (s) until gas evolution ceased and the pH ~9. The resulting aqueous solution was extracted 3x with EtOAc (50 mL) and the combined organic phases were dried with

Na_2SO_4, filtered through celite and then concentrated under reduced pressure. The crude material was purified by column chromatography to afford the desired products.

8.2. Optimization of Electroreductive Alkylation Reaction

General Details: All reactions were performed according to General Procedure 4 on a 1.2 mmol scale unless specified otherwise. Reaction yields were determined by ^{1}H NMR using 1,1,2,2-tetrachloroethylene as an internal standard added after workup.



Deviation from Standard Conditions	*Yield %*
None	63
0.2 M, 10 mA	28
10 mA, 12h	59
30 mA, 1h	58
TMSCl (2 equiv)	58
3.2h (2 equiv of e^-)	63
Mg^0 sacrificial anode	43
Al^0 sacrificial anode	35
TBACl (0.2 M) as electrolyte	51
No $NiCl_2$•dme	0
0 mA	44
Divided Cell, 11.11 mA	37*
Ni^0 sacrifical anode, No $NiCl_2$•dme	50
$CoCl_2$ (10 mol%) as catalyst	53
$MnCl_2$ (10 mol%) as catalyst	7

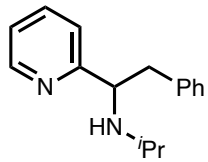
Table S2. Optimization table and control experiments for electroreductive alkylation. * indicates voltage overload due to the high resistance of the divided cell (94% yield based on amount of current passed).

Divided Cell Experiment: Divided cell electrolysis was performed on an H-Cell type electrochemical cell on a 2.0 mmol scale. Due to the high resistance of the divided cell setup,

the reaction reached its safety voltage limit after 3.75 h corresponding limiting the reaction to a 39% theoretical yield based on the amount of electrons passed. Each cell was analyzed individually to ensure there was not significant substrate diffusion over the course of the reaction which was confirmed by finding the anodic cell had <5% of **1a** and no **4m** could be detected.

8.3. Chracterization of Reaction Products: Scheme 2

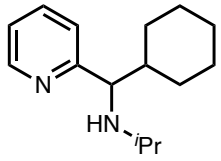
***N*-(2-phenyl-1-(pyridin-2-yl)ethyl)propan-2-amine (3a)**



Prepared from imine **1a** (178 mg, 1.2 mmol, 1 equiv) and benzyl bromide (214 µL, 1.8 mmol, 1.5 equiv) and following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 3:2 w/ 1% Et_3N) afforded **3a** (210 mg, 0.88 mmol, 73%) as a colorless oil.

See Section 4.4 for **3a** characterization.

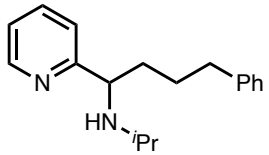
***N*-(cyclohexyl(pyridin-2-yl)methyl)propan-2-amine (4m)**



Prepared from imine **1a** (178 mg, 1.2 mmol, 1 equiv) and cyclohexyliodide (233 µL, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 3:2 w/ 1% Et_3N) afforded **4m** (165 mg, 0.71 mmol, 59%) as a yellow oil.

See Section 4.4 for **4m** characterization.

***N*-isopropyl-4-phenyl-1-(pyridin-2-yl)butan-1-amine (4s)**



Prepared from imine **1a** (178 mg, 1.2 mmol, 1 equiv) and 1-iodo-3-phenylpropane (290 µL, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 3:2 w/ 1% Et_3N) afforded **4s** (164 mg, 0.61 mmol, 51%) as a yellow oil.

R_f = 0.32 (silica, Hex/EtOAc 3:2 w/ 1% Et_3N, UV).

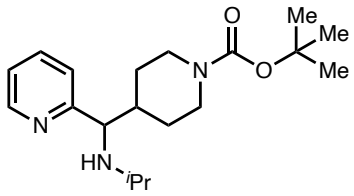
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.56 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.60 (td, J = 7.6, 1.8 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.17 – 7.09 (m, 5H), 3.79 (dd, J = 7.5, 6.3 Hz, 1H), 2.57 (t, J = 7.7 Hz, 2H), 2.52 (p, J = 6.2 Hz, 1H), 1.83 – 1.68 (m, 3H), 1.67 – 1.55 (m, 1H), 1.51 – 1.39 (m, 1H), 1.02 (d, J = 6.1 Hz, 3H), 0.96 (d, J = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 164.66, 149.94, 142.87, 136.53, 128.85, 128.68, 126.10, 122.71, 122.21, 61.69, 46.24, 37.51, 36.40, 28.71, 24.59, 22.64.

FTIR (NaCl, thin film, cm^{-1}): 2960, 2858, 1588, 1432, 1367, 747, 698

HRMS (FD, m/z): calc'd for $C_{18}H_{24}N_2$ $[M]^+$: 268.19340; found: 268.19358.

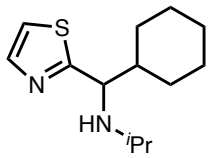
***tert*-butyl 4-((isopropylamino)(pyridin-2-yl)methyl)piperidine-1-carboxylate (4o)**



Prepared from imine **1a** (178 mg, 1.2 mmol, 1 equiv) and 1-boc-4-iodo-piperidine (560 mg, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 3:2 w/ 1% Et_3N) afforded **4o** (173 mg, 0.52 mmol, 43%) as a white solid.

See Section 4.4 for **4o** characterization.

***N*-isopropyl-4-phenyl-1-(pyridin-2-yl)butan-1-amine (4t)**



Prepared from imine **1q** (185 mg, 1.2 mmol, 1 equiv) and cyclohexyliodide (233 μL, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 4:1 w/ 1% Et_3N) afforded **4t** (172 mg, 0.72 mmol, 60%) as a yellow oil.

R_f = 0.67 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

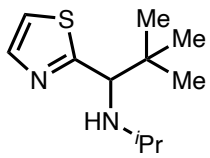
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 3.4 Hz, 1H), 7.22 (d, J = 3.3 Hz, 1H), 3.89 (d, J = 6.0 Hz, 1H), 2.67 (hept, J = 6.3 Hz, 1H), 1.85 – 1.57 (m, 5H), 1.57 – 1.43 (m, 2H), 1.29 – 1.06 (m, 4H), 1.04 (d, J = 6.2 Hz, 3H), 1.02 (d, J = 6.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 178.12, 142.63, 118.76, 63.95, 47.68, 45.04, 30.29, 29.76, 26.86, 26.68, 24.54, 22.75.

FTIR (NaCl, thin film, cm^{-1}): 2958, 2924, 2851, 1497, 1448, 1379, 1365, 1316, 1176, 1121, 1052, 776, 720.

HRMS (FD, m/z): calc'd for $C_{13}H_{22}N_2S$ $[M]^+$: 238.14982; found: 238.15067.

***N*-isopropyl-2,2-dimethyl-1-(thiazol-2-yl)propan-1-amine (4u)**



Prepared from imine **1q** (185 mg, 1.2 mmol, 1 equiv) and 2-iodo-2-methylpropane (215 μL, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 4:1 w/ 1% Et_3N) afforded **4u** (136 mg, 0.64 mmol, 53%) as a yellow oil.

R_f = 0.56 (silica, Hex/EtOAc 1:1 w/ 1% Et_3N, UV).

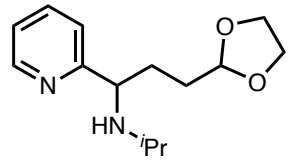
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 3.3 Hz, 1H), 7.23 (d, J = 3.2 Hz, 1H), 3.77 (s, 1H), 2.57 (hept, J = 6.2 Hz, 1H), 1.01 (d, J = 6.1 Hz, 3H), 0.98 (m, 3H), 0.97 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 176.43, 142.29, 118.77, 67.79, 47.62, 35.23, 27.41, 24.61, 22.46.

FTIR (NaCl, thin film, cm^{-1}): 2960, 2866, 1495, 1475, 1367, 1175, 1120, 1089, 1053, 854, 722.

HRMS (FD, m/z): calc'd for $C_{11}H_{20}N_2S$ $[M]^+$: 212.13417; found: 212.13459.

3-(1,3-dioxolan-2-yl)-*N*-isopropyl-1-(pyridin-2-yl)propan-1-amine (4v)



Prepared from imine **1a** (178 mg, 1.2 mmol, 1 equiv) and 2-(2-iodoethyl)-1,3-dioxolane (410 mg, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 3:2 w/ 1% Et_3N) afforded **4v** (158.7 mg, 0.64 mmol, 53%) as a yellow oil.

R_f = 0.24 (silica, Hex/EtOAc 3:2 w/ 1% Et_3N, UV).

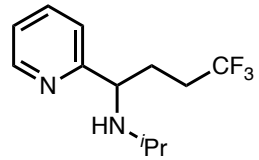
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (ddd, J = 4.9, 1.8, 0.9 Hz, 1H), 7.65 – 7.56 (m, 1H), 7.25 – 7.22 (m, 1H), 7.18 – 7.05 (m, 1H), 4.82 (t, J = 4.6 Hz, 1H), 3.97 – 3.89 (m, 2H), 3.86 (ddd, J = 12.1, 4.6, 0.7 Hz, 1H), 3.81 – 3.76 (m, 2H), 2.56 (hept, J = 6.2 Hz, 1H), 1.90 – 1.72 (m, 3H), 1.73 – 1.60 (m, 1H), 1.57 – 1.43 (m, 1H), 1.02 (d, J = 6.1 Hz, 3H), 0.96 (d, J = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 164.05, 149.61, 136.25, 122.41, 121.94, 104.58, 65.01, 64.98, 61.12, 45.97, 31.50, 30.76, 24.17, 22.44.

FTIR (NaCl, thin film, cm^{-1}): 2960, 2929, 1589, 1569, 1464, 1432, 1365, 1137, 1036, 747.

HRMS (ESI, m/z): calc'd for $C_{14}H_{23}N_2O_2$ [M+H]: 251.1754; found: 251.1857.

4,4,4-trifluoro-*N*-isopropyl-1-(pyridin-2-yl)butan-1-amine (4w)



Prepared from imine **1a** (178 mg, 1.2 mmol, 1 equiv) and 1,1,1-trifluoro-3-iodopropane (211 µL, 1.8 mmol, 1.5 equiv) following General Procedure 4. Purification of the crude residue by silica gel column chromatography (Hex/EtOAc 3:2 w/ 1% Et_3N) afforded **4w** (145 mg, 0.59 mmol, 49%) as a yellow oil.

R_f = 0.53 (silica, Hex/EtOAc 3:2 w/ 1% Et_3N, UV).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (ddd, J = 4.8, 1.8, 1.0 Hz, 1H), 7.64 (td, J = 7.6, 1.8 Hz, 1H), 7.21 (dt, J = 7.8, 1.1 Hz, 1H), 7.17 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 3.77 (t, J = 6.8 Hz, 1H), 2.54 (hept, J = 6.2 Hz, 1H), 2.35 – 2.11 (m, 1H), 2.11 – 1.96 (m, 1H), 1.96 – 1.84 (m, 2H), 1.75 (s, 1H), 1.01 (d, J = 6.1 Hz, 3H), 0.96 (d, J = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.97, 149.91, 136.52, 127.73 (q, J = 277.4 Hz), 122.35, 122.28, 59.88, 45.84, 30.86 (q, J = 28.6 Hz), 29.46 (q, J = 2.8 Hz), 24.18, 22.34.

^{19}F NMR (282 MHz, $CDCl_3$): -66.2 (t, J = 10.8 Hz).

FTIR (NaCl, thin film, cm^{-1}): 3309, 2996, 2964, 1590, 1571, 1471, 1452, 1434, 1382, 1337, 1289, 1251, 1134, 1091, 1023, 787, 749

HRMS (ESI, m/z): calc'd for $C_{12}H_{18}N_2F_3$ [M+H]: 247.1417; found: 247.1851

9. Computational Details

General Details: All density functional theory (DFT) calculations were carried out using the ORCA 4.2 software package.[12] Geometry optimizations and numerical frequency calculations were carried out using the B3LYP hybrid functional.[13] 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[14] approximation was used for the exchange integrals (RIJCOSX). Weigend's coulomb fitting auxiliary basis set[15] (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 keywords. Broken symmetry calculations were performed using the method described by Ginsberg[16] and Noodleman *et al*[17]. The broken symmetry notation (*m,n*)[18] 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[19] and orbital/density surfaces with the program *ChemCraft*.[20]

9.1. 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
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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)

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! 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
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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

```
! 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

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)

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

% pal nprocs 16 # num of processors
end
```

```
%maxcore 9000
%method
Z_solver DIIS
end


* xyz 0 2
28      1.820504000     2.710304000    -0.462278000
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
6       3.241551000     0.241976000    -0.535267000
7       3.314755000     1.482274000    -1.009712000
6       4.399285000     1.933652000    -1.871706000
7       0.466660000     4.144535000     0.430781000
6       0.969791000     5.074446000     1.436590000
6      -0.587175594     4.338434098    -0.251245236
6      -0.871256000     3.368339000    -1.353266000
7       0.128340000     2.503397000    -1.621594000
6       0.003177000     1.612616000    -2.606858000
6      -1.145336000     1.530870000    -3.398371000
6      -2.189476000     2.420140000    -3.141325000
6      -2.051919000     3.353557000    -2.110629000
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1       2.465272000    -2.155223000     0.648204000
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1       6.319969000     2.956801000    -1.734309000
1       5.134877000     3.404343000    -0.479095000
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1       3.872757602    -0.666009171    -0.718639988
*
```

Optimized coordinates – $(1a)_2Ni^{I}Cl$

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
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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
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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
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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

9.2. Calculated Geometries of 9 and 9^{ox}

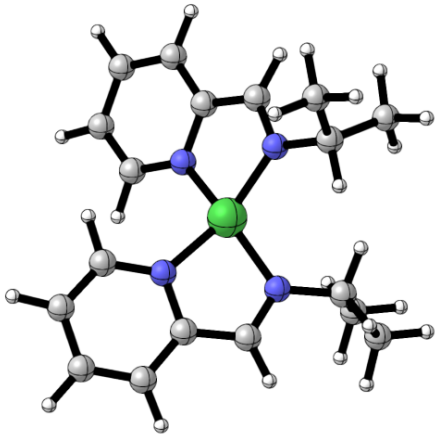

Figure S25: "BS(0,0)" low spin optimized geometry of **9**.

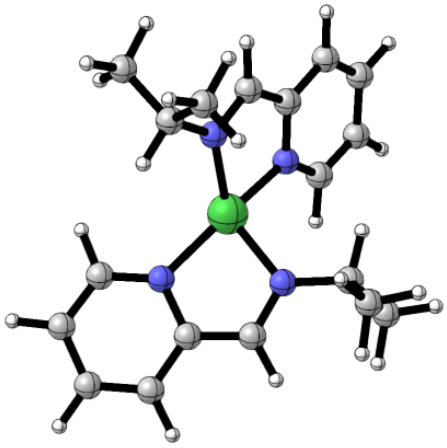

Figure S26: "BS(0,0)" high spin optimized geometry of **9**.

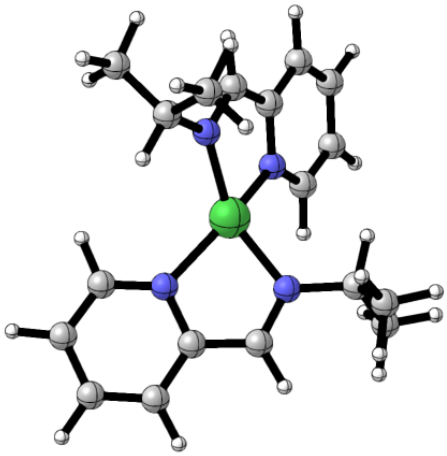

Figure S27: BS(2,2) optimized geometry of **9**.

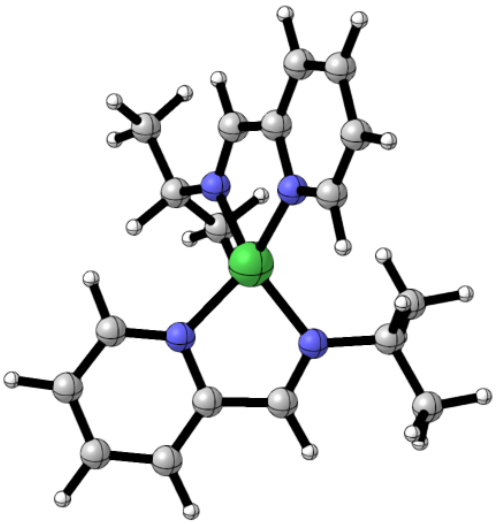

Figure S28: Optimized geometry of **9^{ox}** cation.

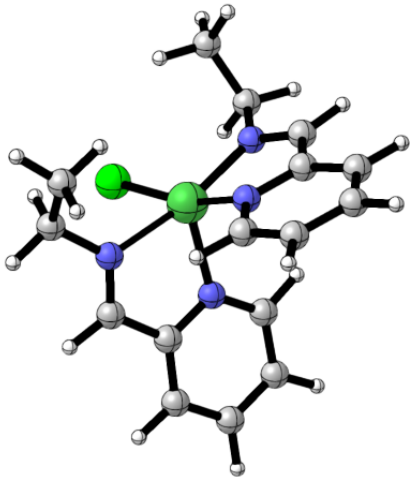

Figure S29: Optimized geometry of neutral **9^{ox}-Cl** complex (not featured in text).

9.3. Qualitative MO diagram of BS(2,2) 9

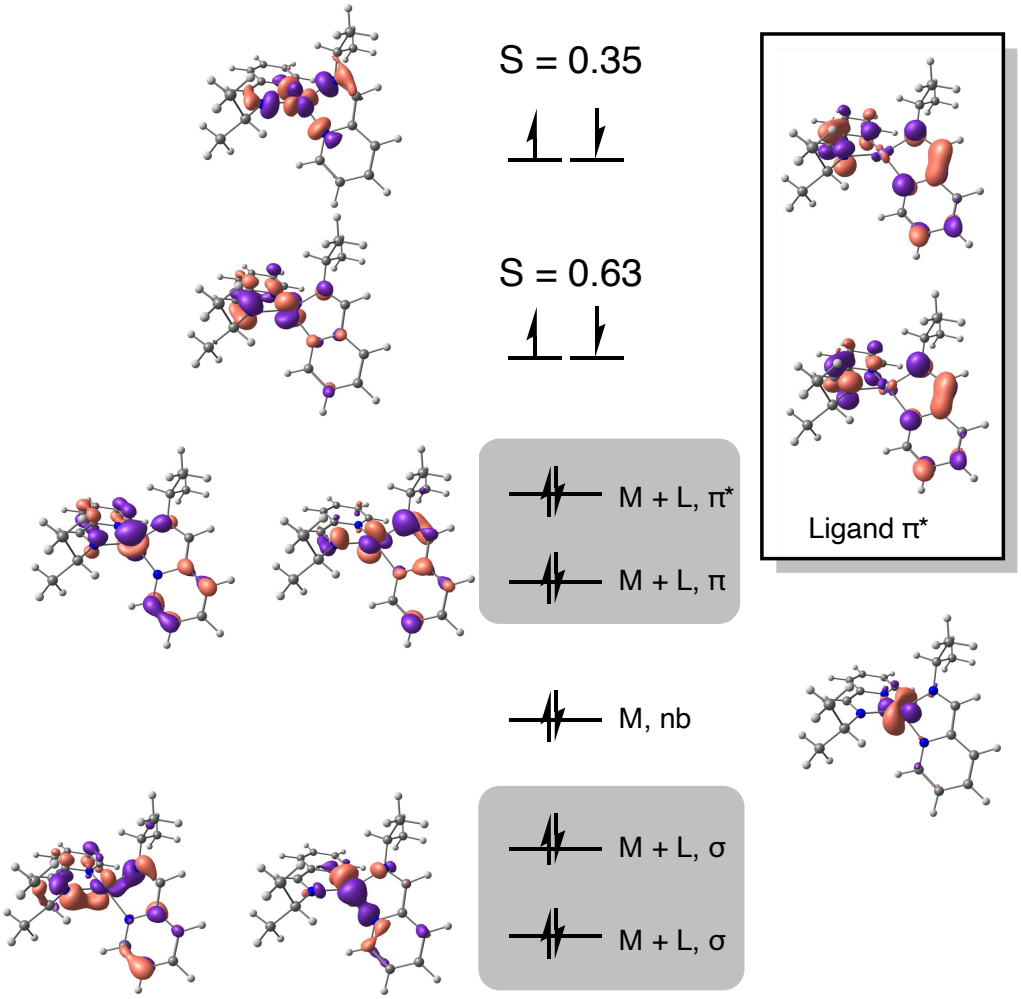

Figure S30: Qualitative MO diagram of BS(2,2) **9** with spatial overlap values for S<0.999. Assignments of M (metal-based) or L (ligand-based) are made based on Ni d character or the corresponding orbital.

10. X-Ray Diffraction Data

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 Cu K_α radiation (λ = 1.54178 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.[21] Absorption corrections were applied using SADABS.[22] The structure was solved by intrinsic phasing using SHELXT[23] and refined against F2 on all data by full-matrix least squares with SHELXL-2017[24] using established refinement techniques.[25] 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'**, **10**, and **11** 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.[26]

Table S3: 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] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(Fo^2)^2]]^{1/2}$.

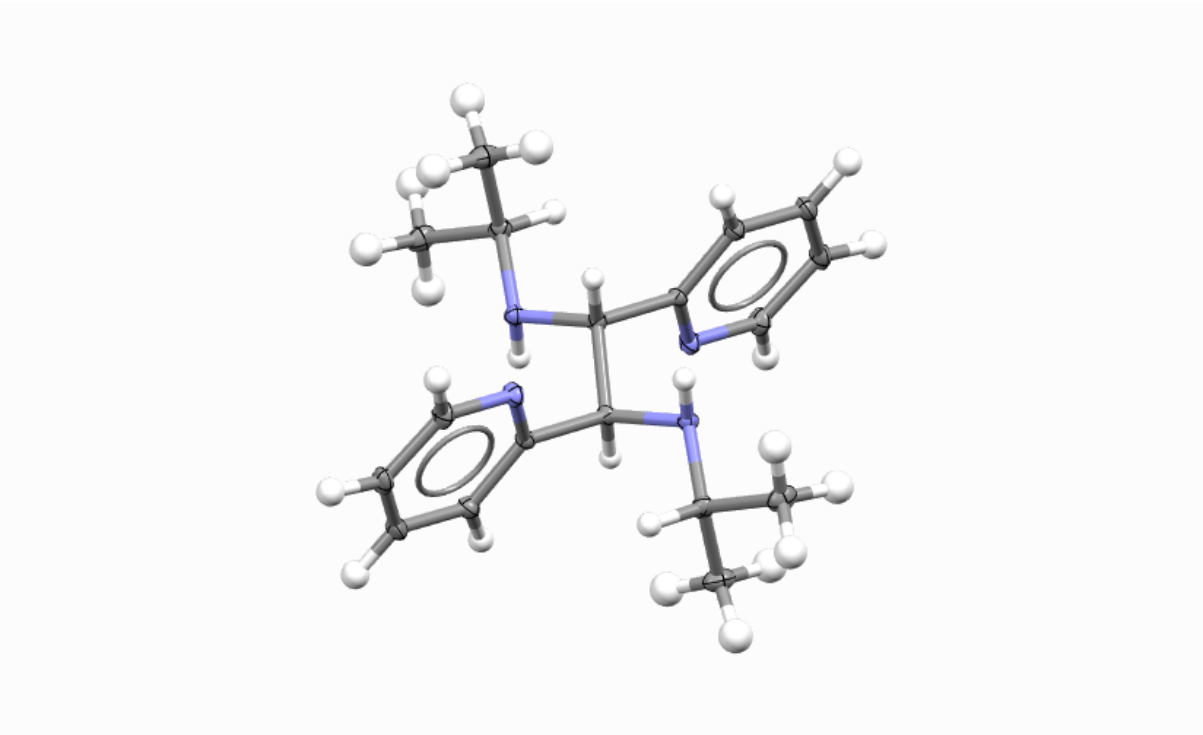

Figure S31: Structure of **1a'**with 50% probability anisotropic displacement ellipsoids.

Table S4: Crystal and Refinement Data for 10

CCDC Number	2117478
Formula	$C_{18}H_{24}N_4Cl_2Ni$
Formula Weight	426.02
Crystal System	monoclinic
Space Group	$P2_1/c$
a, Å	14.142(5)
b, Å	25.845(7)
c, Å	11.136(4)
α, °	90
β, °	91.374(17)
γ, °	90
Volume, Å	4069(2)
T (K)	100
d_{calc}, g/cm ^{3}	1.391
Z	8
R_1,[a] wR_2,[b] [I>2σ(I)]	0.0549, 0.1487
GOF	1.033

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

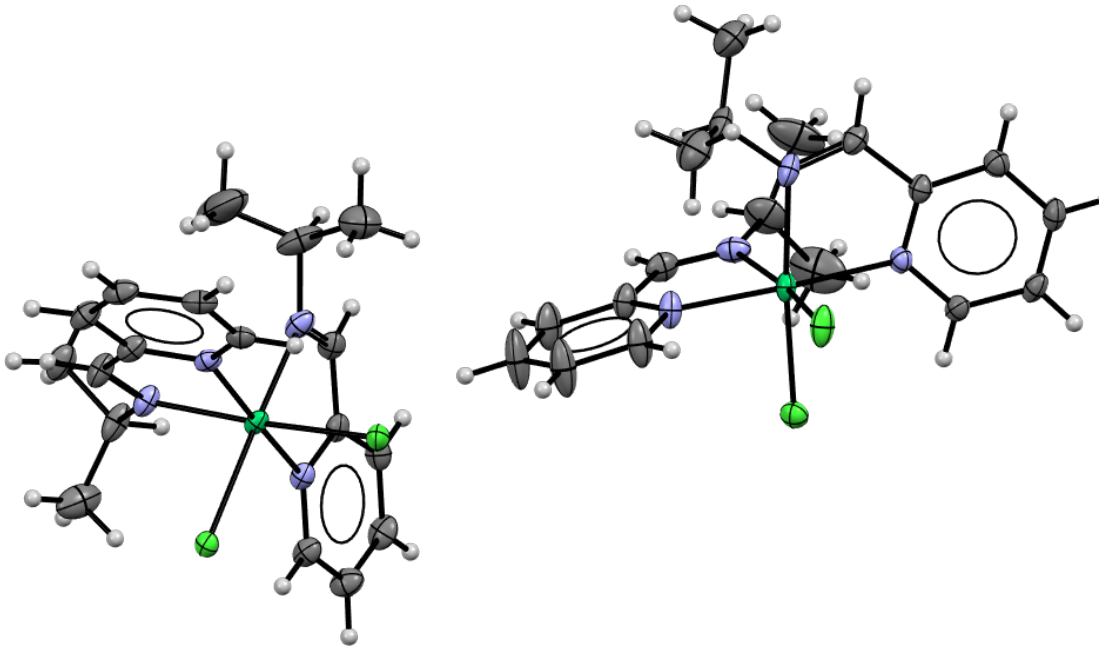

Figure S32: Structure of **10** with 50% probability anisotropic displacement ellipsoids. compound crystallized with two molecules in the asymmetric unit.

Table S5: Crystal and Refinement Data for 11

CCDC Number	2117477
Formula	$C_{18}H_{24}N_4Cl_2Mn$
Formula Weight	422.261
Crystal System	Orthorhombic
Space Group	$P2_12_12_1$
a, Å	11.185(6)
b, Å	13.024(7)
c, Å	13.725(11)
α, °	90
β, °	90
γ, °	90
Volume, Å	1999(2)
T (K)	100
d_{calc}, g/cm ^{3}	1.403
Z	4
R_1,[a] wR_2,[b] [I>2σ(I)]	0.0486, 0.0819
GOF	1.010

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

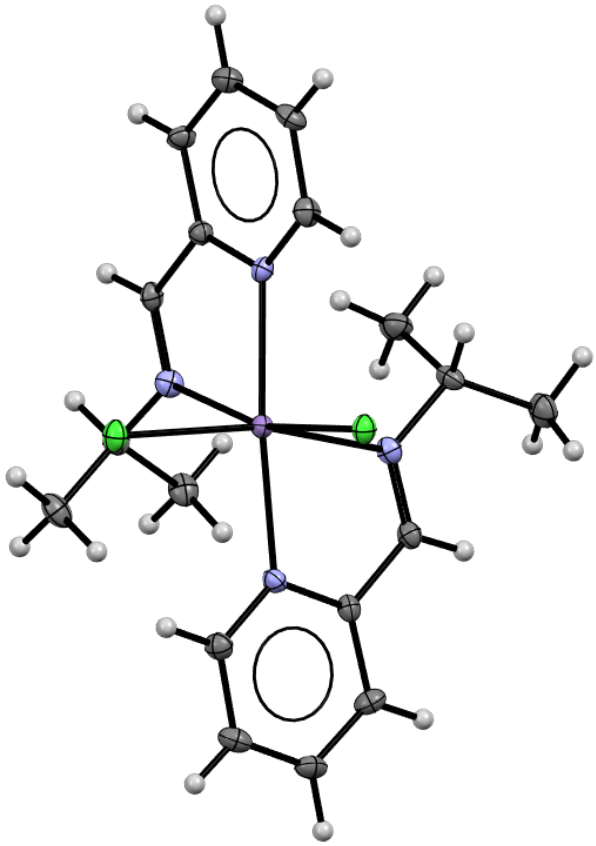

Figure S33: Structure of **11** with 50% probability anisotropic displacement ellipsoids.

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 **S34**) and amount of trace Ni in sample A was corrected for matrix/digestion effects determined by samples B and C.

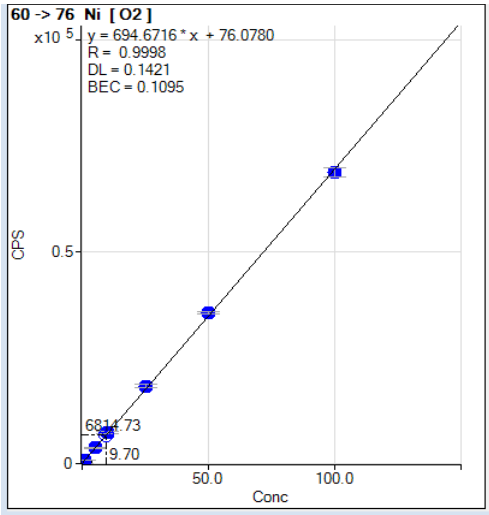

Figure S34: Ni calibration curve of measured counts/s against concentration in ppb.

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 S6: 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, each reaction on a 0.3 mmol scale described by general procedure 3 has ~900 ng of nickel species (0.005 mol%) added through the addition of our Mn^0 reductant.

12. References

[1] W. C. Still, M. Kahn, A. Mitra, *J. Org. Chem.* **1978**, *43*, 2923–2925.
[2] N. Suzuki, J. L. Hofstra, K. E. Poremba, S. E. Reisman, *Org. Lett.* **2017**, *19*, 2150–2153.
[3] L. M. Kammer, A. Rahman, T. Opatz, *Molecules* **2018**, *23*, 764.
[4] Y. Jiang, J. Pan, T. Yang, Y. Zhao, M. J. Koh, *Chem* **2021**, *7*, 993–1005.
[5] L. R. Mills, C. Zhou, E. Fung, S. A. L. Rousseaux, *Org. Lett.* **2019**, *21*, 8805–8809.

[6] Z. Peng, P. Knochel, *Org. Lett.* **2011**, *13*, 3198–3201.

[7] J. Roberto Pioquinto-Mendoza, D. Martínez-Otero, N. Andrade-López, J. G. Alvarado-Rodríguez, V. Salazar-Pereda, G. Sánchez-Cabrera, F. J. Zuno-Cruz, *Polyhedron* **2013**, *50*, 289–296.
[8] S. Daniele, M. Martelli, G. Bontempelli, *Inorganica Chimica Acta* **1991**, *179*, 105–111.
[9] C. Sandford, L. R. Fries, T. E. Ball, S. D. Minteer, M. S. Sigman, *J. Am. Chem. Soc.* **2019**, *141*, 18877–18889.
[10] S. Hoops, S. Sahle, R. Gauges, C. Lee, J. Pahle, N. Simus, M. Singhal, L. Xu, P. Mendes, U. Kummer, *Bioinformatics* **2006**, *22*, 3067–3074.
[11] C. C. Lu, E. Bill, T. Weyhermüller, E. Bothe, K. Wieghardt, *J. Am. Chem. Soc.* **2008**, *130*, 3181–3197.
[12] F. Neese, *WIREs Computational Molecular Science* **2012**, *2*, 73–78; b) F. Neese, *WIREs Computational Molecular Science* **2018**, *8*, e1327.
[13] A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652.
[14] F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chemical Physics* **2009**, *356*, 98–109.
[15] F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057–1065.
[16] A. P. Ginsberg, *J. Am. Chem. Soc.* **1980**, *102*, 111–117.
[17] L. Noodleman, C. Y. Peng, D. A. Case, J.-M. Mouesca, *Coordination Chemistry Reviews* **1995**, *144*, 199–244.
[18] B. Kirchner, F. Wennmohs, S. Ye, F. Neese, *Current Opinion in Chemical Biology* **2007**, *11*, 134–141.
[19] C. Y. Legault, CYLview, 1.0b; Université de Sherbrooke: Québec, Montreal, Canada, **2009**; http://www.cylview.org
[20] Chemcraft - graphical software for visualization of quantum chemistry computations. https://www.chemcraftprog.com
[21]G. M. Sheldrick, "SADABS (version 2008/1): Program for Absorption Correction for Data from Area Detector Frames", University of Göttingen, **2008.**
[22] G. M. Sheldrick, SADABS (version 2008/1): Program for Absorption Correction for Data from Area Detector Frames. University of Göttingen, **2008**.
[23] G. M. Sheldrick, **2008** *Acta Cryst*., 64, 112-122.
[24] G. M. Sheldrick, **2015**, *Acta Cryst.,* A71, 3–8.
[25] P. Müller, *Crystallography Reviews* **2009**, *15*, 57–83.
[26] C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler, P. A. Wood, **2020**. *J. Appl. Cryst*. 53, 226-235.

13. NMR Data

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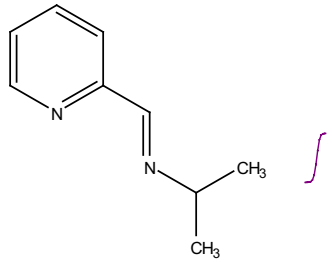

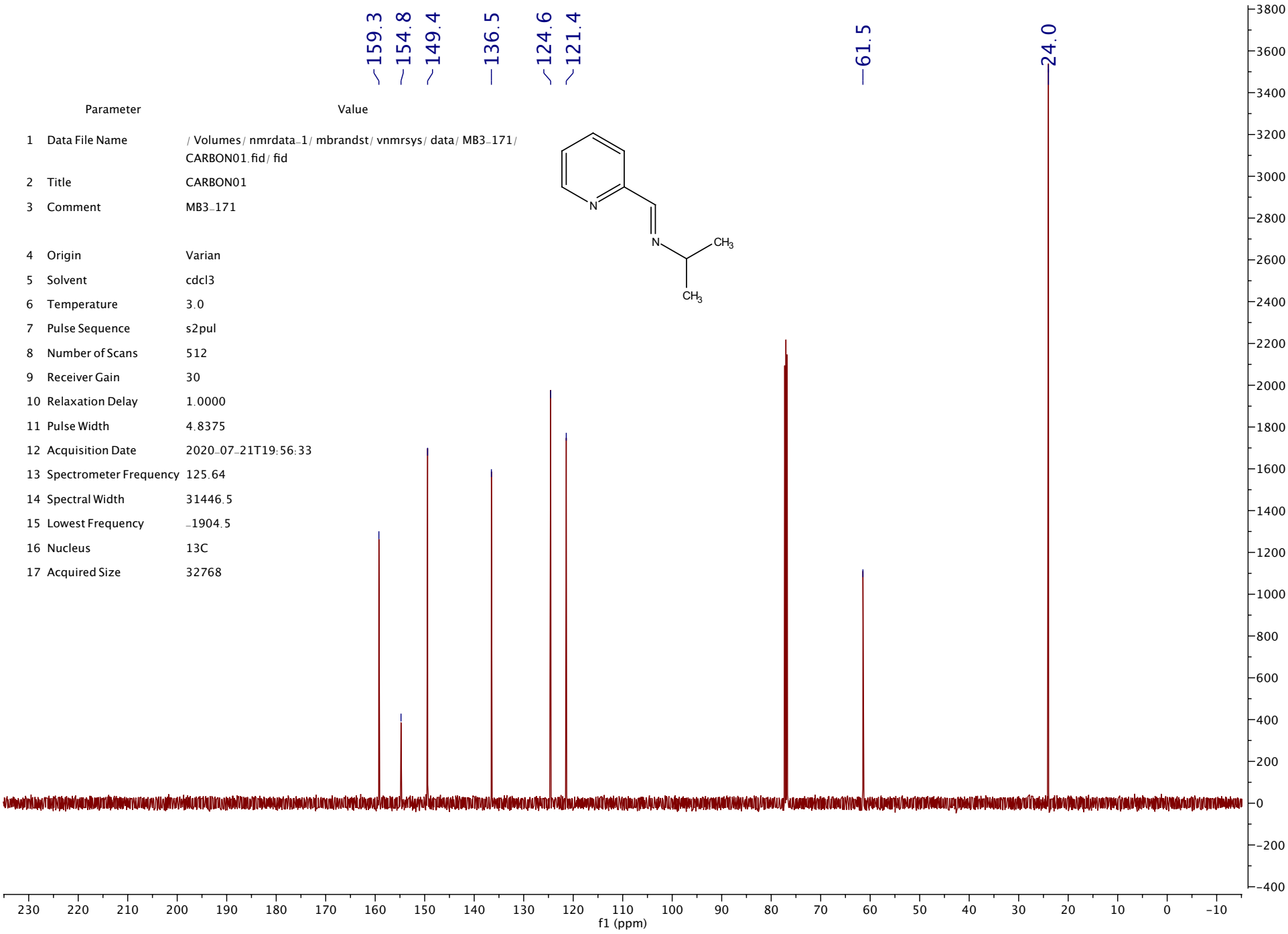

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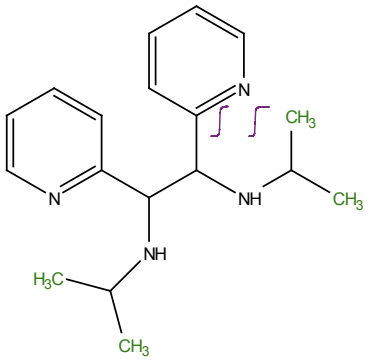

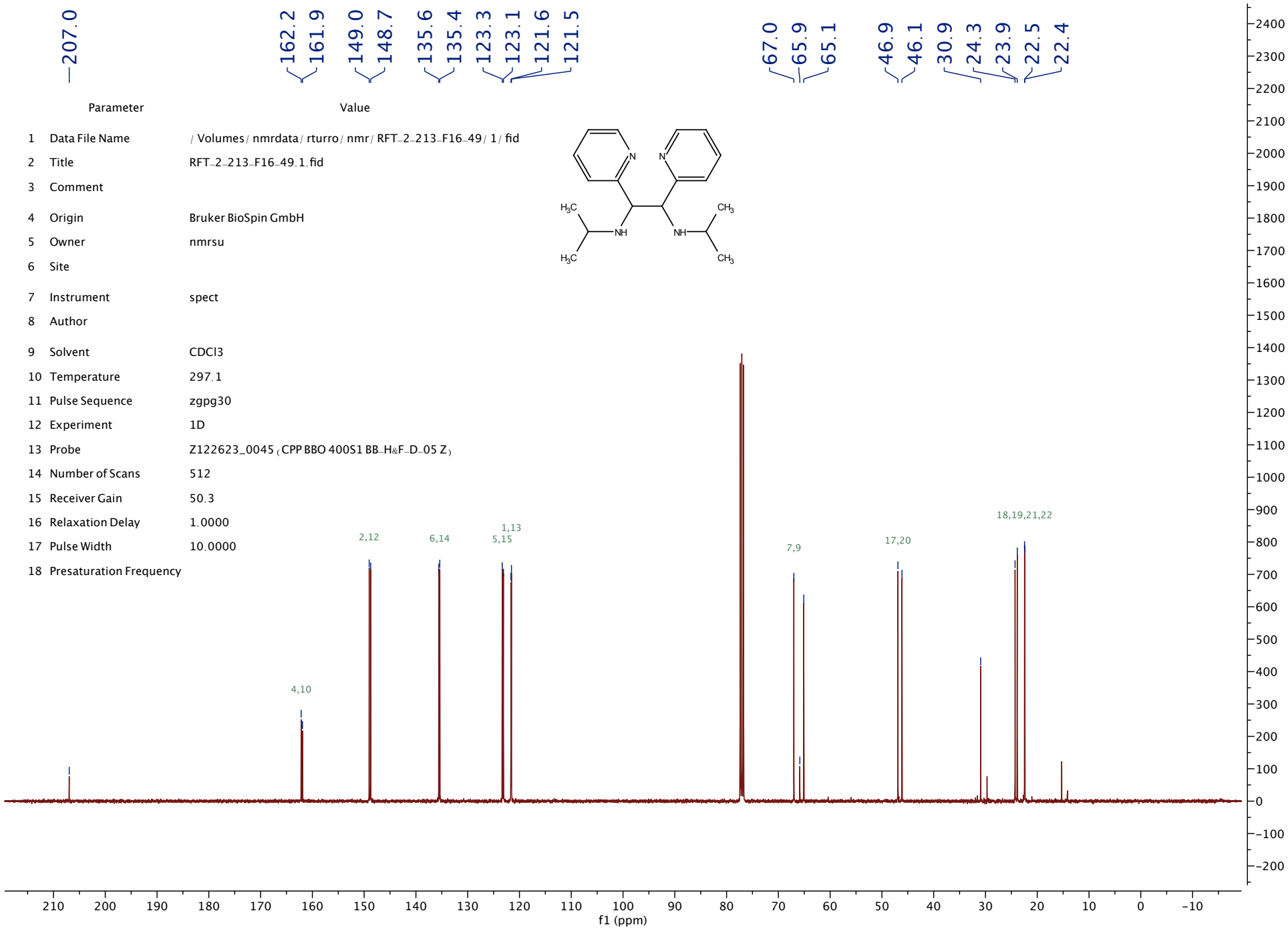
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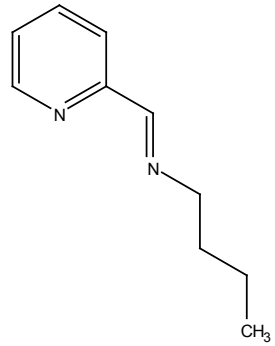
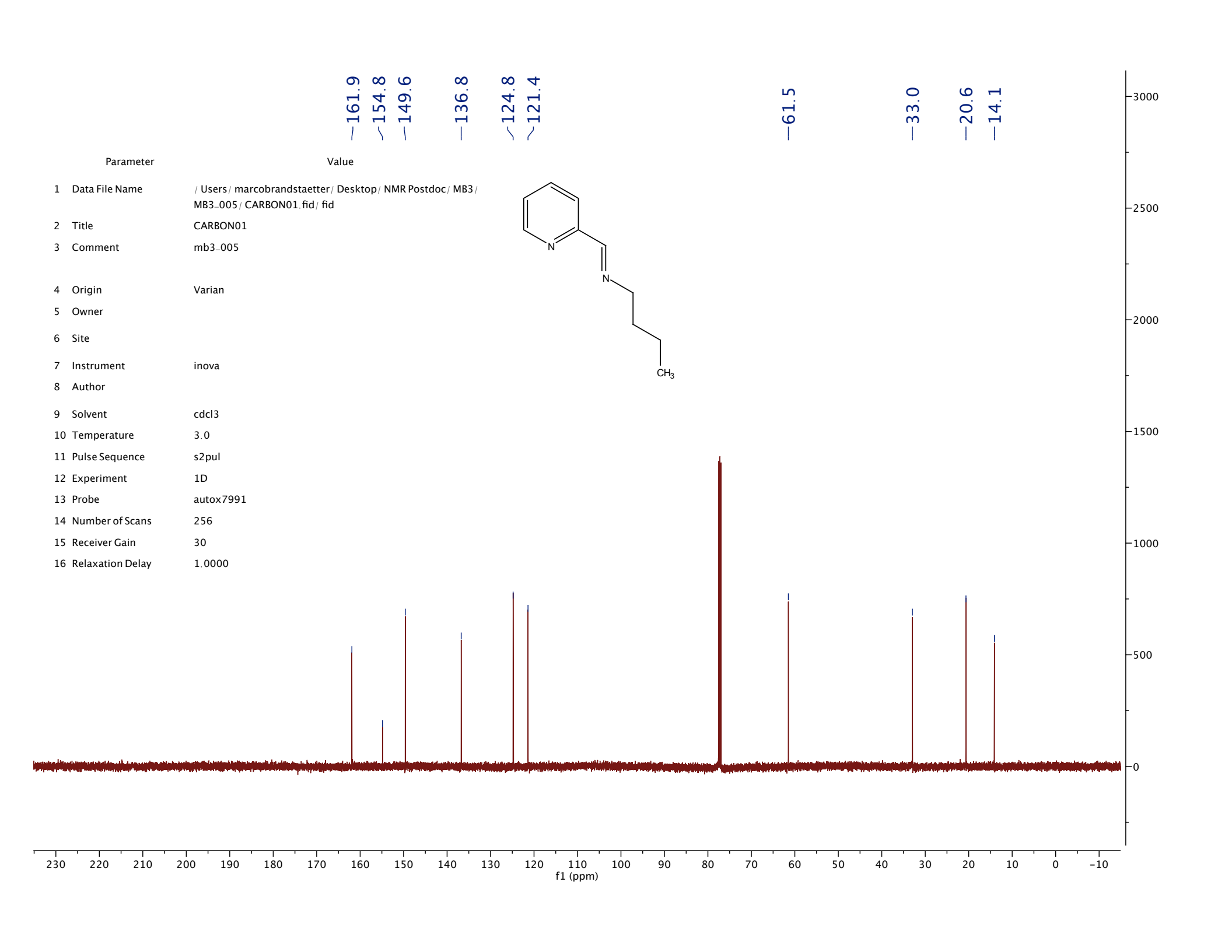
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	52
16	Relaxation Delay	1.0000




161.9
154.8
149.6
136.8
124.8
121.4
61.5
33.0
20.6
14.1
Parameter
Value
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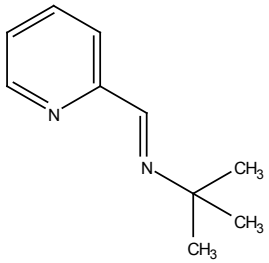
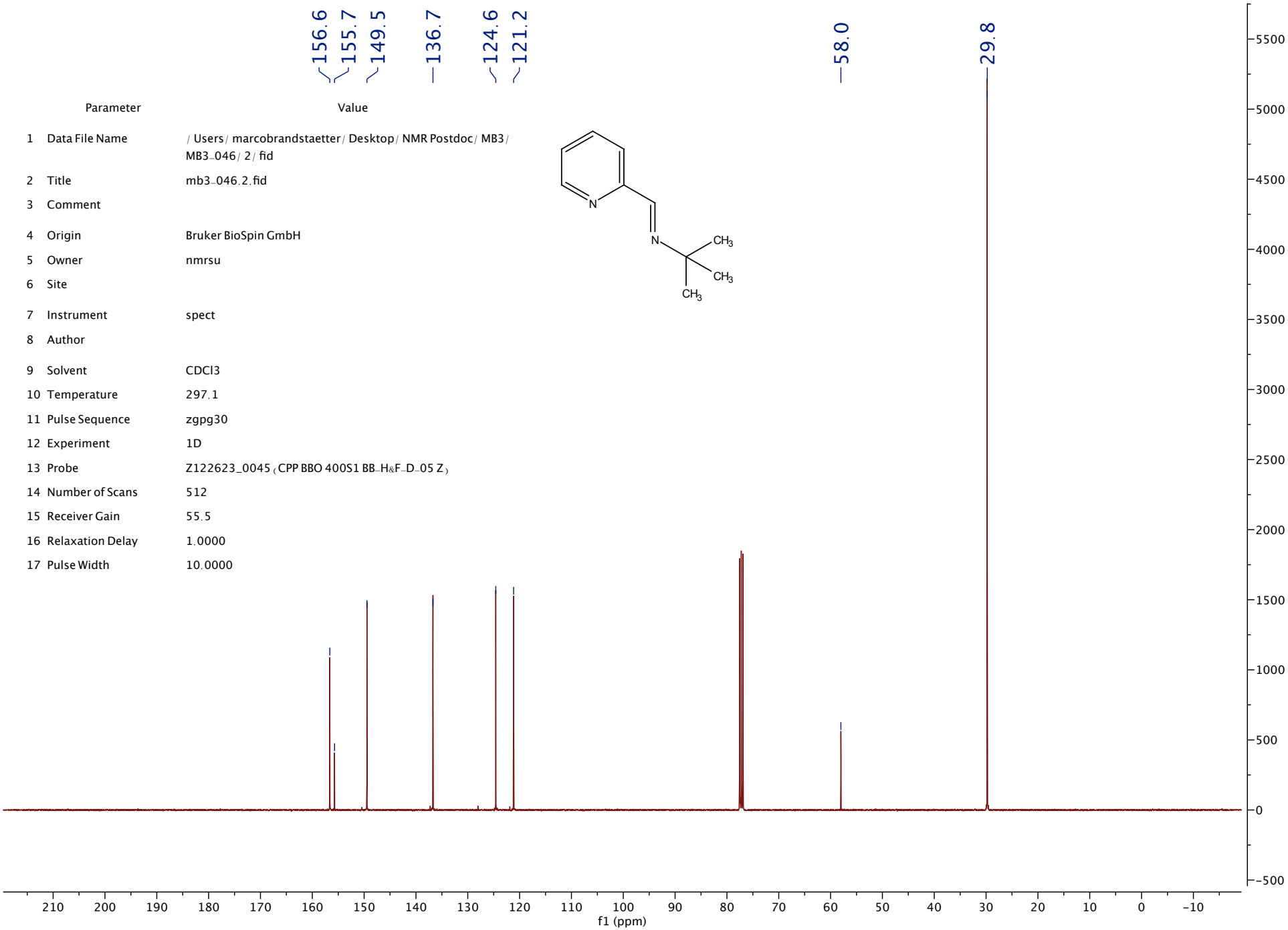
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_005 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
mb3_005
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
N
N
CH3
3000
2500
2000
1500
1000
500
0
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)

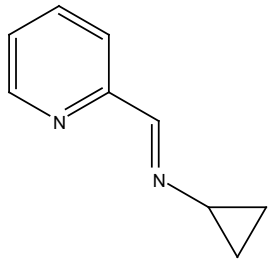
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_046 / 1 / fid
2	Title	mb3_046.1.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
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

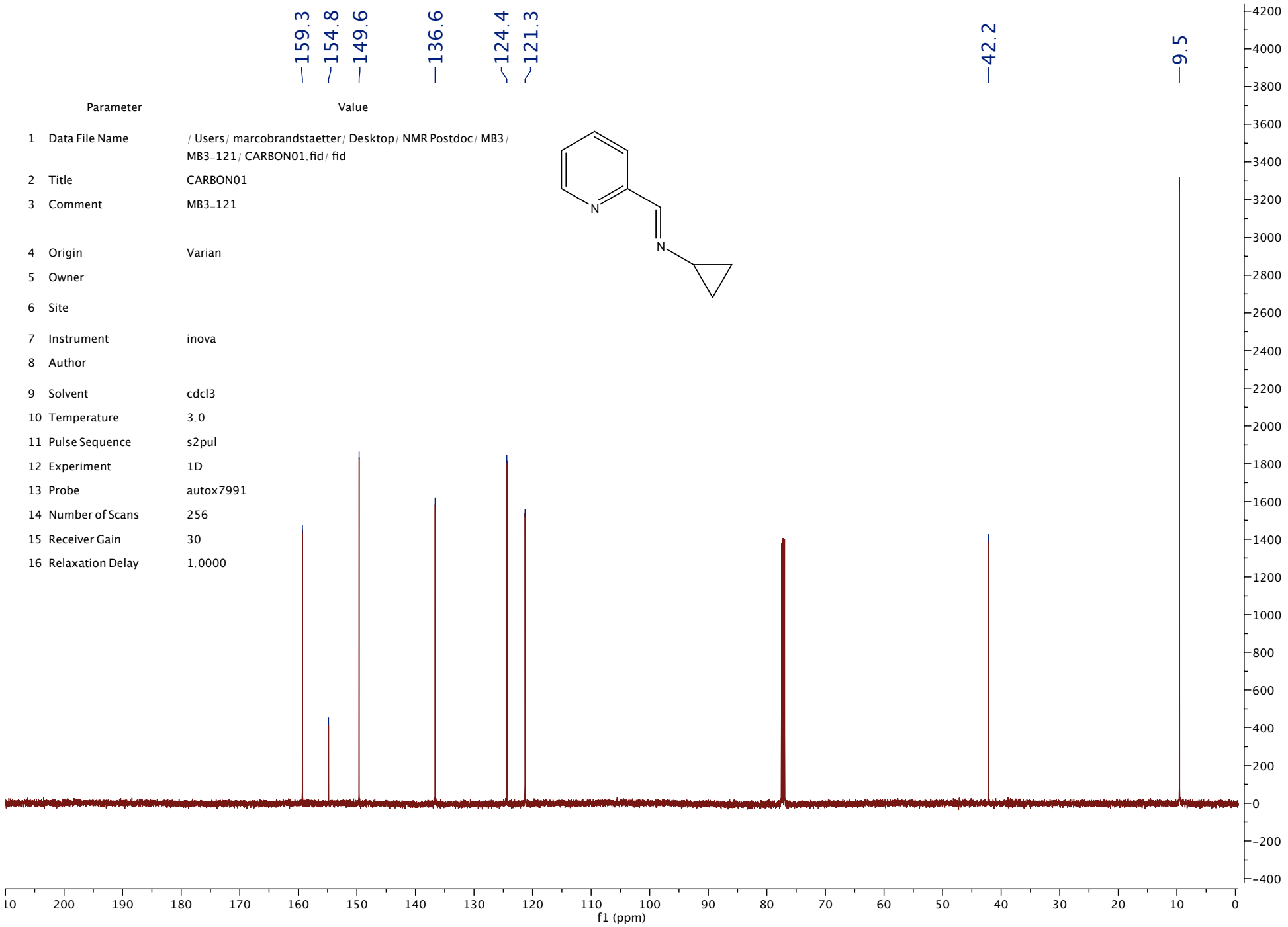




Parameter		Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_046 / 2 / fid
2	Title	mb3_046.2.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.1
11	Pulse Sequence	zgpg30
12	Experiment	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




159.3
154.8
149.6
136.6
124.4
121.3
42.2
9.5
Parameter
Value
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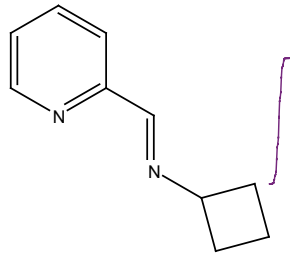
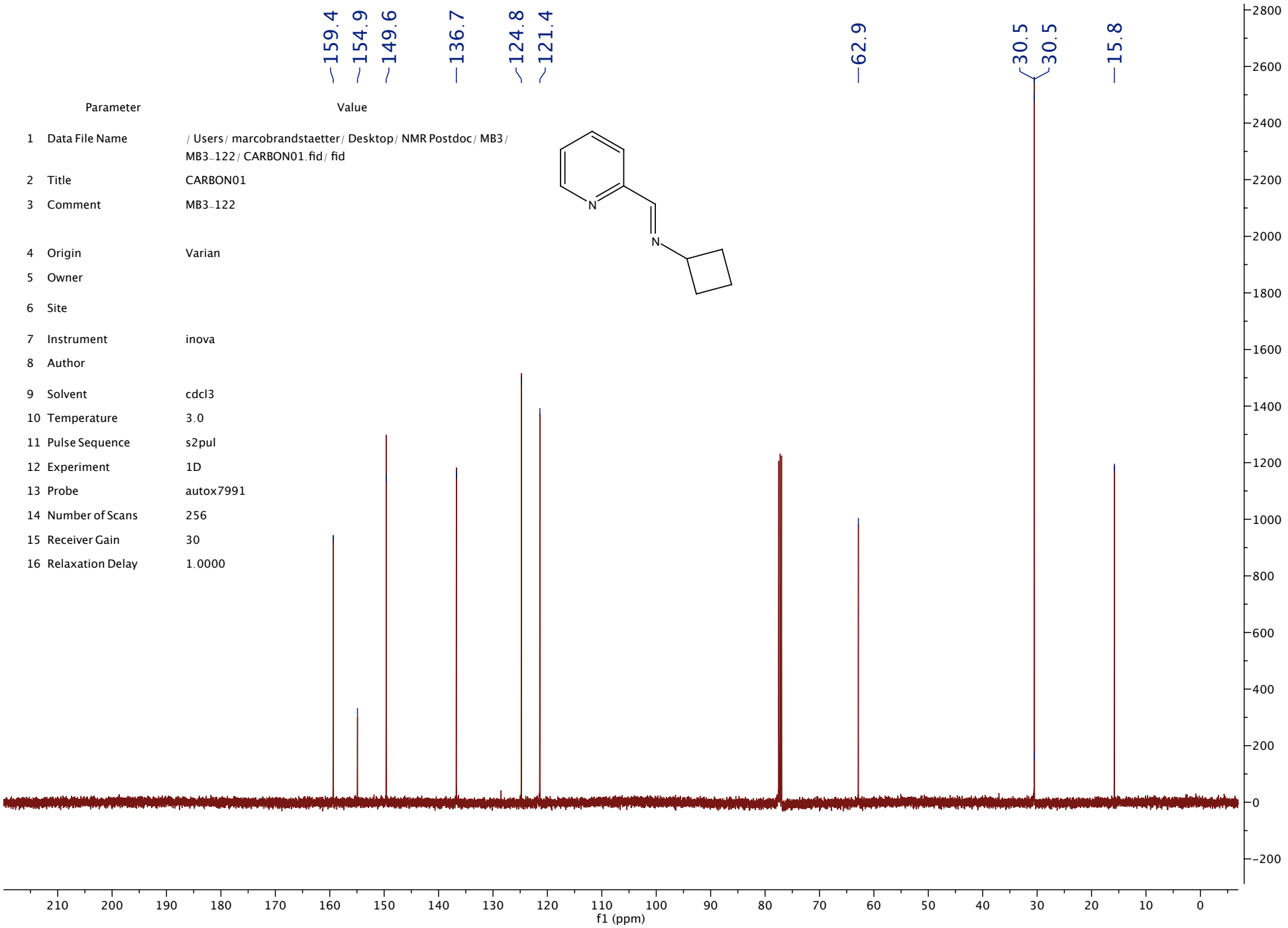
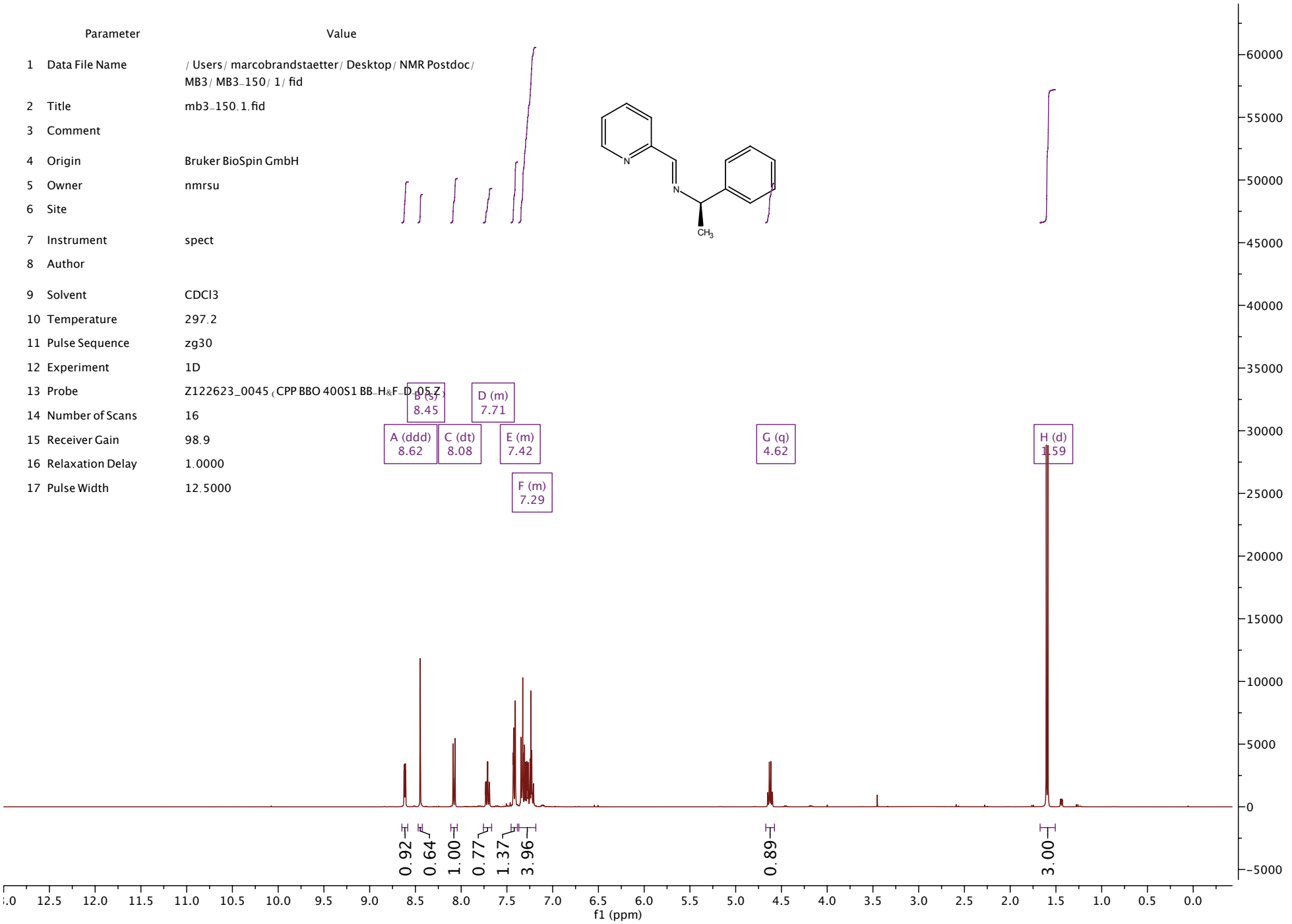
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_121 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
MB3_121
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 Receiver Gain
30
16 Relaxation Delay
1.0000
N
N
f1 (ppm)

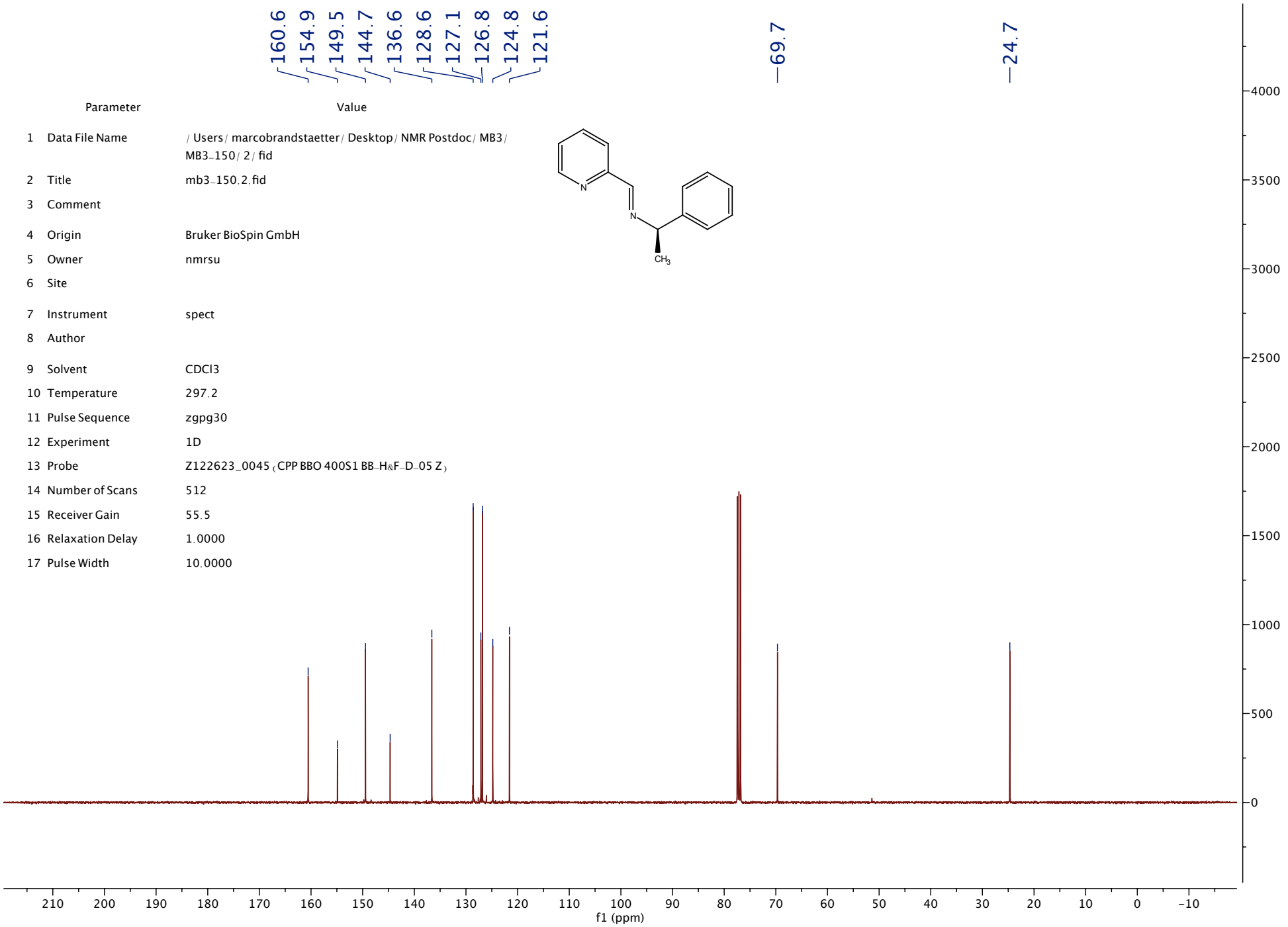
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_122 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB3_122
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe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



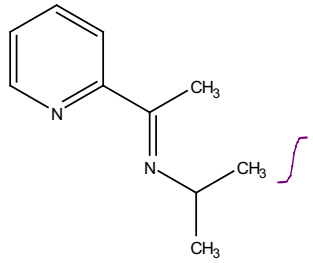

159.4
154.9
149.6
136.7
124.8
121.4
62.9
30.5
30.5
15.8
Parameter
Value
1 Data File Name
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_122 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
MB3_122
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
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
N
N
f1 (ppm)

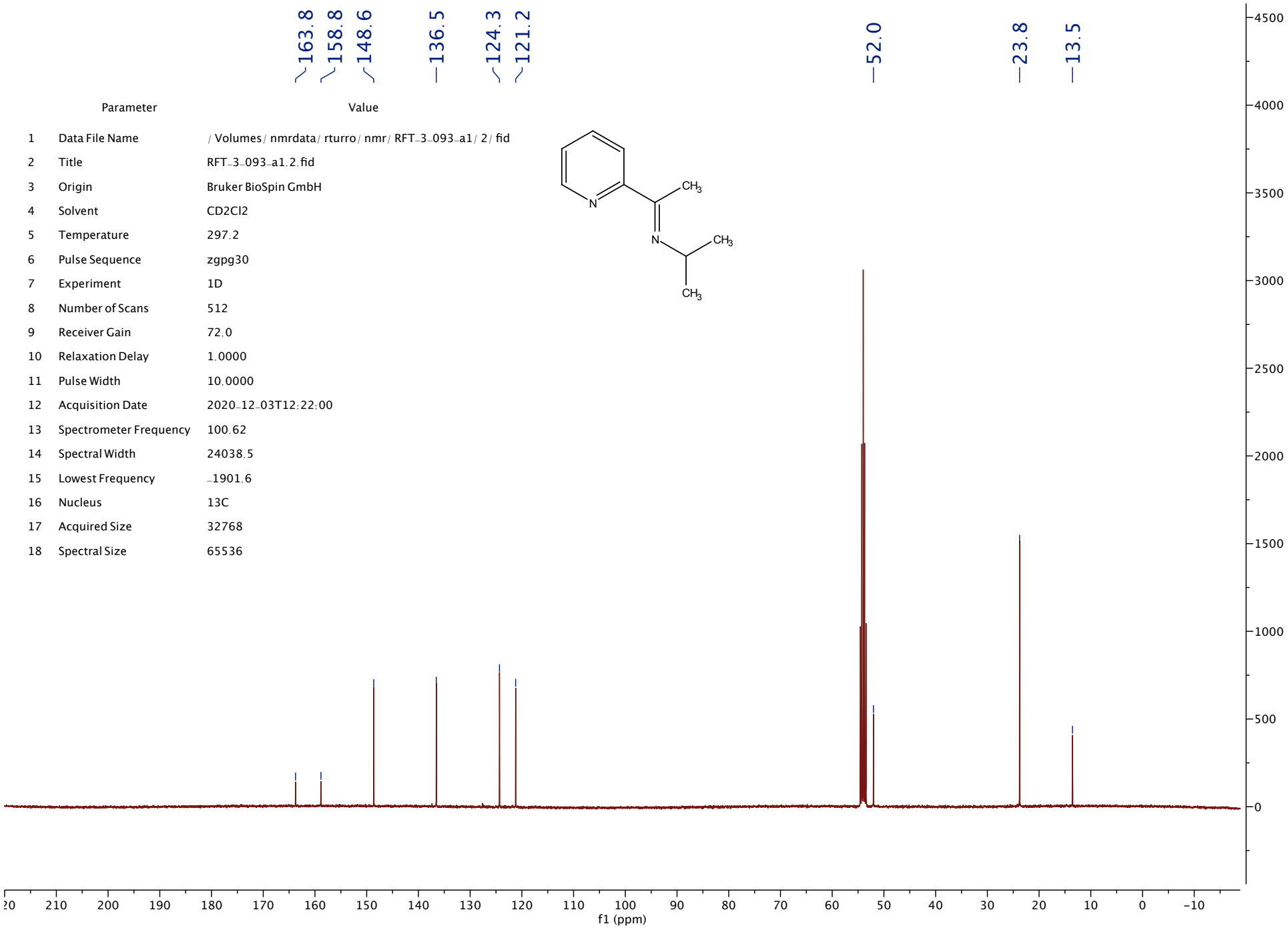
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_150 / 1 / fid
2	Title	mb3_150.1.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
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



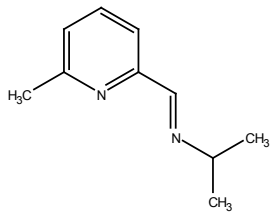

160.6
154.9
149.5
144.7
136.6
128.6
127.1
126.8
124.8
121.6
69.7
24.7
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_150 / 2 / fid
2 Title mb3_150.2.fid
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Instrument spect
8 Author
9 Solvent 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)

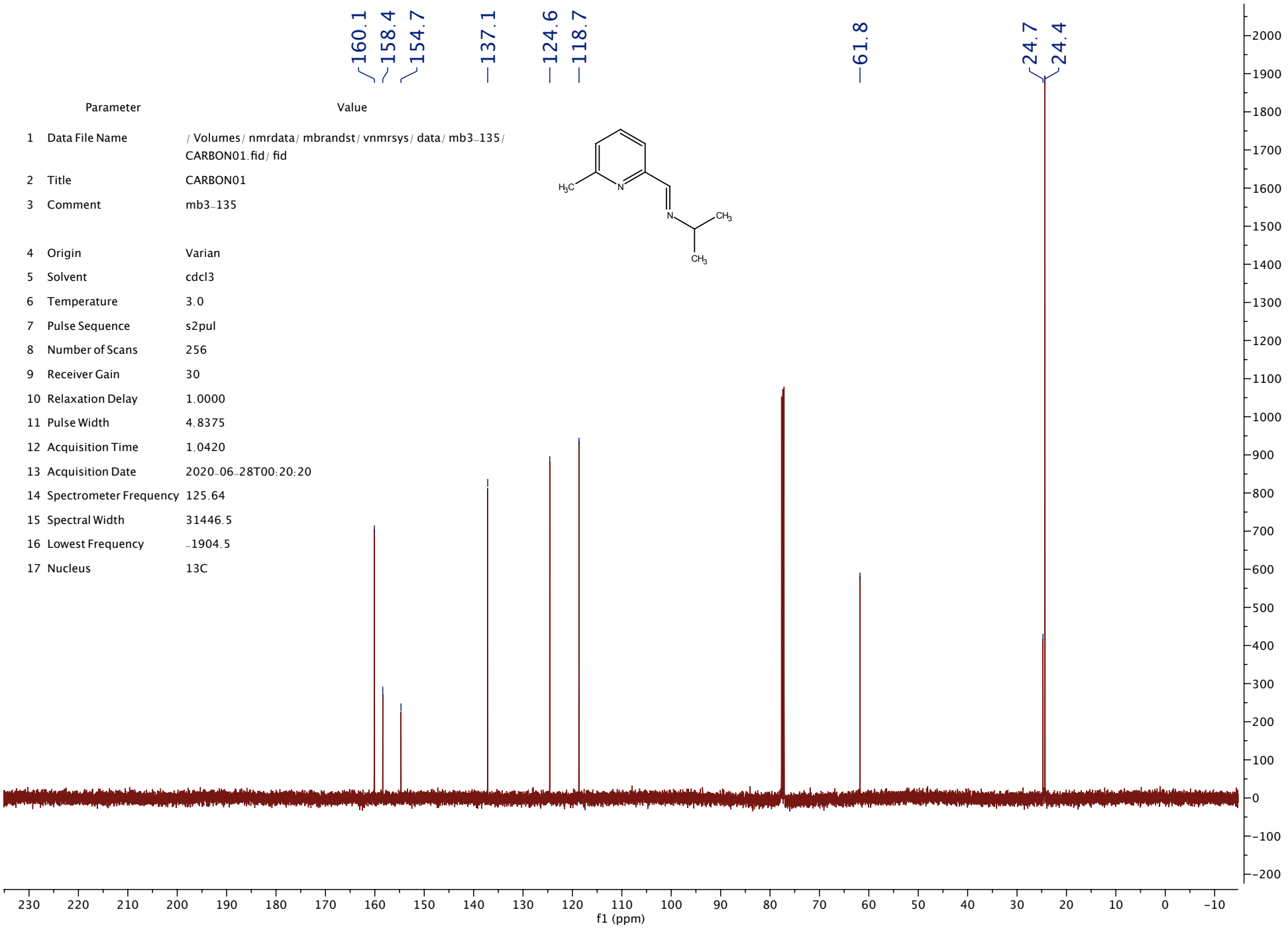
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_093_a1/1/fid
2	Title	RFT_3_093_a1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CD2Cl2
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	127.1
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
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



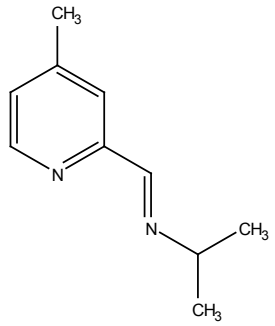

163.8
158.8
148.6
136.5
124.3
121.2
52.0
23.8
13.5
Parameter
Value
1 Data File Name / Volumes/ nmrdata/ rturro/ nmr/ RFT_3_093_a1/ 2/ fid
2 Title RFT_3_093_a1.2.fid
3 Origin Bruker BioSpin GmbH
4 Solvent CD2Cl2
5 Temperature 297.2
6 Pulse Sequence zgpg30
7 Experiment 1D
8 Number of Scans 512
9 Receiver 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
N
CH3
N
CH3
CH3
4500
4000
3500
3000
2500
2000
1500
1000
500
0
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)

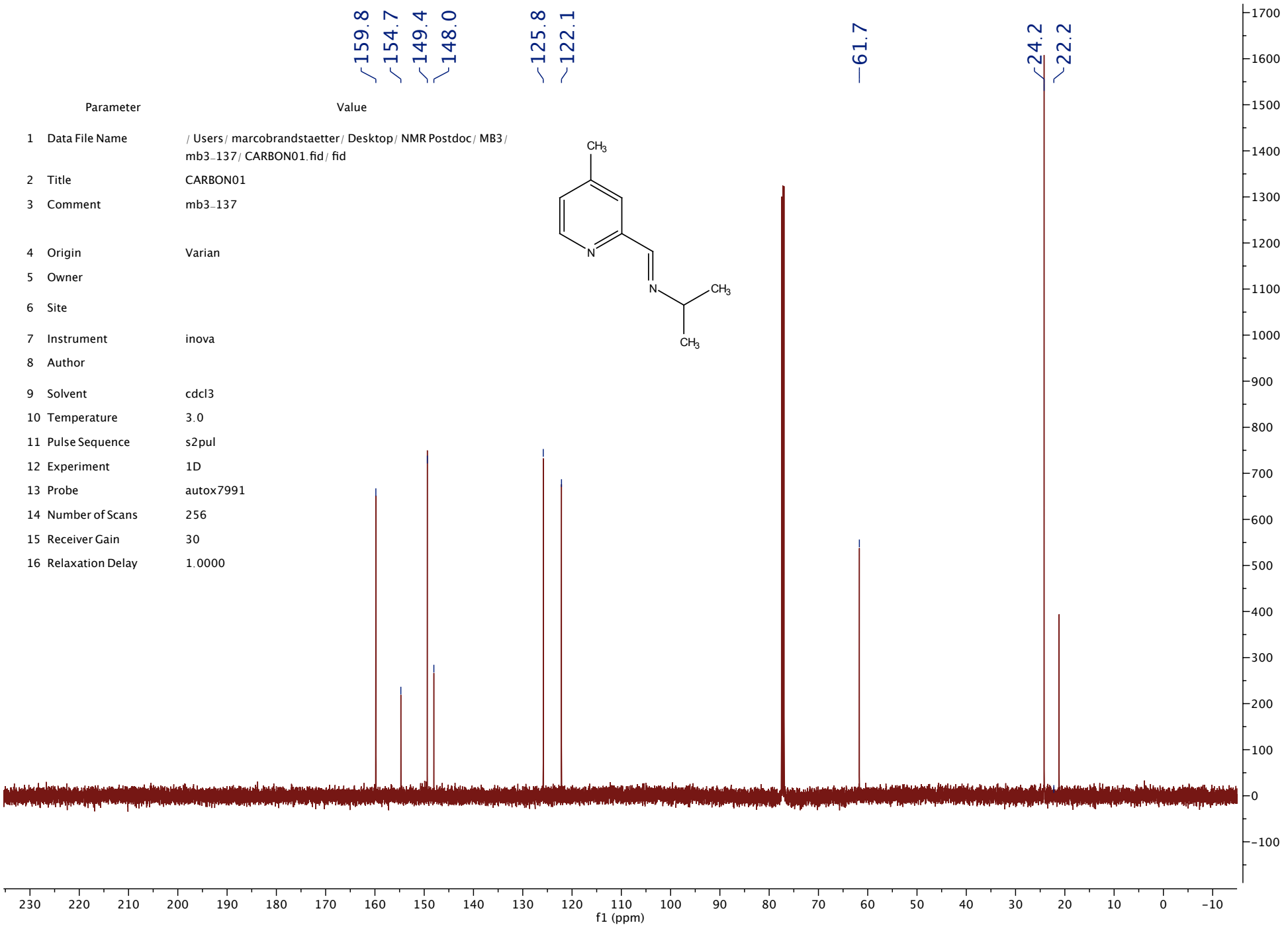
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ mbrandst/ vnmrsys/ data/ mb3_135/ PROTON01.fid/ fid
2	Title	PROTON01
3	Comment	mb3_135
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Time	3.0000
13	Acquisition Date	2020_06_28T00:19:31
14	Spectrometer Frequency	499.60
15	Spectral Width	8000.0
16	Lowest Frequency	_1002.4
17	Nucleus	1H



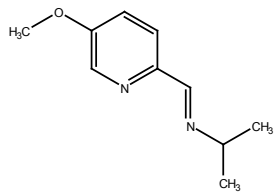

160.1
158.4
154.7
137.1
124.6
118.7
61.8
24.7
24.4
Parameter
Value
1 Data File Name / Volumes/ nmrdata/ mbrandst/ vnmrsys/ data/ mb3_135/ CARBON01.fid/ fid
2 Title CARBON01
3 Comment mb3_135
4 Origin Varian
5 Solvent cdcl3
6 Temperature 3.0
7 Pulse Sequence s2pul
8 Number of Scans 256
9 Receiver Gain 30
10 Relaxation Delay 1.0000
11 Pulse Width 4.8375
12 Acquisition Time 1.0420
13 Acquisition Date 2020_06_28T00:20:20
14 Spectrometer Frequency 125.64
15 Spectral Width 31446.5
16 Lowest Frequency _1904.5
17 Nucleus 13C
H3C
N
N
CH3
CH3
f1 (ppm)

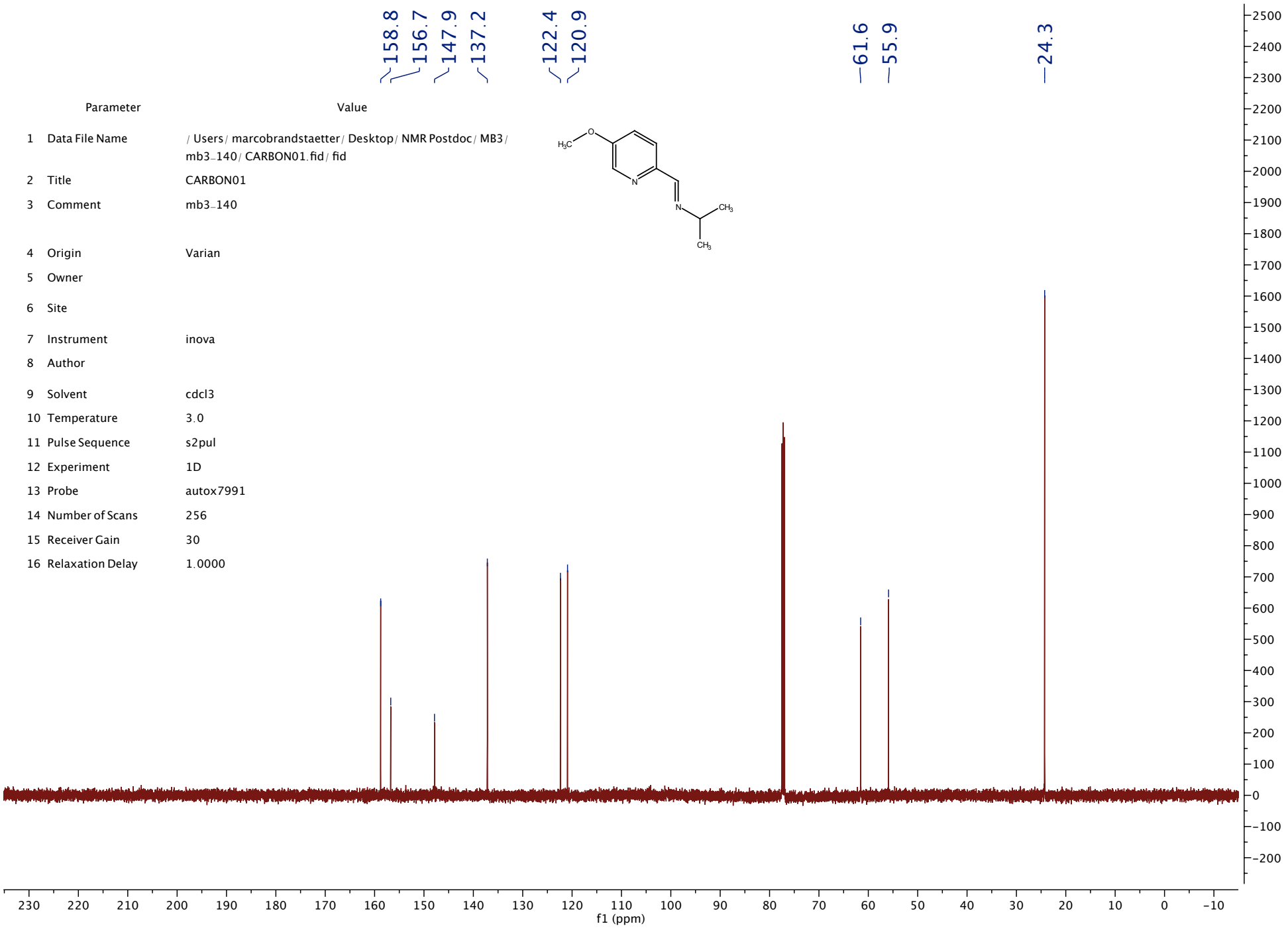
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_137 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb3_137
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe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



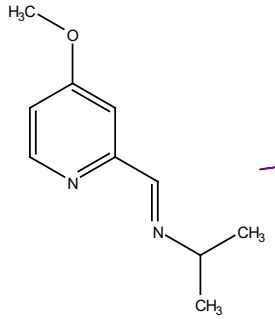

159.8
154.7
149.4
148.0
125.8
122.1
61.7
24.2
22.2
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_137 / CARBON01.fid / fid
2 Title CARBON01
3 Comment mb3_137
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
10 Temperature 3.0
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)

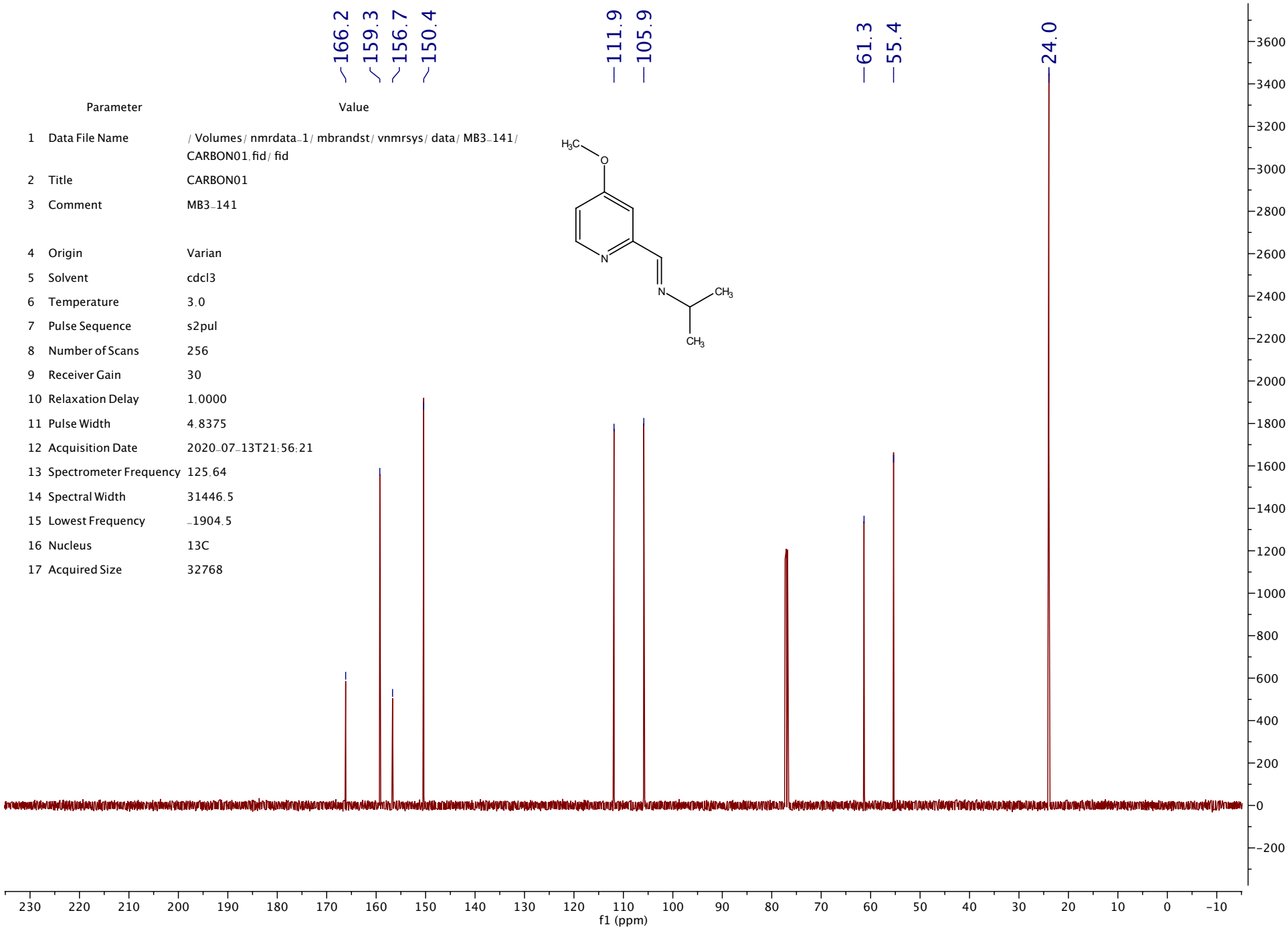
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_140 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb3_140
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	50
16	Relaxation Delay	1.0000




158.8
156.7
147.9
137.2
122.4
120.9
61.6
55.9
24.3
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_140 / CARBON01.fid / fid
2 Title CARBON01
3 Comment mb3_140
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
N
CH3
CH3
f1 (ppm)

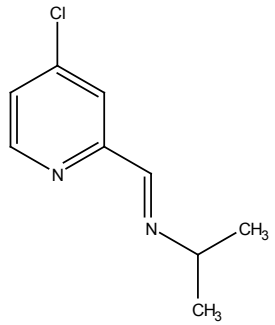
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_141/PROTON02.fid/fid
2	Title	PROTON02
3	Comment	MB3_141
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	42
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition 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

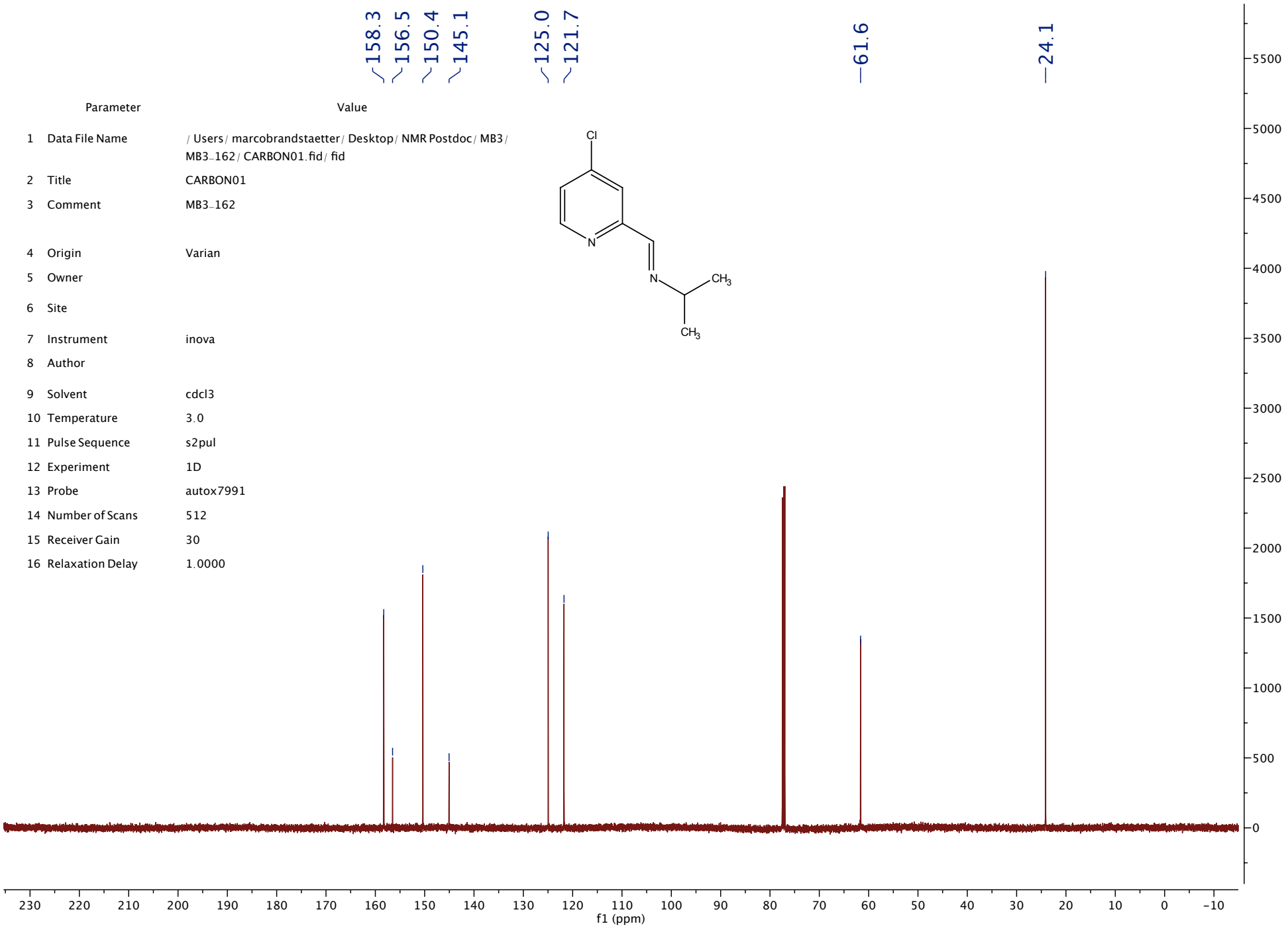




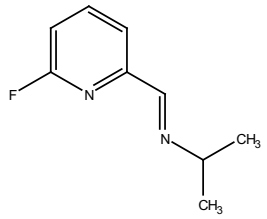
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_141/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3_141
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition 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

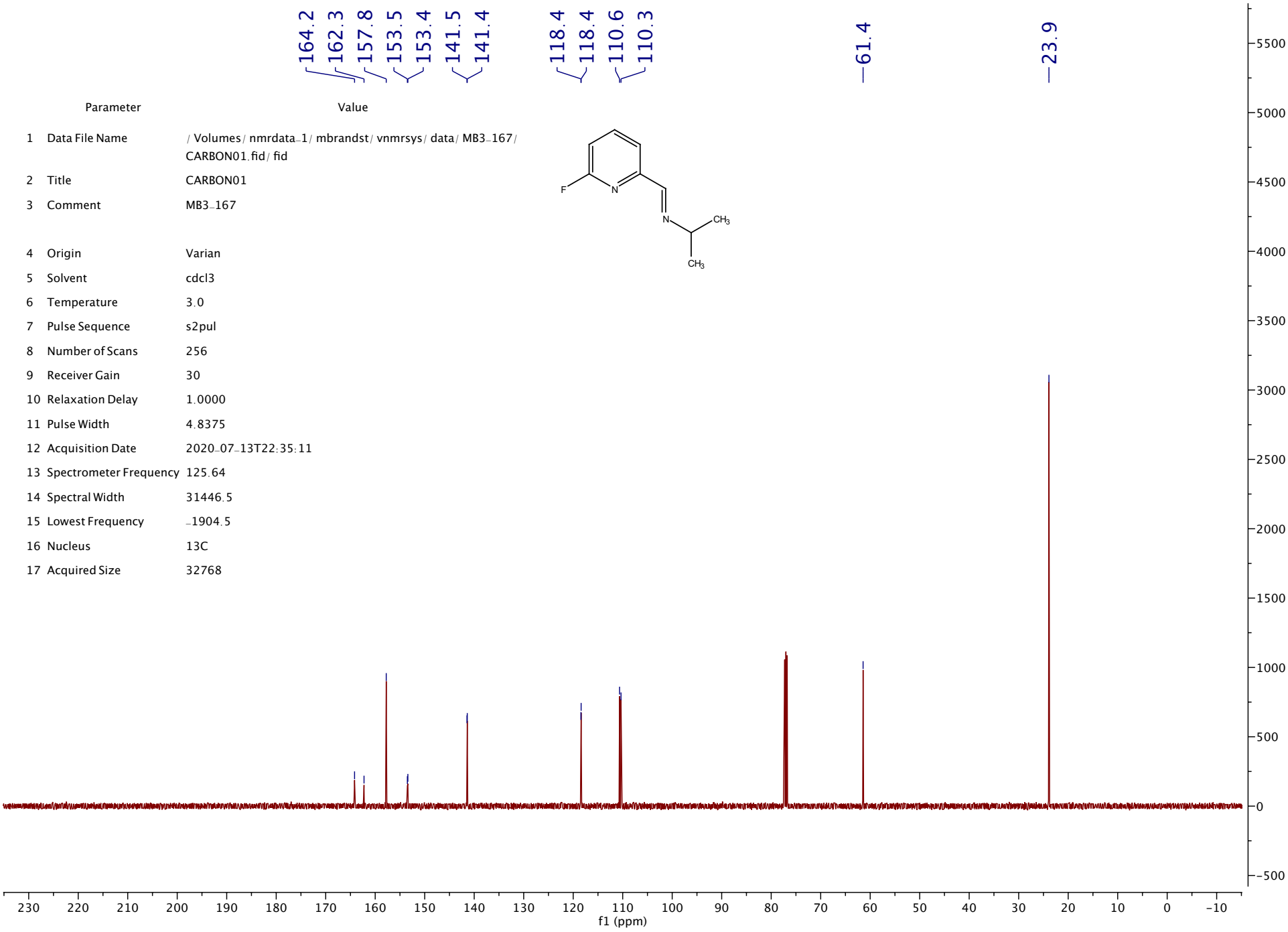
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_162 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB3_162
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	16
15	Receiver Gain	50
16	Relaxation Delay	1.0000




158.3
156.5
150.4
145.1
125.0
121.7
61.6
24.1
Parameter
Value
1 Data File Name
/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_162 / CARBON01.fid / fid
2 Title
CARBON01
3 Comment
MB3_162
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
Cl
N
N
CH3
CH3
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
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_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

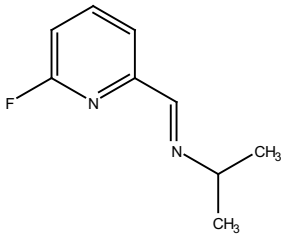




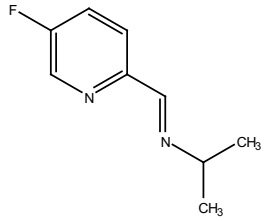
Parameter	Value
1 Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_167/CARBON01.fid/fid
2 Title	CARBON01
3 Comment	MB3_167
4 Origin	Varian
5 Solvent	cdcl3
6 Temperature	3.0
7 Pulse Sequence	s2pul
8 Number of Scans	256
9 Receiver Gain	30
10 Relaxation Delay	1.0000
11 Pulse Width	4.8375
12 Acquisition 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

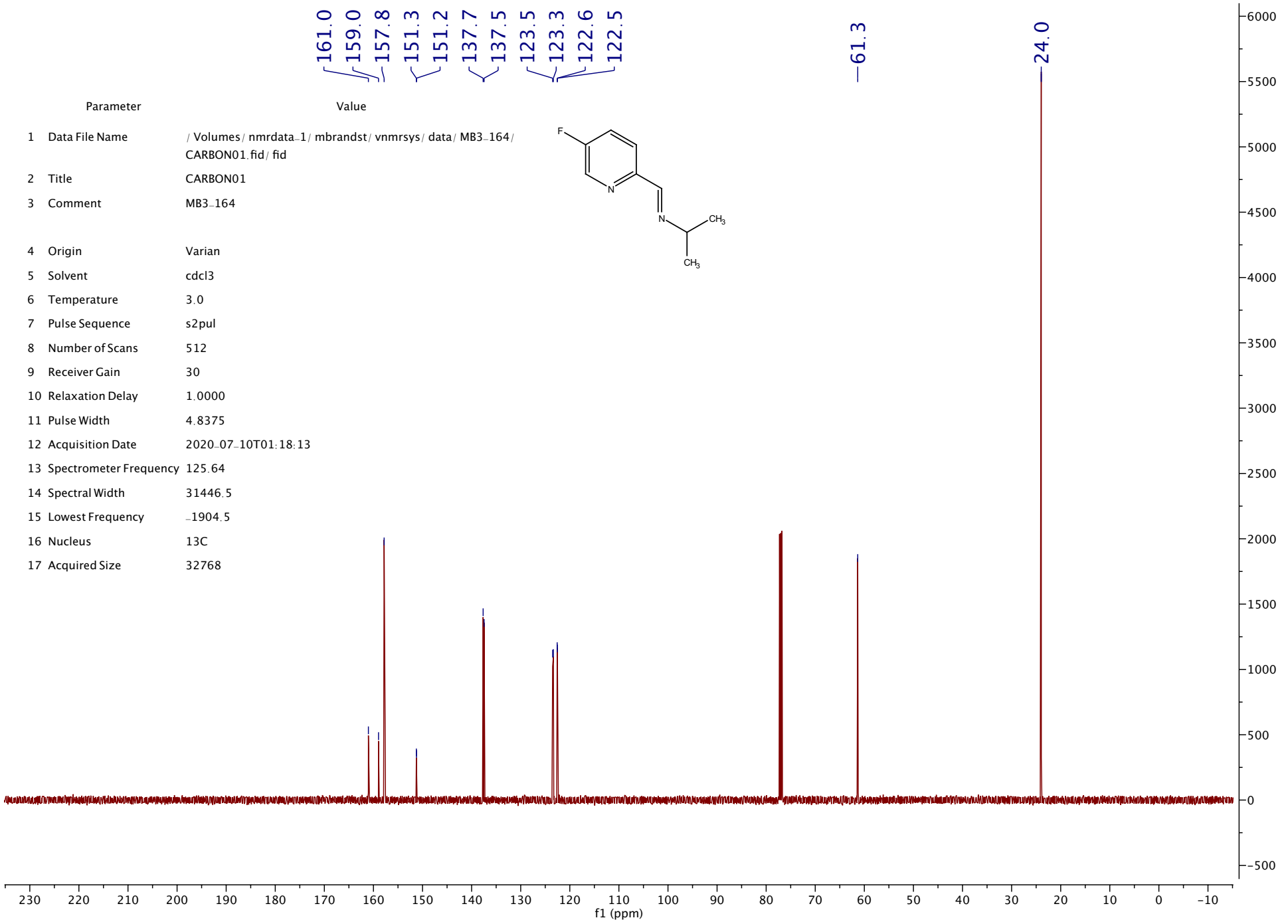
−67.8

	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/vnmrsys/data/MB3_167/FLUORINE01.fid/fid
2	Title	FLUORINE01
3	Comment	MB3_167
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	6.3333
12	Acquisition Time	0.9856
13	Acquisition Date	2022_06_16T17:15:26
14	Spectrometer Frequency	282.34
15	Spectral Width	64935.1
16	Lowest Frequency	_56468.7
17	Nucleus	19F



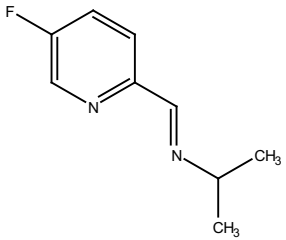
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB3_164 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB3_164
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	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



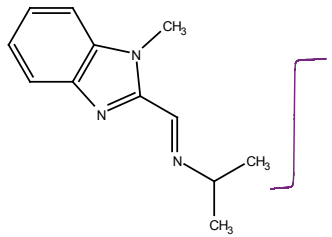


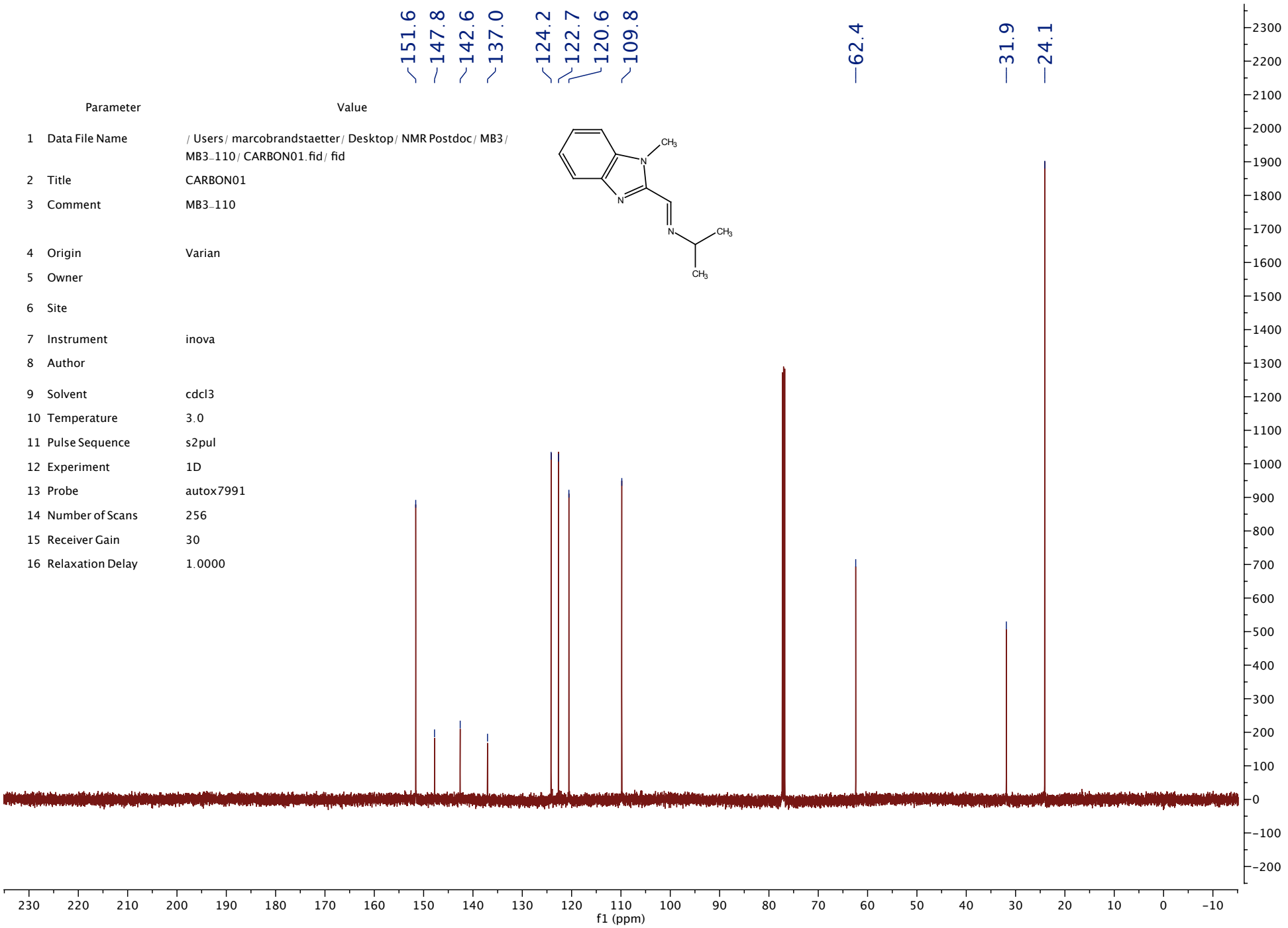
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_164/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3_164
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition 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	/Volumes/nmrdata/rturro/vnmrsys/data/MB3-164/FLUORINE01.fid/fid
2	Title	FLUORINE01
3	Comment	MB3-164
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	6.3333
12	Acquisition Time	0.9856
13	Acquisition Date	2022-06-16T17:23:34
14	Spectrometer Frequency	282.34
15	Spectral Width	64935.1
16	Lowest Frequency	-56468.7
17	Nucleus	19F

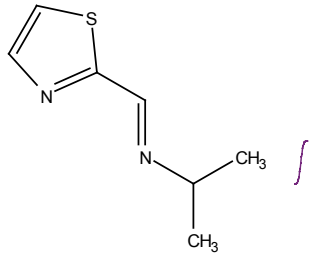


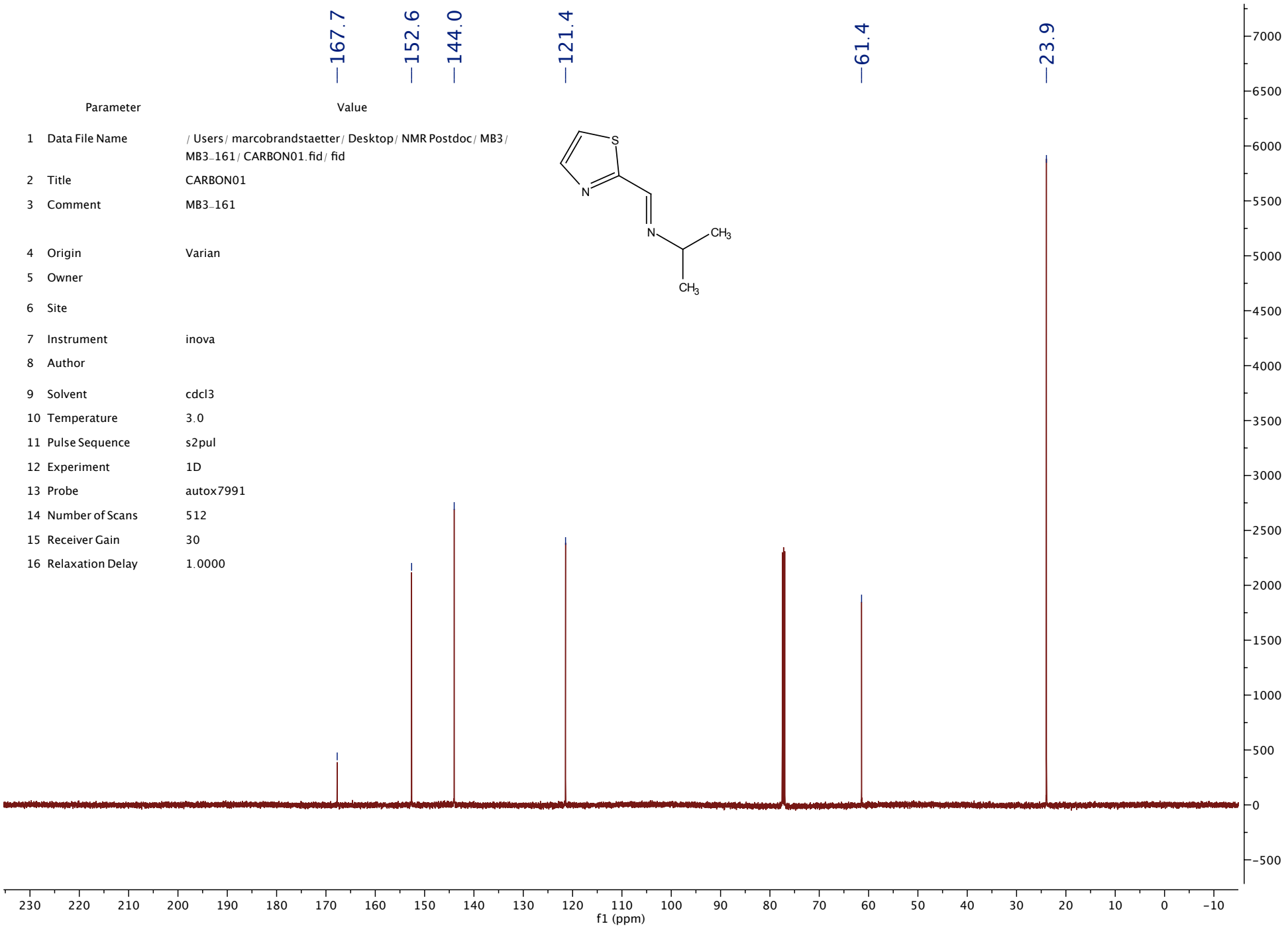
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_110 / PROTON03.fid / fid
2	Title	PROTON03
3	Comment	MB3_110
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe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



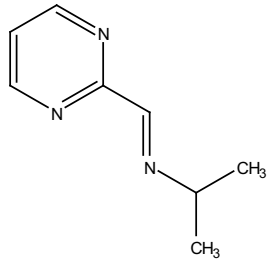

151.6
147.8
142.6
137.0
124.2
122.7
120.6
109.8
62.4
31.9
24.1
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_110 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB3_110
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
10 Temperature 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




167.7
152.6
144.0
121.4
61.4
23.9
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
S
N
N
CH3
CH3
7000
6500
6000
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)

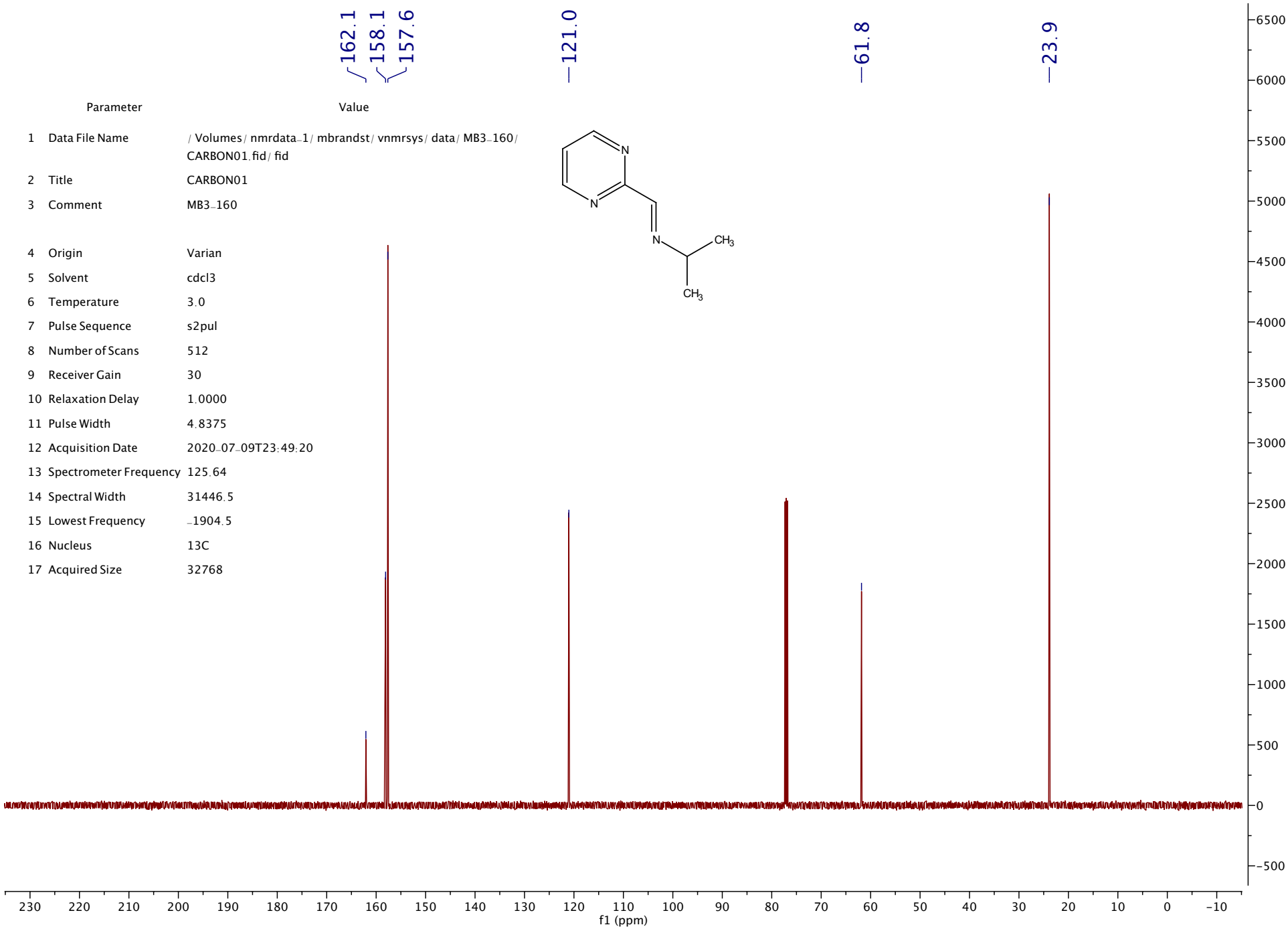
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_160/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB3_160
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition 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



C (dd) 8.84
B (s) 8.43
A (td) 7.29
D (hept) 3.72
E (dd) 1.33

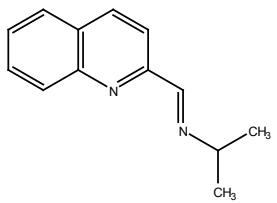
1.88
0.66
1.00
1.09
6.45

f1 (ppm)



	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

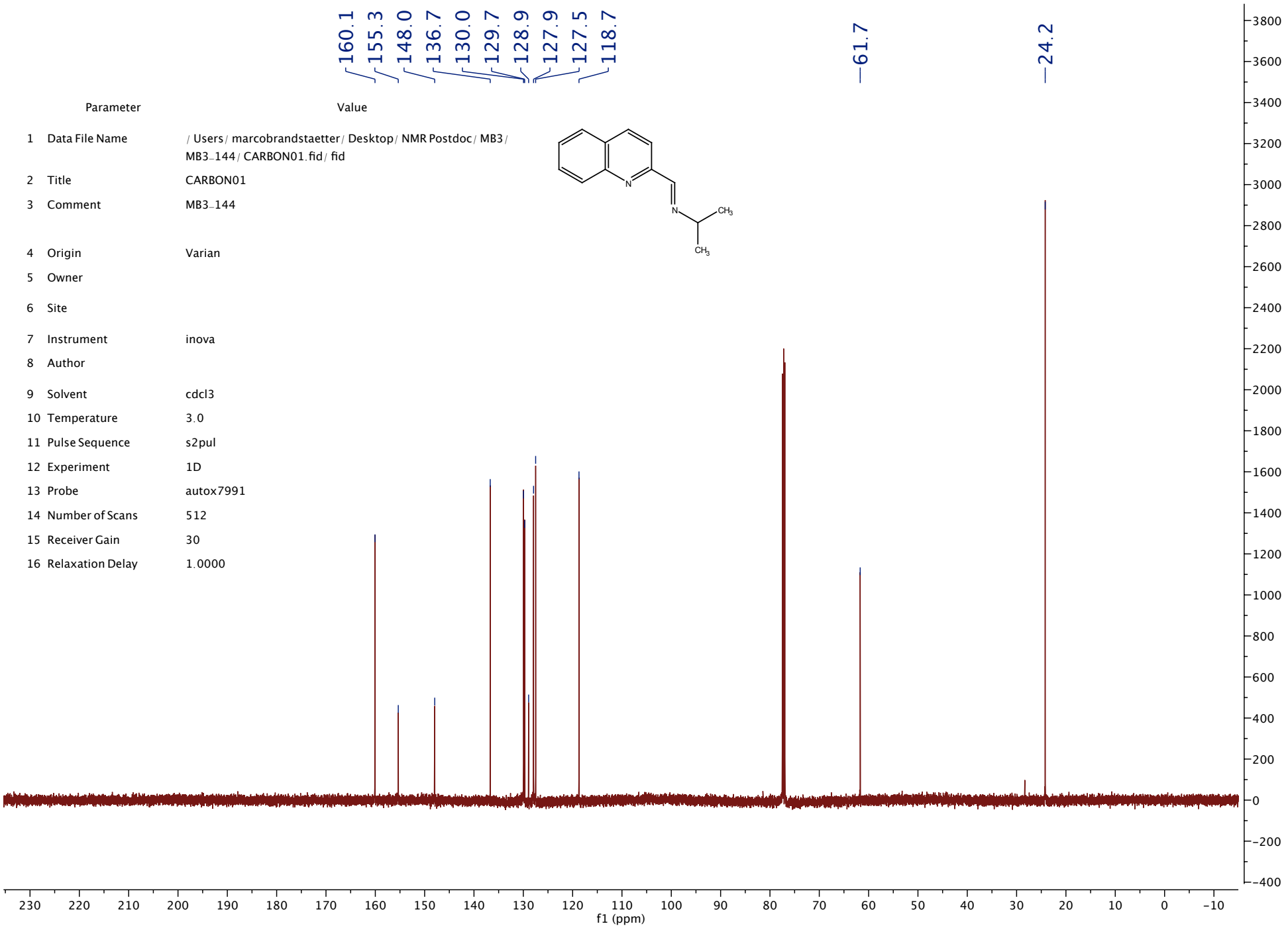
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_144 / PROTON02.fid / fid
2	Title	PROTON02
3	Comment	MB3_144
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	16
15	Receiver Gain	50
16	Relaxation Delay	1.0000



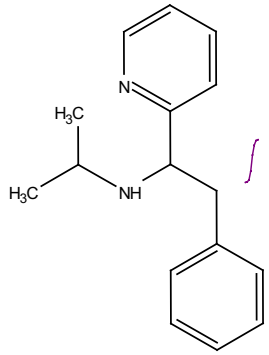
H (s) 8.17
D (t) 7.73
F (s) 8.56
G (d) 8.12
C (t) 7.57
E (d) 7.83
A (hept) 3.73
B (d) 1.33

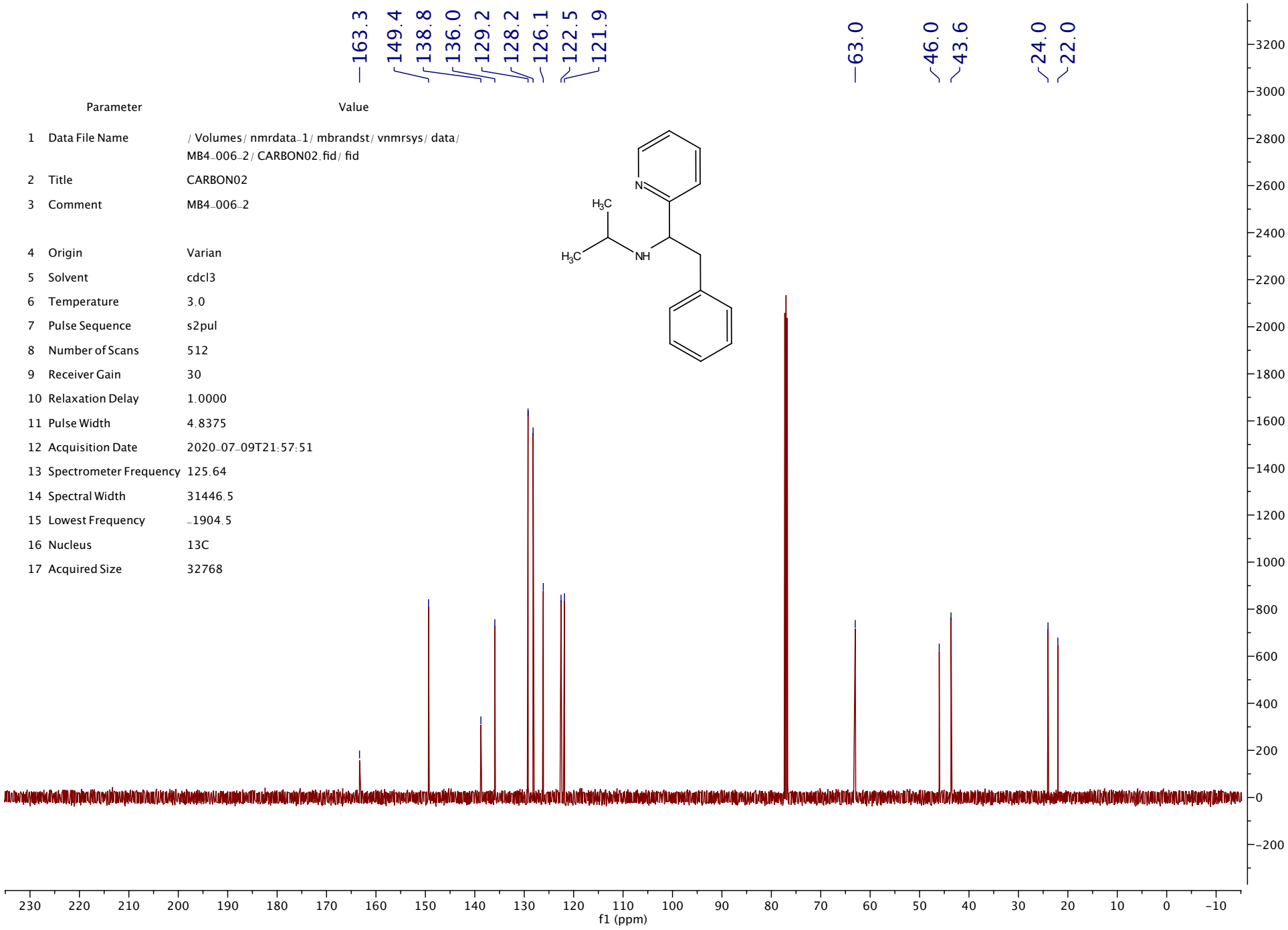
0.95 1.86 0.90 1.00 1.00 0.93 1.00 6.00

f1 (ppm)


160.1
155.3
148.0
136.7
130.0
129.7
128.9
127.9
127.5
118.7
61.7
24.2
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_144 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB3_144
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
f1 (ppm)

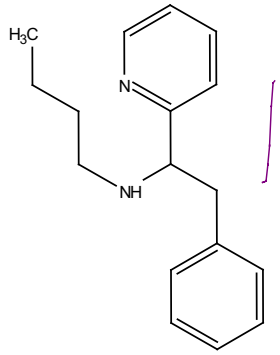
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_006_2 / PROTON02.fid / fid
2	Title	PROTON02
3	Comment	MB4_006_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	34
10	Relaxation Delay	1.0000
11	Pulse 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

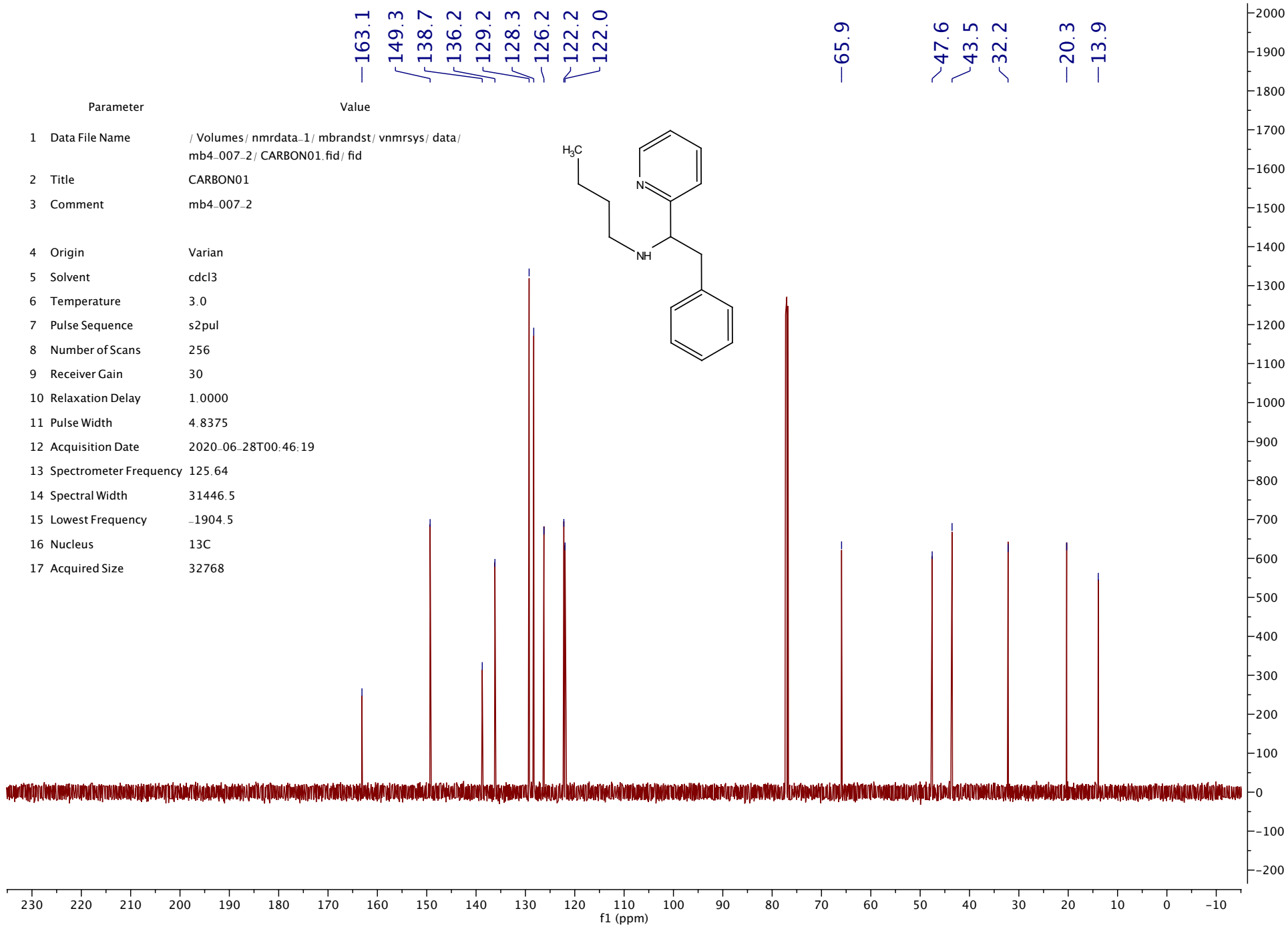




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_006_2 / CARBON02.fid / fid
2	Title	CARBON02
3	Comment	MB4_006_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse 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

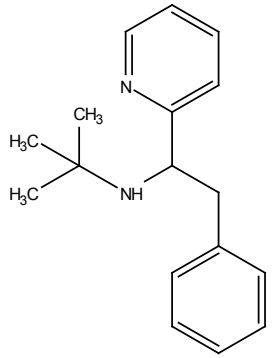
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_007_2/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb4_007_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	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

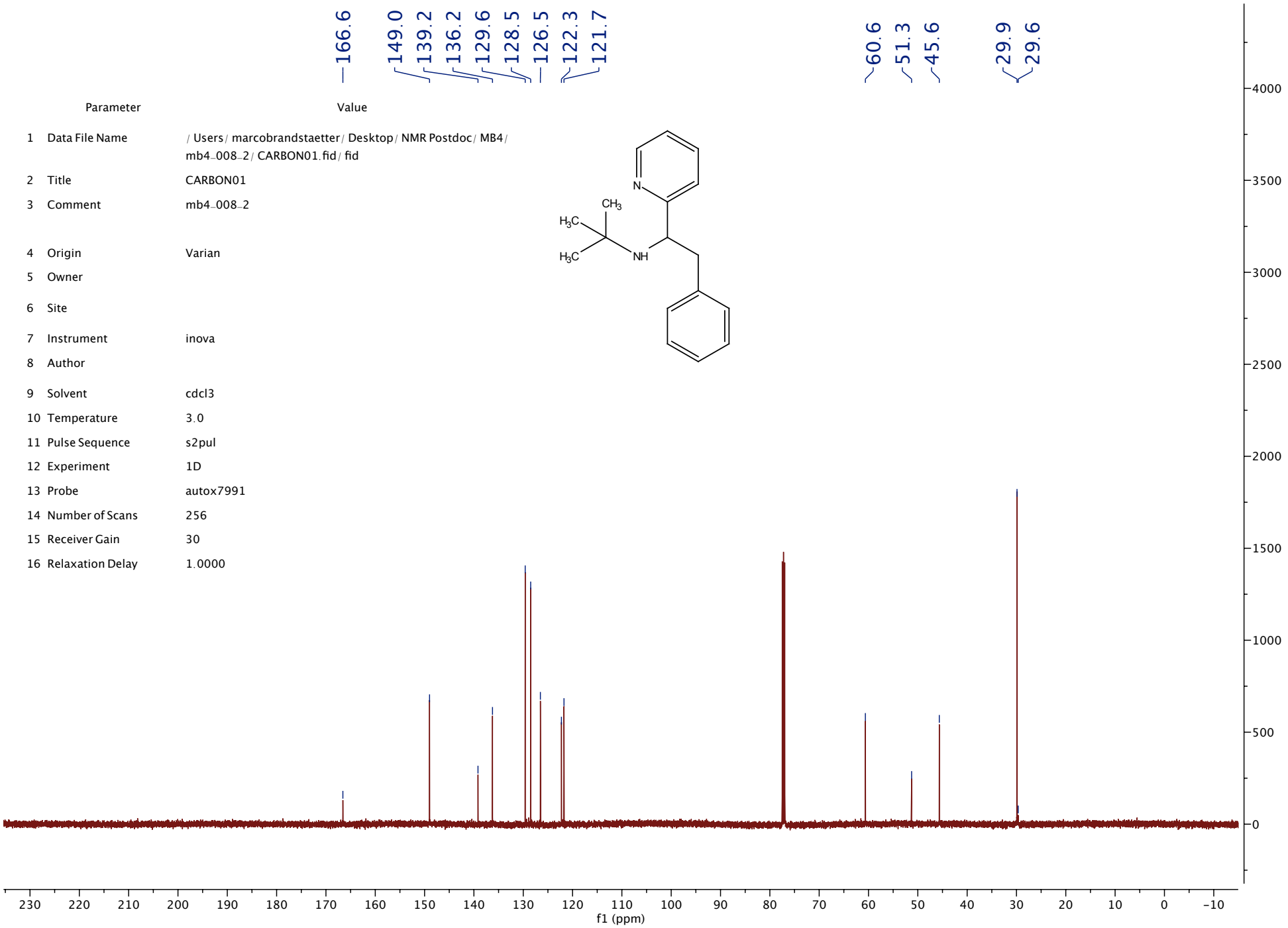




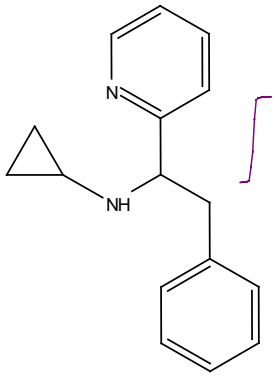
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / mb4_007_2 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	mb4_007_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse 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

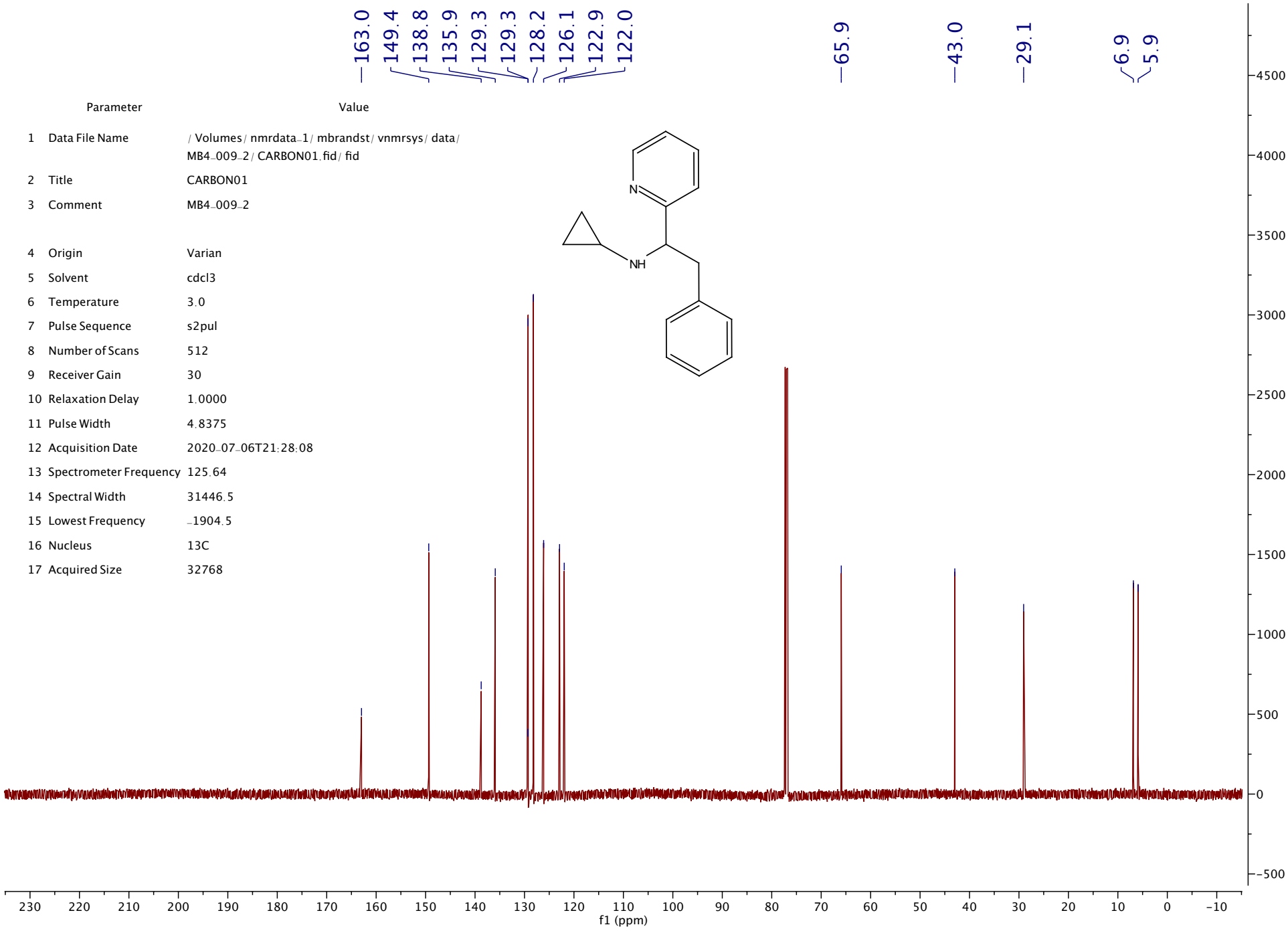
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / mb4_008_2 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb4_008_2
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	48
16	Relaxation Delay	1.0000




166.6
149.0
139.2
136.2
129.6
128.5
126.5
122.3
121.7
60.6
51.3
45.6
29.9
29.6
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / mb4_008_2 / CARBON01.fid / fid
2 Title CARBON01
3 Comment mb4_008_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
N
CH3
H3C
H3C
NH
4000
3500
3000
2500
2000
1500
1000
500
0
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)

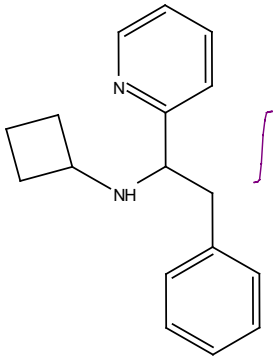
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_009_2 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_009_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse 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

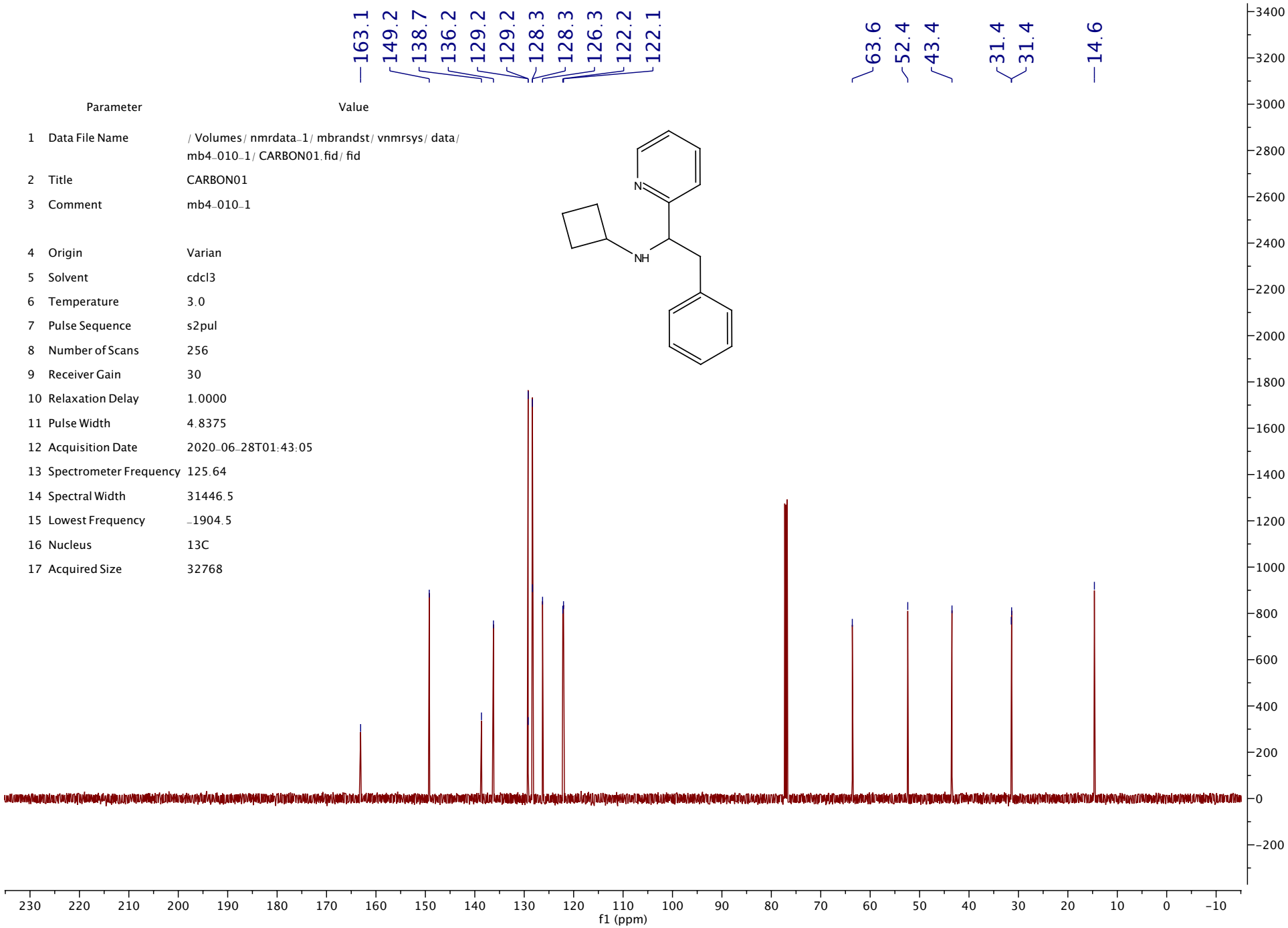




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_009_2/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB4_009_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
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

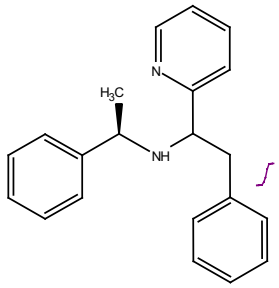
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/mb4_010_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	mb4_010_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	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

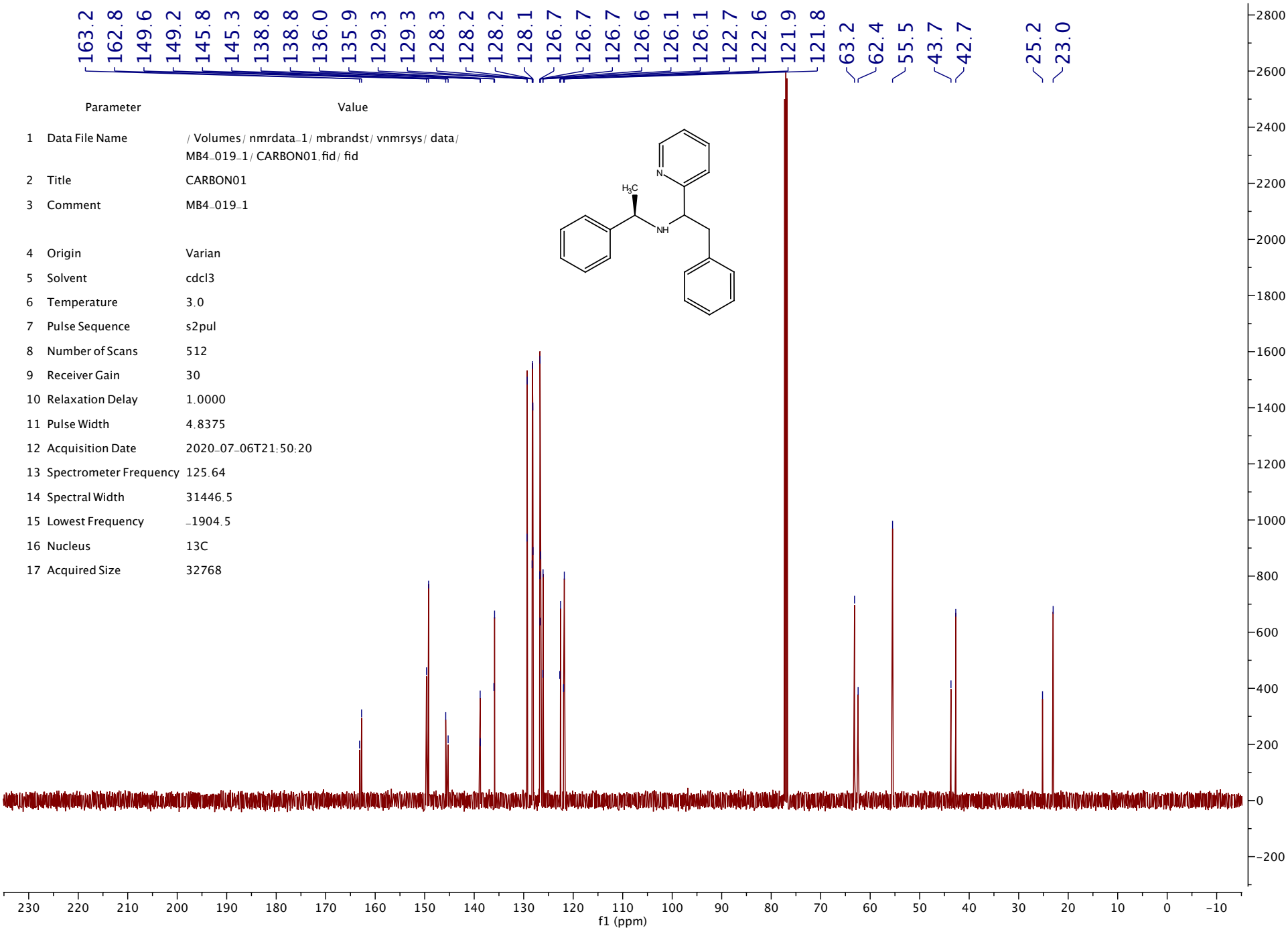




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / mb4_010_1 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	mb4_010_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse 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

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162.8
149.6
149.2
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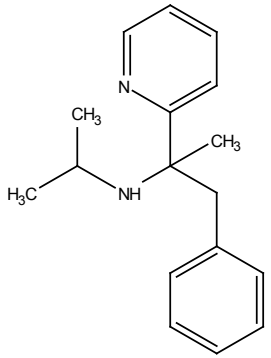
145.3
138.8
138.8
136.0
135.9
129.3
129.3
128.3
128.2
128.2
128.1
126.7
126.7
126.7
126.6
126.1
126.1
122.7
122.6
121.9
121.8
63.2
62.4
55.5
43.7
42.7
25.2
23.0
Parameter
Value
1 Data File Name / Volumes/ nmrdata_1/ mbrandst/ vnmrsys/ data/ MB4_019_1/ CARBON01.fid/ fid
2 Title CARBON01
3 Comment MB4_019_1
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
H3C
NH
N
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)

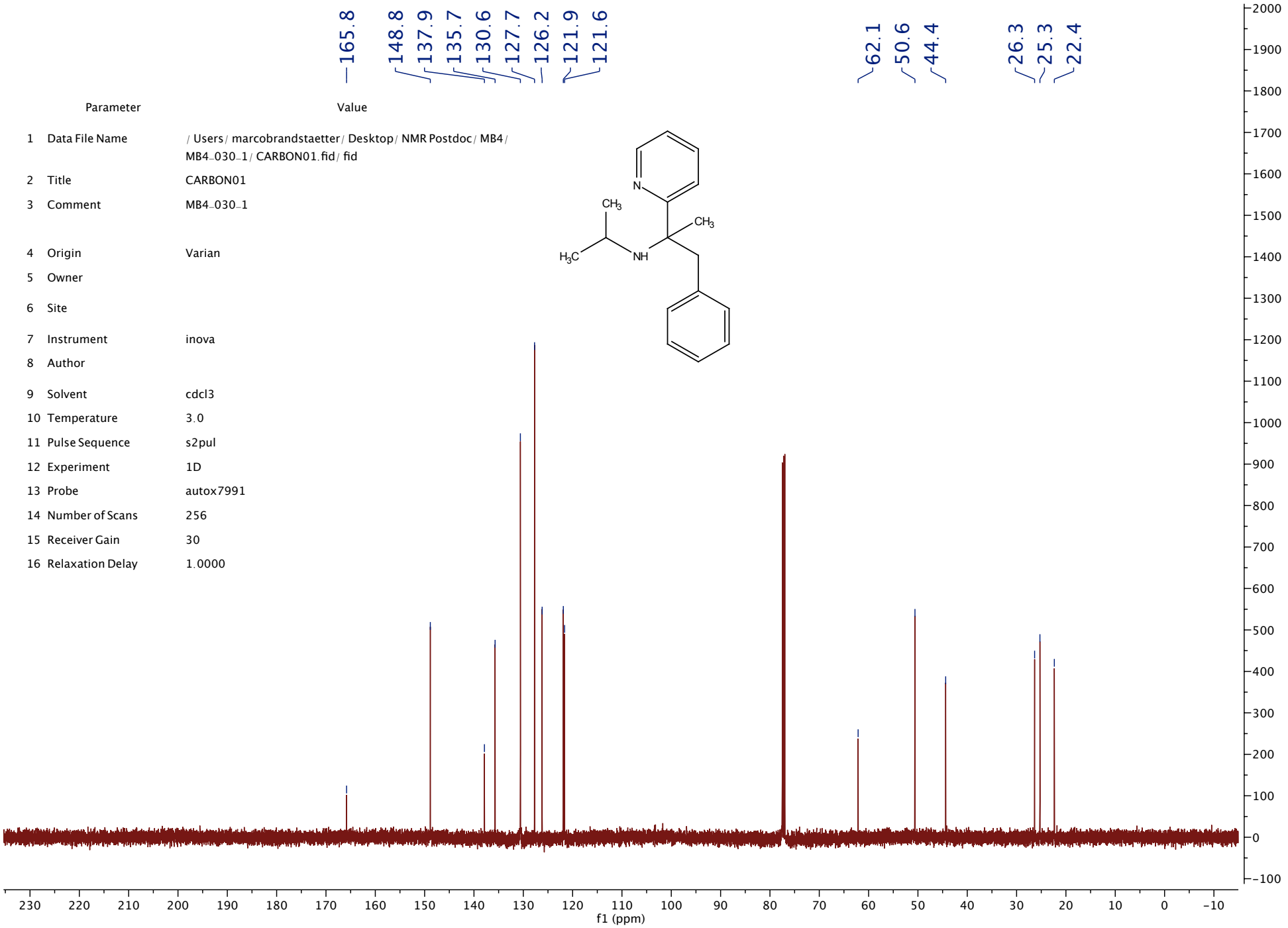
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_030_1 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_030_1
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	48
16	Relaxation Delay	1.0000



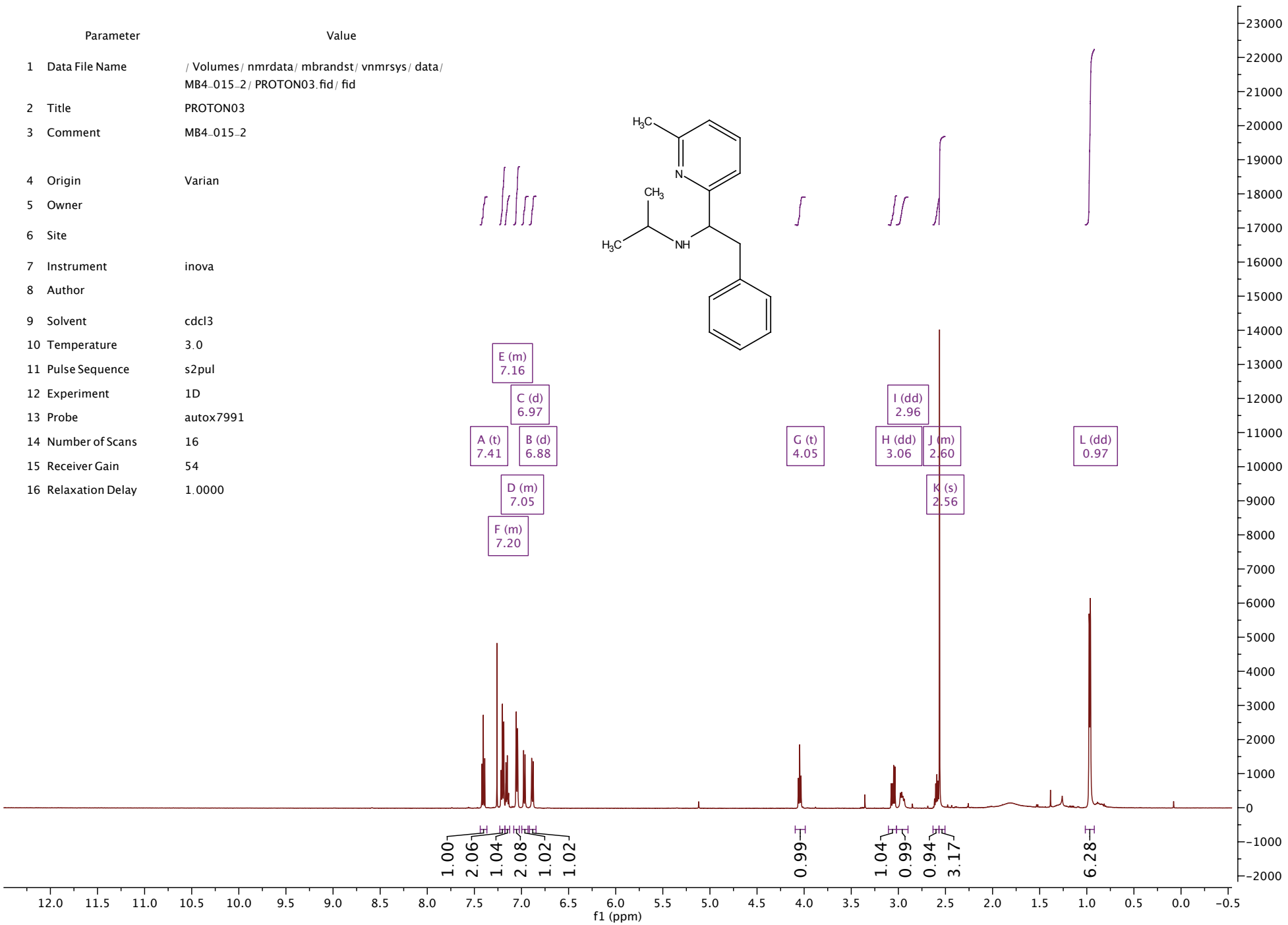
H (d) 8.65
K (m) 7.12
I (t) 7.48
J (d) 6.65
L (dt) 7.06
B (d) 2.95
D (s) 2.32
G (d) 0.84
A (d) 3.17
C (hept) 2.66
E (s) 1.50
F (d) 1.08

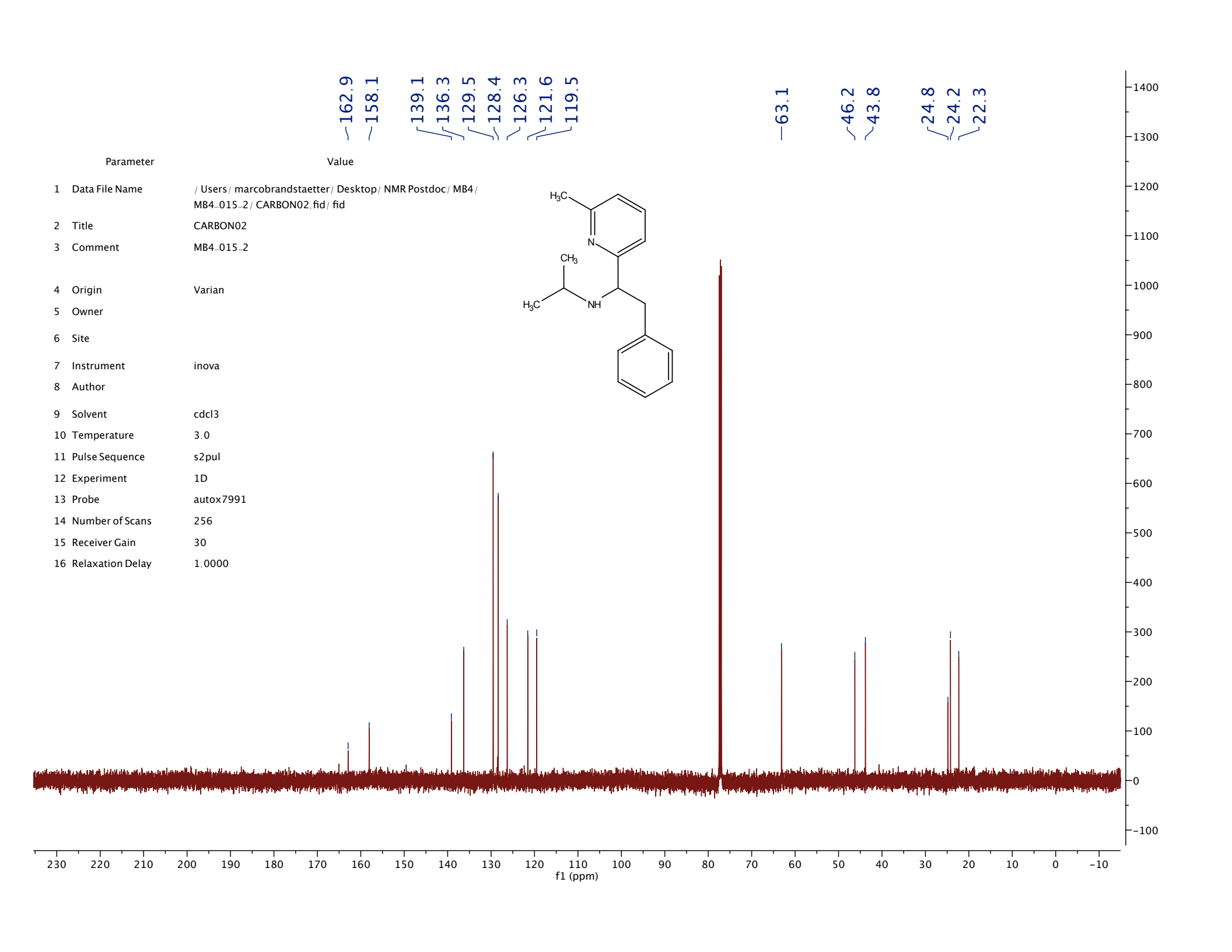
0.92 1.00 1.19 4.14 2.04 1.00 1.05 0.99 1.43 3.26 3.17 3.24

f1 (ppm)

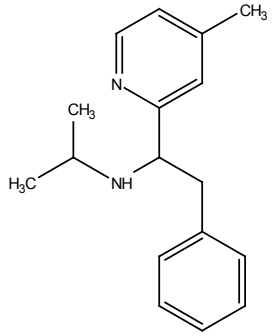

165.8
148.8
137.9
135.7
130.6
127.7
126.2
121.9
121.6
62.1
50.6
44.4
26.3
25.3
22.4
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_030_1 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB4_030_1
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
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
N
CH3
CH3
H3C
NH
f1 (ppm)

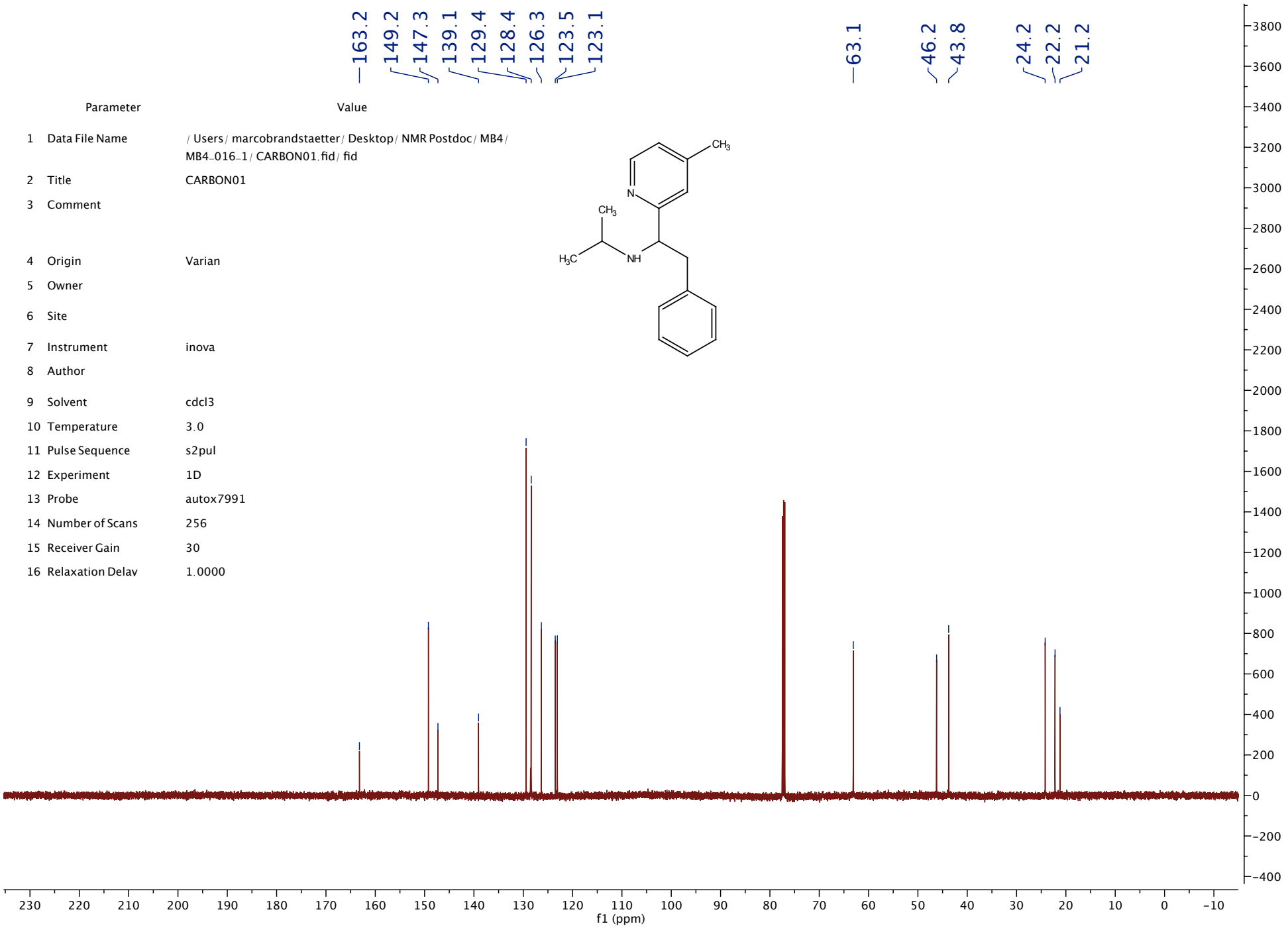
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ mbrandst/ vnmrsys/ data/ MB4_015_2/ PROTON03.fid/ fid
2	Title	PROTON03
3	Comment	MB4_015_2
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	16
15	Receiver Gain	54
16	Relaxation Delay	1.0000



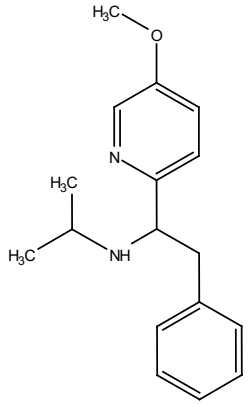

162.9
158.1
139.1
136.3
129.5
128.4
126.3
121.6
119.5
63.1
46.2
43.8
24.8
24.2
22.3
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_015_2 / CARBON02.fid / fid
2 Title CARBON02
3 Comment MB4_015_2
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
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
N
CH3
H3C
NH
f1 (ppm)

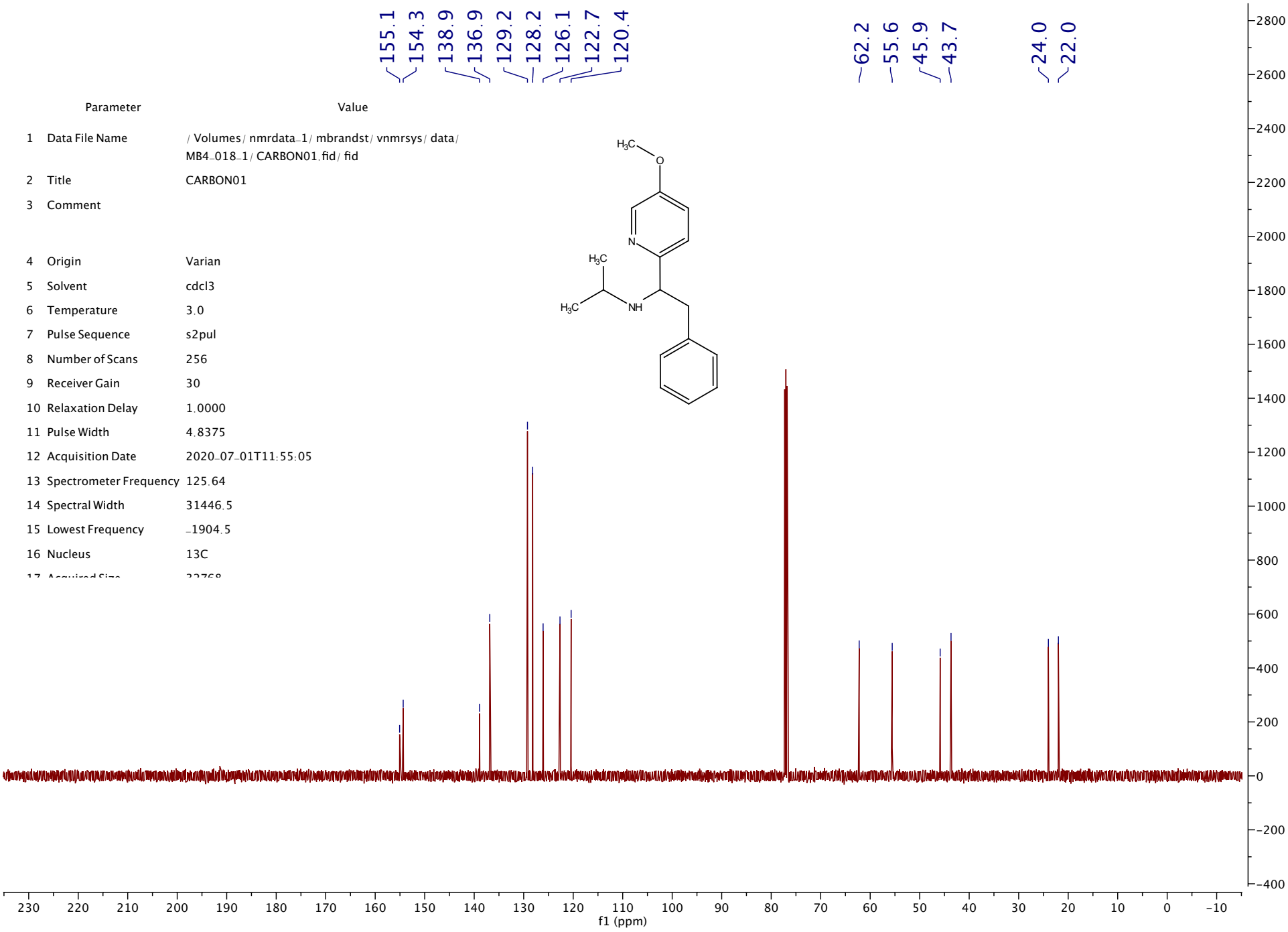
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_016_1 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	46
16	Relaxation Delay	1.0000




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
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_016_1 / CARBON01.fid / fid
2 Title CARBON01
3 Comment
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
CH3
H3C
NH
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





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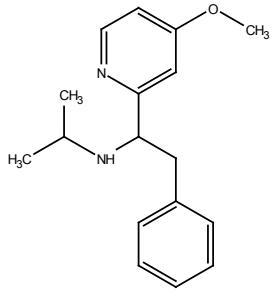
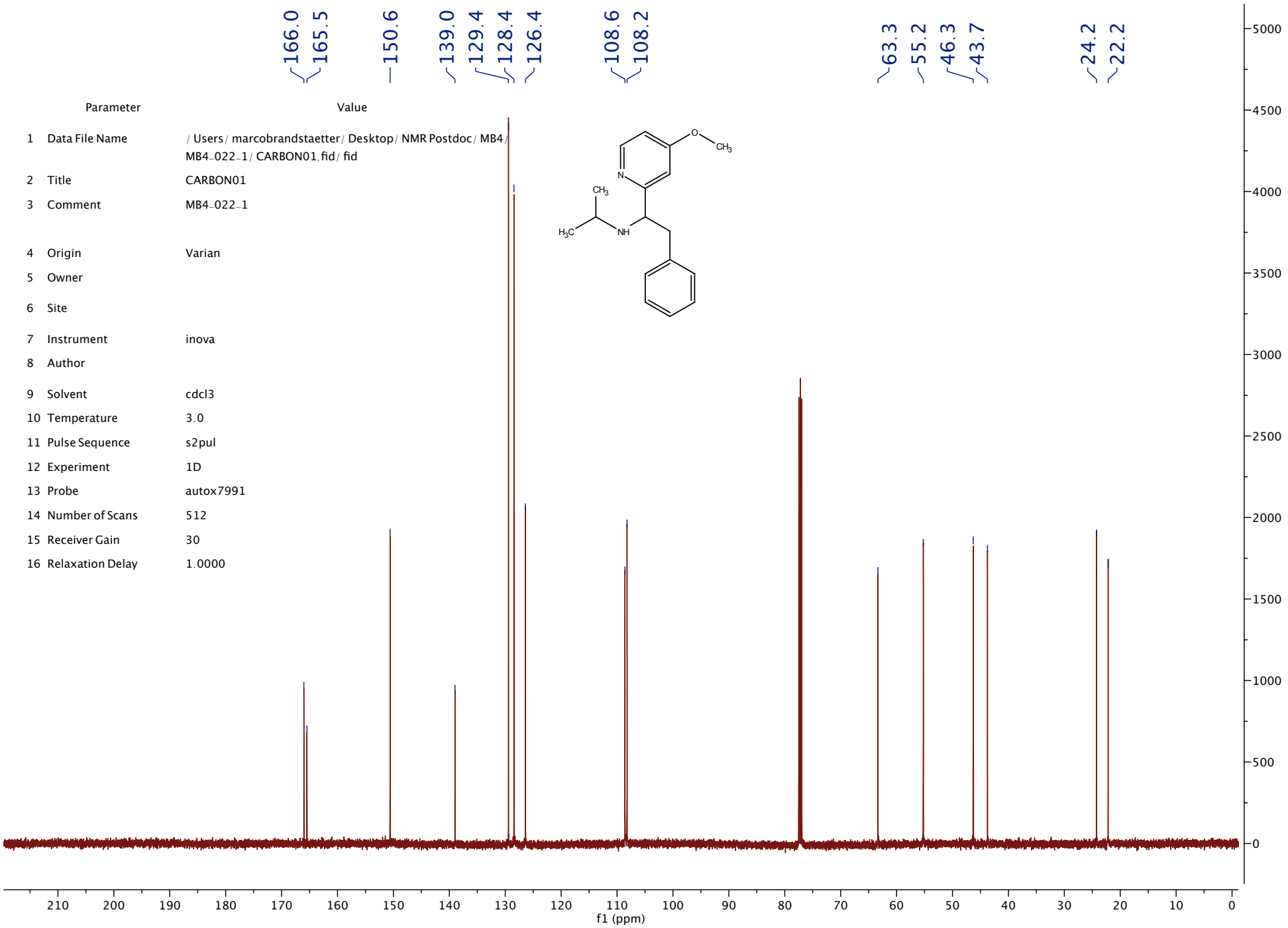
2	Title	CARBON01
3	Comment	
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_01T11:55:05
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency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

	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_022_1 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_022_1
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	36
16	Relaxation Delay	1.0000




166.0
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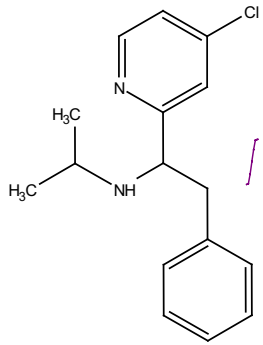
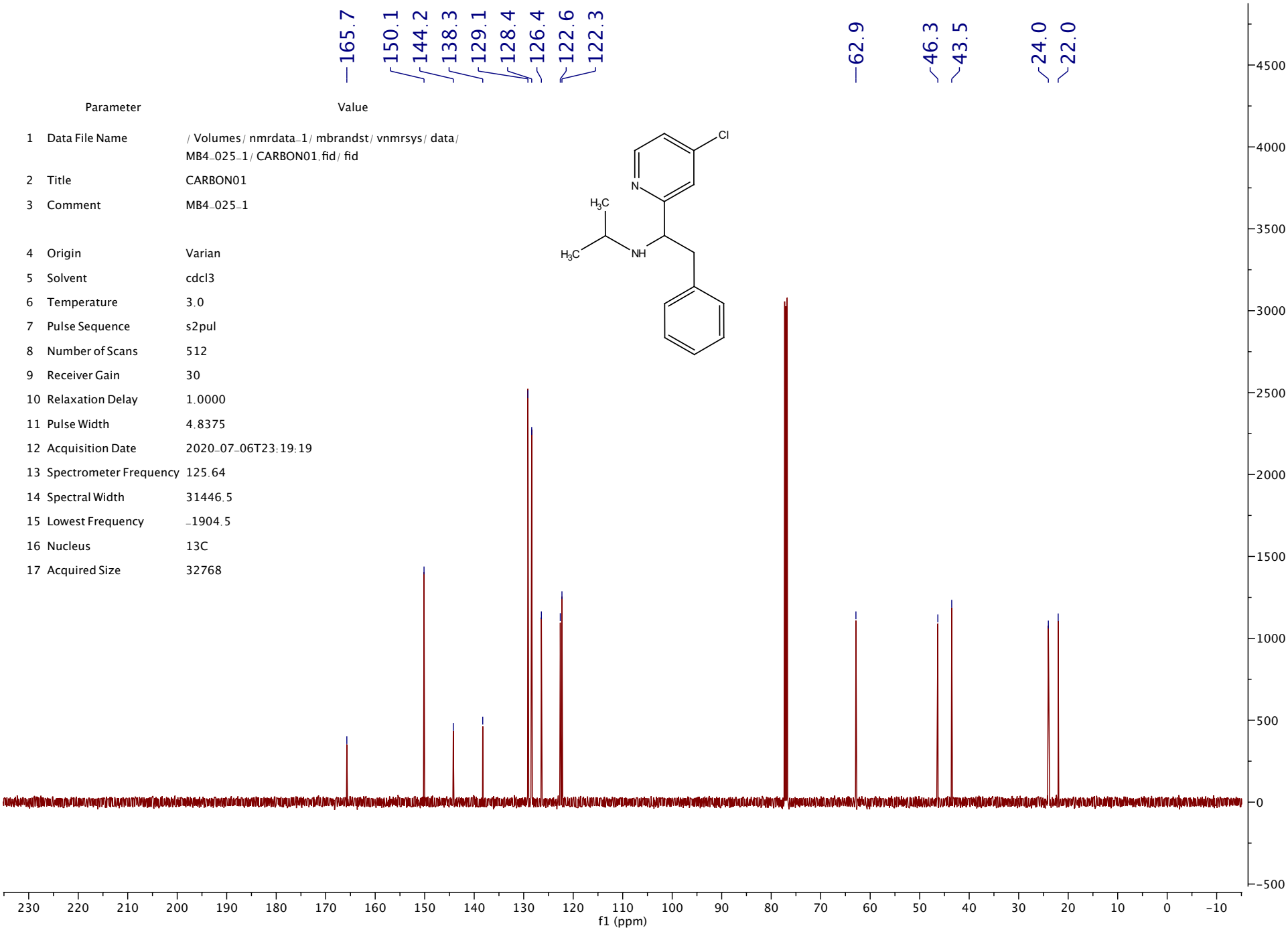
139.0
129.4
128.4
126.4
108.6
108.2
63.3
55.2
46.3
43.7
24.2
22.2
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_022_1 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB4_022_1
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
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
O
CH3
CH3
H3C
NH
5000
4500
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
f1 (ppm)

	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
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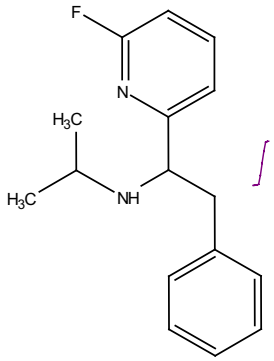
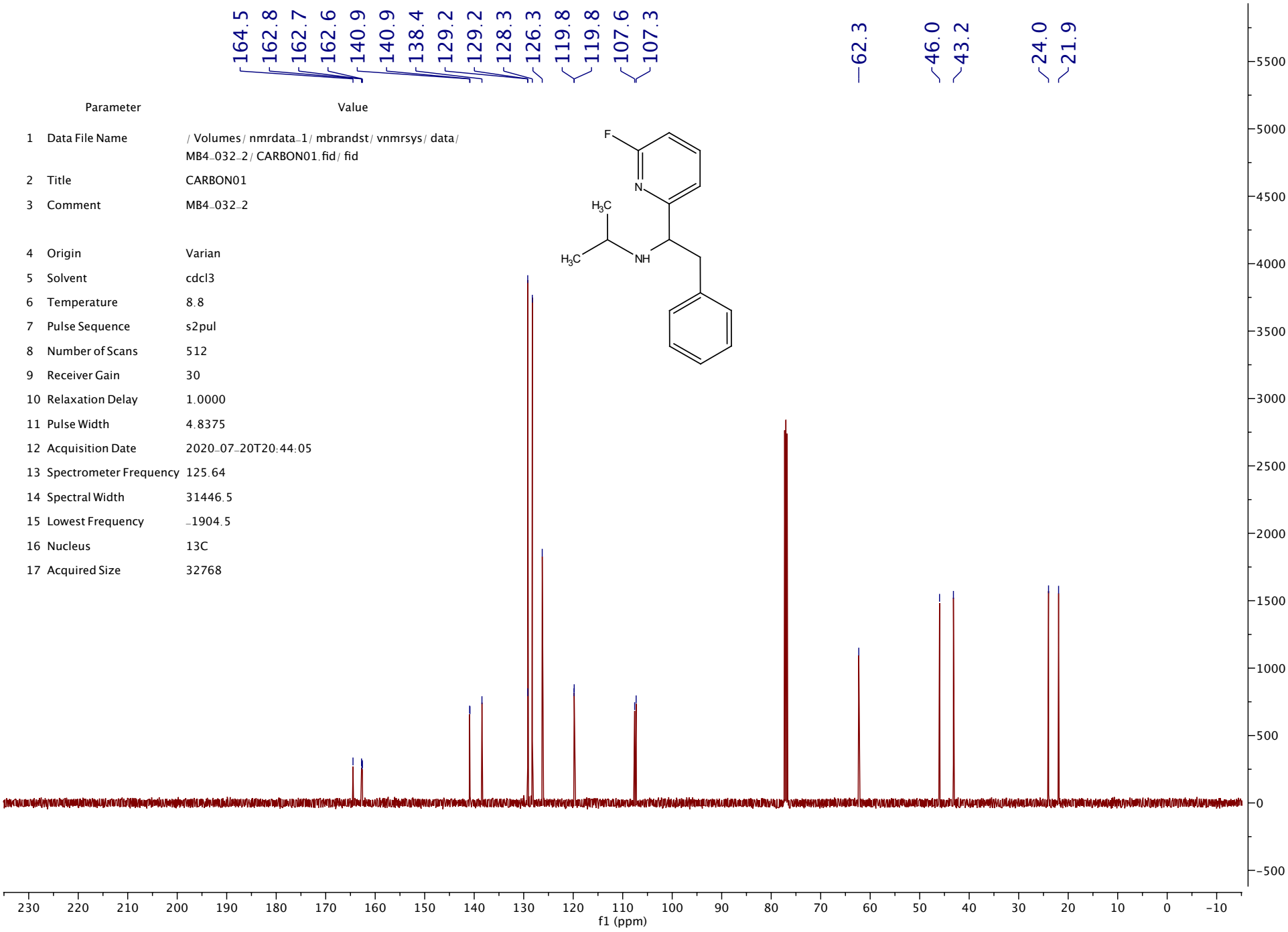
2	Title	CARBON01
3	Comment	MB4_025_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_06T23:19:19
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	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
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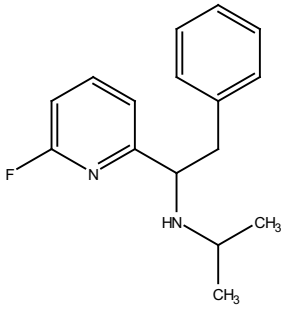
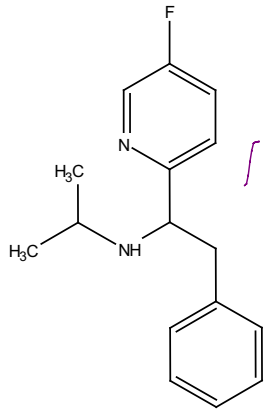
2	Title	CARBON01
3	Comment	MB4_032_2
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	8.8
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition Date	2020_07_20T20:44:05
13	Spectrometer Frequency	125.64
14	Spectral Width	31446.5
15	Lowest Frequency	-1904.5
16	Nucleus	13C
17	Acquired Size	32768

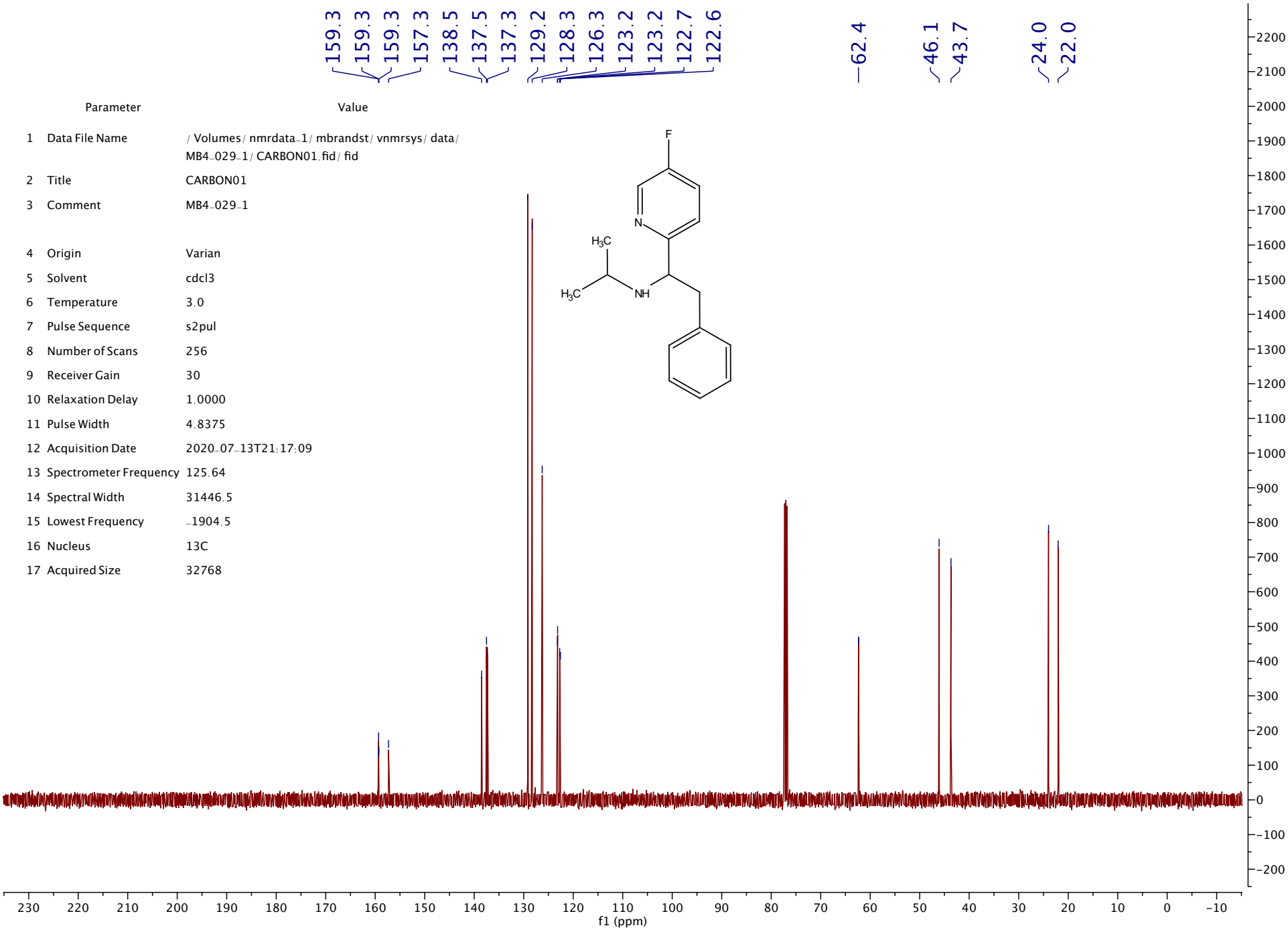
-67.6 -67.6 -67.6 -67.6 -67.6 -67.6

	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/vnmrsys/data/MB4_032/FLUORINE01.fid/fid
2	Title	FLUORINE01
3	Comment	MB4_032
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	6.3333
12	Acquisition Time	0.9856
13	Acquisition Date	2022_06_16T17:27:26
14	Spectrometer Frequency	282.34
15	Spectral Width	64935.1
16	Lowest Frequency	_56468.7
17	Nucleus	19F



	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

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159.3
157.3
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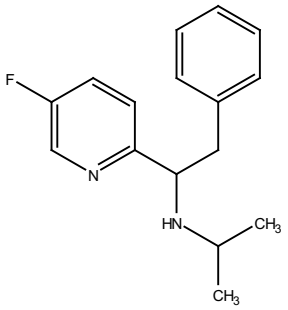
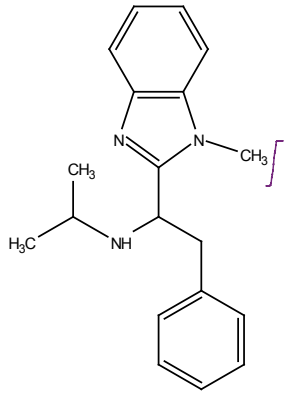
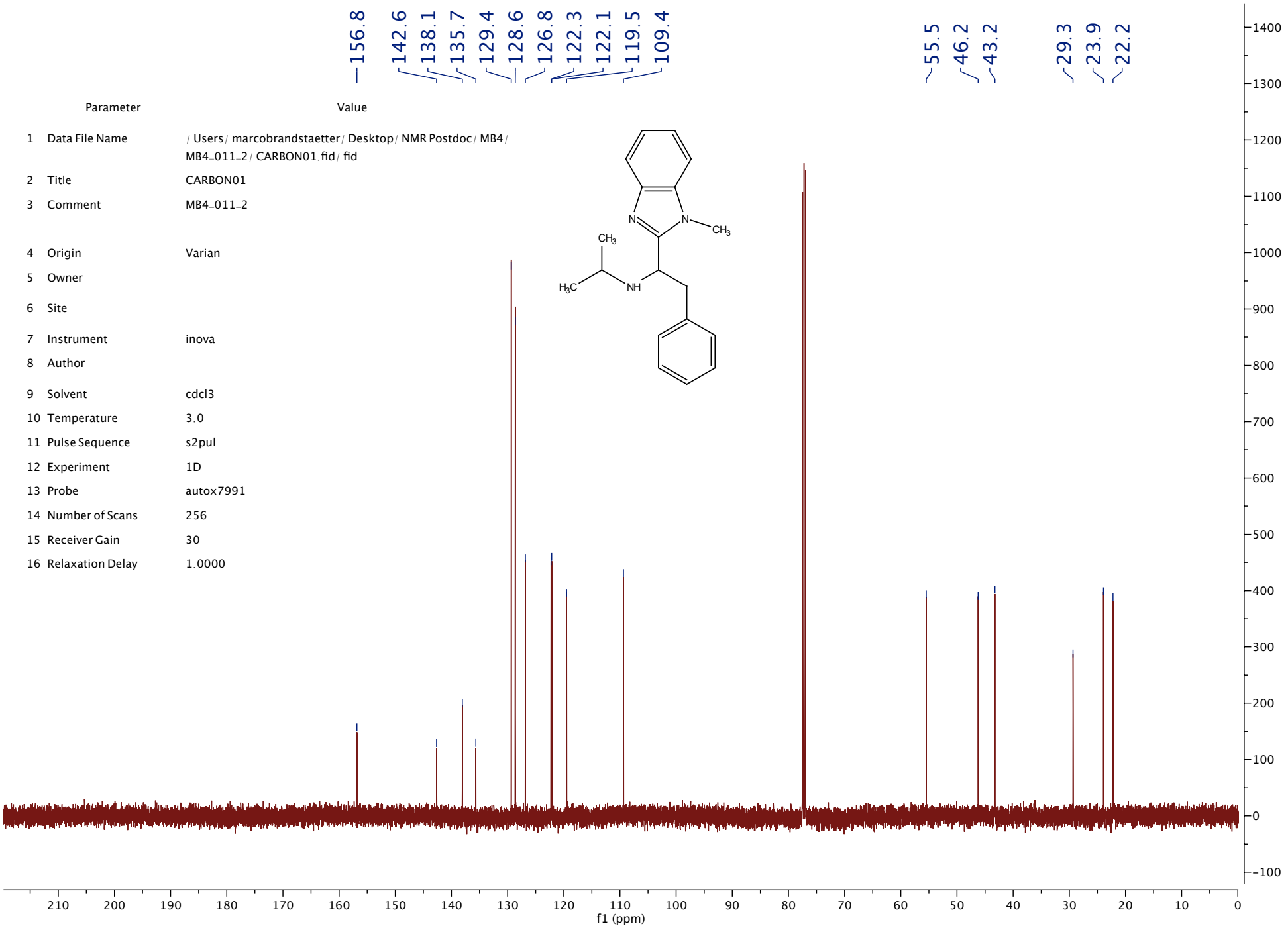
137.5
137.3
129.2
128.3
126.3
123.2
123.2
122.7
122.6
62.4
46.1
43.7
24.0
22.0
F
N
H3C
H3C
NH
Parameter
Value
1 Data File Name / Volumes/ nmrdata_1/ mbrandst/ vnmrsys/ data/ MB4_029_1/ CARBON01.fid/ fid
2 Title CARBON01
3 Comment MB4_029_1
4 Origin Varian
5 Solvent cdcl3
6 Temperature 3.0
7 Pulse Sequence 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
f1 (ppm)

	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/vnmrsys/data/MB3_292/FLUORINE01.fid/fid
2	Title	FLUORINE01
3	Comment	MB3_292
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	6.3333
12	Acquisition Time	0.9856
13	Acquisition Date	2022_06_16T17:31:25
14	Spectrometer Frequency	282.34
15	Spectral Width	64935.1
16	Lowest Frequency	_56468.7
17	Nucleus	19F

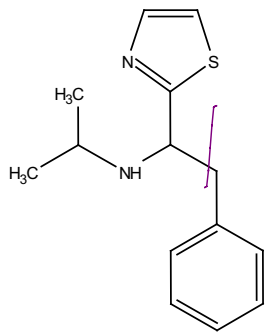


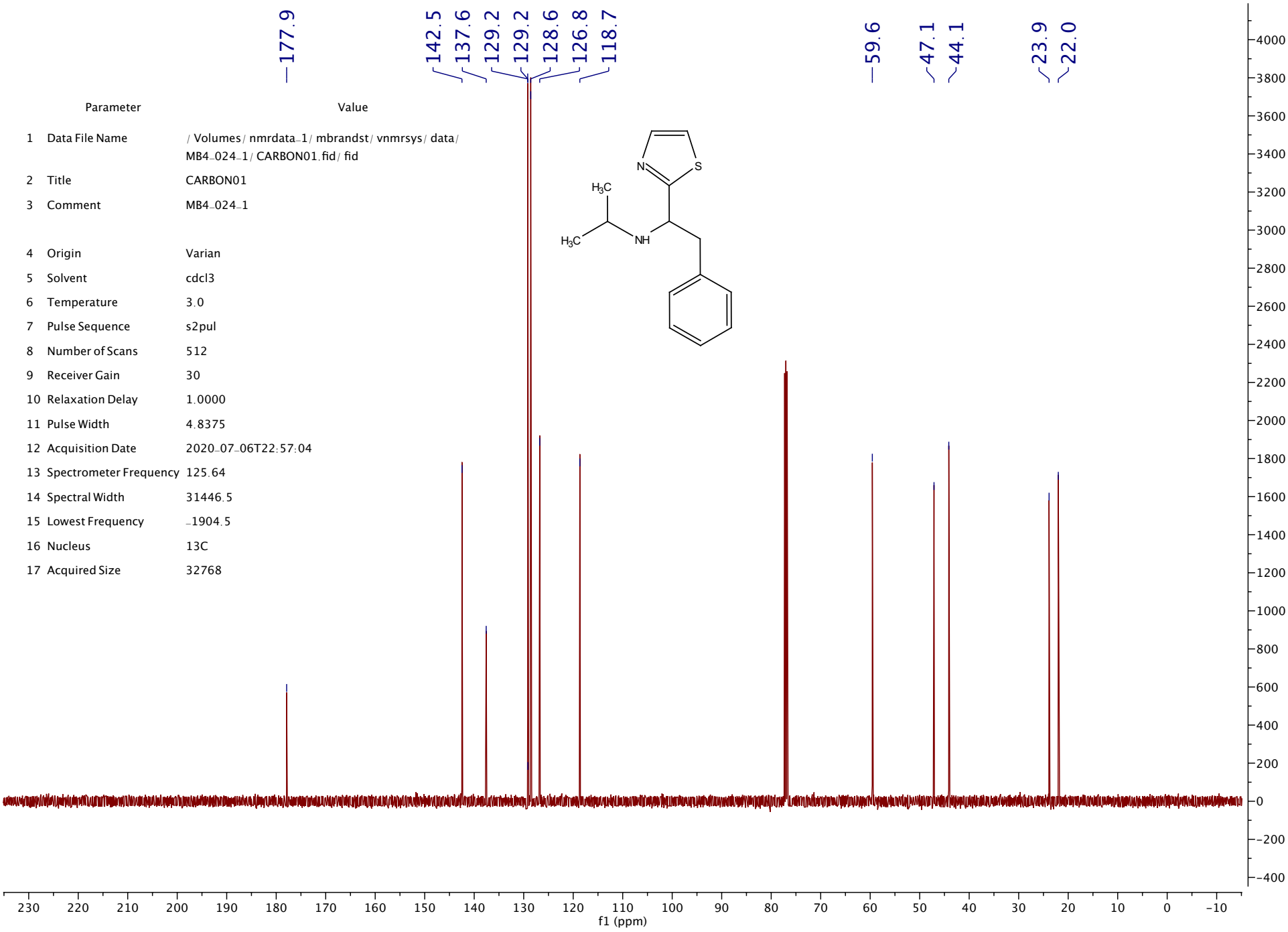
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_011_2 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_011_2
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	autox7991
14	Number of Scans	8
15	Receiver Gain	36
16	Relaxation Delay	1.0000




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
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB4 / MB4_011_2 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB4_011_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
N
N
CH3
CH3
H3C
NH
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

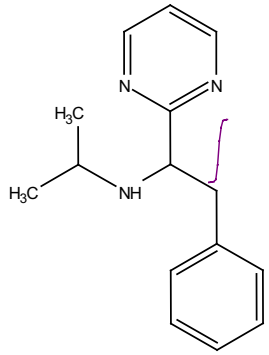
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_024_1/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB4_024_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	40
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	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

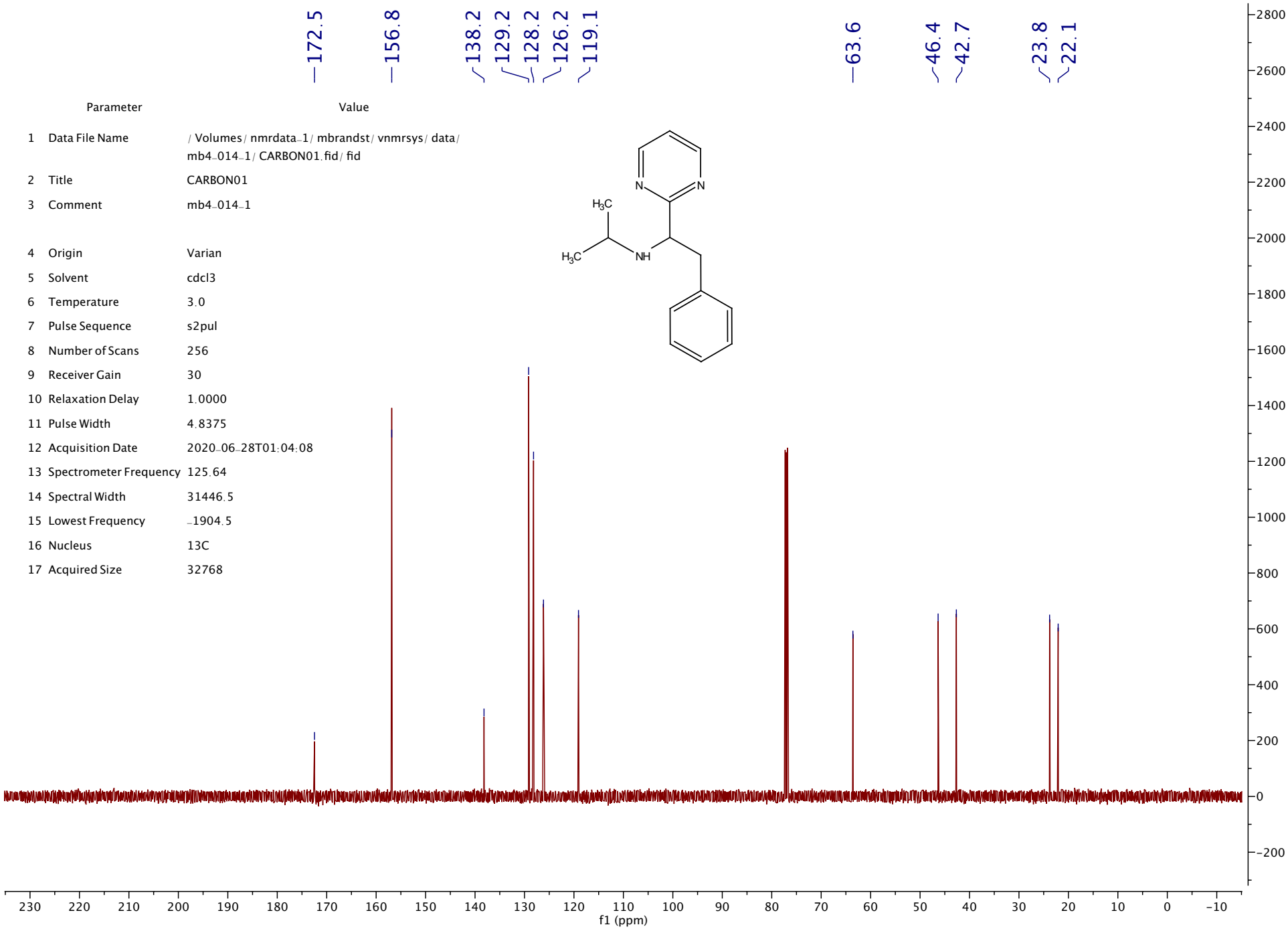




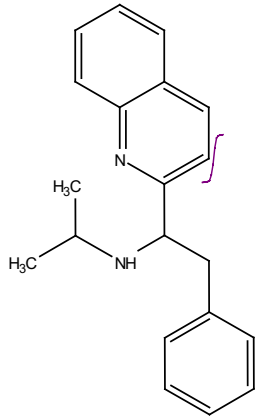
Parameter		Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_024_1 / CARBON01.fid / fid
2	Title	CARBON01
3	Comment	MB4_024_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse 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

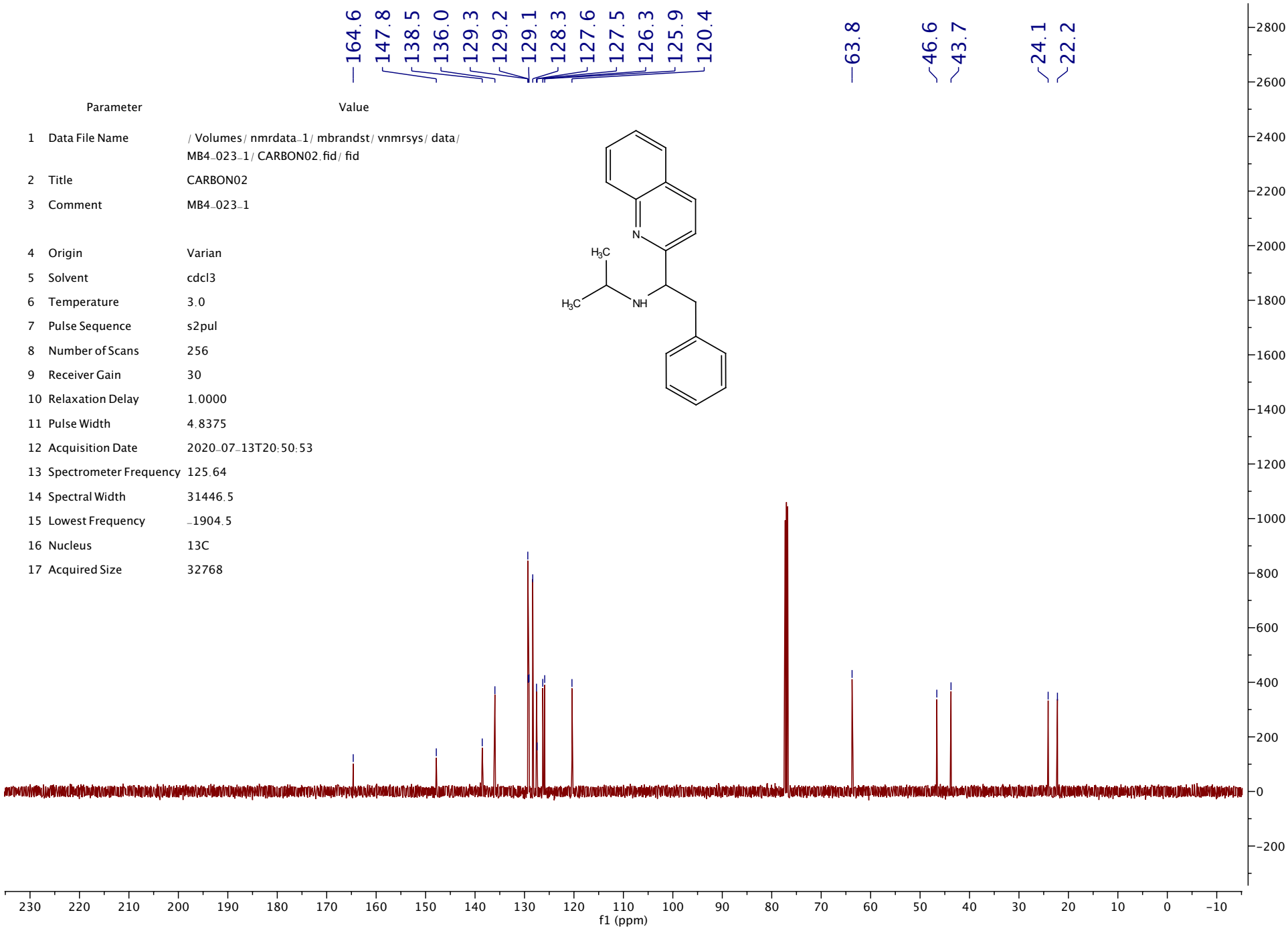
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / mb4_014_1 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb4_014_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse 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)

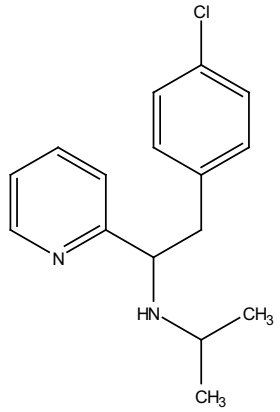
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB4_023_1/PROTON02.fid/fid
2	Title	PROTON02
3	Comment	MB4_023_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	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

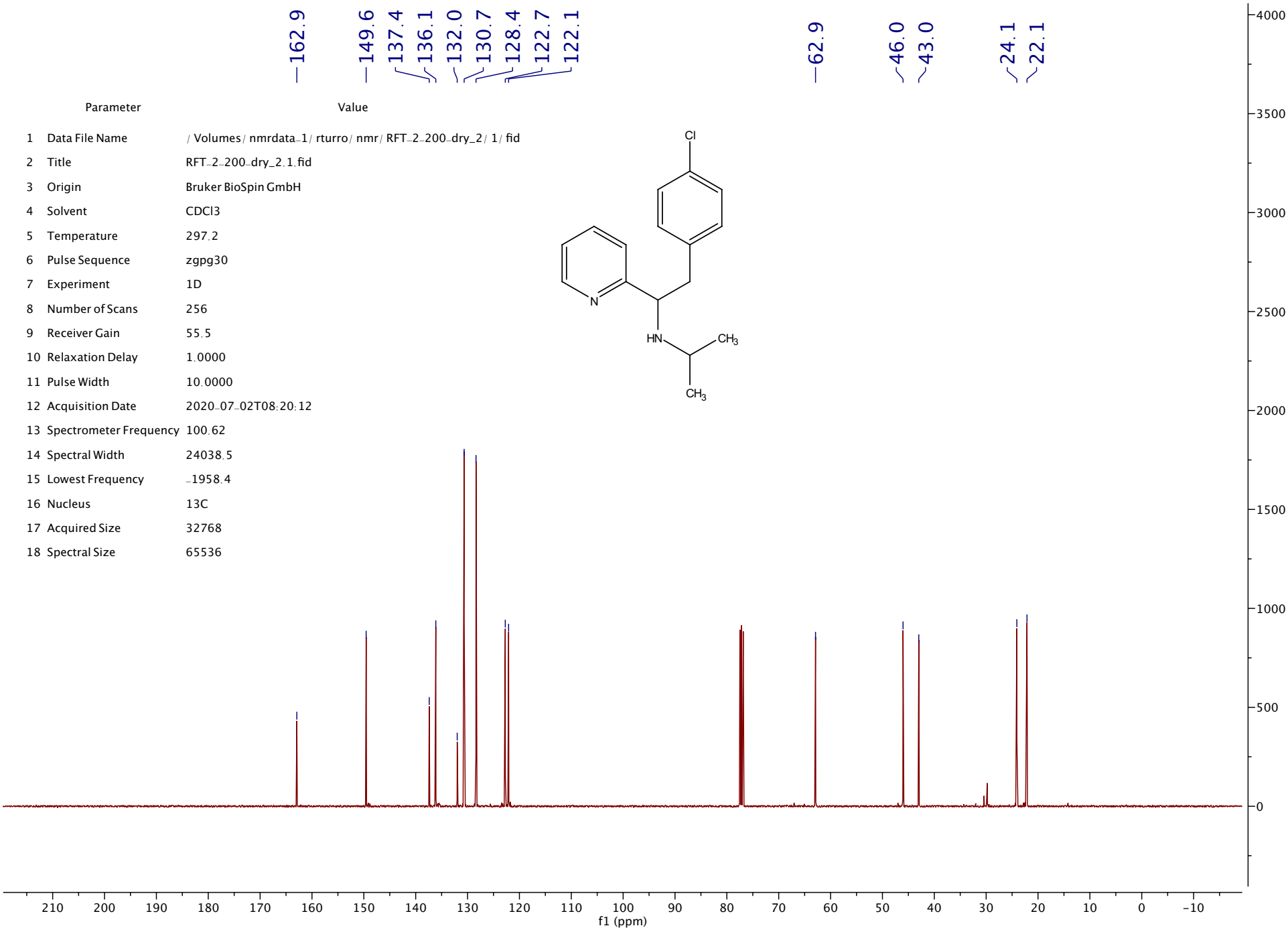




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_023_1 / CARBON02.fid / fid
2	Title	CARBON02
3	Comment	MB4_023_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse 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

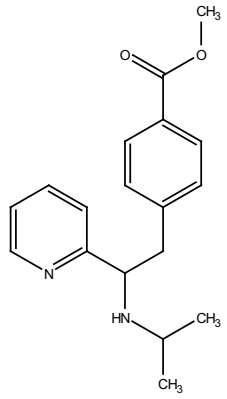
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_228_F2 / 1 / fid
2	Title	RFT_2_228_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	32
9	Receiver Gain	21.4
10	Relaxation Delay	1.0000
11	Pulse 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

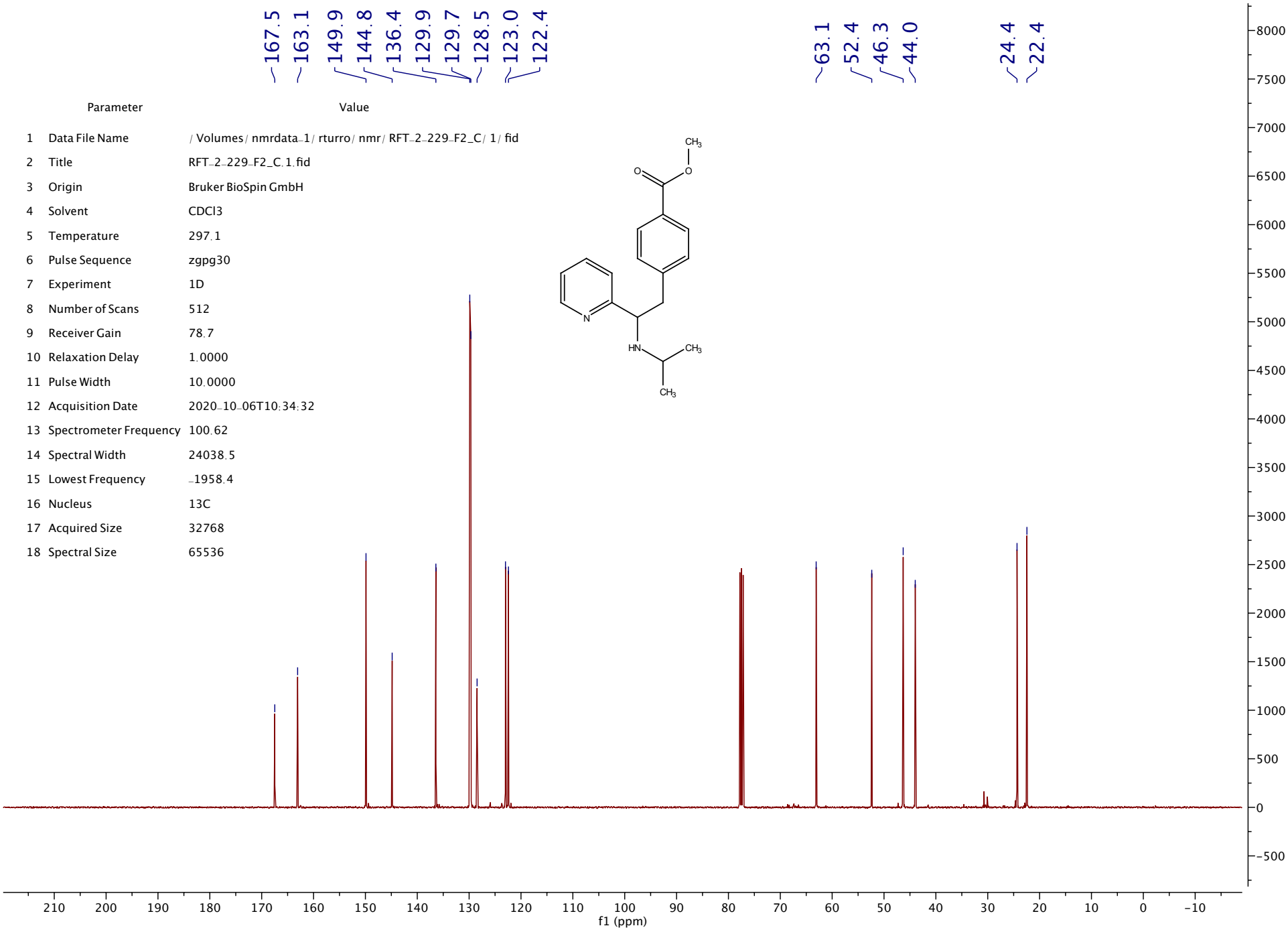




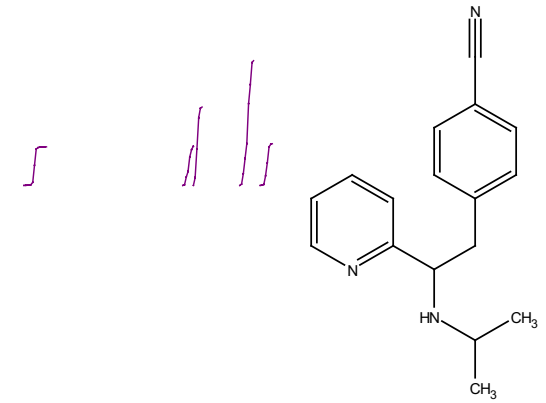
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_200_dry_2 / 1 / fid
2	Title	RFT_2_200_dry_2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	256
9	Receiver Gain	55.5
10	Relaxation Delay	1.0000
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

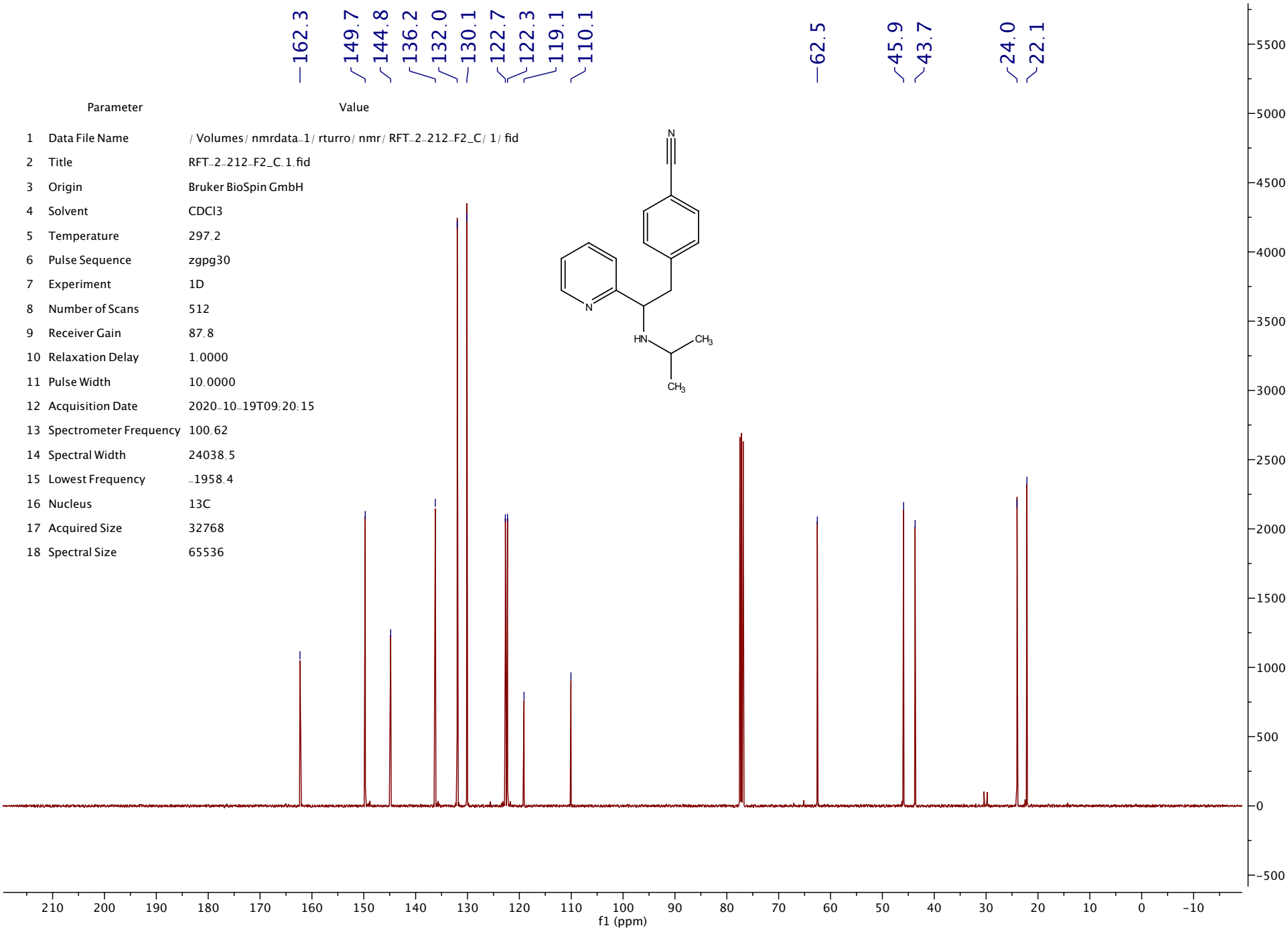
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_229_F2 / 1 / fid
2	Title	RFT_2_229_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	21.4
10	Relaxation Delay	1.0000
11	Pulse 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



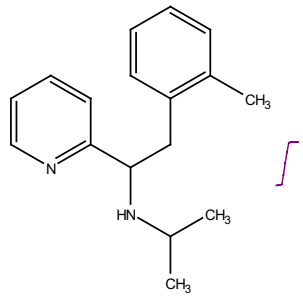

167.5
163.1
149.9
144.8
136.4
129.9
129.7
128.5
123.0
122.4
63.1
52.4
46.3
44.0
24.4
22.4
Parameter
Value
1 Data File Name / Volumes / nmrdata_1 / rturro / nmr / RFT_2_229_F2_C / 1 / fid
2 Title RFT_2_229_F2_C.1.fid
3 Origin Bruker BioSpin GmbH
4 Solvent CDCl3
5 Temperature 297.1
6 Pulse Sequence zgpg30
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
CH3
O
O
N
HN
CH3
CH3
8000
7500
7000
6500
6000
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)

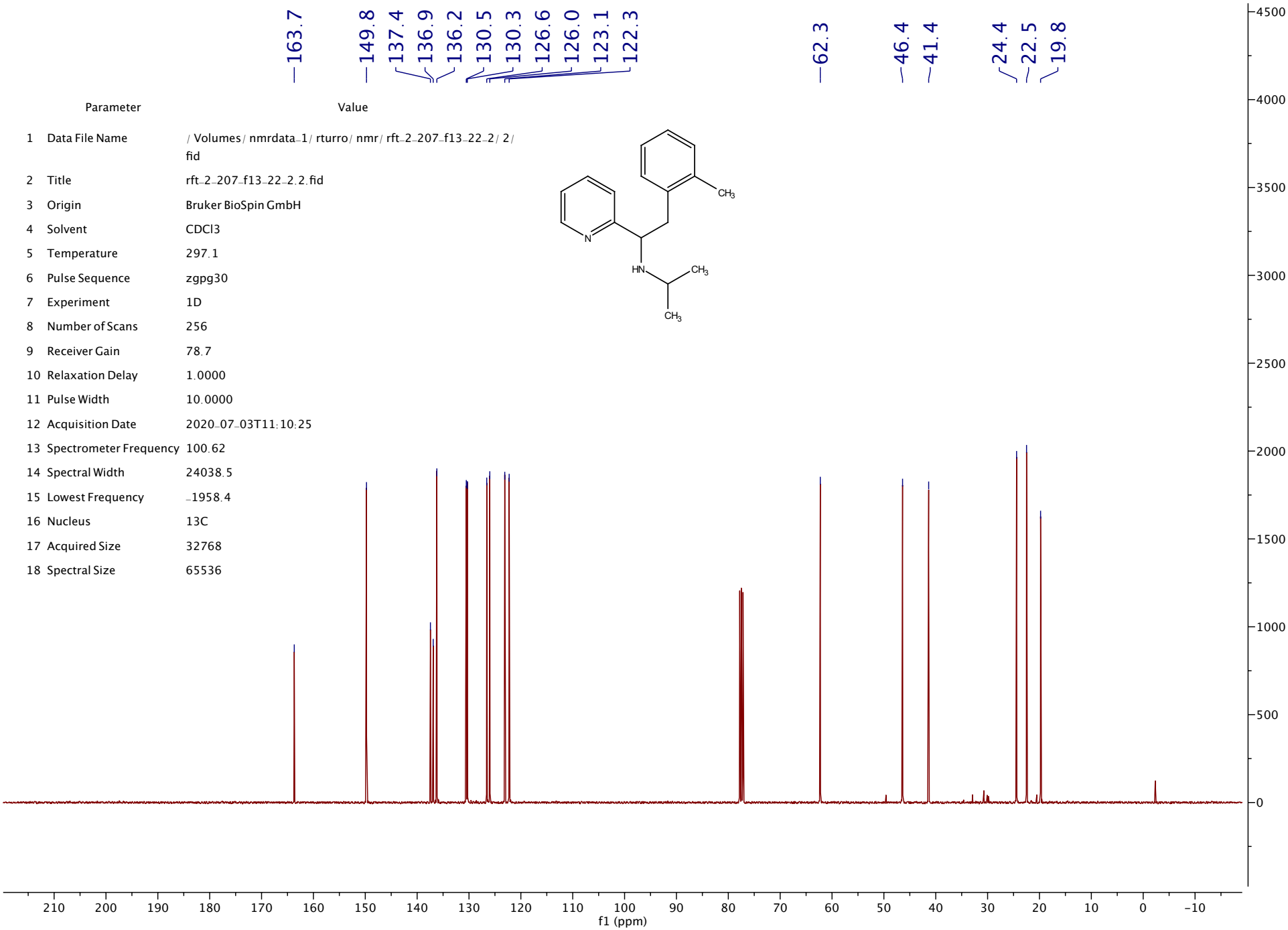
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_212_F2 / 1 / fid
2	Title	RFT_2_212_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse 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)

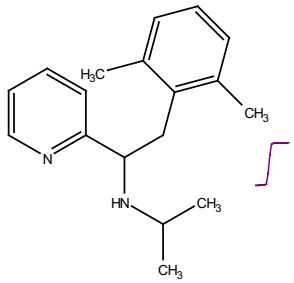
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_207_C2_F13_32 / 1 / fid
2	Title	RFT_2_207_C2_F13_32.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	17.5
10	Relaxation Delay	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

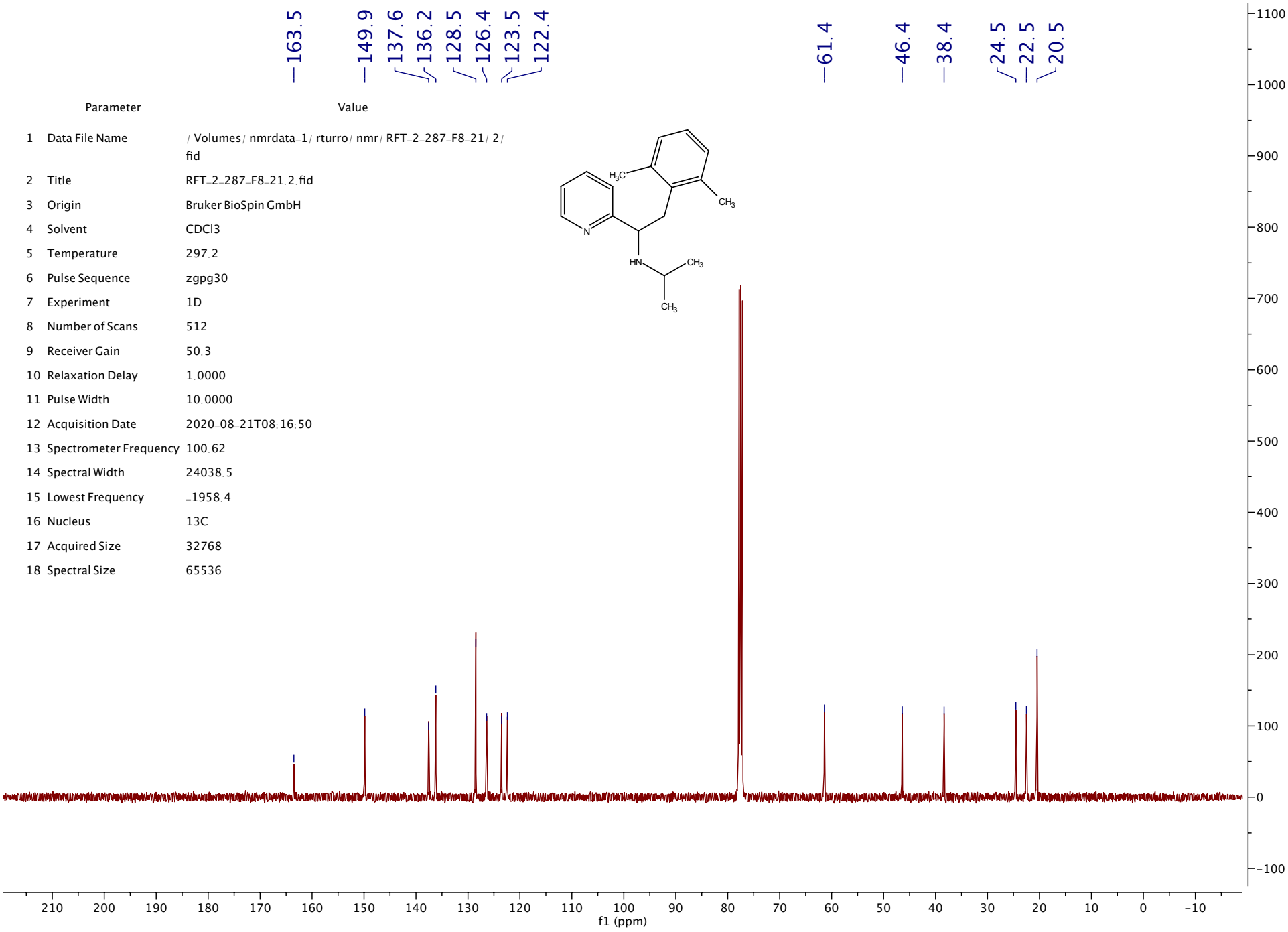




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / rft_2_207_f13_22_2 / 2 / fid
2	Title	rft_2_207_f13_22_2.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	256
9	Receiver Gain	78.7
10	Relaxation Delay	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

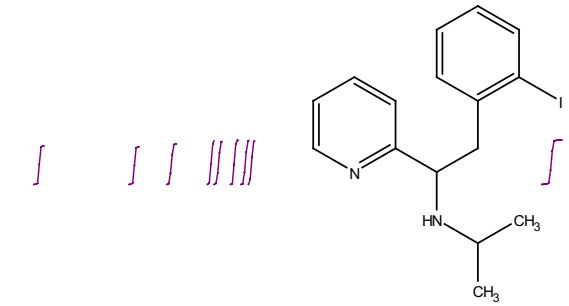
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_2_287_F8_21 / 1 / fid
2	Title	RFT_2_287_F8_21.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	98.9
10	Relaxation Delay	1.0000
11	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

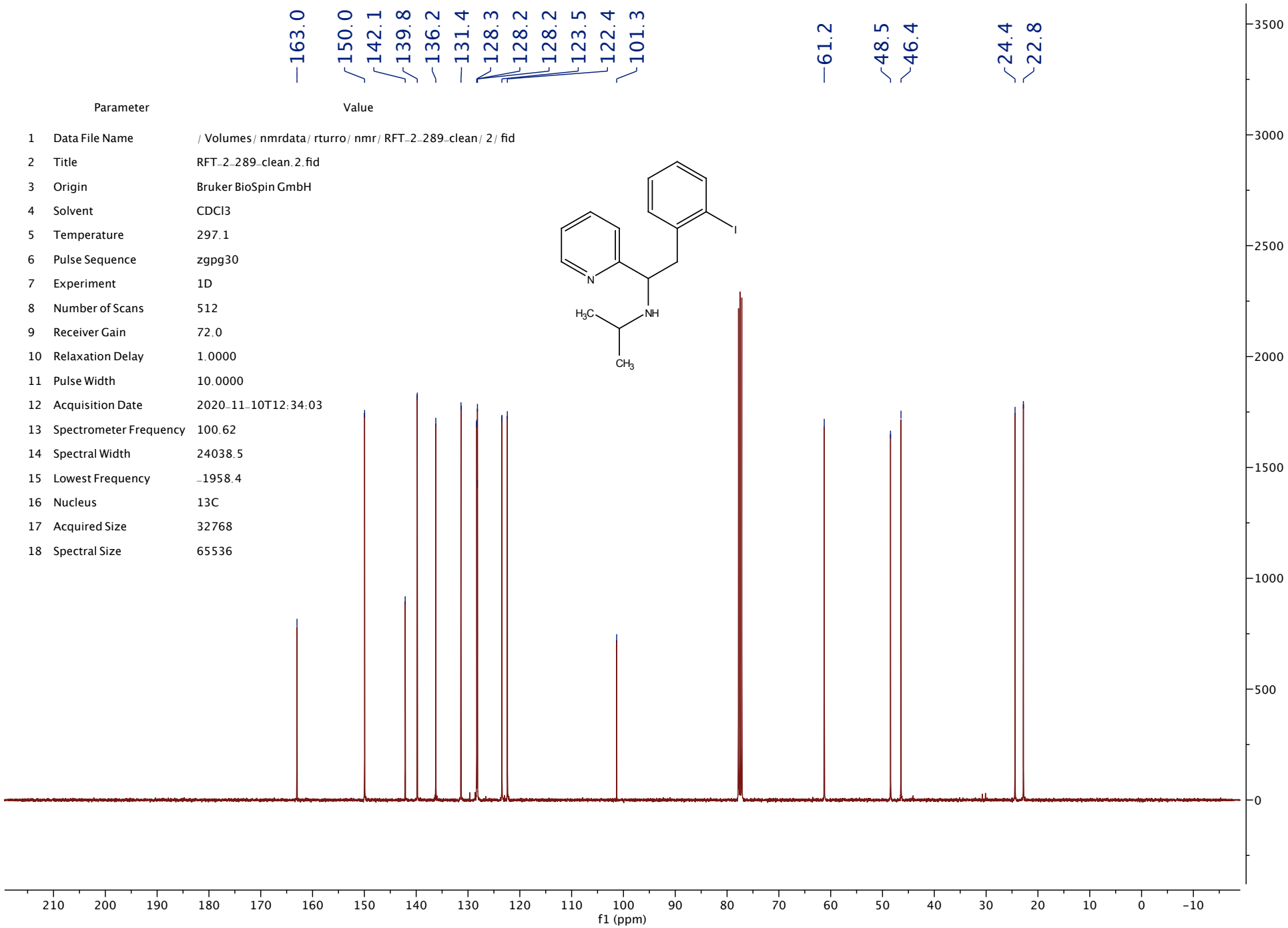




	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata_1/ rturro/ nmr/ RFT_2_287_F8_21/ 2/ fid
2	Title	RFT_2_287_F8_21.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse 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

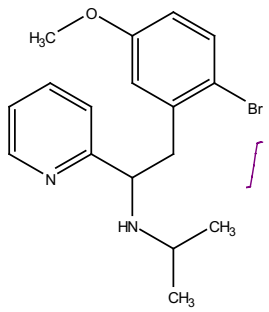
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/vnmrsys/data/RFT_2_289_F8_21/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	RFT_2_289_F8_21
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	23.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	56
10	Relaxation Delay	1.0000
11	Pulse Width	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

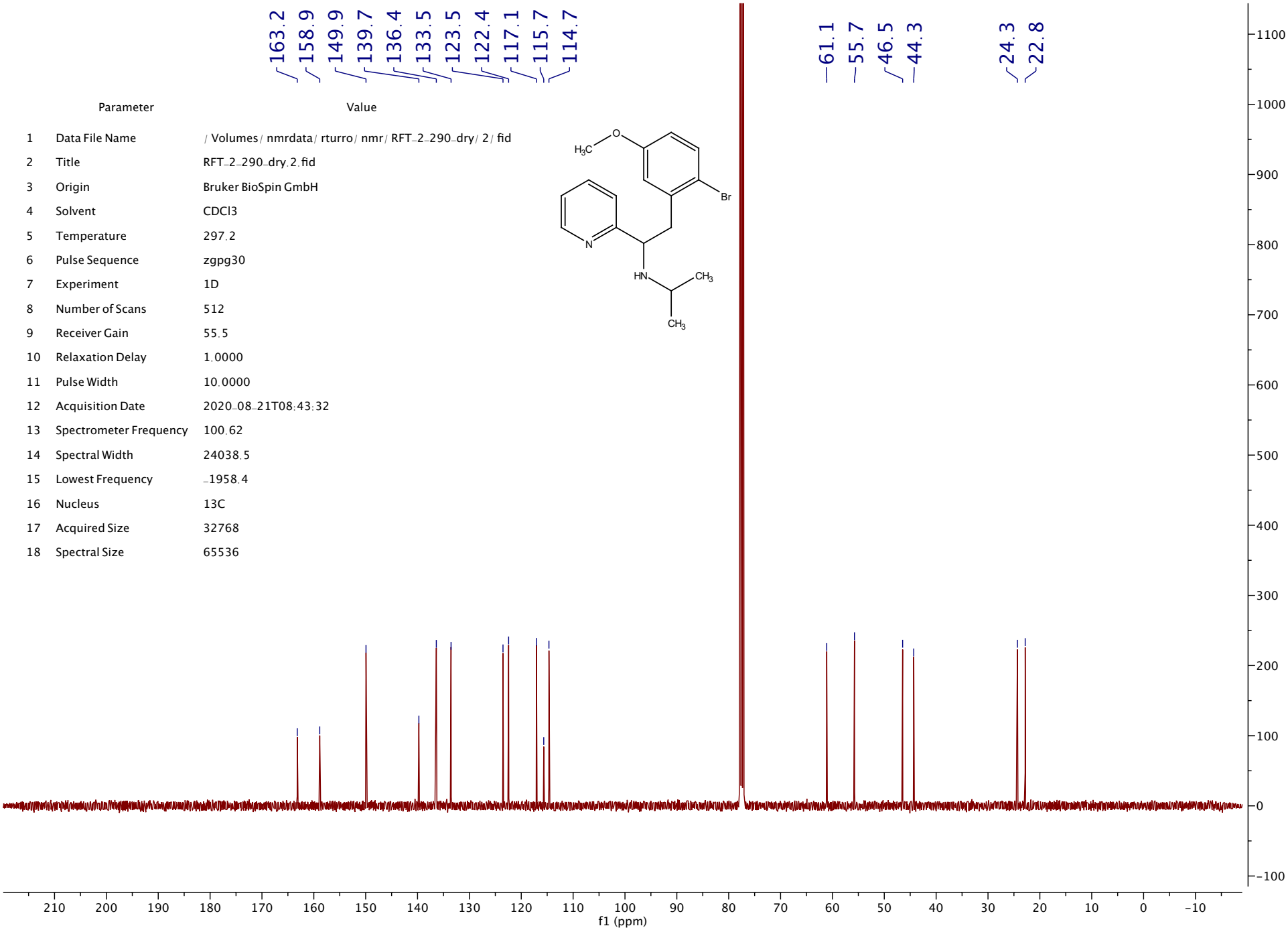




	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ RFT_2_289_clean/ 2/ fid
2	Title	RFT_2_289_clean.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	72.0
10	Relaxation Delay	1.0000
11	Pulse 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

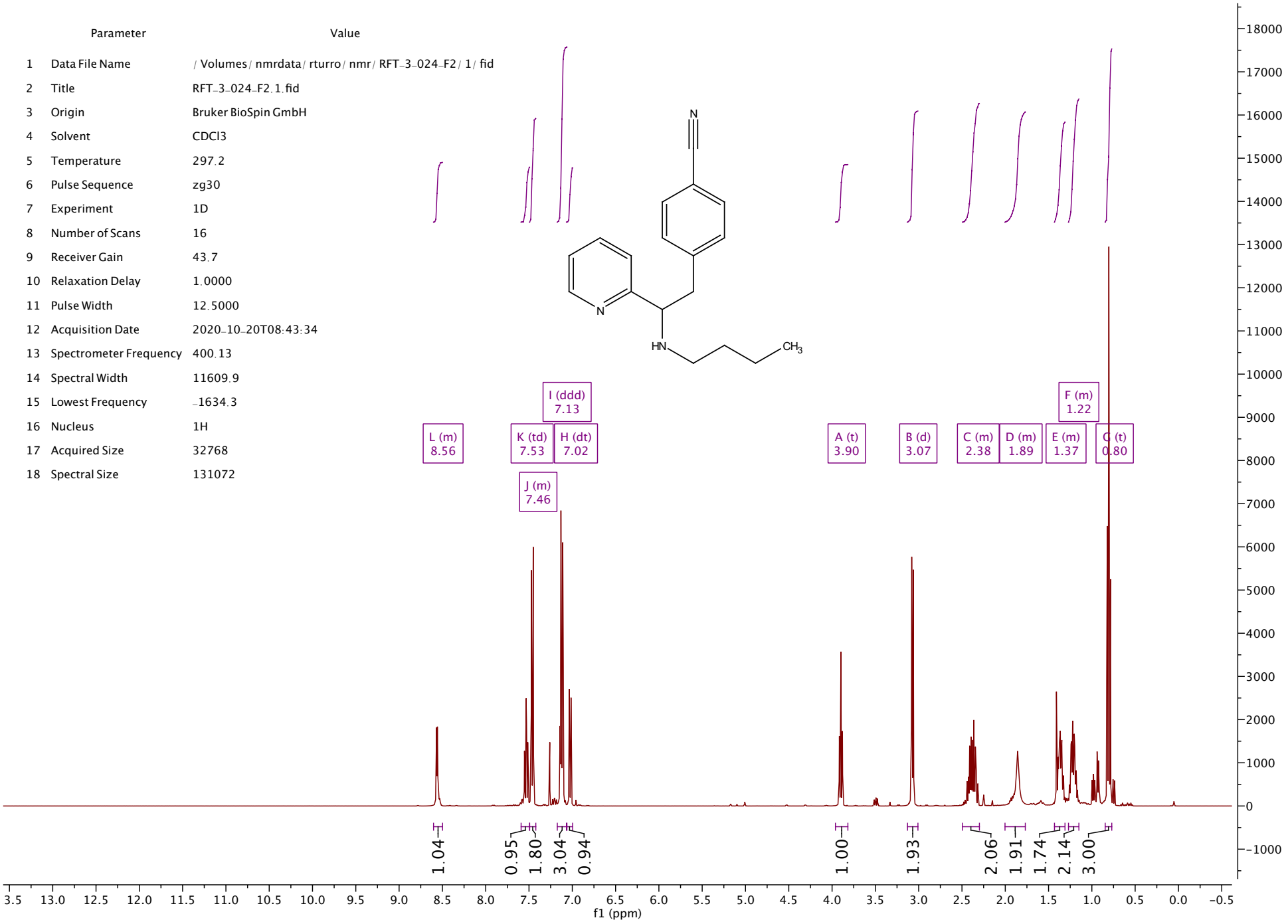
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_2_290_dry / 1 / fid
2	Title	RFT_2_290_dry.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse 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

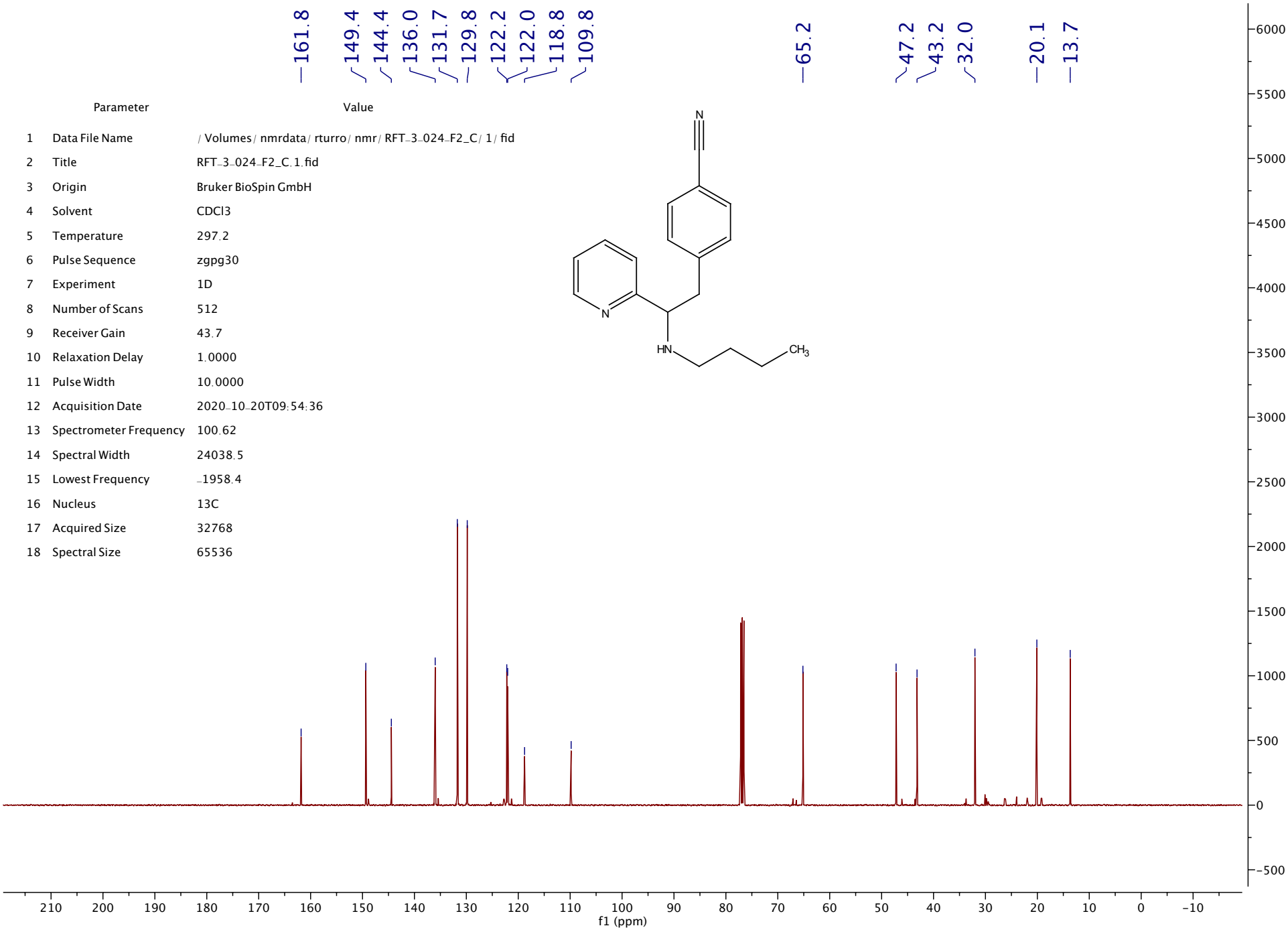




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_2_290_dry/2/fid
2	Title	RFT_2_290_dry.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	55.5
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
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

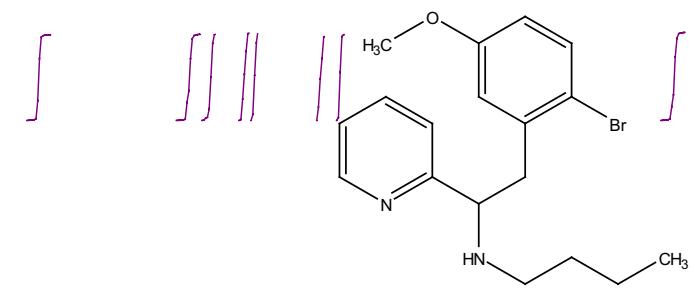
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_024_F2 / 1 / fid
2	Title	RFT_3_024_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse 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

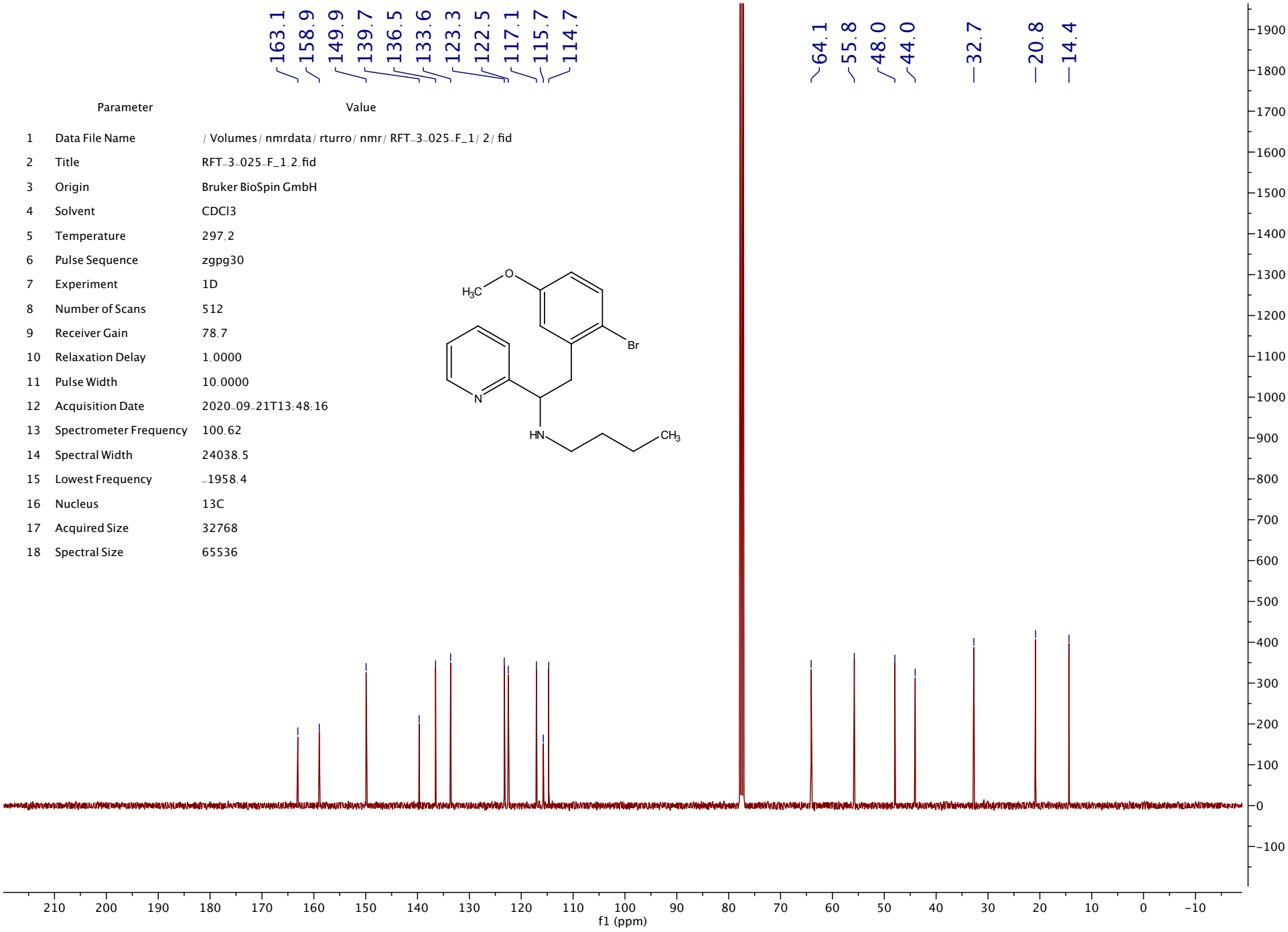




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_024_F2_C/1/fid
2	Title	RFT_3_024_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	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

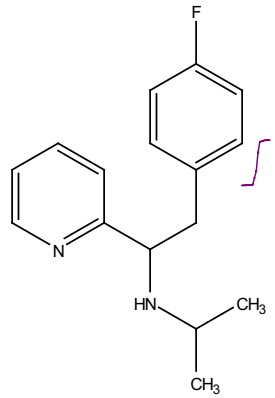
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_025_F_1 / 1 / fid
2	Title	RFT_3_025_F_1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse 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

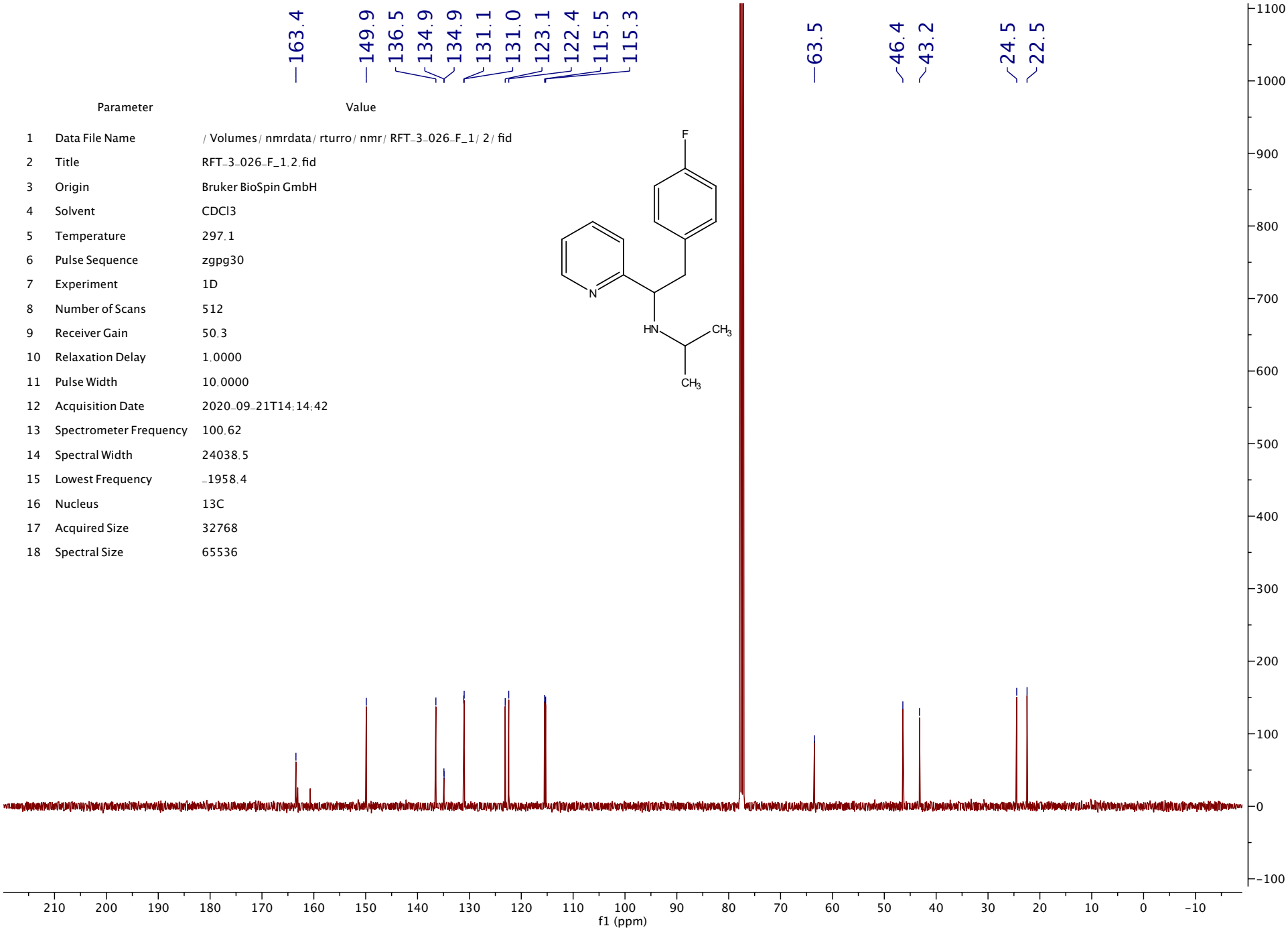




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_025_F_1/2/fid
2	Title	RFT_3_025_F_1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	78.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
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

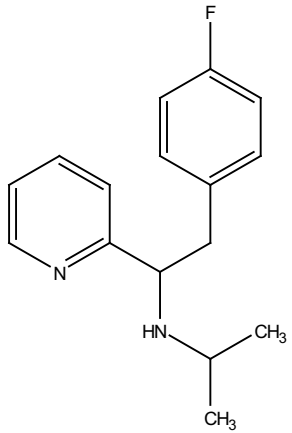
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_026_F_1 / 1 / fid
2	Title	RFT_3_026_F_1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	197.4
10	Relaxation Delay	1.0000
11	Pulse 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



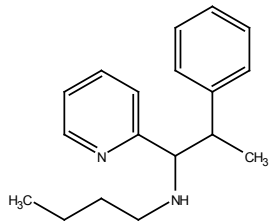


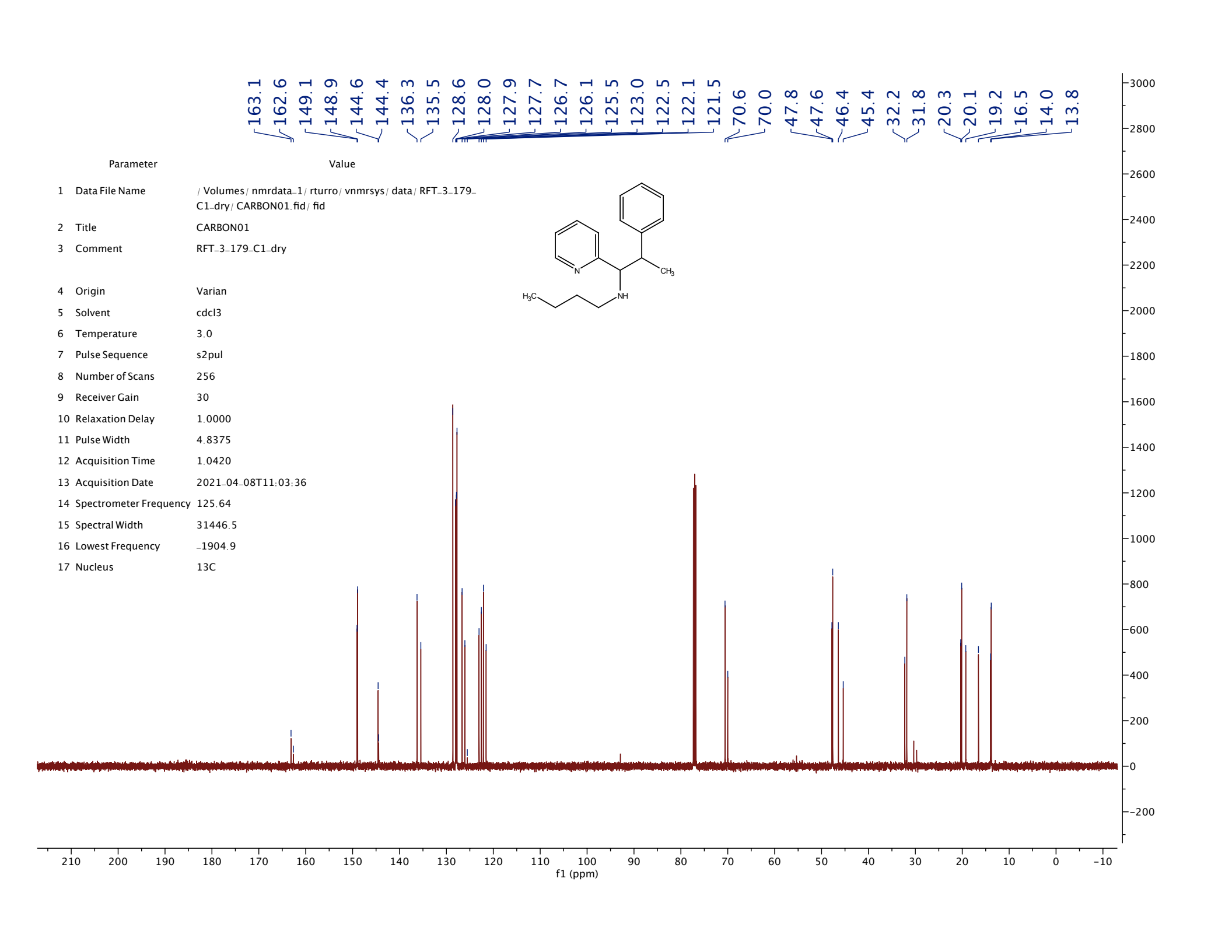
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_026_F_1/2/fid
2	Title	RFT_3_026_F_1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
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/rturro/vnmrsys/data/RFT_3_026/FLUORINE01.fid/fid
2	Title	FLUORINE01
3	Comment	RFT_3_026
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	6.3333
12	Acquisition Time	0.9856
13	Acquisition Date	2022_06_16T17:19:51
14	Spectrometer Frequency	282.34
15	Spectral Width	64935.1
16	Lowest Frequency	_56468.7
17	Nucleus	19F

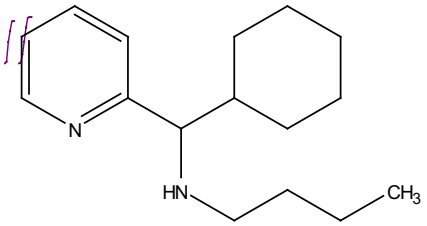


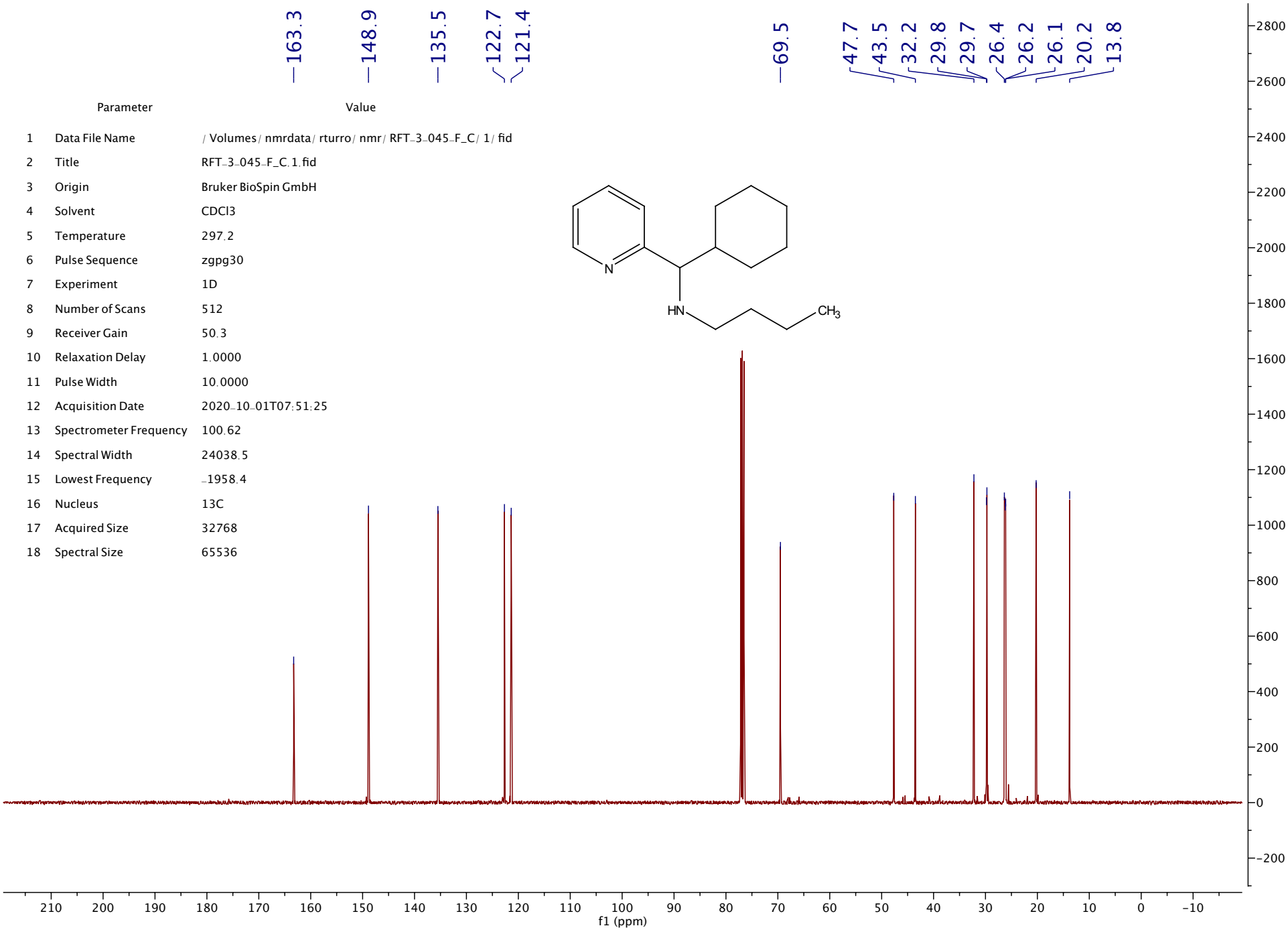
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / vnmrsys / data / RFT_3_179_C1_dry / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	RFT_3_179_C1_dry
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	1
9	Receiver Gain	42
10	Relaxation Delay	10.0000
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




163.1
162.6
149.1
148.9
144.6
144.4
136.3
135.5
128.6
128.0
127.9
127.7
126.7
126.1
125.5
123.0
122.5
122.1
121.5
70.6
70.0
47.8
47.6
46.4
45.4
32.2
31.8
20.3
20.1
19.2
16.5
14.0
13.8
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
N
CH3
H3C
NH
f1 (ppm)

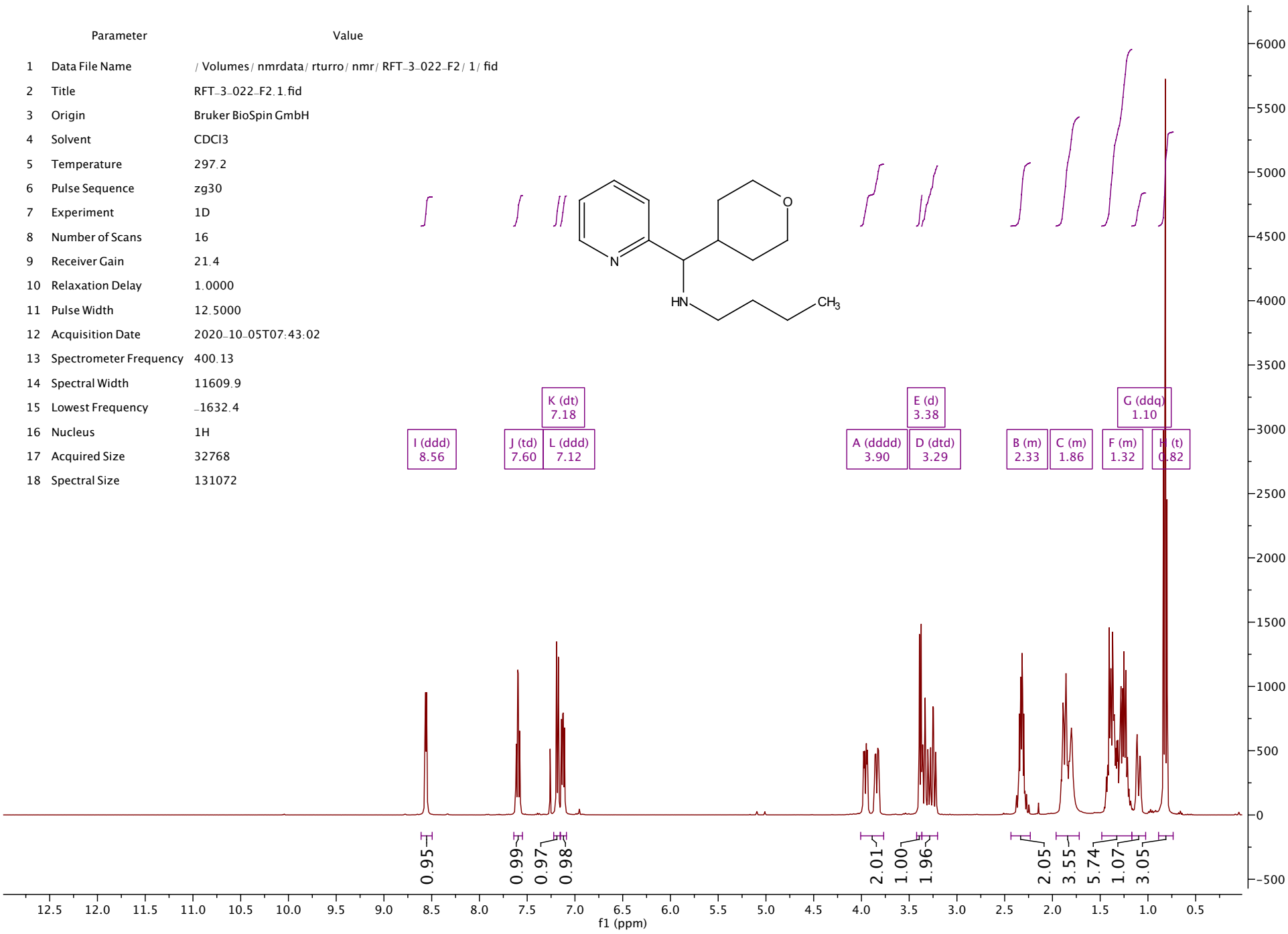
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_045_F/1/fid
2	Title	RFT_3_045_F.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	24.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	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

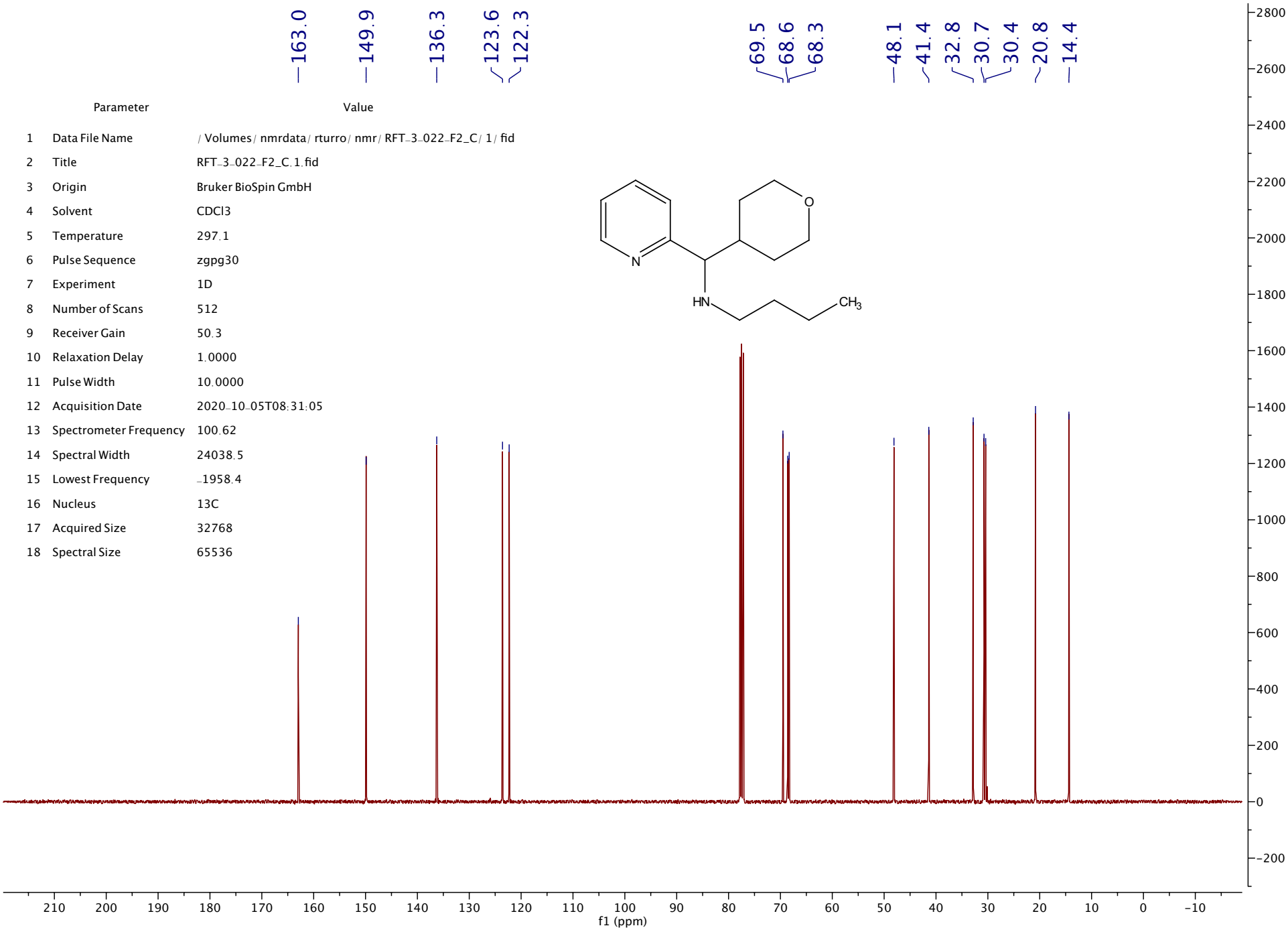




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_045_F_C/1/fid
2	Title	RFT_3_045_F_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
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

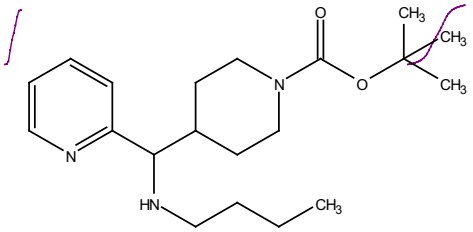
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_022_F2 / 1 / fid
2	Title	RFT_3_022_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	21.4
10	Relaxation Delay	1.0000
11	Pulse 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

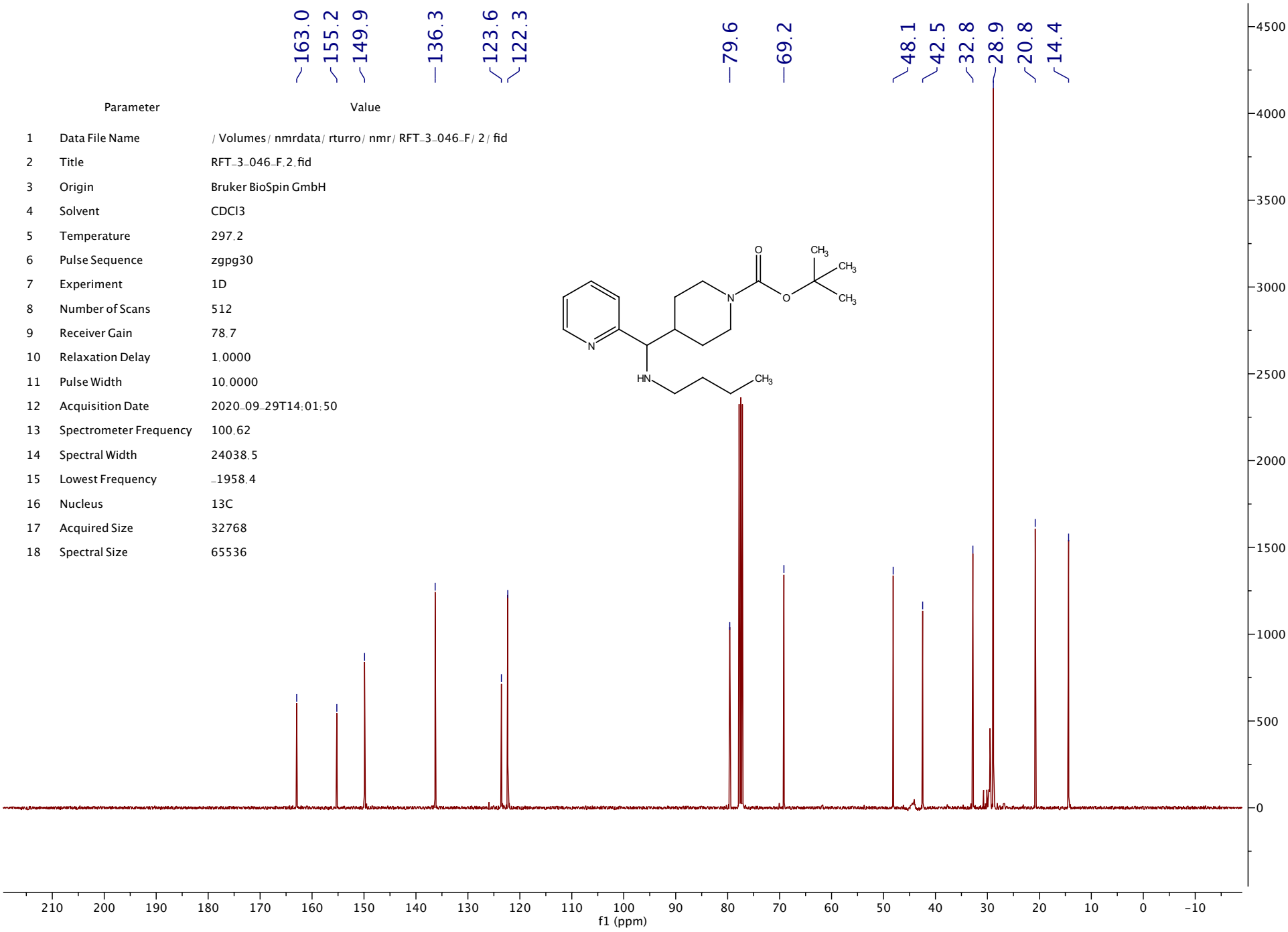




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_022_F2_C / 1 / fid
2	Title	RFT_3_022_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	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

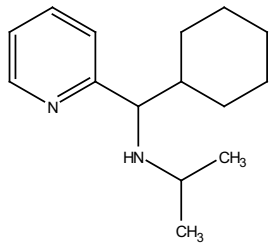
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_047_F/1/fid
2	Title	RFT_3_047_F.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	38.0
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	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

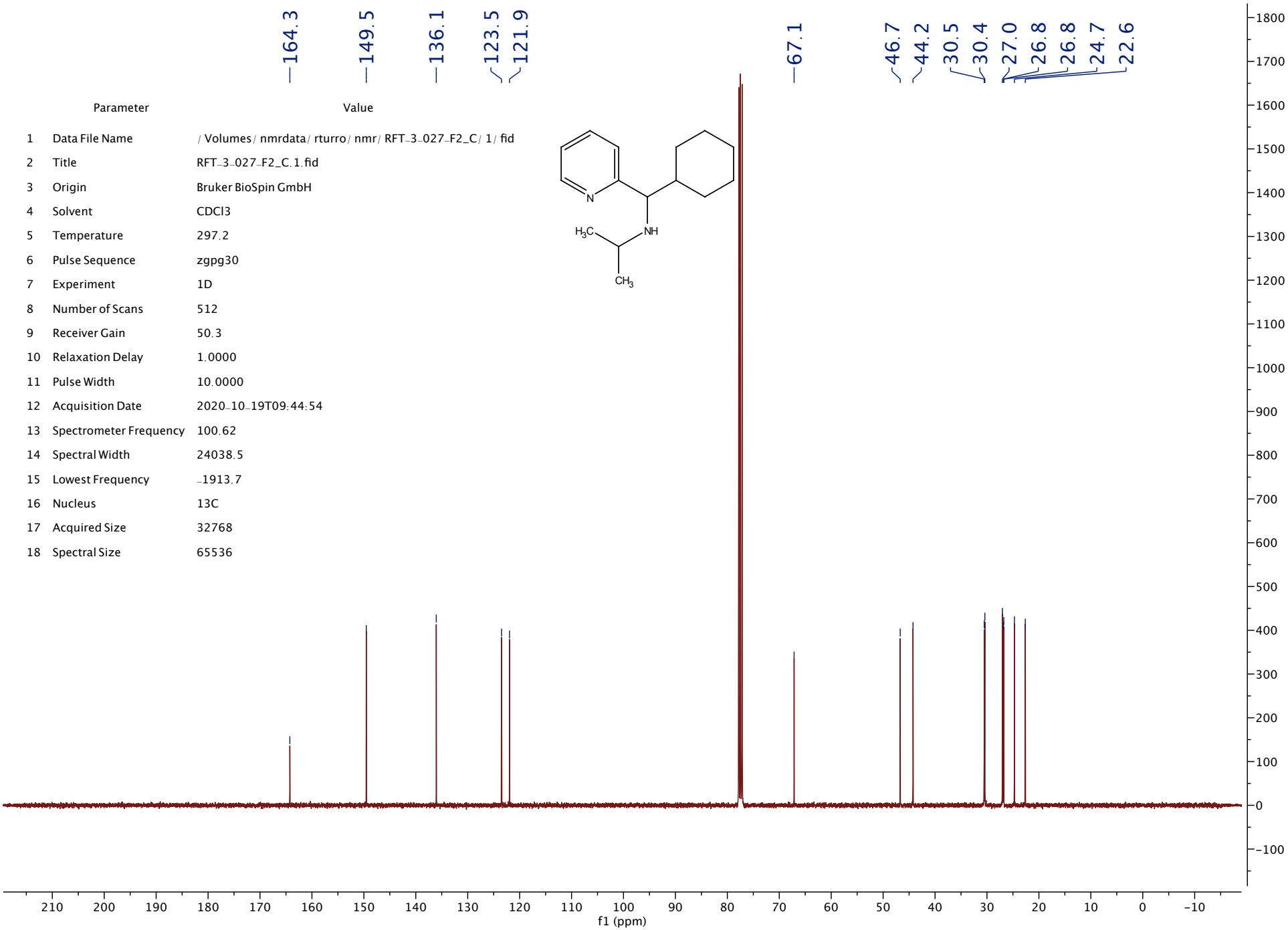




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_046_F / 2 / fid
2	Title	RFT_3_046_F.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	78.7
10	Relaxation Delay	1.0000
11	Pulse 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

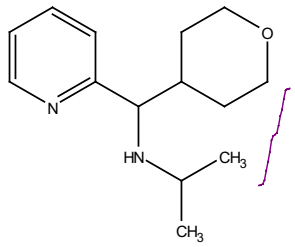
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_027_F2 / 1 / fid
2	Title	RFT_3_027_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	32
9	Receiver Gain	112.8
10	Relaxation Delay	1.0000
11	Pulse 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

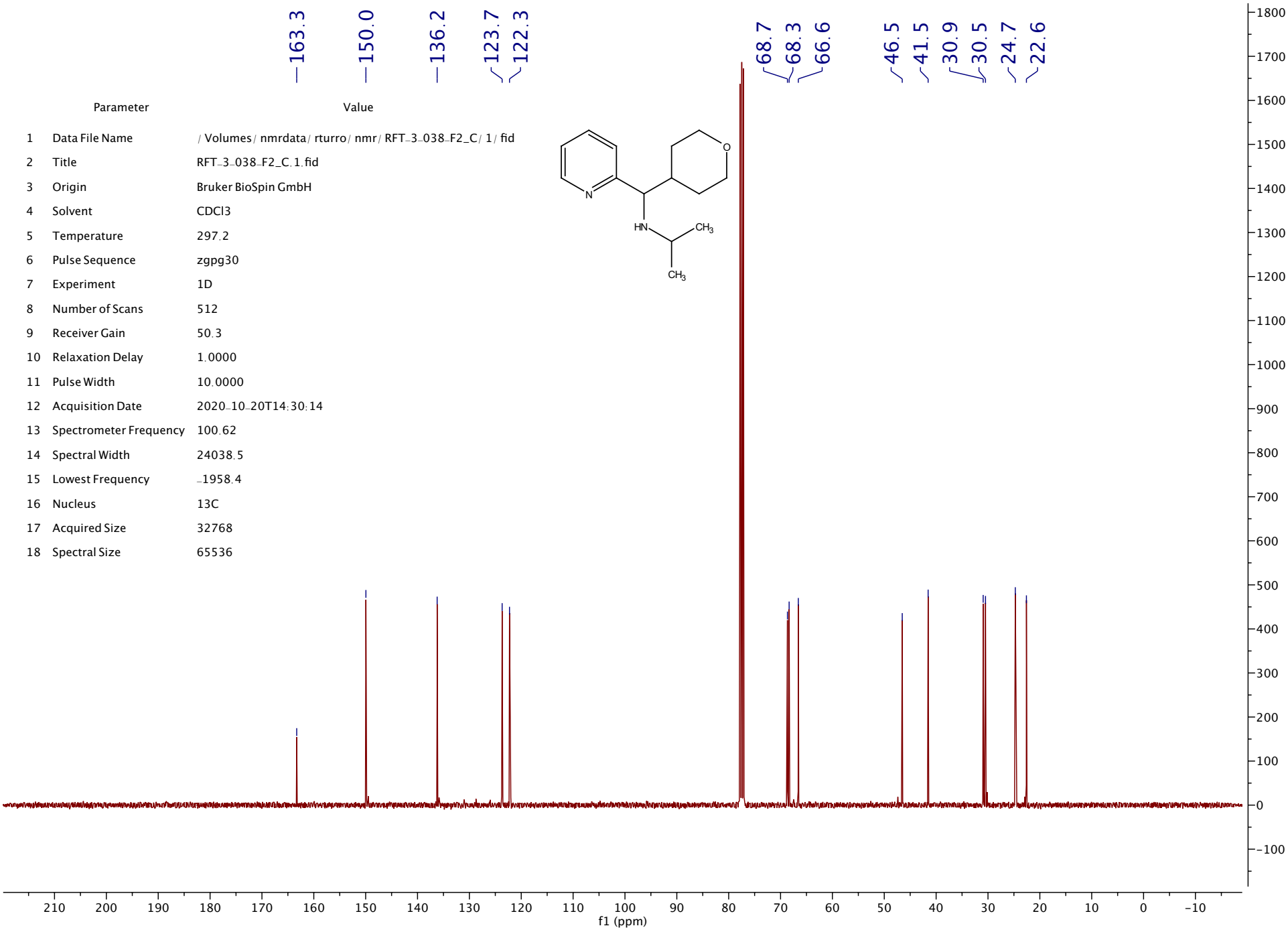




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_027_F2_C/1/fid
2	Title	RFT_3_027_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	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

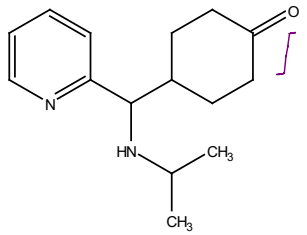
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_2/rturro/vnmrsys/data/RFT_3_038_F2_DCM/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	RFT_3_038_F2_DCM
4	Origin	Varian
5	Solvent	CDCl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	22
10	Relaxation Delay	1.0000
11	Pulse Width	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

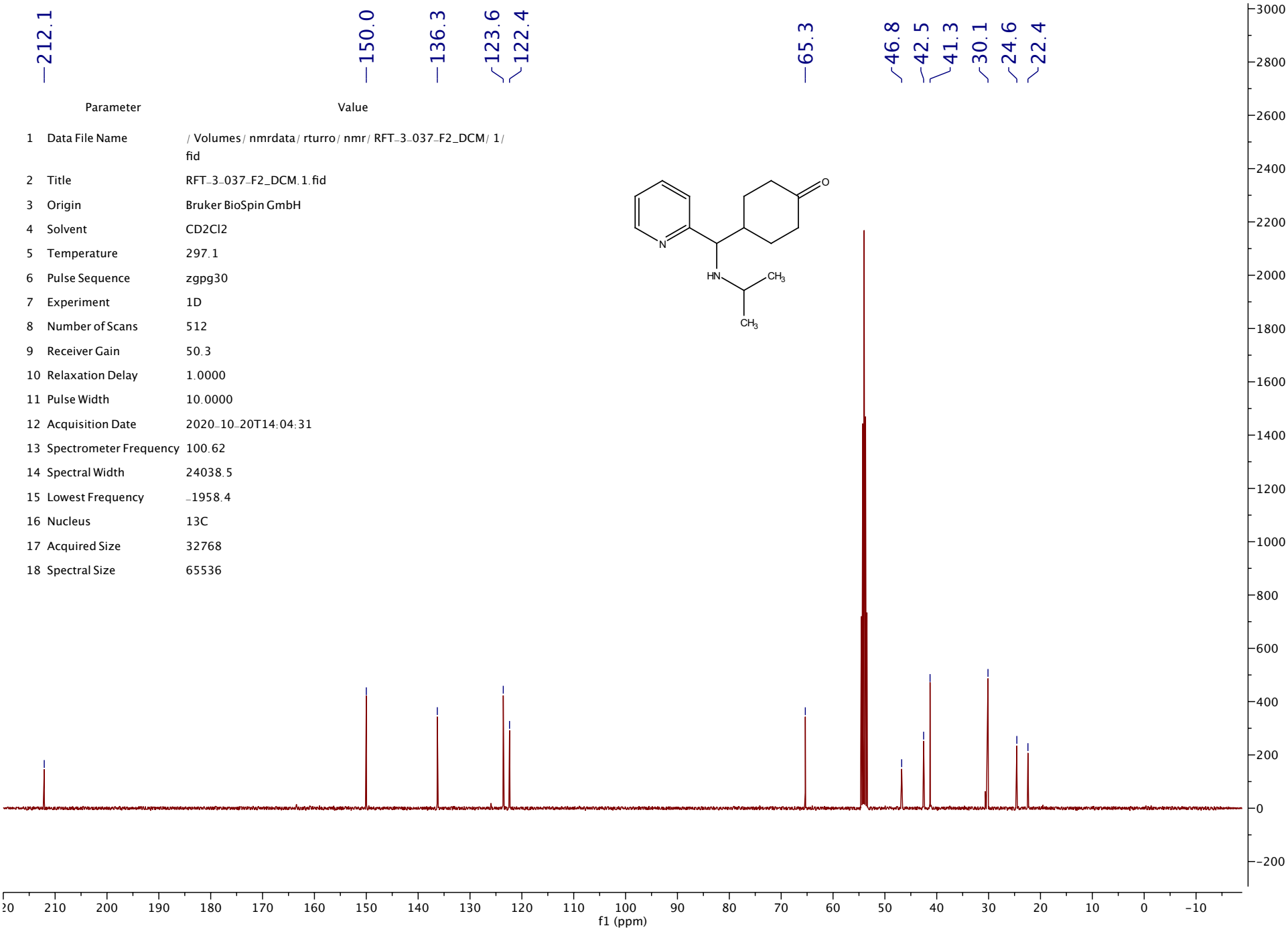




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_038_F2_C / 1 / fid
2	Title	RFT_3_038_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	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

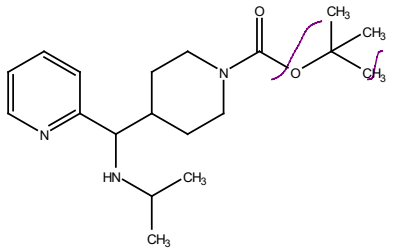
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_038_F2 / 1 / fid
2	Title	RFT_3_038_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse 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

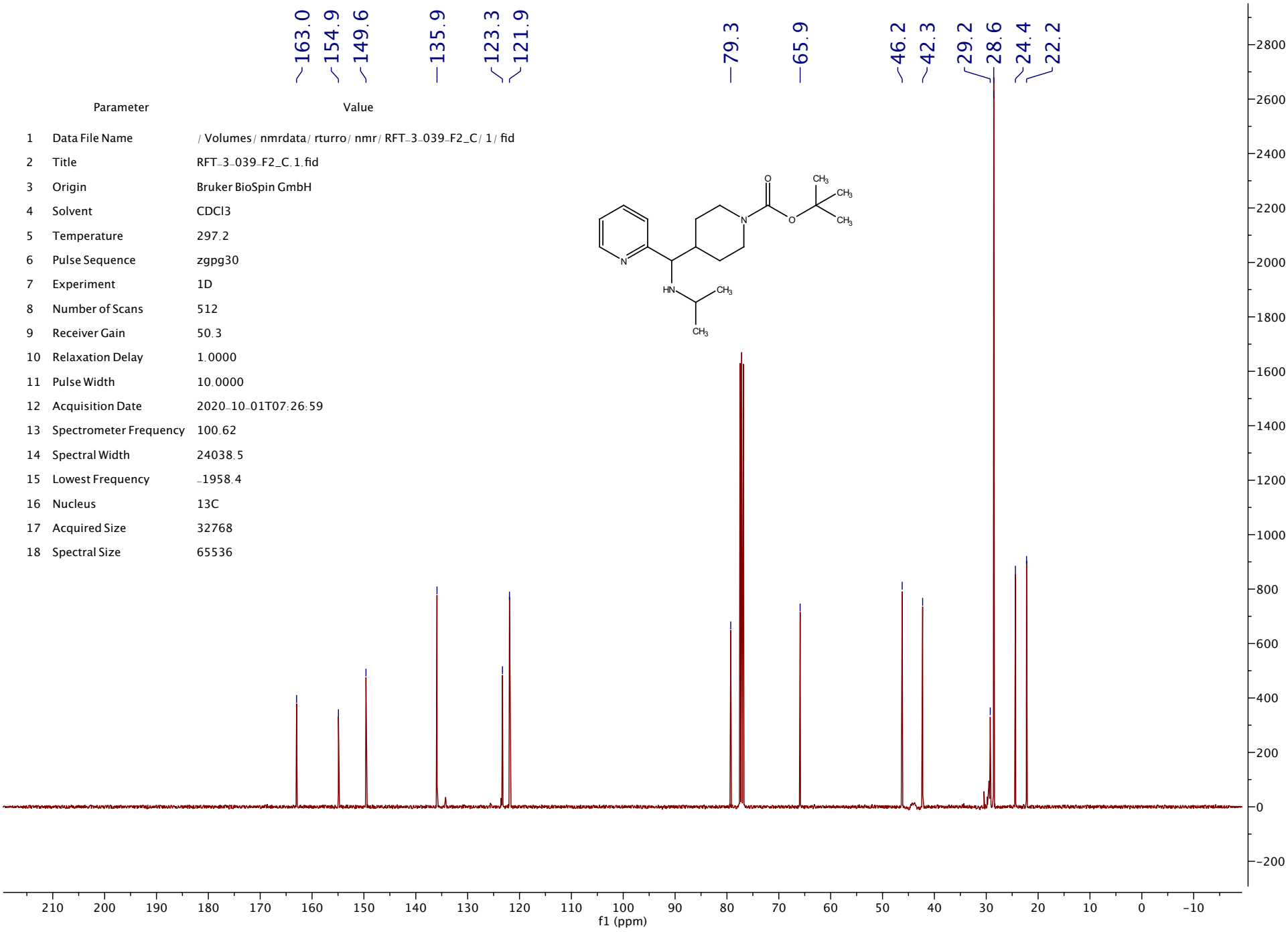




	Parameter	Value
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / RFT_3_037_F2_DCM / 1 / fid
2	Title	RFT_3_037_F2_DCM.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CD2Cl2
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
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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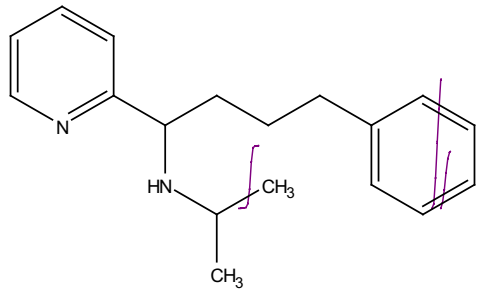
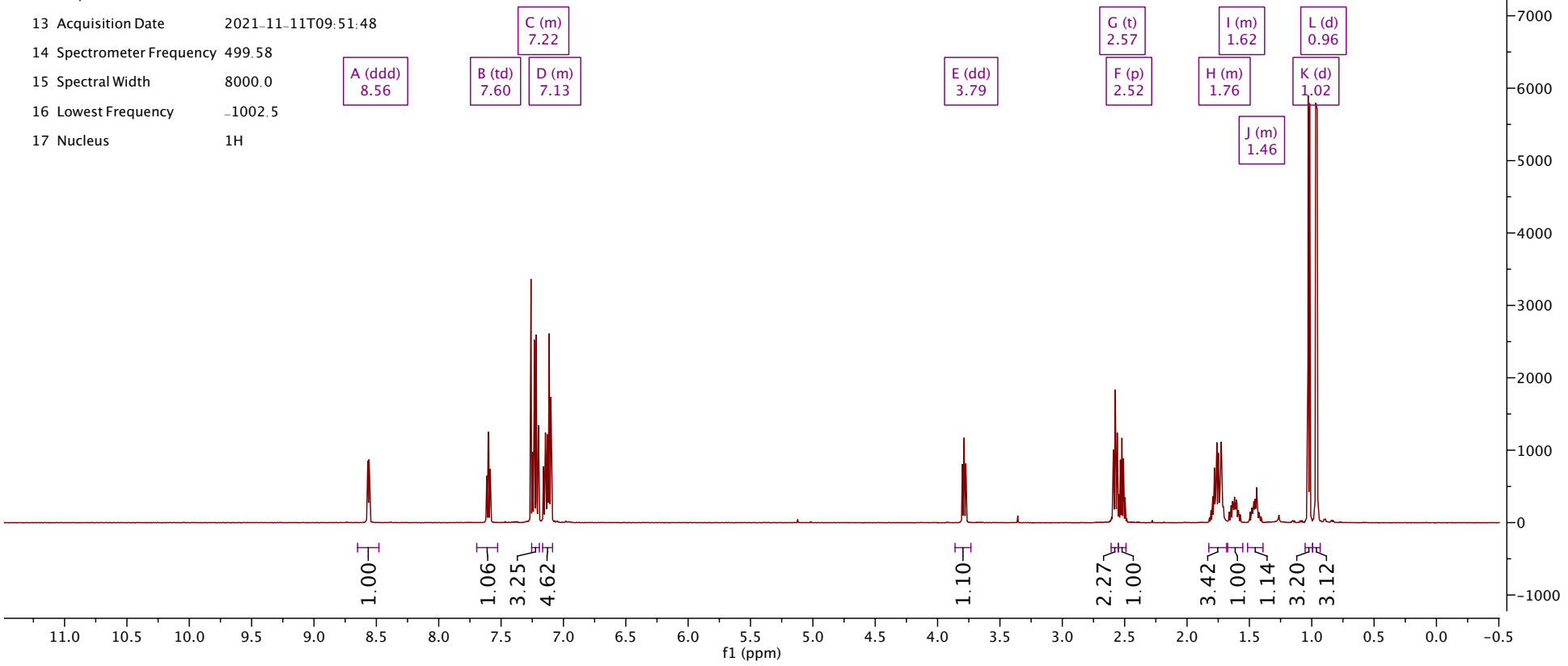
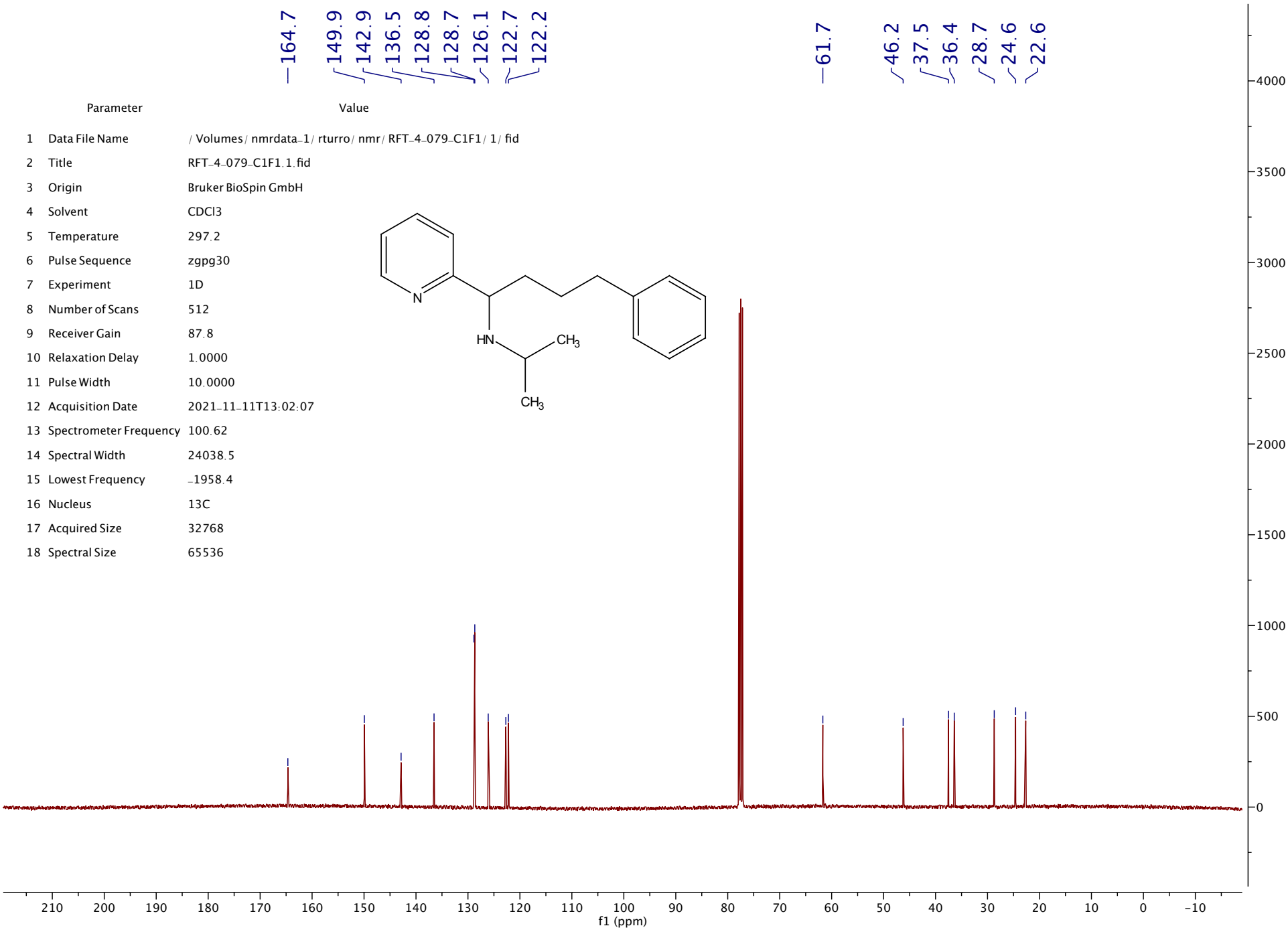
1	Data File Name	/Volumes/nmrdata/rturro/nmr/RFT_3_039_F2_C/1/fid
2	Title	RFT_3_039_F2_C.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	50.3
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2020_10_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 / rturro / vnmrsys / data / RFT_4_079_C1F1 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	RFT_4_079_C1F1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	54
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Time	3.0000
13	Acquisition Date	2021_11_11T09:51:48
14	Spectrometer Frequency	499.58
15	Spectral Width	8000.0
16	Lowest Frequency	-1002.5
17	Nucleus	1H

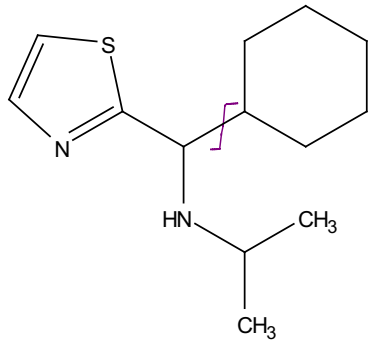


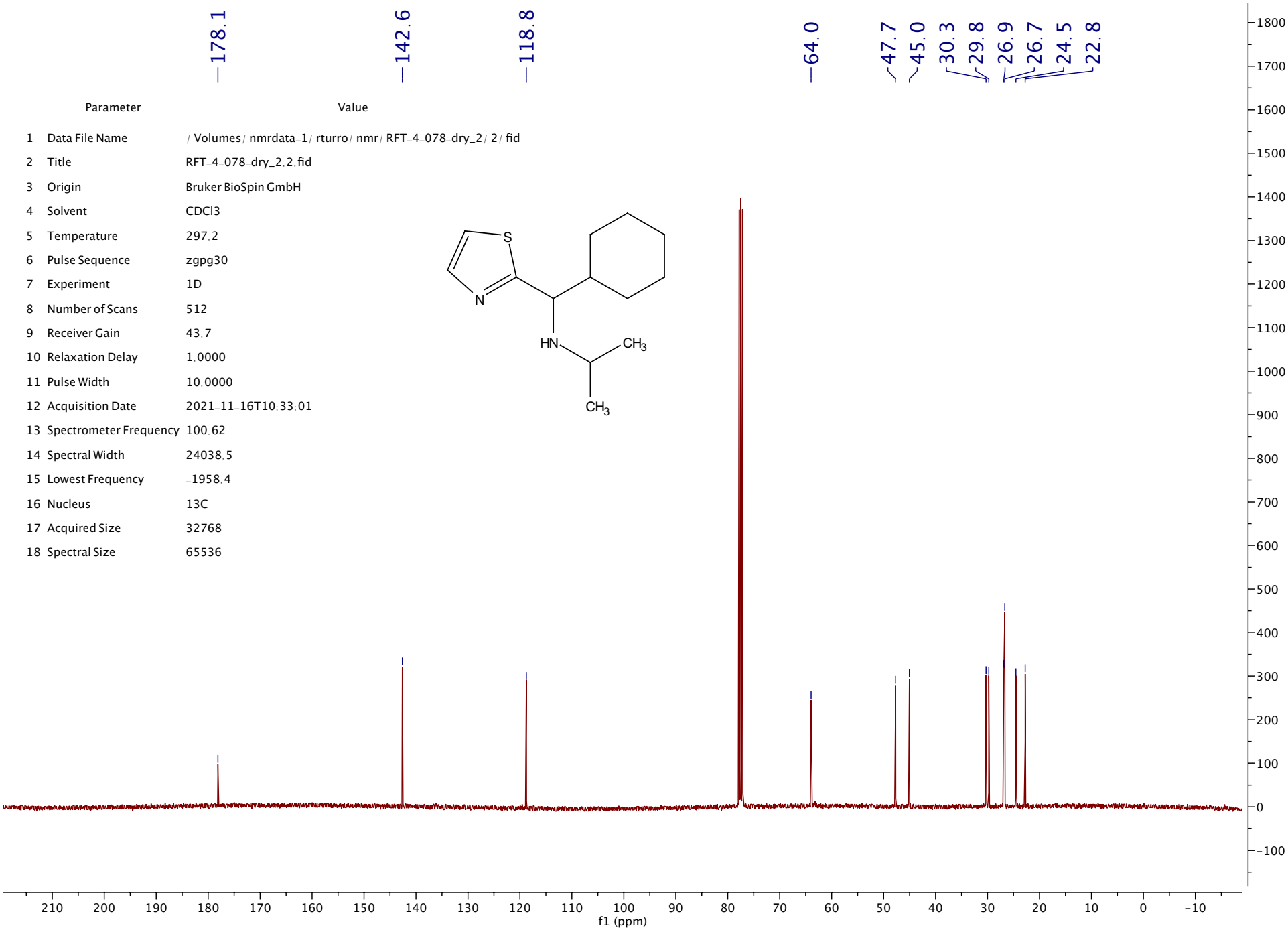




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/rturro/nmr/RFT_4_079_C1F1/1/fid
2	Title	RFT_4_079_C1F1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	87.8
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2021_11_11T13:02:07
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

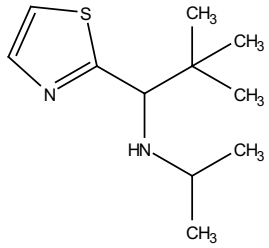
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_4_078_dry_2 / 1 / fid
2	Title	RFT_4_078_dry_2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	127.1
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2021_11_16T10:10:50
13	Spectrometer Frequency	400.13
14	Spectral Width	8012.8
15	Lowest Frequency	_1535.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536

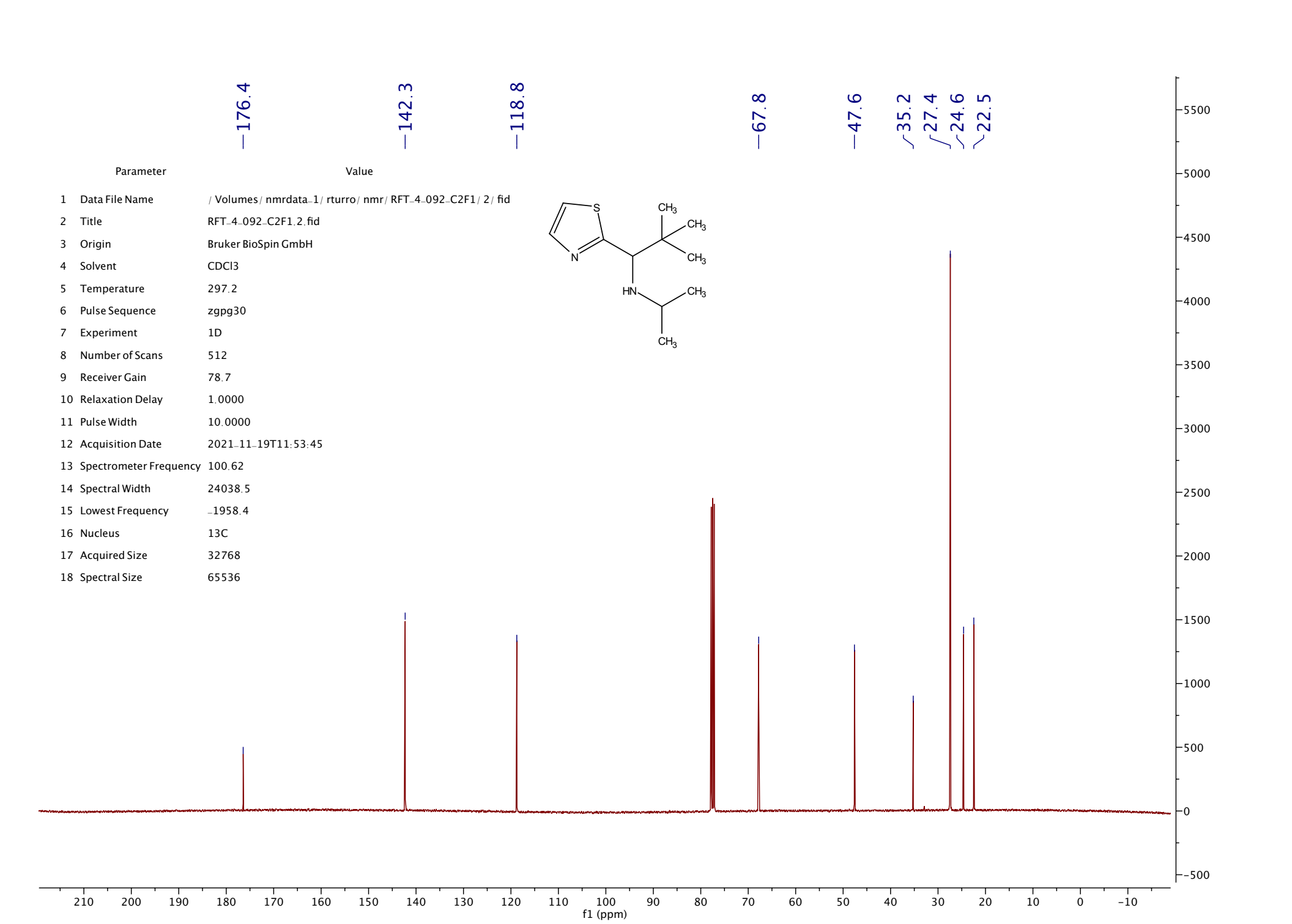




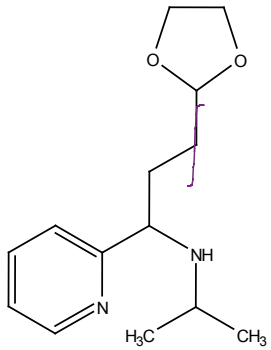
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_4_078_dry_2 / 2 / fid
2	Title	RFT_4_078_dry_2.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	43.7
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2021_11_16T10:33:01
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

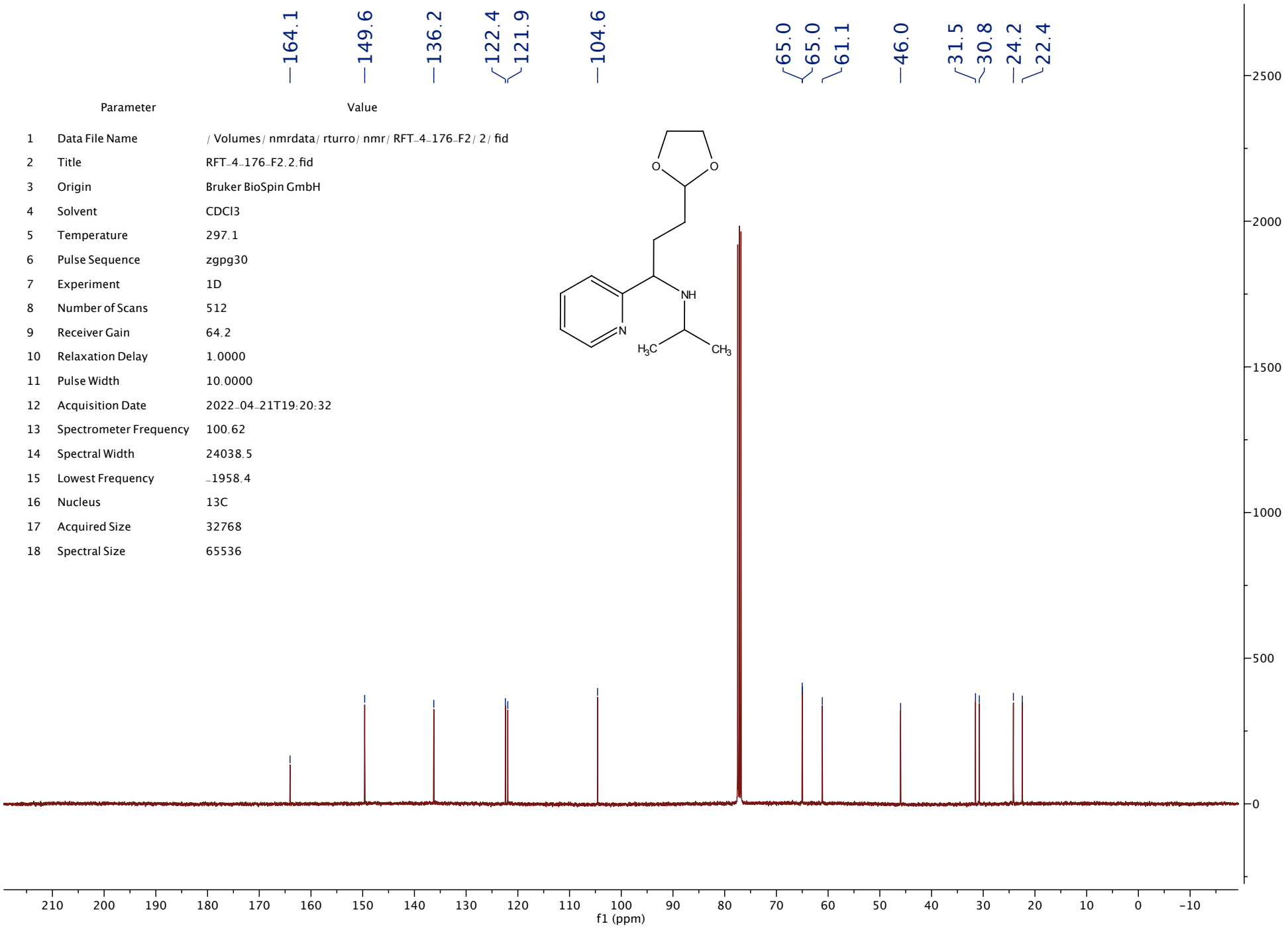
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / rturro / nmr / RFT_4_092_C2F1 / 1 / fid
2	Title	RFT_4_092_C2F1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	64.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2021_11_19T11:31:30
13	Spectrometer Frequency	400.13
14	Spectral Width	8012.8
15	Lowest Frequency	_1569.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536




176.4
142.3
118.8
67.8
47.6
35.2
27.4
24.6
22.5
Parameter
Value
1 Data File Name / Volumes / nmrdata_1 / rturro / nmr / RFT_4_092_C2F1 / 2 / fid
2 Title RFT_4_092_C2F1.2.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 2021_11_19T11:53:45
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
S
N
HN
CH3
CH3
CH3
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)

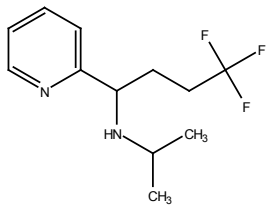
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ RFT_4_176_F2/ 1/ fid
2	Title	RFT_4_176_F2.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2022_04_21T18:58:32
13	Spectrometer Frequency	400.13
14	Spectral Width	8012.8
15	Lowest Frequency	_1535.4
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536

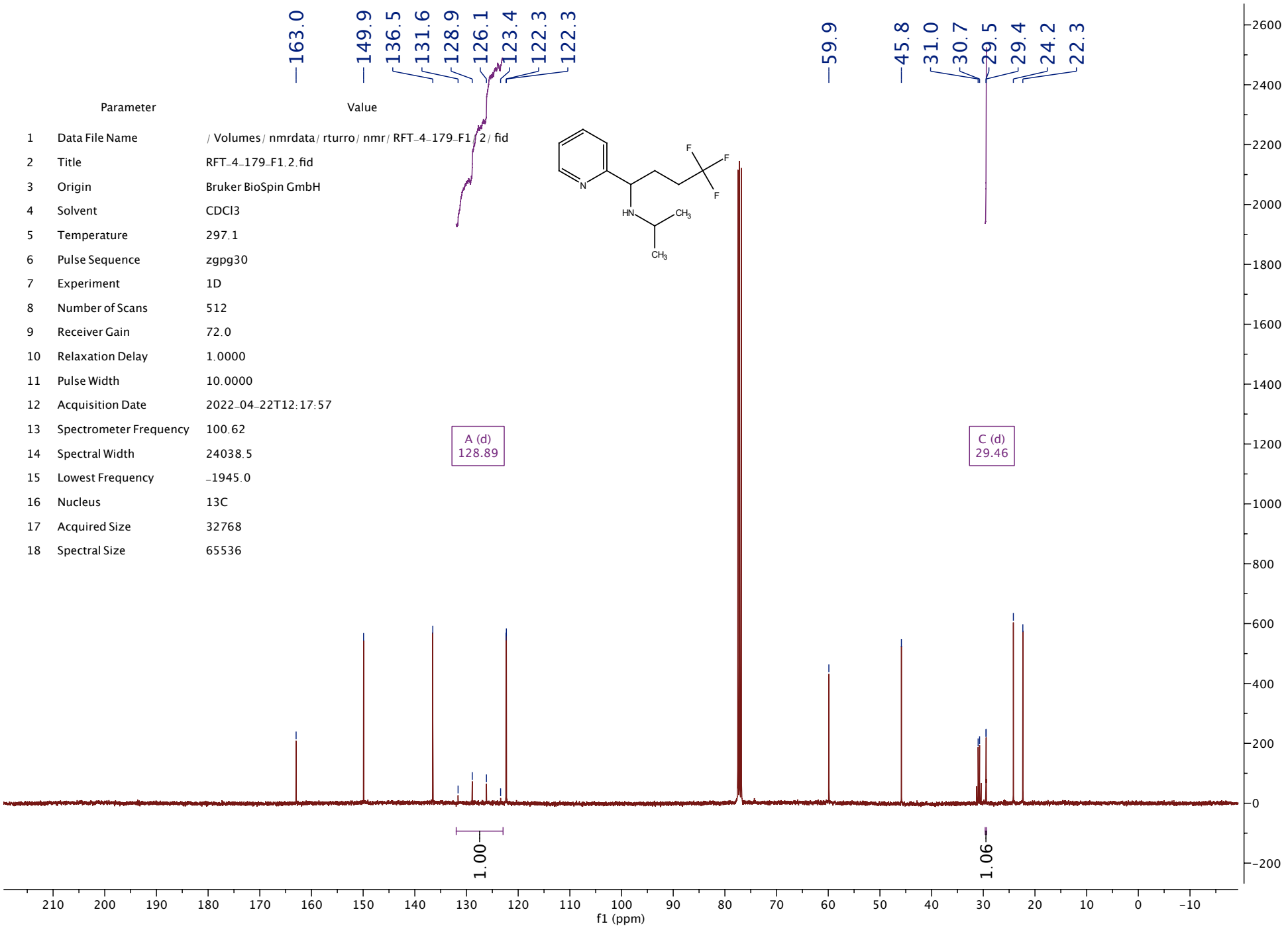




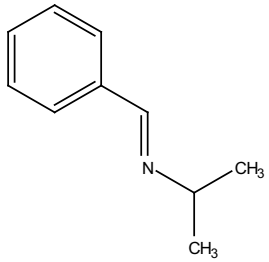
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ RFT_4_176_F2/ 2/ fid
2	Title	RFT_4_176_F2.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	64.2
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
12	Acquisition Date	2022_04_21T19:20:32
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

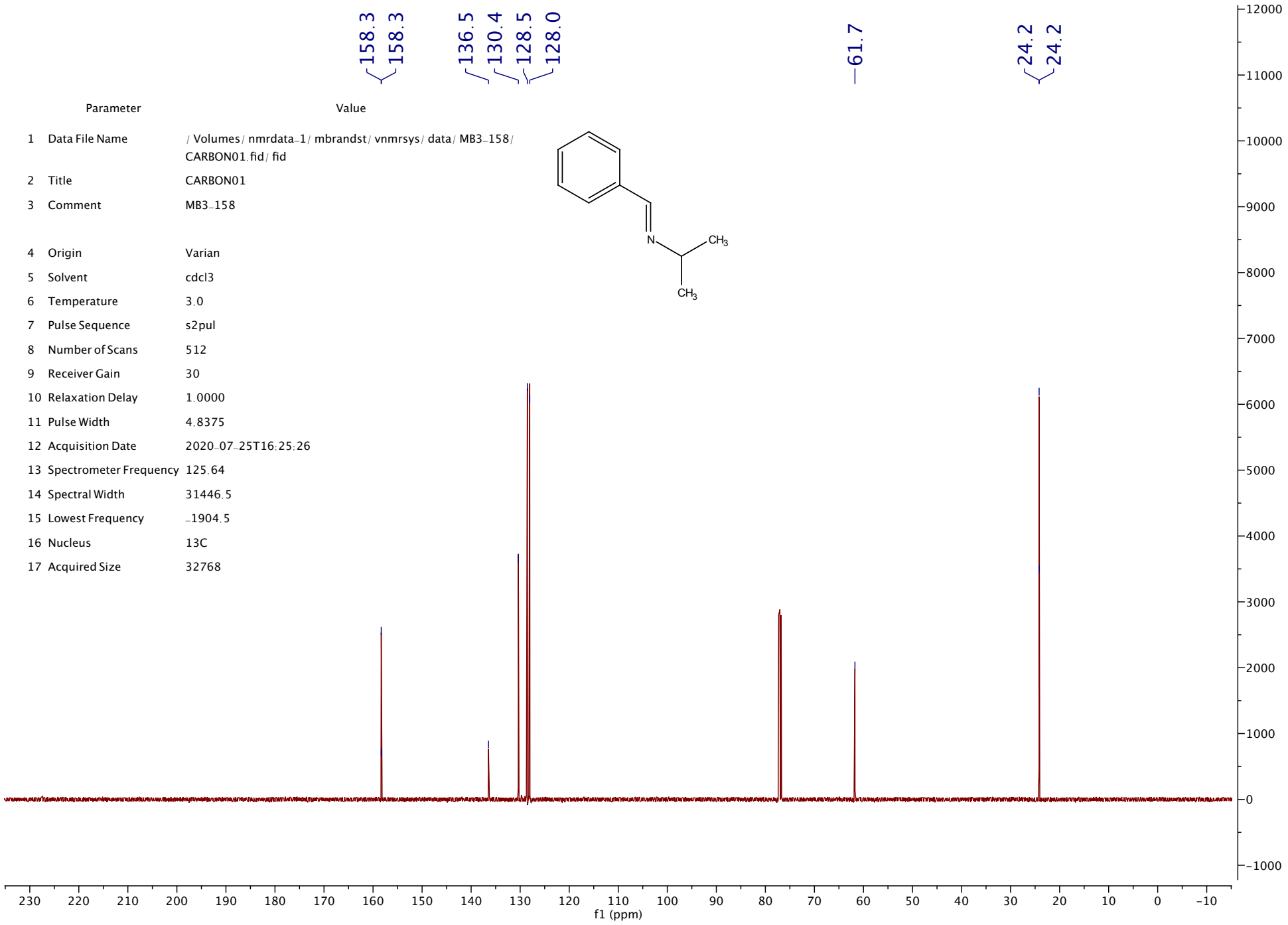
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ RFT_4_179_F1/ 1/ fid
2	Title	RFT_4_179_F1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	142.8
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	Acquisition Date	2022_04_22T11:56:44
13	Spectrometer Frequency	400.13
14	Spectral Width	8012.8
15	Lowest Frequency	_1545.3
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536




163.0
149.9
136.5
131.6
128.9
126.1
123.4
122.3
122.3
59.9
45.8
31.0
30.7
29.5
29.4
24.2
22.3
Parameter
Value
1 Data File Name / Volumes/ nmrdata/ rturro/ nmr/ RFT_4_179_F1/ 2/ fid
2 Title RFT_4_179_F1.2.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 2022_04_22T12:17:57
13 Spectrometer Frequency 100.62
14 Spectral Width 24038.5
15 Lowest Frequency _1945.0
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
F
F
F
N
HN
CH3
CH3
A (d)
128.89
C (d)
29.46
1.00
1.06
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
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)

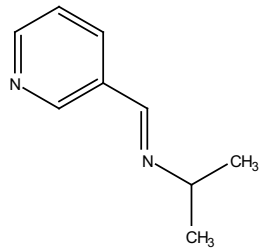
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_158/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB3_158
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	46
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition 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

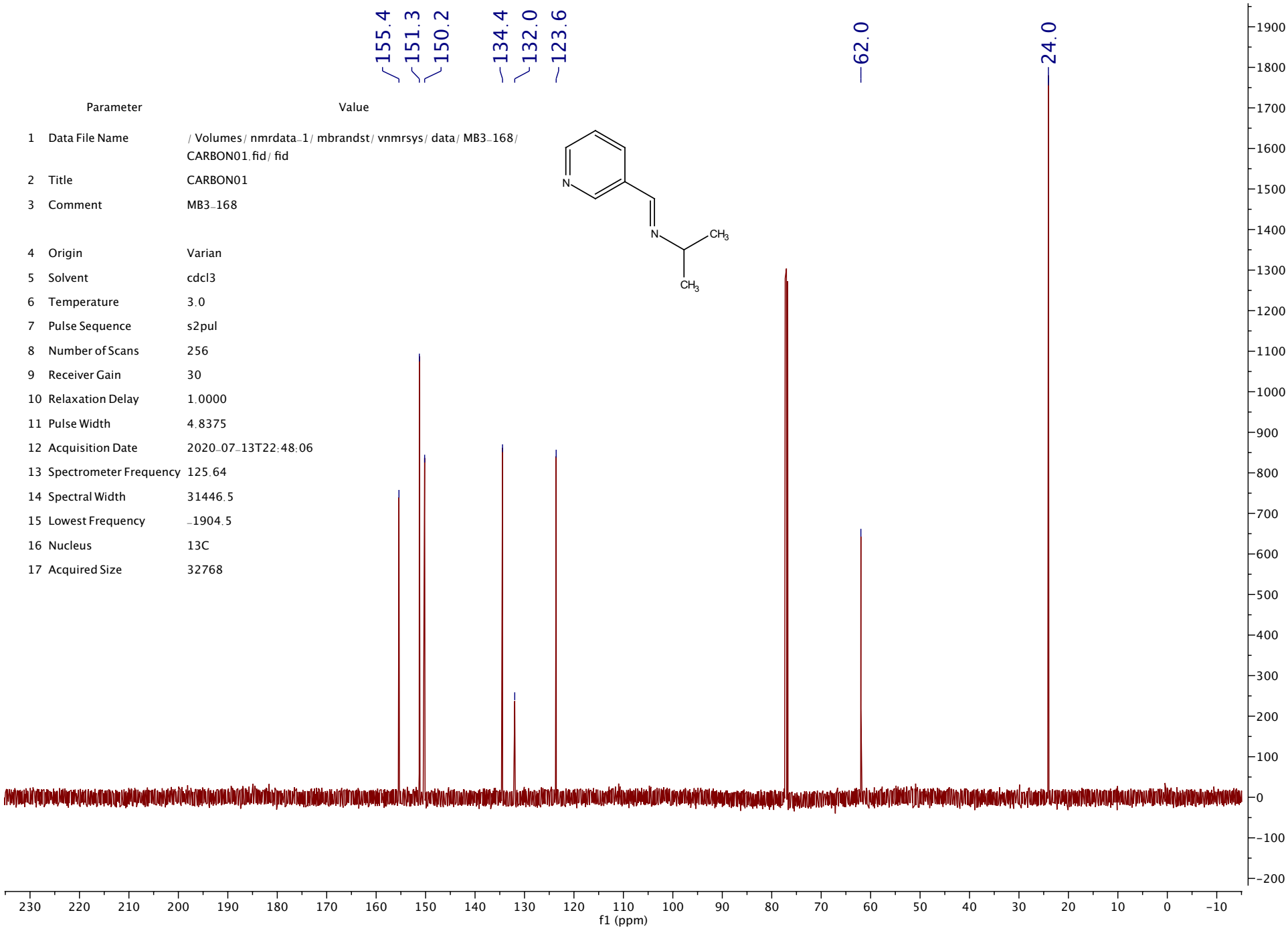




	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_158/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3_158
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	512
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition 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

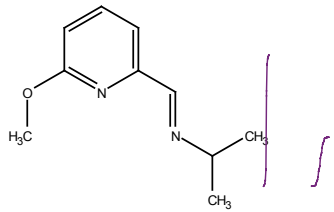
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_168/PROTON01.fid/fid
2	Title	PROTON01
3	Comment	MB3_168
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition 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

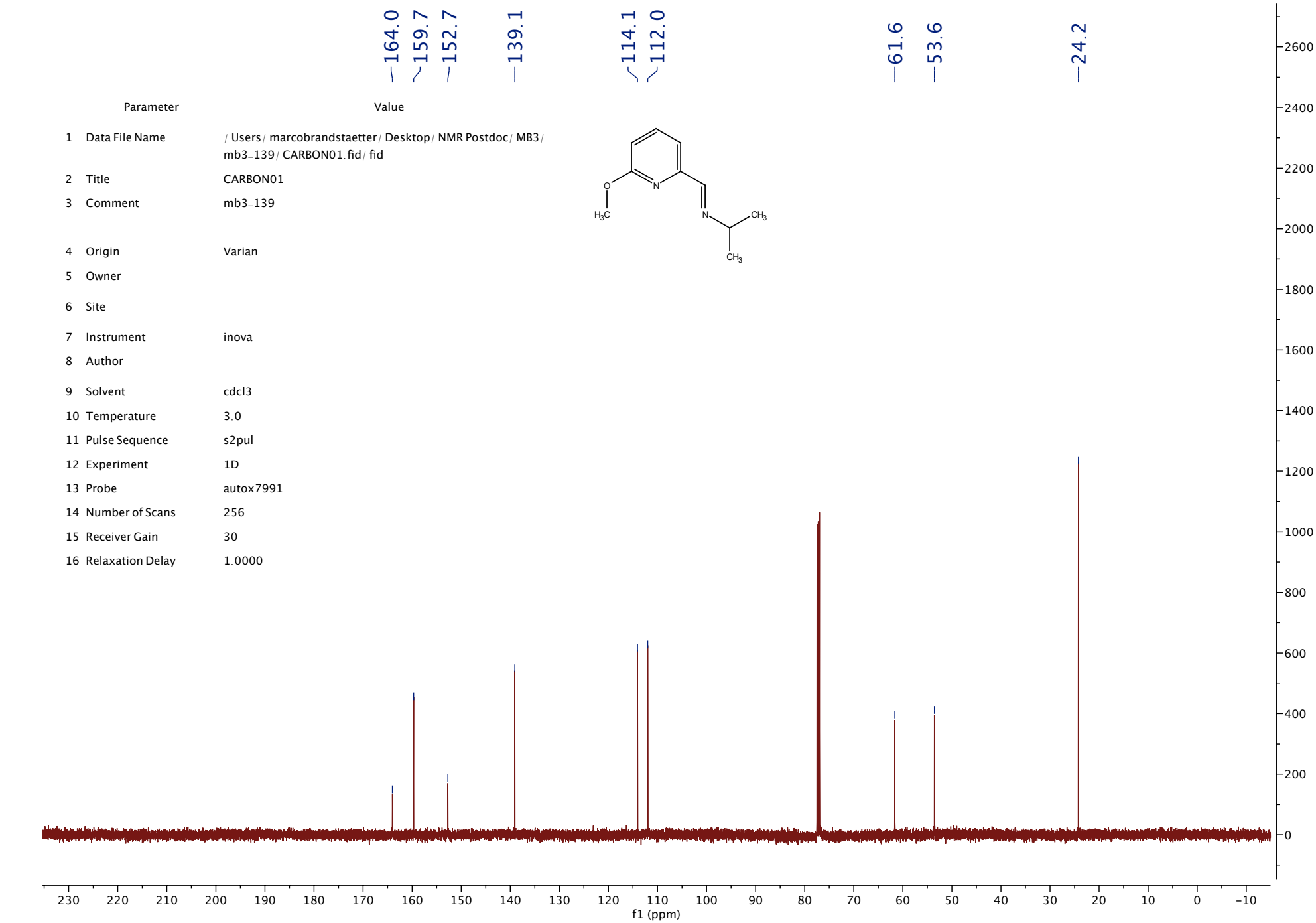




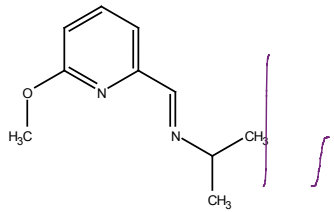
	Parameter	Value
1	Data File Name	/Volumes/nmrdata_1/mbrandst/vnmrsys/data/MB3_168/CARBON01.fid/fid
2	Title	CARBON01
3	Comment	MB3_168
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	256
9	Receiver Gain	30
10	Relaxation Delay	1.0000
11	Pulse Width	4.8375
12	Acquisition 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

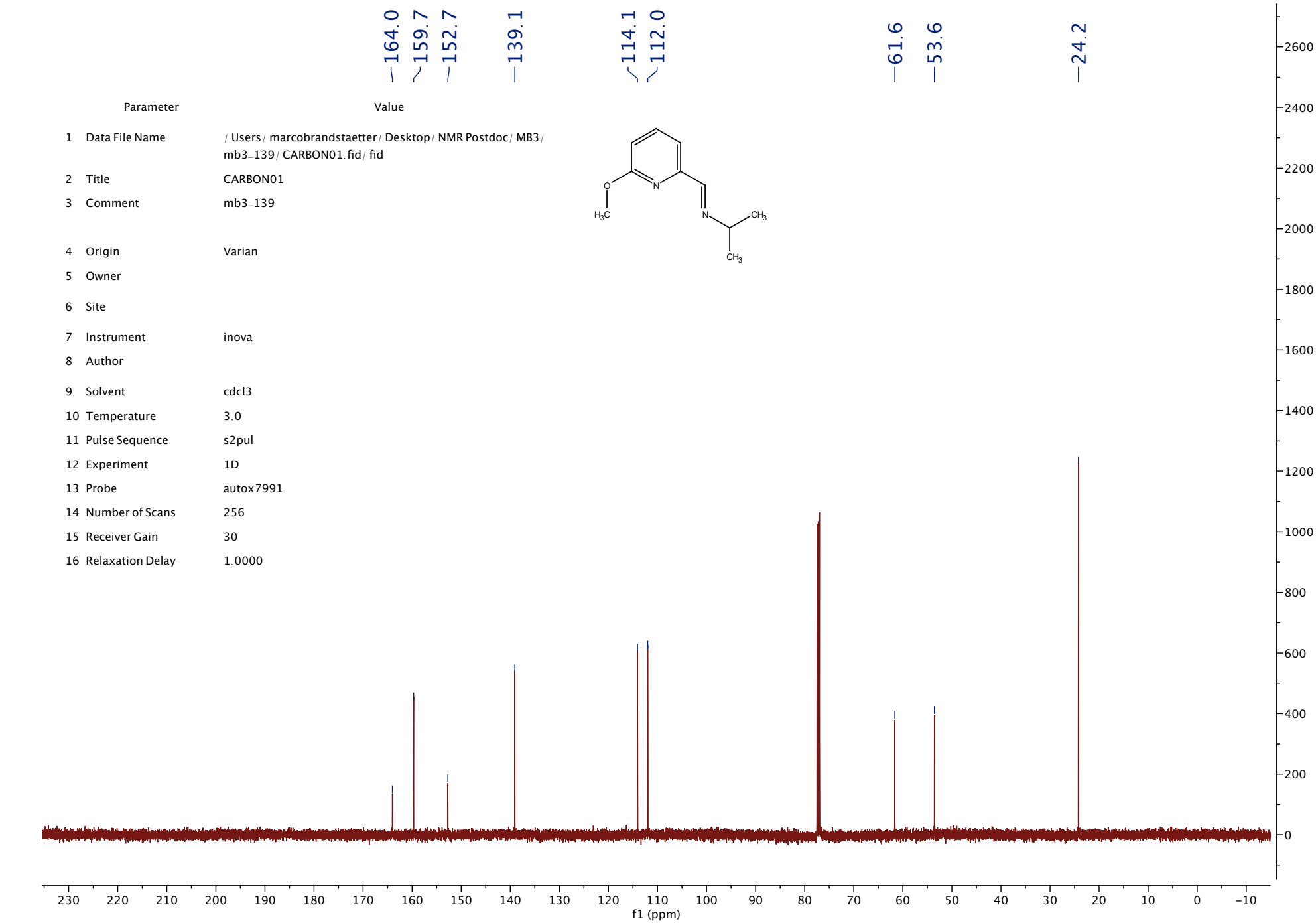
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_139 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	mb3_139
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe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



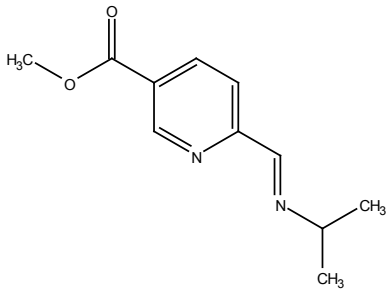

164.0
159.7
152.7
139.1
114.1
112.0
61.6
53.6
24.2
Parameter
Value
1 Data File Name / Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / mb3_139 / CARBON01.fid / fid
2 Title CARBON01
3 Comment mb3_139
4 Origin Varian
5 Owner
6 Site
7 Instrument inova
8 Author
9 Solvent cdcl3
10 Temperature 3.0
11 Pulse Sequence s2pul
12 Experiment 1D
13 Probe autox7991
14 Number of Scans 256
15 Receiver Gain 30
16 Relaxation Delay 1.0000
O
N
H3C
N
CH3
CH3
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
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_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




164.0
159.7
152.7
139.1
114.1
112.0
61.6
53.6
24.2
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
O
N
H3C
N
CH3
CH3
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
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)

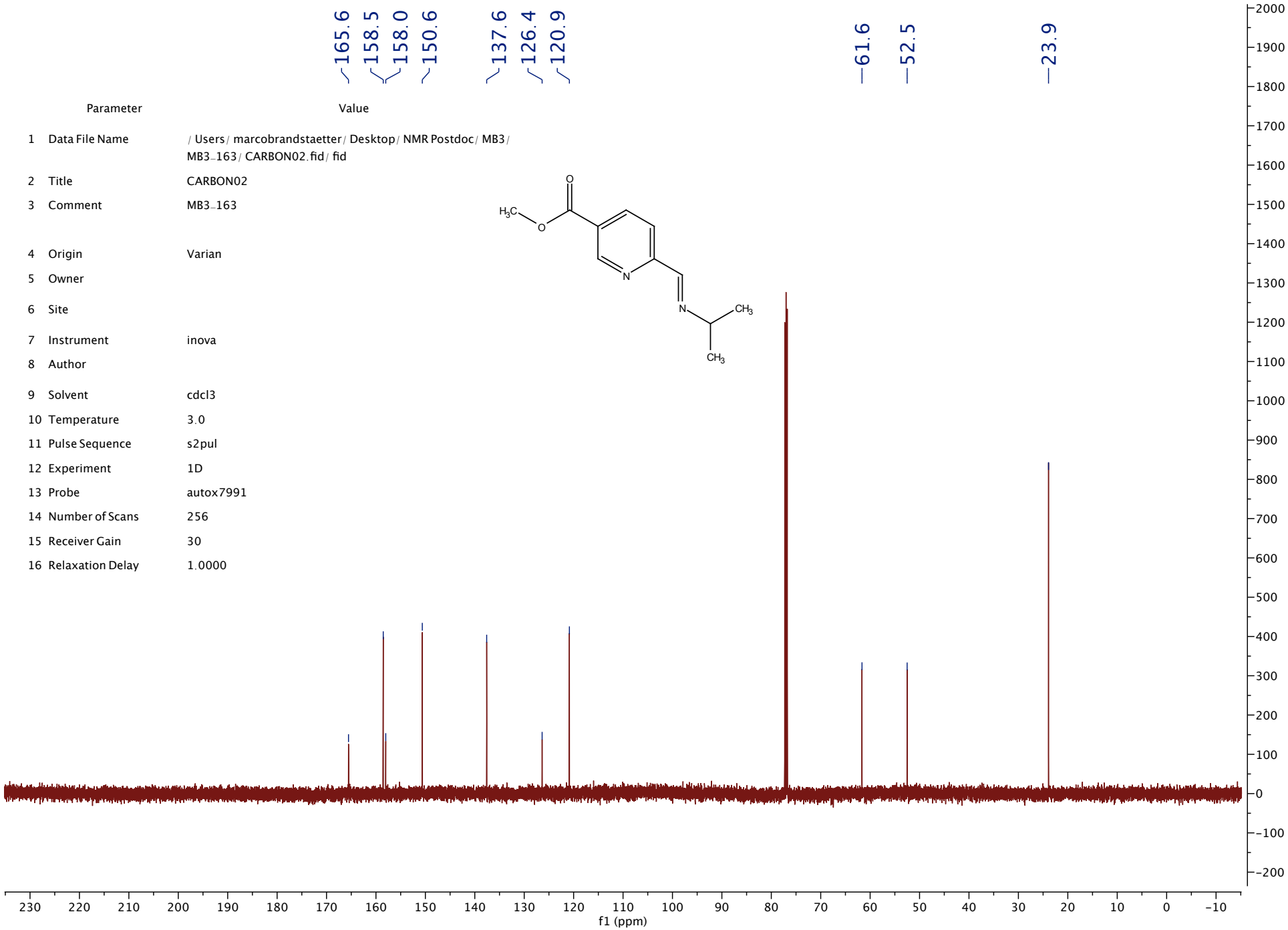
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_163 / PROTON02.fid / fid
2	Title	PROTON02
3	Comment	MB3_163
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe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



A (s) 9.22
B (s) 8.43
C (d) 8.32
D (d) 8.08
E (s) 3.97
G (hept) 3.68
F (d) 1.30

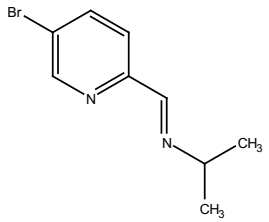
1.00 1.16 1.18 0.74 1.19 1.59 2.70

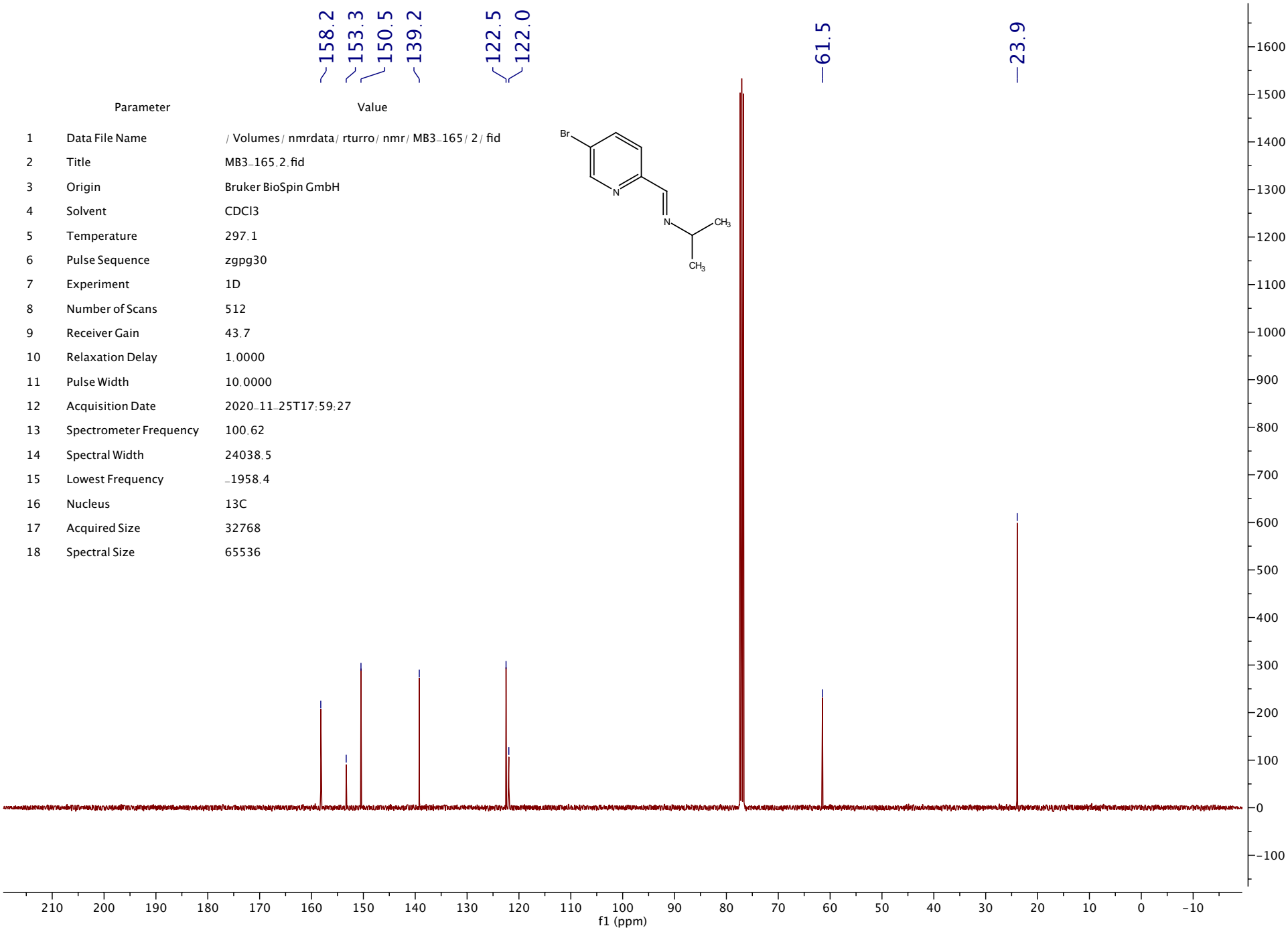
f1 (ppm)



	Parameter	Value
1	Data File Name	/ 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

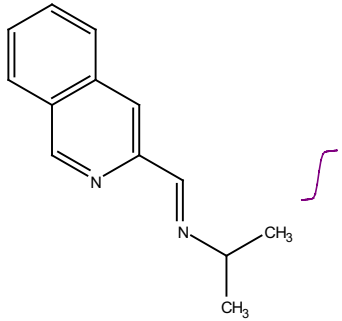
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ rturro/ nmr/ MB3_165/ 1/ fid
2	Title	MB3_165.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.2
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	197.4
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	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
1	Data File Name	/ Volumes / nmrdata / rturro / nmr / MB3_165 / 2 / fid
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

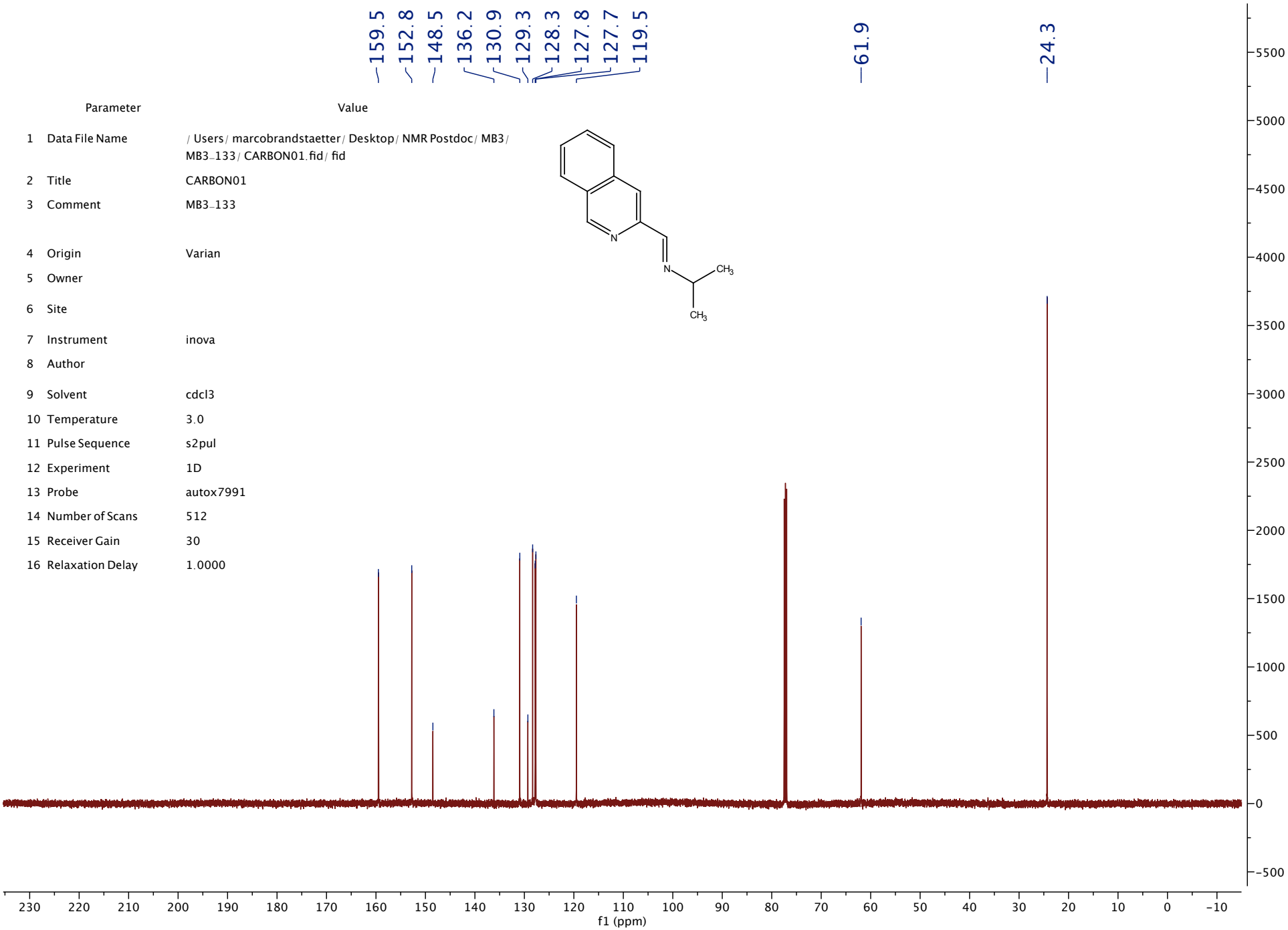
	Parameter	Value
1	Data File Name	/ Volumes/ nmrdata/ mbrandst/ vnmrsys/ data/ MB3_133/ PROTON03.fid/ fid
2	Title	PROTON03
3	Comment	MB3_133
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse Width	5.6500
12	Acquisition Time	3.0000
13	Acquisition Date	2020_07_09T23:03:34
14	Spectrometer Frequency	499.60
15	Spectral Width	8000.0
16	Lowest Frequency	-1002.4
17	Nucleus	1H



C (s) 9.28
D (d) 8.57
E (s) 8.26
F (d) 7.98
G (d) 7.89
H (ddd) 7.70
I (td) 7.63
A (m) 3.69
B (dd) 1.34

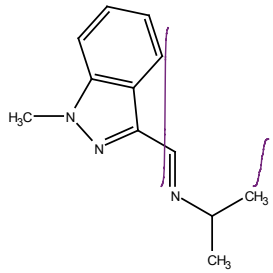
0.85 0.93 0.87 0.93 0.93 0.91 0.90 1.00 5.81

f1 (ppm)



	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

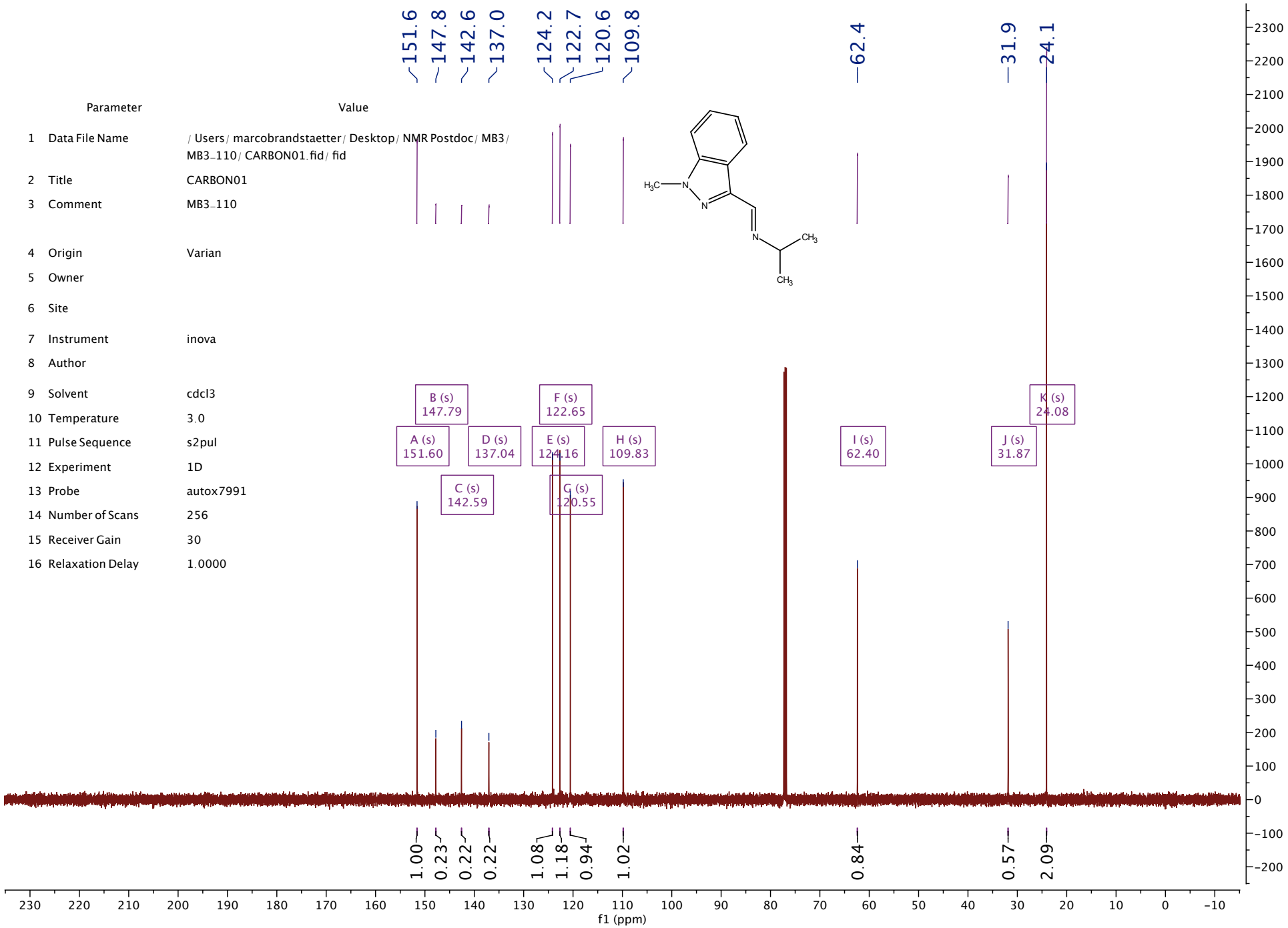
	Parameter	Value
1	Data File Name	/ Users / marcobrandstaetter / Desktop / NMR Postdoc / MB3 / MB3_110 / PROTON03.fid / fid
2	Title	PROTON03
3	Comment	MB3_110
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	inova
8	Author	
9	Solvent	cdcl3
10	Temperature	3.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe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

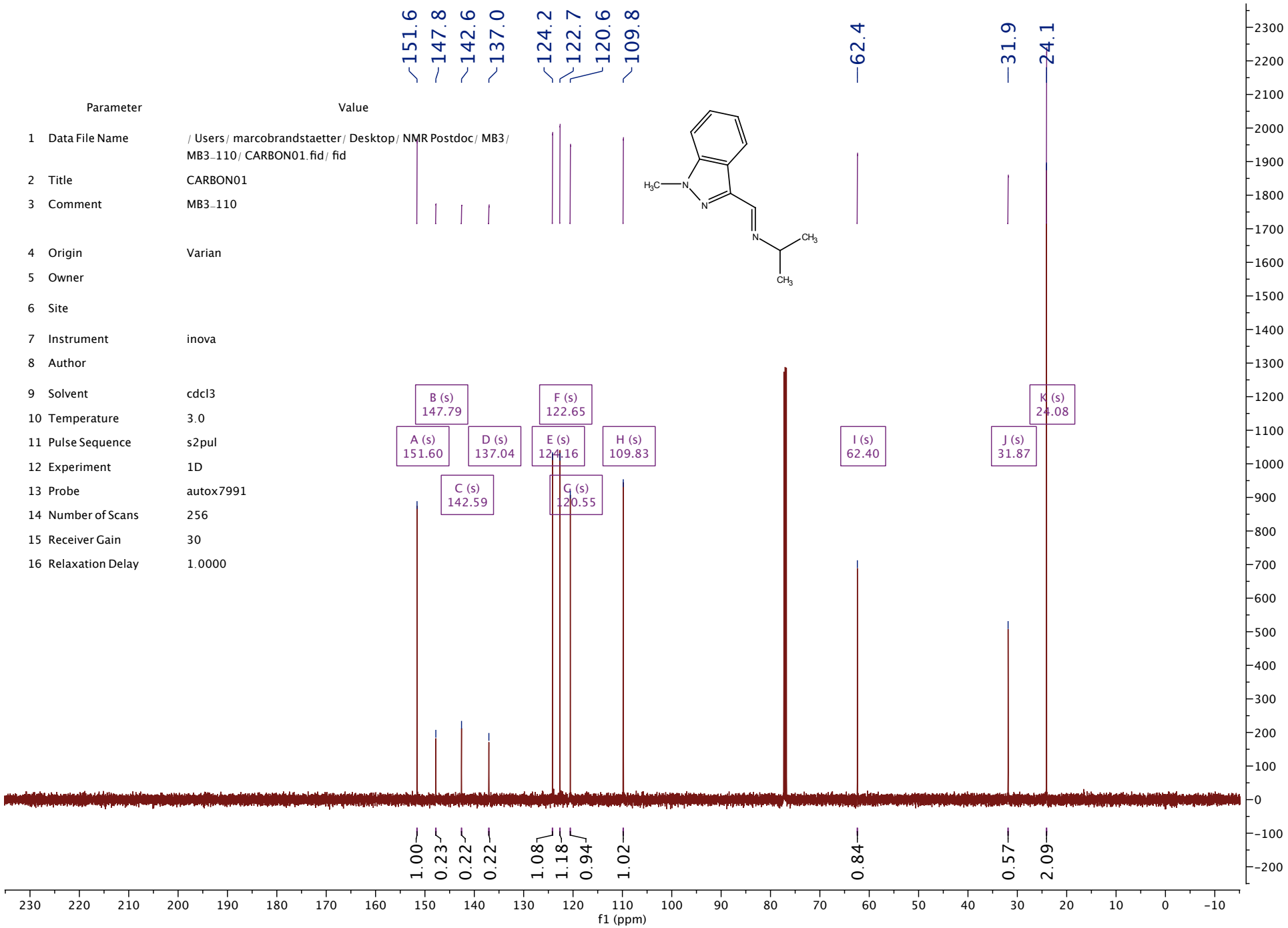


A (s) 8.53
B (d) 7.80
C (d) 7.40
D (m) 7.35
E (t) 7.29
H (s) 4.18
G (m) 3.61
F (d) 1.30

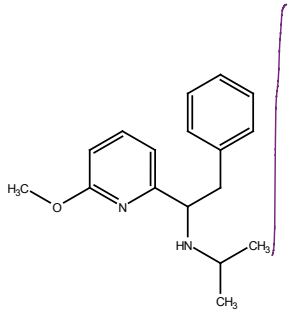
1.00 2.01 2.15 1.69 1.76 3.23 0.96 5.37

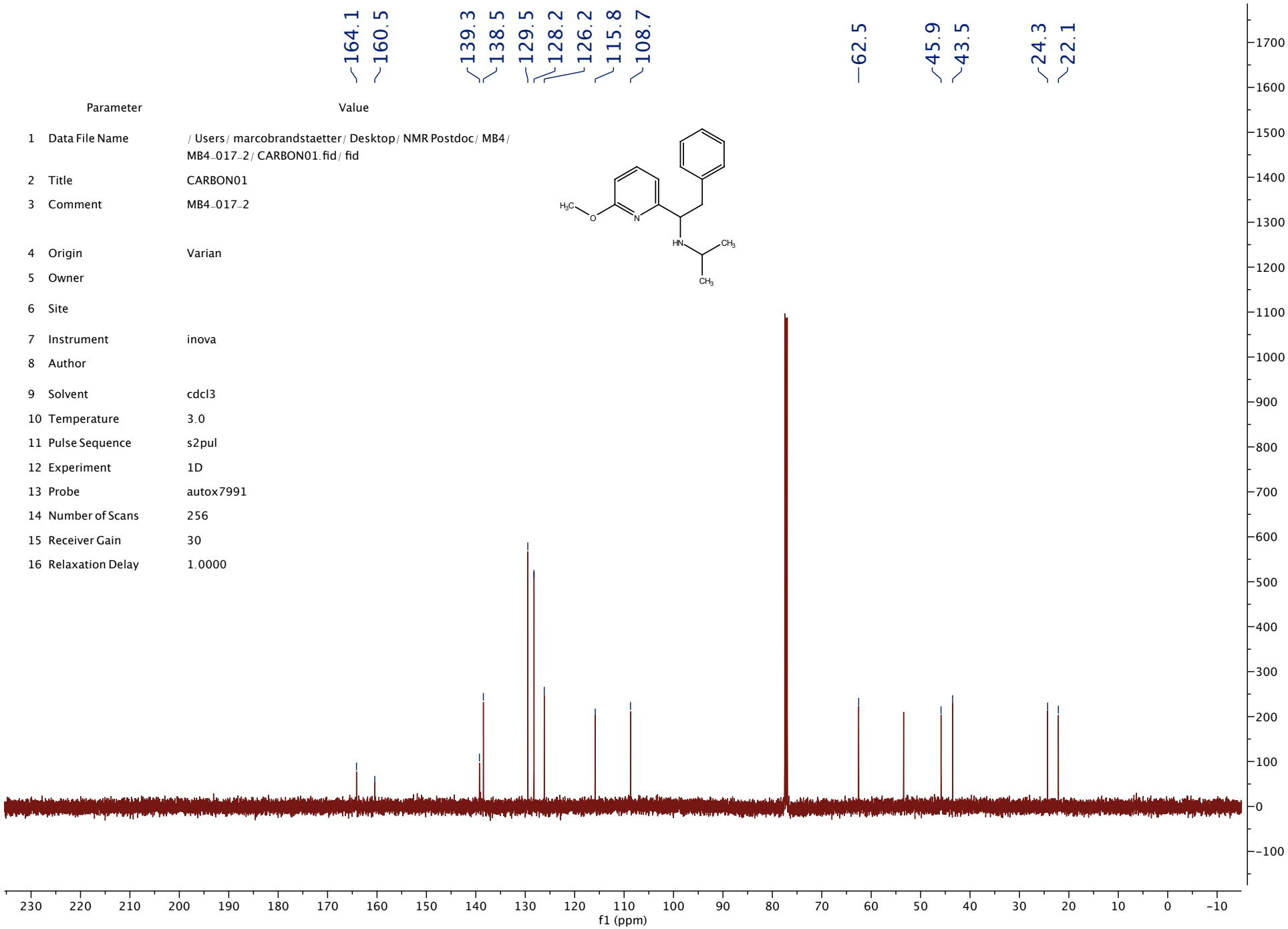
f1 (ppm)


151.6
147.8
142.6
137.0
124.2
122.7
120.6
109.8
62.4
31.9
24.1
Parameter
Value
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
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)


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
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
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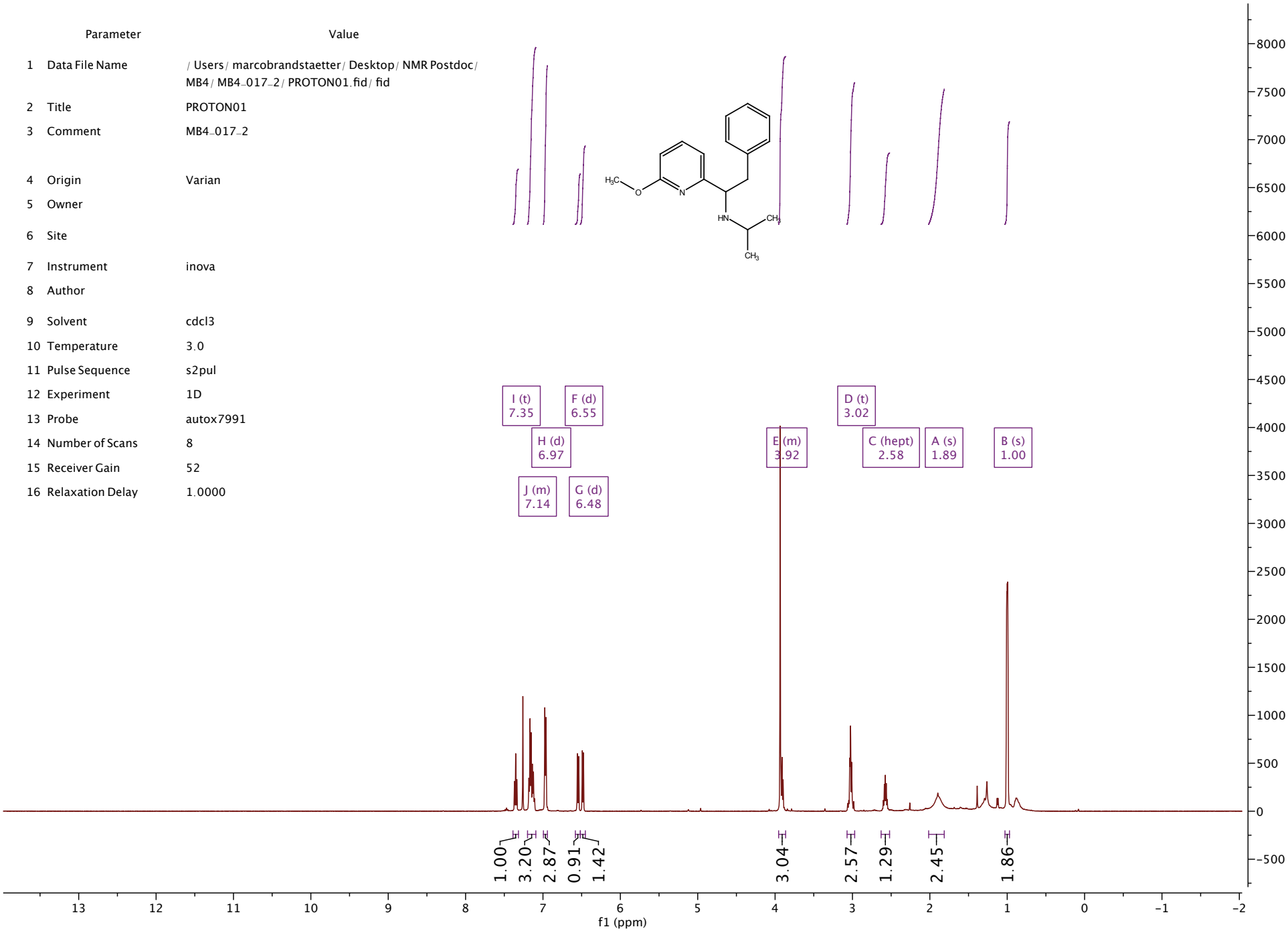
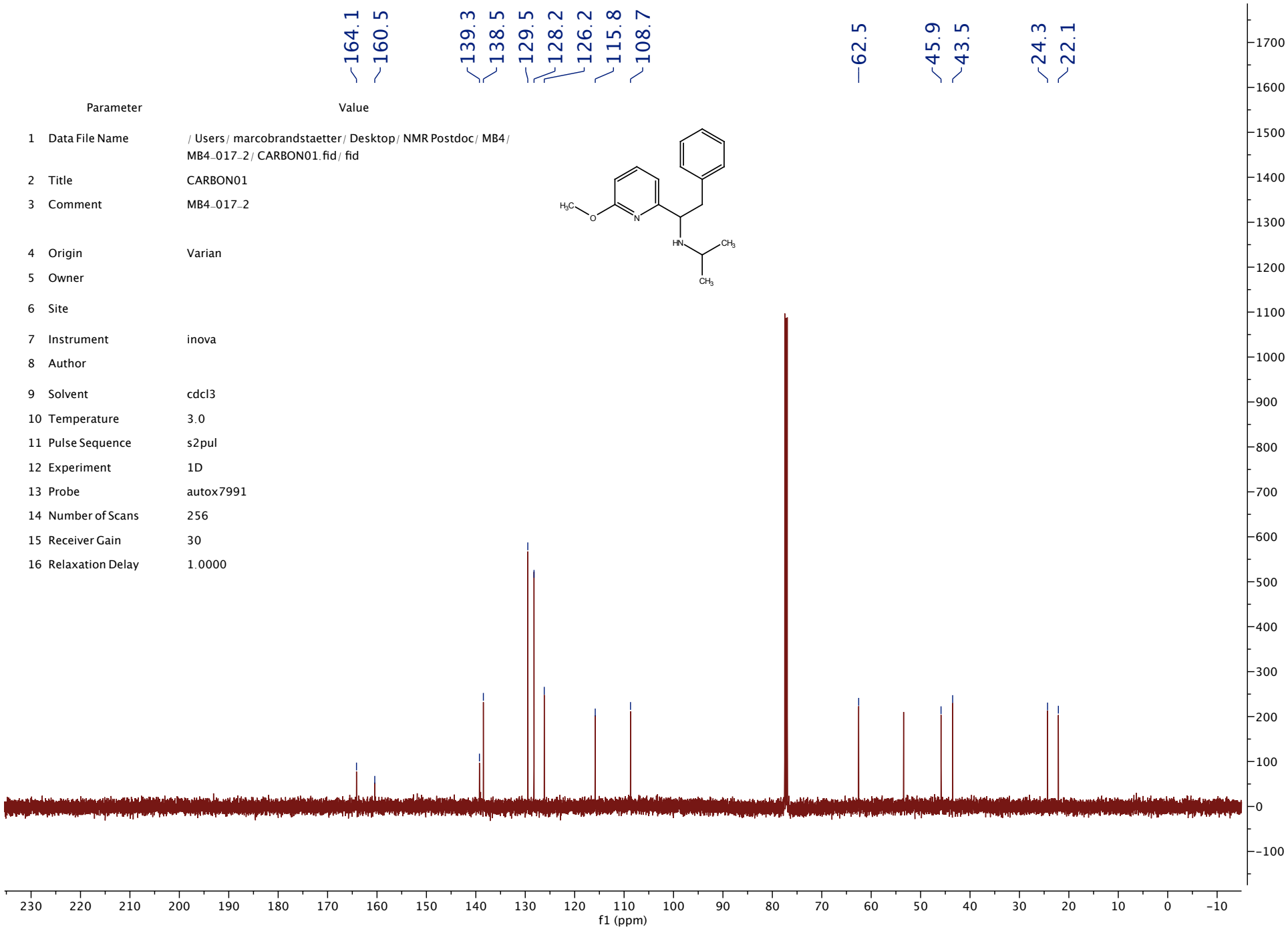
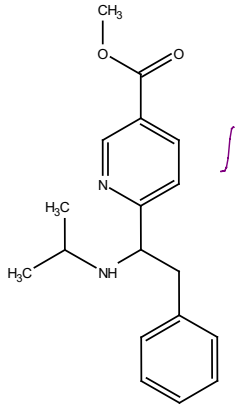
/ Users/ marcobrandstaetter/ Desktop/ NMR Postdoc/ MB4/ MB4_017_2/ CARBON01.fid/ fid
2 Title
CARBON01
3 Comment
MB4_017_2
4 Origin
Varian
5 Owner
6 Site
7 Instrument
inova
8 Author
9 Solvent
cdcl3
10 Temperature
3.0
11 Pulse Sequence
s2pul
12 Experiment
1D
13 Probe
autox7991
14 Number of Scans
256
15 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)

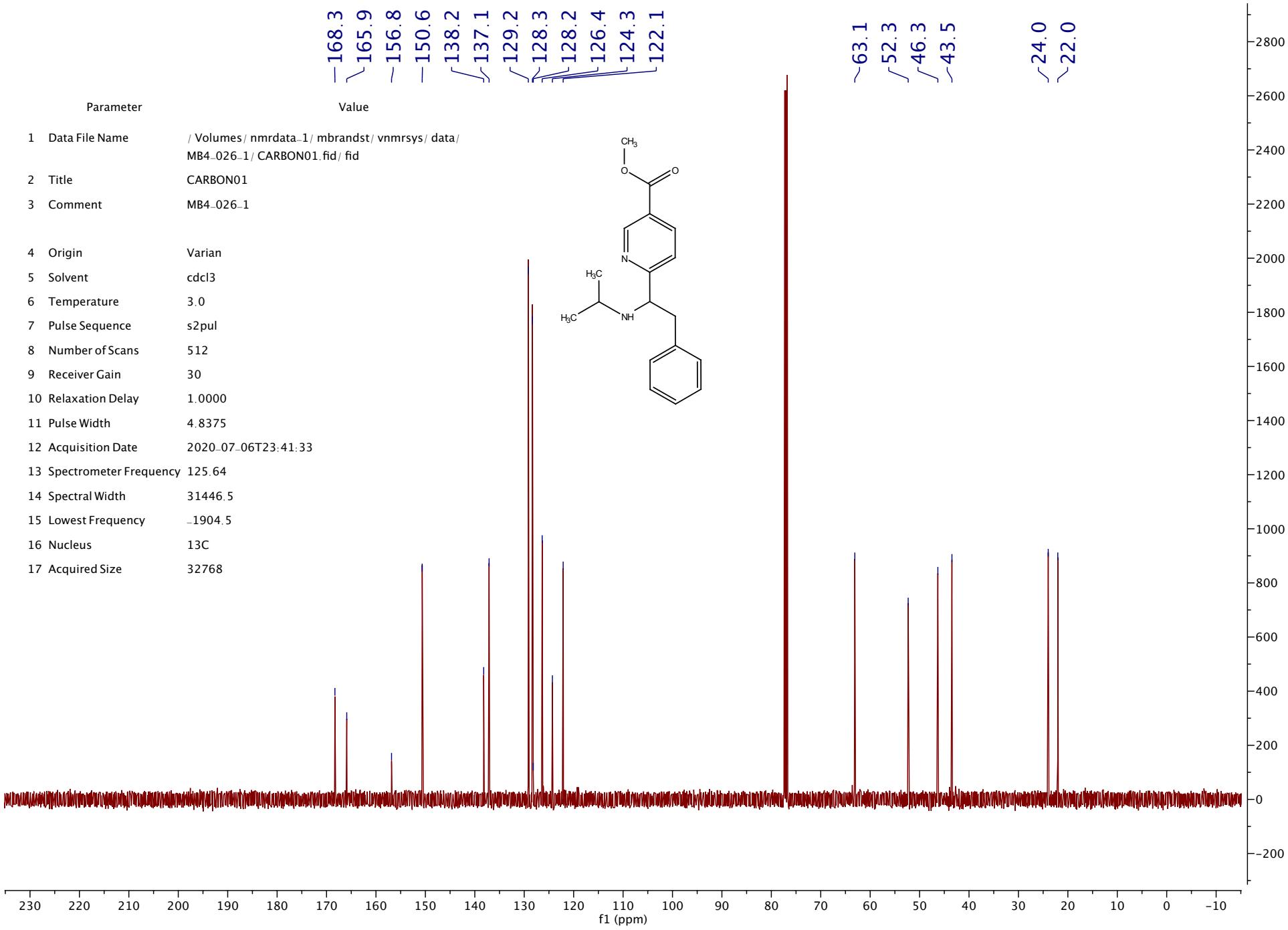
	Parameter	Value
1	Data File Name	/ Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_026_1 / PROTON01.fid / fid
2	Title	PROTON01
3	Comment	MB4_026_1
4	Origin	Varian
5	Solvent	cdcl3
6	Temperature	3.0
7	Pulse Sequence	s2pul
8	Number of Scans	16
9	Receiver Gain	48
10	Relaxation Delay	1.0000
11	Pulse 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



G (d) 9.20
H (dd) 8.15
J (m) 7.05
I (m) 7.21
B (s) 3.97
A (t) 4.17
C (m) 3.04
D (dt) 2.57
E (s) 1.81
F (d) 0.98

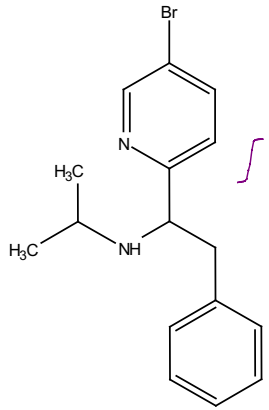
0.78 0.93 4.39 2.29 1.00 2.87 2.22 1.10 2.56 5.95

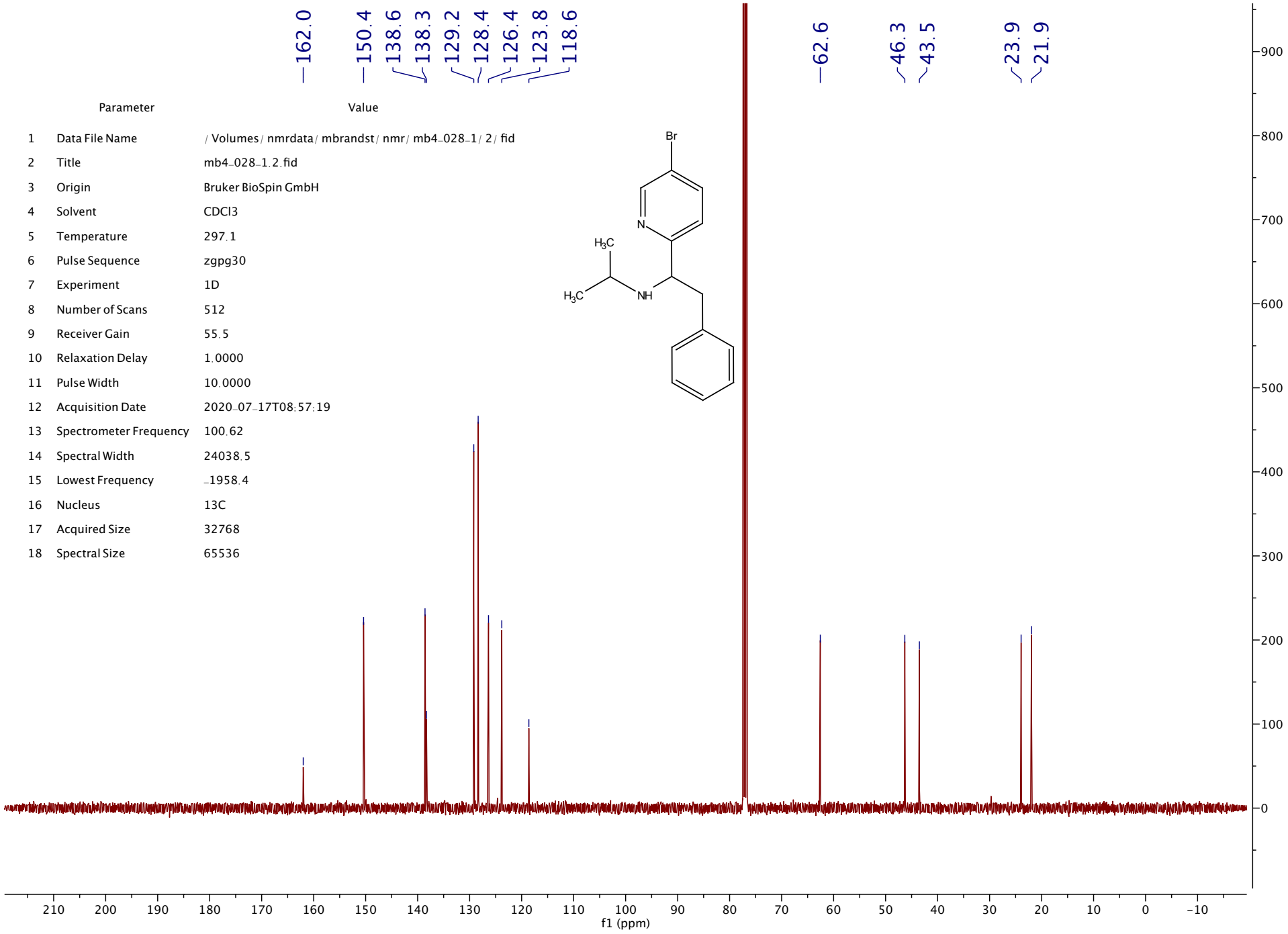
f1 (ppm)



	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

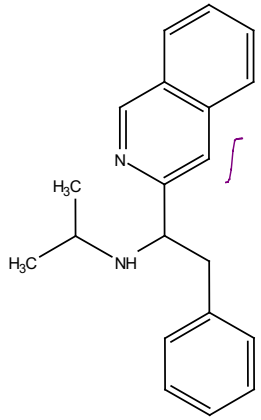
	Parameter	Value
1	Data File Name	/Volumes/nmrdata/mbrandst/nmr/mb4_028_1/1/fid
2	Title	mb4_028_1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zg30
7	Experiment	1D
8	Number of Scans	16
9	Receiver Gain	156.2
10	Relaxation Delay	1.0000
11	Pulse Width	12.5000
12	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

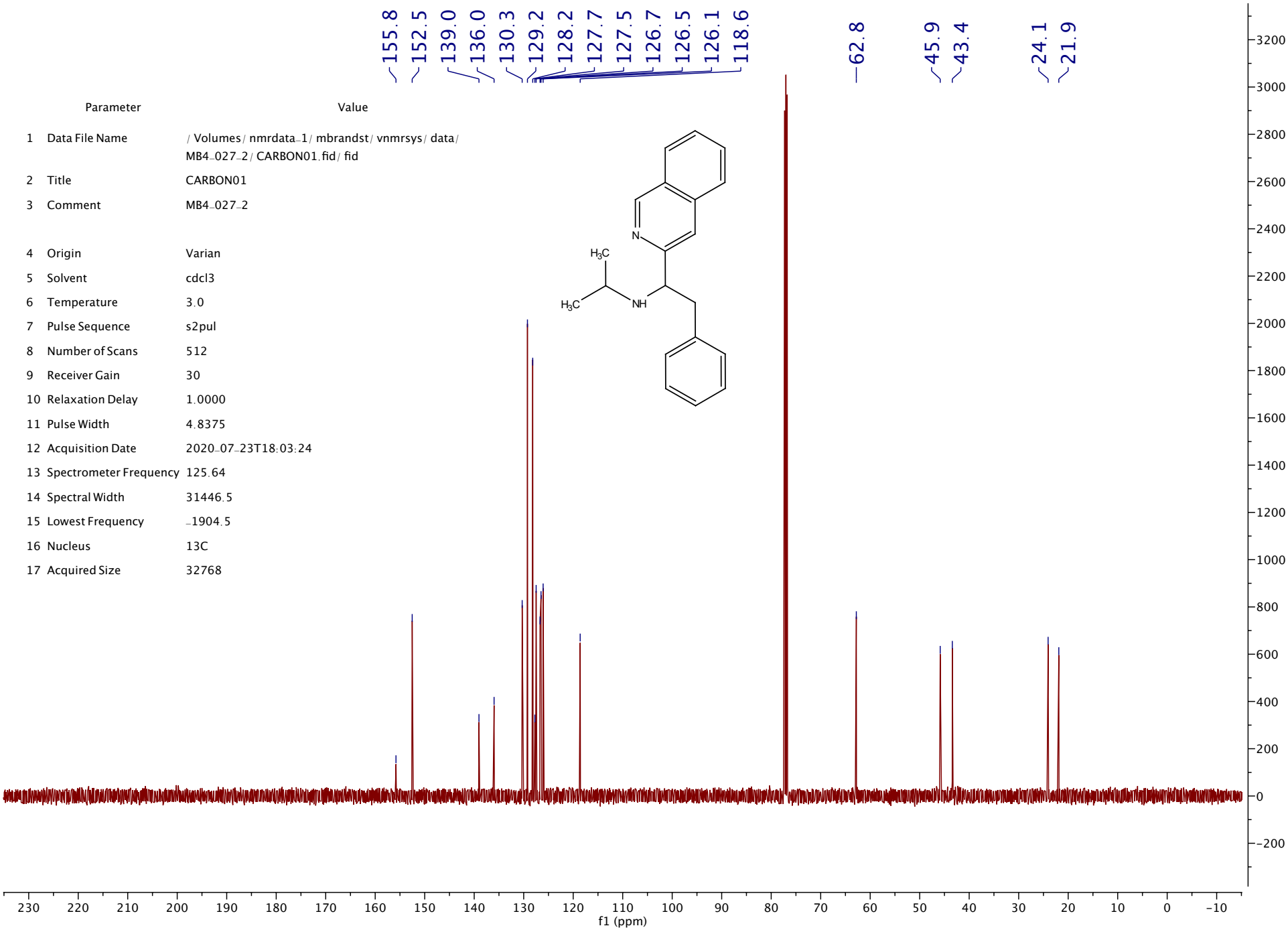




	Parameter	Value
1	Data File Name	/Volumes/nmrdata/mbrandst/nmr/mb4_028_1/2/fid
2	Title	mb4_028_1.2.fid
3	Origin	Bruker BioSpin GmbH
4	Solvent	CDCl3
5	Temperature	297.1
6	Pulse Sequence	zgpg30
7	Experiment	1D
8	Number of Scans	512
9	Receiver Gain	55.5
10	Relaxation Delay	1.0000
11	Pulse Width	10.0000
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

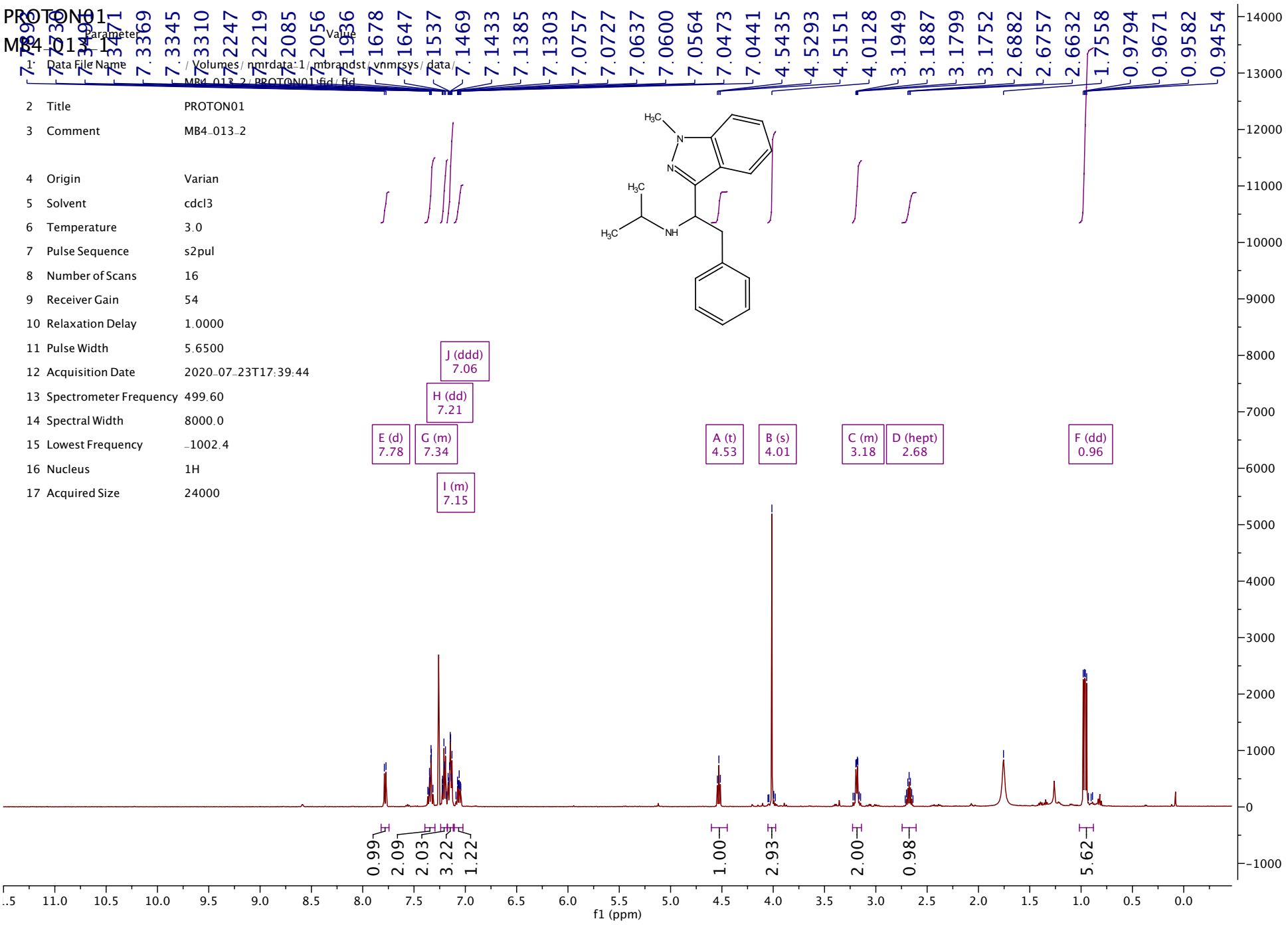


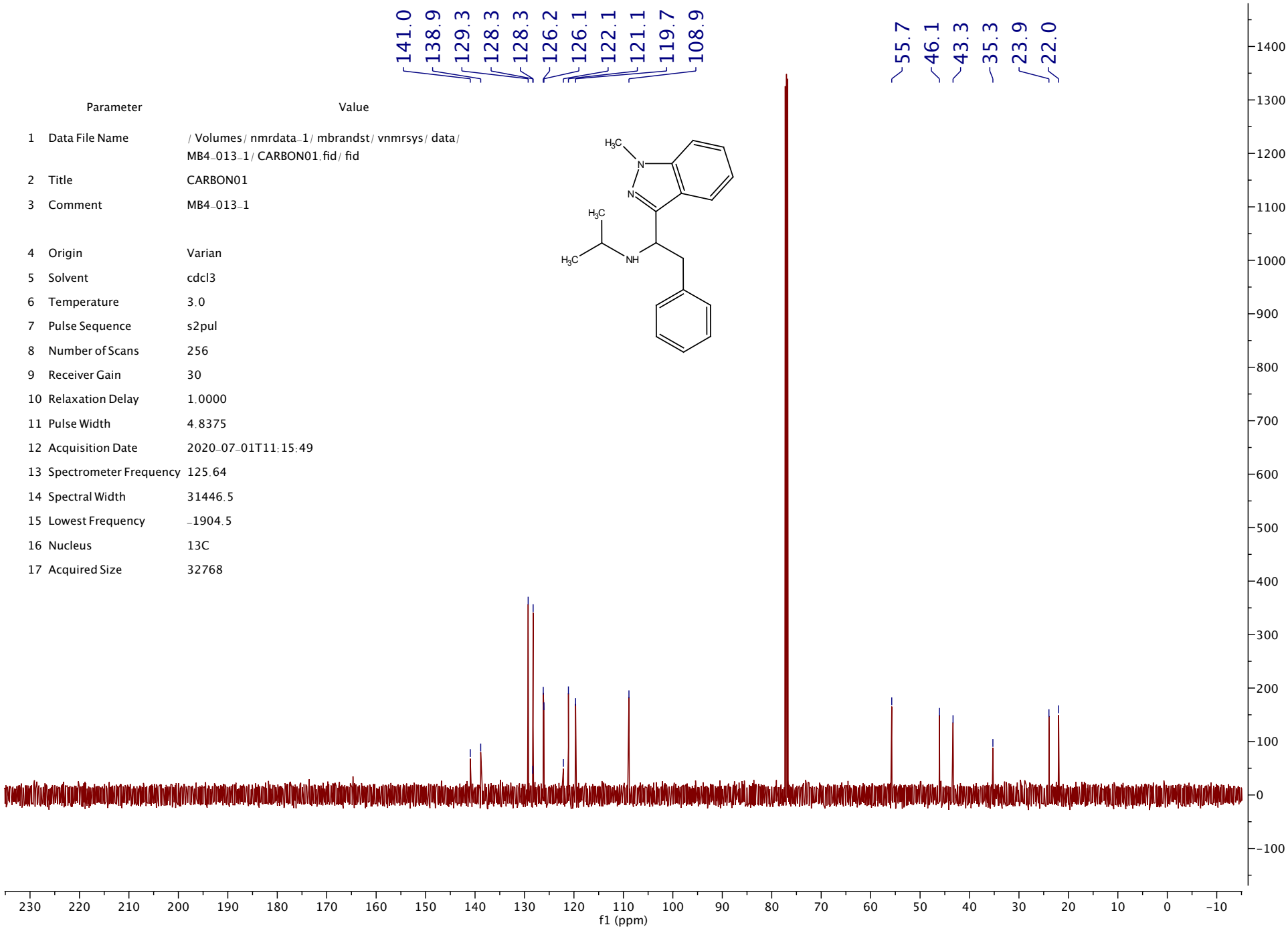

155.8
152.5
139.0
136.0
130.3
129.2
128.2
127.7
127.5
126.7
126.5
126.1
118.6
62.8
45.9
43.4
24.1
21.9
Parameter
Value
1 Data File Name / Volumes / nmrdata_1 / mbrandst / vnmrsys / data / MB4_027_2 / CARBON01.fid / fid
2 Title CARBON01
3 Comment MB4_027_2
4 Origin Varian
5 Solvent cdcl3
6 Temperature 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
N
H3C
H3C
NH
f1 (ppm)

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





	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