Supporting Information

3-Aminooxetanes: Versatile 1,3-Amphoteric Molecules for Intermolecular Annulation Reactions

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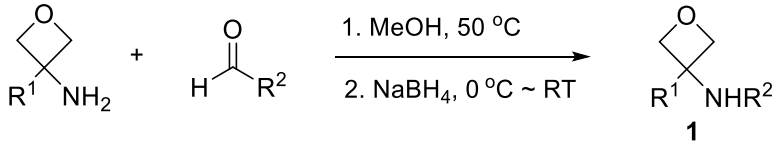
I. General Information

All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using dry solvents. Flash column chromatography was performed over silica gel (230-400 mesh) purchased from Qindao Puke Co., China. Anhydrous dichloromethane and tetrahydrofuran were purified by the Innovative® solvent purification system. ^{1}H and ^{13}C NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, acetone-d_6 at 2.09 ppm, DMSO-d_6 at 2.51 ppm, and CD_3OD at 3.34 ppm. ^{13}C NMR: $CDCl_3$ at 77.0 ppm, acetone-d_6 at 206.0 ppm, DMSO-d_6 at 39.8 ppm, and CD_3OD at 48.8 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, or a MALDI Micro MX mass spectrometer, or an API QSTAR XL System.

II. Substrate Preparation

3-Aminooxatanes were synthesized according to the following procedures. Siloxy alkynes used in this work are all known compounds.[1]

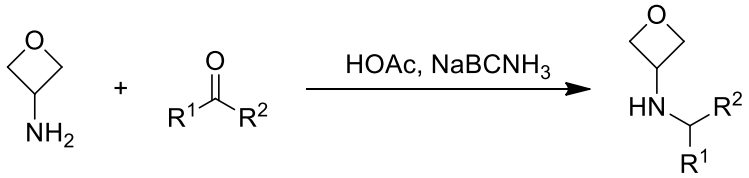
General Procedure A



1

A mixture of the oxetane (3 mmol) and the aldehyde (3.6 mmol) in MeOH (10 mL) was stirred at 50 °C overnight. The mixture was then cooled to 0 °C, to which $NaBH_4$ (125 mg, 3.3 mmol) was added slowly. Next, the reaction mixture was allowed to warm to room temperature and stirred for 1 h before it was quenched with saturated NH_4Cl (10 mL). The mixture was extracted with EtOAc (20 mL×3). The combined organic layers were washed with brine (20 mL), dried with anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column silica gel chromatography (eluent: hexanes/EtOAc = 2:1) to afford the desired product **1**.

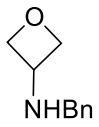
General Procedure B



At room temperature, to a solution of oxetan-3-amine (0.7 mL, 10 mmol) and the aldehyde or ketone (12 mmol, 1.2 equiv) in DCE (25 mL) were added $NaBH_3CN$ (0.94 g, 15 mmol) and AcOH (0.7 mL, 12 mmol). The mixture was stirred overnight, and an aqueous solution of NaOH (1M, 15 mL) was added

1 A. Wu, Q. Feng, H. H. Y. Sung, I. D. Williams, J. Sun, *Angew. Chem., Int. Ed.*, 2019, **58**, 6776 – 6780.

to quench the reaction. The layers were separated, and the aqueous layer was extracted with EtOAc (15 mL×3). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to afford the secondary amine.



1b

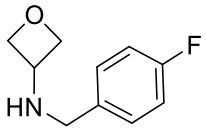
***N*-Benzyloxetan-3-amine (1b)** was prepared as colorless oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.18 (m, 5H), 4.76 (t, J = 6.9 Hz, 2H), 4.40 (t, J = 6.4 Hz, 2H), 4.08 – 3.91 (m, 1H), 3.73 (s, 2H), 1.90 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 128.4, 127.9, 127.1, 79.5, 53.0, 51.3.

IR (neat) 3421, 2953, 2872, 1664, 1375, 967, 848, 745, 702 cm^{-1}.

HRMS (EI+) calcd for $C_{10}H_{14}NO$ $[M+H]^+$: 164.1075, found 164.1069.



1c

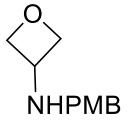
***N*-(4-Fluorobenzyl)oxetan-3-amine (1c)** was prepared as colorless oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.21 (m, 2H), 7.06 – 7.00 (m, 2H), 4.80 (t, J = 6.9 Hz, 2H), 4.43 (t, J = 6.4 Hz, 2H), 4.09 – 3.95 (m, 1H), 3.73 (s, 2H), 1.83 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1 (d, $J_{C\text{-}F}$ = 244.0 Hz), 135.4, 129.7 (d, $J_{C\text{-}F}$ = 8.0 Hz), 115.4 (d, $J_{C\text{-}F}$ = 22.0 Hz), 79.6, 53.1, 50.7.

IR (neat) 3421, 2957, 2875, 1604, 1510, 1221, 968, 828 cm^{-1}.

HRMS (EI+) calcd for $C_{10}H_{13}FNO$ $[M+H]^+$: 182.0981, found 182.0947.



1d

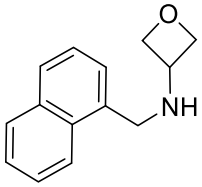
***N*-(4-Methoxybenzyl)oxetan-3-amine (1d)** was prepared as colorless oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, J = 8.5 Hz, 2H), 6.86 (d, J = 8.6 Hz, 2H), 4.76 (t, J = 6.8 Hz, 2H), 4.39 (t, J = 6.3 Hz, 2H), 4.02-3.98 (m, 1H), 3.80 (s, 3H), 3.68 (s, 2H), 1.81 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 131.7, 129.3, 113.9, 79.7, 55.3, 53.0, 50.9.

IR (neat) 3421, 2958, 1612, 1513, 1247, 1178, 1032, 965, 820 cm^{-1}.

HRMS (EI+) calcd for $C_{11}H_{16}NO_2$ $[M+H]^+$: 194.1181, found 194.1182.



1e

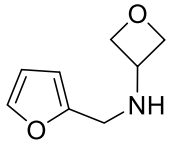
***N*-(Naphthalen-1-ylmethyl)oxetan-3-amine (1e)** was prepared as colorless oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.3 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.84 – 7.73 (m, 1H), 7.54 (m, 2H), 7.45 – 7.42 (m, 2H), 4.77 (dd, J = 6.4, 6.6 Hz, 2H), 4.40 (dd, J = 6.4, 6.6 Hz, 2H), 4.20 (s, 2H), 4.15 – 4.04 (m, 1H), 2.03 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 135.2, 133.9, 131.6, 128.8, 128.2, 126.3, 126.2, 125.8, 125.4, 123.4, 79.7, 53.5, 49.1.

IR (neat) 3441, 2952, 2869, 1637, 1460, 1263, 969, 779 cm^{-1}.

HRMS (EI+) calcd for $C_{14}H_{16}NO$ $[M+H]^+$: 214.1232, found 214.1237.



1f

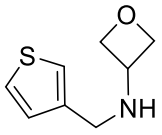
***N*-(Furan-2-ylmethyl)oxetan-3-amine (1f)** was prepared as brown oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (s, 1H), 6.29 (s, 1H), 6.13 (d, J = 2.4 Hz, 1H), 4.72 (dd, J = 6.4, 6.6 Hz, 2H), 4.29 (t, J = 6.4, 6.6 Hz, 2H), 3.99 – 3.93(m, 1H), 3.74 (s, 2H), 2.02 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 142.0, 110.3, 107.1, 79.7, 53.1, 43.9.

IR (neat) 3425, 2358, 1637, 1148, 962 cm^{-1}.

HRMS (EI+) calcd for $C_8H_{12}NO_2$ $[M+H]^+$: 154.0868, found 154.0866.



1g

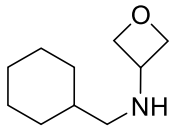
***N*-(Thiophen-3-ylmethyl)oxetan-3-amine (1g)** was prepared as brown oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, J = 4.8, 3.0 Hz, 1H), 7.14 – 7.07 (m, 1H), 7.02 (d, J = 4.9 Hz, 1H), 4.76 (t, J = 6.8 Hz, 2H), 4.39 (t, J = 6.4 Hz, 2H), 4.10 – 3.89 (m, 1H), 3.76 (s, 2 H), 1.94 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 127.4, 126.1, 121.8, 79.6, 53.1, 46.2.

IR (neat) 3425, 2955, 2874, 1643, 1469, 965, 785 cm^{-1}.

HRMS (EI+) calcd for $C_8H_{12}NOS$ $[M+H]^+$: 170.0640, found 170.0638.



1h

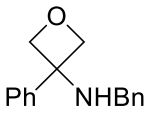
***N*-(Cyclohexylmethyl)oxetan-3-amine (1h)** was prepared as colorless oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.77 (t, J = 6.7 Hz, 2H), 4.39 (t, J = 6.2 Hz, 2H), 3.89 (m, 1H), 2.33 (d, J = 6.6 Hz, 2H), 1.72 – 1.62 (m, 6H), 1.38 – 1.28 (m, 1H), 1.26 – 1.00 (m, 3H), 0.99 – 0.69 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 79.6, 53.8, 53.6, 38.2, 31.3, 26.5, 25.9.

IR (neat) 3429, 2924, 2855, 1642, 1454, 1144, 968 cm^{-1}.

HRMS (EI+) calcd for $C_{10}H_{20}NO$ $[M+H]^+$:170.1545, found 170.1546.



1i

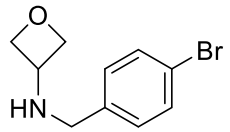
***N*-Benzyl-3-phenyloxetan-3-amine (1i)** was prepared as colorless oil according to the General Procedure A (purification by flash column chromatography: hexanes/EtOAc = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.50 (m, 2H), 7.48 – 7.44 (m, 2H), 7.38 – 7.34 (m, 5H), 7.31 – 7.26 (m, 1H), 5.02 (d, J = 6.4 Hz, 2H), 4.82 (d, J = 6.4 Hz, 2H), 3.59 (s, 2H), 2.11 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 142.0, 139.9, 128.6, 128.5, 128.1, 127.4, 127.1, 126.2, 82.4, 63.5, 47.9.

IR (neat) 3445, 2949, 2871, 2357, 1636, 1455, 980, 700 cm^{-1}.

HRMS (EI+) calcd for $C_{16}H_{18}NO$ $[M+H]^+$: 240.1388, found 240.1391.



1j

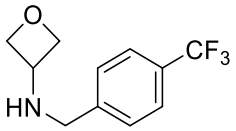
***N*-(4-Bromobenzyl)oxetan-3-amine (1j)** was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, J = 6.9 Hz, 2H), 7.17 (d, J = 7.2 Hz, 2H), 4.76 (t, J = 6.7 Hz, 2H), 4.39 (t, J = 6.2 Hz, 2H), 4.03 – 3.90 (m, 1H), 3.68 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 131.5, 129.7, 121.0, 79.5, 53.0, 50.6.

IR (thin film) 3048, 2952, 2868, 1481, 1266, 970 cm^{-1}.

HRMS (CI+) Calcd for $C_{10}H_{13}BrNO$ $[M+H]^+$: 242.0181, Found: 242.0187.



1k

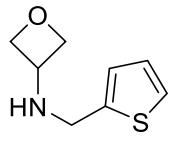
***N*-(4-(Trifluoromethyl)benzyl)oxetan-3-amine (1k)** was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 7.7 Hz, 2H), 7.43 (d, J = 7.7 Hz, 2H), 4.79 (t, J = 6.6 Hz, 2H), 4.42 (t, J = 6.0 Hz, 2H), 4.06 – 3.91 (m, 1H), 3.80 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 129.5 (q, J = 34.0 Hz), 128.3, 125.4 (q, J = 4.0 Hz), 124.1 (q, J = 271.0 Hz), 79.5, 53.1, 50.8.

IR (thin film) 3052, 2954, 2870, 1322, 1116, 970 cm^{-1}.

HRMS (CI+) Calcd for $C_{11}H_{13}F_3NO$ $[M+H]^+$: 232.0949, Found: 232.0954.



1l

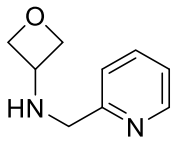
***N*-(Thiophen-2-ylmethyl)oxetan-3-amine (1l)** was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (dd, J = 5.1, 1.2 Hz, 1H), 6.93 (dd, J = 5.0, 3.5 Hz, 1H), 6.89 (dd, J = 3.3, 0.9 Hz, 1H), 4.76 (t, J = 6.9 Hz, 2H), 4.39 (t, J = 6.4 Hz, 2H), 4.08 – 3.98 (m, 1H), 3.94 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 126.7, 125.1, 124.7, 79.5, 52.9, 45.9.

IR (thin film) 3050, 2952, 2868, 1466, 1267, 969 cm^{-1}.

HRMS (CI+) Calcd for $C_8H_{12}NOS$ $[M+H]^+$: 170.0636, Found: 170.0640.



1m

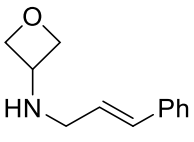
***N*-(Pyridin-2-ylmethyl)oxetan-3-amine (1m)** was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 – 8.45 (m, 1H), 7.62 (td, J = 7.7, 1.8 Hz, 1H), 7.35 – 7.20 (m, 1H), 7.23 – 7.03 (m, 1H), 4.73 (t, J = 6.9 Hz, 2H), 4.41 (t, J = 6.5 Hz, 2H), 4.10 – 3.91 (m, 1H), 3.84 (s, 2H), 2.34 (s, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 149.3, 136.6, 122.2 (2C), 79.5, 53.3, 52.7.

IR (thin film) 3052, 2952, 2870, 1590, 1472, 967 cm^{-1}.

HRMS (CI+) Calcd for $C_9H_{13}N_2O$ $[M+H]^+$: 165.1028, Found: 165.1026.



1n

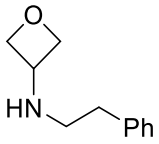
***N*-Cinnamyloxetan-3-amine (1n)** was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.27 (m, 4H), 7.27 – 7.19 (m, 1H), 6.51 (d, *J* = 15.8 Hz, 1H), 6.21 (dt, *J* = 15.8, 6.4 Hz, 1H), 4.82 (t, *J* = 6.9 Hz, 2H), 4.46 (t, *J* = 6.5 Hz, 2H), 4.11 – 3.92 (m, 1H), 3.36 (dd, *J* = 6.4, 1.3 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 131.7, 128.5, 127.6, 127.5, 126.2, 79.8, 53.1, 49.3.

IR (thin film) 3045, 2953, 2869, 1456, 1266, 968 cm^{-1}.

HRMS (CI+) Calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, Found: 190.1233.



1o

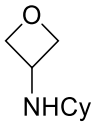
***N*-Phenethyloxetan-3-amine (1o)** was prepared according to the General Procedure B.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 2H), 7.24 – 7.14 (m, 3H), 4.77 (t, *J* = 6.8 Hz, 2H), 4.37 (t, *J* = 6.4 Hz, 2H), 4.03 – 3.85 (m, 1H), 2.91 – 2.61 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 128.43, 128.39, 126.2, 79.4, 53.3, 48.1, 36.4.

IR (thin film) 3047, 2950, 2868, 1459, 1267, 969 cm^{-1}.

HRMS (CI+) Calcd for $C_{11}H_{16}NO$ $[M+H]^+$: 178.1237, Found: 178.1232.



1p

***N*-Cyclohexyloxetan-3-amine (1p)** was prepared according to the General Procedure B.

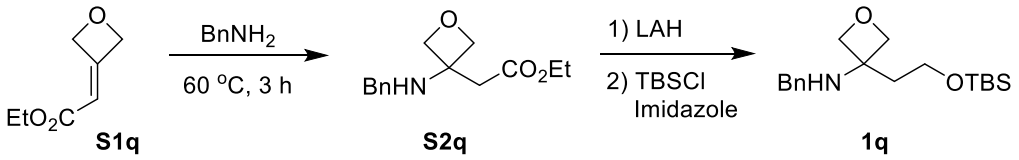
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.80 (t, *J* = 6.9 Hz, 2H), 4.40 (t, *J* = 6.5 Hz, 2H), 4.13 – 3.93 (m, 1H), 2.47 – 2.31 (m, 1H), 1.81 – 1.63 (m, 4H), 1.61 – 1.55 (m, 1H),

1.33 – 1.10 (m, 3H), 1.08 – 0.89 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 80.8, 55.6, 51.5, 34.0, 25.8, 24.9.

IR (thin film) 2928, 2857, 1453, 1266, 969 cm^{-1}.

HRMS (CI+) Calcd for $C_9H_{18}NO$ $[M+H]^+$: 156.1388, Found: 156.1392.



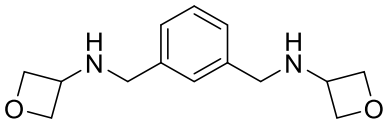
***N*-Benzyl-3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)oxetan-3-amine (1q).** A miture of **S1q** (1.4 g, 10 mmol, 1.0 equiv) and $BnNH_2$ (1.2 mL, 11 mmol, 1.1 equiv) was stirred (without solvent) at 60 °C for 3 h to afford **S2q**. Next, dry THF (20 mL) was added to dissolve the crude **S2q**. The mixture was cooled to 0 °C and $LiAlH_4$ (312 mg, 8 mmol, 0.8 equiv) was added in portions. Then the mixture was allowed to stir at room temperature for 1.5 h before $Na_2SO_4 \bullet 10H_2O$ was added to quench the reaction. The mixture was filtered and washed with EtOAc (10 mL×3). The filtrate was concentrated under reduced pressure. The residue was dissolved in DCM (20 mL), to which imidazole (817 mg, 12 mmol, 1.2 equiv) was added. The mixture was cooled to 0 °C, and TBSCl (1.3 g, 8.8 mmol, 0.88 equiv) was added in portions. The reaction mixture was stirred overnight at room temperature, and then water (30 mL) was added to quench the reaction. The layers were separated, and the aqueous layer was extracted with DCM (15 mL×3). The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: 20% Et_2O in hexanes) to afford the pure **1q** as a pale yellow oil (2.1 g, 65% for 3 steps).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.29 (m, 4H), 7.29 – 7.22 (m, 1H), 4.61 (d, J = 6.5 Hz, 2H), 4.53 (d, J = 6.6 Hz, 2H), 3.87 – 3.72 (m, 4H), 2.15 (t, J = 6.2 Hz, 2H), 0.86 (s, 9H), 0.04 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 128.5, 128.1, 127.1, 81.6, 59.7, 59.3, 47.3, 38.0, 25.9, 18.2, –5.5.

IR (thin film) 3055, 2938, 2862, 1464, 1258, 1092 cm^{-1}.

HRMS (CI+) Calcd for $C_{18}H_{32}NO_2Si$ $[M+H]^+$: 322.2202, Found: 322.2210.



1r

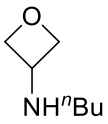
***N,N′*-(1,3-Phenylenebis(methylene))bis(oxetan-3-amine) (1r)** was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.22 (m, 2H), 7.17 (d, J = 7.5 Hz, 2H), 4.75 (t, J = 6.8 Hz, 4H), 4.39 (t, J = 6.3 Hz, 4H), 4.07 – 3.88 (m, 2H), 3.70 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 128.7, 127.8, 127.0, 79.6, 53.1, 51.2.

IR (thin film) 3045, 2948, 2865, 1471, 1172, 966 cm^{-1}.

HRMS (CI+) Calcd for $C_{14}H_{21}N_2O_2$ $[M+H]^+$: 249.1603, Found: 249.1600.



1s

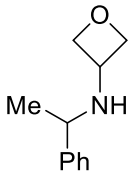
***N*-Butyloxetan-3-amine (1s)** was prepared according to the General Procedure B.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.83 (t, J = 6.9 Hz, 2H), 4.45 (t, J = 6.4 Hz, 2H), 4.01 – 3.91 (m, 1H), 2.56 (t, J = 8.0 Hz, 2H), 1.49 – 1.42 (m, 2H), 1.41 – 1.29 (m, 2H), 0.92 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 79.8, 53.5, 46.8, 32.4, 20.3, 13.9.

IR (thin film) 2956, 2870, 2330, 1465, 1131, 964 cm^{-1}.

HRMS (CI+) Calcd for $C_{13}H_{16}NO_3$ $[M+H]^+$: 130.1232, Found:130.1236.



1t

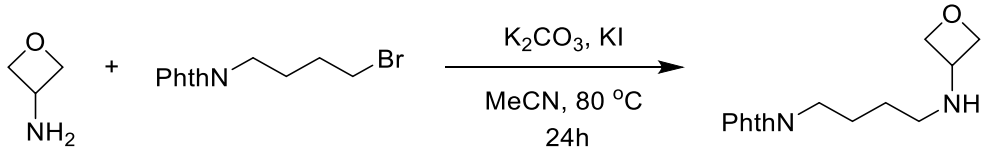
(*R*)-*N*-(1-Phenylethyl)oxetan-3-amine (1t) was prepared according to the General Procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.30 (m, 2H), 7.27 – 7.23 (m, 3H), 4.76 (t, *J* = 6.7 Hz, 1H), 4.51 (t, *J* = 6.8 Hz, 1H), 4.44 (t, *J* = 6.3 Hz, 1H), 4.20 (t, *J* = 6.4 Hz, 1H), 3.87 (p, *J* = 6.7 Hz, 1H), 3.72 (q, *J* = 6.6 Hz, 1H), 1.80 (s, 1H), 1.37 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 128.5, 127.2, 126.4, 80.1, 80.0, 56.5, 51.8, 23.8.

IR (thin film) 3029, 2963, 2869, 1265, 970 cm^{-1}.

HRMS (CI+) Calcd for $C_{11}H_{16}NO$ $[M+H]^+$: 178.1232, Found: 178.1234.



S1u **1u**

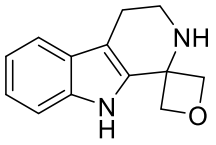
2-(4-(Oxetan-3-ylamino)butyl)isoindoline-1,3-dione (1u). A 100-mL flask was charged with **S1u** (2.2 g, 7.8 mmol, 1.3 equiv), K_2CO_3 (1.7 g, 12 mmol, 2.0 equiv) and KI (2.0 g, 12 mmol, 2.0 equiv), to which MeCN (30 mL) and oxetan-3-amine (0.42 mL, 6.0 mmol, 1.0 equiv) were sequentially added. The mixture was stirred at 80 °C for 24 h, and then water (30 mL) was added. The mixture was extracted with EtOAc (20 mL×3). The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: 5% MeOH in DCM) to afford pure **1u** as a pale yellow solid (612 mg, 37%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.73 (m, 2H), 7.72 – 7.60 (m, 2H), 4.76 (t, *J* = 6.7 Hz, 2H), 4.37 (t, *J* = 6.2 Hz, 2H), 3.90 (p, *J* = 6.4 Hz, 1H), 3.66 (t, *J* = 7.1 Hz, 2H), 2.55 (t, *J* = 7.2 Hz, 2H), 1.74 – 1.64 (m, 2H), 1.54 – 1.38 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 133.8, 131.9, 123.1, 79.6, 53.4, 46.4, 37.5, 27.4, 26.2.

IR (thin film) 3055, 2946, 2867, 1707, 1440, 1267, 969 cm^{-1}.

HRMS (CI+) Calcd for $C_{15}H_{19}N_2O_3$ $[M+H]^+$: 275.1396, Found: 275.1395.



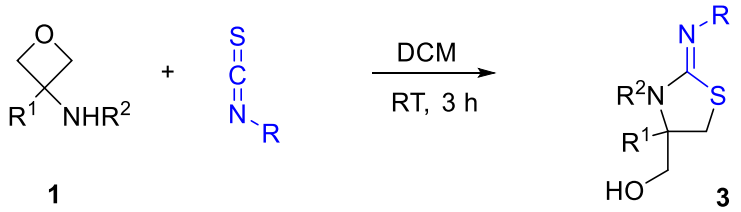
1v

Oxetane **1v** is a known compound. It was prepared according to literature procedure.[2]

2 B. O. Beasley, A. Alli-Balogun, G. J. Clarkson, M. Shipman, *Tetrahedron Lett.*, 2014, **55**, 541–543.

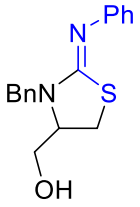
III. [3+2] Annulation with Isothiocyanates

General Procedure C



1 **3**

To a stirred solution of 3-aminooxetane (0.3 mmol) in DCM (3 mL) was added isothiocyanate (0.33 mmol) at room temperature. The reaction was stirred for ~3 h at the same temperature before it was concentrated under reduced pressure and purified by silica gel flash chromatography to afford the desired product.



3a

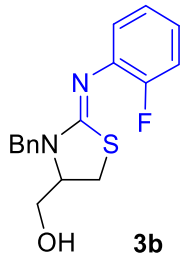
(*Z*)-(3-Benzyl-2-(phenylimino)thiazolidin-4-yl)methanol (3a) was prepared as colorless oil according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 86.7 mg, 97% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.27 (m, 7H), 7.18 – 6.99 (m, 3H), 5.40 (d, *J* = 15.5 Hz, 1H), 4.56 (d, *J* = 15.5 Hz, 1H), 4.05 – 3.72 (m, 3H), 3.67 (dd, *J* = 11.6, 3.5 Hz, 1H), 3.26 (dd, *J* = 12.0, 8.0 Hz, 1H), 3.20 (dd, *J* = 11.2, 9.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 149.7, 137.0, 128.9, 128.82, 127.8, 127.7, 123.9, 122.5, 62.4, 60.9, 49.1, 29.0.

IR (neat) 3366, 2933, 2358, 1618, 1489, 1221, 1062, 696 cm^{-1}.

HRMS (EI+) calcd for $C_{17}H_{19}N_2OS$ $[M+H]^+$: 299.1218, found 299.1216.



3b

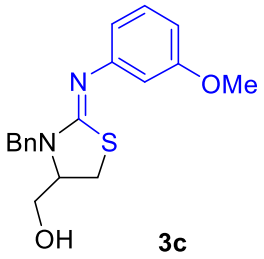
(*Z*)-(3-Benzyl-2-((2-fluorophenyl)imino)thiazolidin-4-yl)methanol (3b) was prepared as white solid according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 93.9 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.34 (m, 4H), 7.31 – 7.28 (m, 1H), 7.14 – 6.94 (m, 4H), 5.15 (d, J = 15.4 Hz, 1H), 4.46 (d, J = 15.4 Hz, 1H), 3.83 – 3.76 (m, 2H), 3.62 (d, J = 8.5 Hz, 1H), 3.27 – 3.00 (m, 2H), 2.33 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 156.2, 153.7, 139.4 (d, $J_{C\text{-}F}$ = 12.2 Hz), 137.2, 128.8, 127.8, 127.6, 124.2, 124.1, 115.8 (d, $J_{C\text{-}F}$ = 20.2 Hz), 62.1, 60.9, 48.6, 28.9.

IR (neat) 3394, 2358, 1605, 1491, 1230, 1044, 750 cm^{-1}.

HRMS (EI+) calcd for $C_{17}H_{18}FN_2OS$ $[M+H]^+$: 317.1124, found 317.1110.



3c

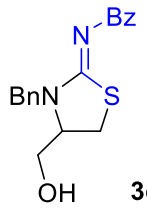
(*Z*)-(3-Benzyl-2-((3-methoxyphenyl)imino)thiazolidin-4-yl)methanol (3c) was prepared as white solid according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 97.4 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.24 (m, 5H), 7.20 (t, J = 8.0 Hz, 1H), 6.70 – 6.36 (m, 3H), 5.10 (d, J = 15.5 Hz, 1H), 4.40 (d, J = 15.5 Hz, 1H), 3.79 (s, 3H), 3.76 – 3.66 (m, 2H), 3.59 (d, J = 8.0 Hz, 1H), 3.11 (d, J = 4.9 Hz, 2H), 2.64 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 152.8, 137.3, 129.5 (2C), 128.7, 127.6, 127.5, 114.5, 109.0, 107.7, 61.7, 60.8, 55.1, 48.5, 28.9.

IR (neat) 3382, 2942, 2358, 1582, 1481, 1273, 1043, 947, 778 cm^{-1}.

HRMS (EI+) calcd for $C_{18}H_{21}N_2O_2S$ $[M+H]^+$: 329.1324, found 329.1322.



3d

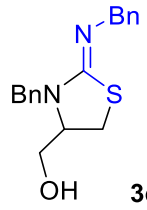
(*Z*)-*N*-(3-Benzyl-4-(hydroxymethyl)thiazolidin-2-ylidene)benzamide (3d) was prepared as colorless oil according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 90.0 mg, 92% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 7.8 Hz, 2H), 7.49 (t, J = 7.1 Hz, 1H), 7.40 (t, J = 7.5 Hz, 2H), 7.33 – 7.29 (m, 5H), 5.51 (d, J = 15.0 Hz, 1H), 4.59 (d, J = 15.0 Hz, 1H), 3.98 – 3.87 (m, 1H), 3.83 (dd, J = 11.3, 8.6 Hz, 1H), 3.75 (dd, J = 11.6, 7.8 Hz, 1H), 3.27 – 3.10 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.1, 172.7, 136.5, 136.4, 132.0, 129.6, 128.9, 128.0, 128.0, 127.8, 60.8, 60.6, 45.0, 29.6.

IR (neat) 3701, 2924, 1566, 1402, 1318, 1063, 720 cm^{-1}.

HRMS (EI+) calcd for $C_{18}H_{19}N_2O_2S$ $[M+H]^+$: 327.1167, found 327.1161.



3e

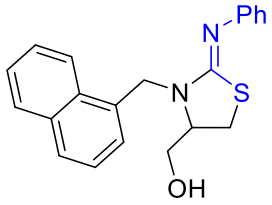
(*Z*)-(3-Benzyl-2-(benzylimino)thiazolidin-4-yl)methanol (3e) was prepared as colorless oil according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 92.7 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.10 (m, 10H), 5.08 (d, J = 15.5 Hz, 1H), 4.61 – 4.41 (m, 2H), 4.31 (d, J = 15.5 Hz, 1H), 3.72 – 3.57 (m, 2H), 3.49 (dd, J = 10.7, 2.5 Hz, 1H), 3.35 (br s, 1H), 3.25 – 3.04 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 140.9, 137.7, 128.6, 128.1, 127.6, 127.4, 127.3, 126.4, 61.5, 60.5, 58.2, 48.5, 28.9.

IR (neat) 3407, 2358, 1622, 1522, 1445, 1043, 699 cm^{-1}.

HRMS (EI+) calcd for $C_{18}H_{20}N_2OS$ $[M]^+$: 312.1296, found 312.1293.



3f

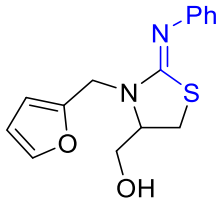
(*Z*)-(3-(Naphthalen-1-ylmethyl)-2-(phenylimino)thiazolidin-4-yl)methanol (3f) was prepared as white solid according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 102.3 mg, 98% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.3 Hz, 1H), 7.90 (d, J = 7.5 Hz, 1H), 7.83 (d, J = 7.9 Hz, 1H), 7.63 – 7.48 (m, 2H), 7.48 – 7.37 (m, 2H), 7.33 (t, J = 7.7 Hz, 2H), 7.15 – 6.97 (m, 3H), 5.68 (d, J = 15.3 Hz, 1H), 4.67 (d, J = 15.3 Hz, 1H), 3.71 – 3.43 (m, 3H), 3.03 (br s, 1H), 2.94 (d, J = 4.5 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 151.6, 133.8, 132.5, 131.5, 128.9, 128.7, 128.5, 126.5, 126.4, 126.0, 125.1, 123.7, 123.3, 122.2, 60.8, 60.5, 46.9, 28.8.

IR (neat) 3394, 2357, 1616, 1482, 1209, 1057, 778 cm^{-1}.

HRMS (EI+) calcd for $C_{21}H_{21}N_2OS$ $[M+H]^+$: 349.1375, found 349.1367.



3g

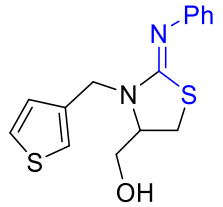
(*Z*)-(3-(Furan-2-ylmethyl)-2-(phenylimino)thiazolidin-4-yl)methanol (3g) was prepared as colorless oil according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 85.5 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.31 (t, J = 7.7 Hz, 2H), 7.08 (t, J = 7.3 Hz, 1H), 6.98 (d, J = 8.1 Hz, 2H), 6.38 (s, 2H), 5.04 (d, J = 15.8 Hz, 1H), 4.44 (d, J = 15.8 Hz, 1H), 3.93 – 3.76 (m, 2H), 3.70 (dd, J = 10.9, 2.9 Hz, 1H), 3.31 – 3.07 (m, 2H), 2.99 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 151.4, 150.6, 142.1, 128.8, 123.3, 122.0, 110.5, 108.7, 62.0, 60.8, 41.5, 28.8.

IR (neat) 3390, 2358, 1618, 1490, 1215, 1062, 739 cm^{-1}.

HRMS (EI+) calcd for $C_{15}H_{17}N_2O_2S$ $[M+H]^+$: 289.1011, found 289.1003.



3h

(*Z*)-(2-(Phenylimino)-3-(thiophen-3-ylmethyl)thiazolidin-4-yl)methanol (3h) was prepared as colorless oil according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 90.3 mg, 99% yield).

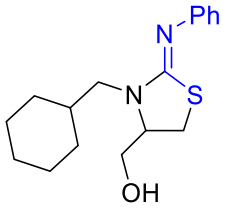
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dd, J = 10.0, 5.2 Hz, 3H), 7.19 (s, 1H), 7.12 (d, J = 4.9 Hz, 1H), 7.08 (t, J = 7.3 Hz, 1H), 6.99 (d, J = 7.9 Hz, 2H), 5.05 (d, J =

15.4 Hz, 1H), 4.38 (d, *J* = 15.4 Hz, 1H), 3.71 – 3.68 (m, 2H), 3.60 – 3.56 (m, 1H), 3.10 – 3.02 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 151.4, 137.9, 128.8, 127.5, 126.3, 123.3, 122.6, 122.1, 61.7, 60.8, 43.8, 28.8.

IR (neat) 3379, 2937, 2358, 1616, 1437, 1215, 1058, 771 cm^{-1}.

HRMS (EI+) calcd for $C_{15}H_{17}N_2OS_2$ $[M+H]^+$: 305.0782, found 305.0789.



3i

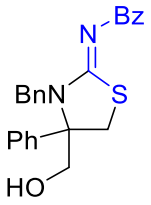
(*Z*)-(3-(Cyclohexylmethyl)-2-(phenylimino)thiazolidin-4-yl)methanol (3i) was prepared as white solid according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 90.3 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.6 Hz, 2H), 7.06 (t, *J* = 7.3 Hz, 1H), 6.93 (d, *J* = 8.1 Hz, 2H), 3.86 – 3.77 (m, 2H), 3.75 – 3.60 (m, 2H), 3.27 (br s, 1H), 3.21 (dd, *J* = 10.9, 7.1 Hz, 1H), 3.11 (dd, *J* = 11.0, 3.1 Hz, 1H), 2.91 (dd, *J* = 13.9, 6.4 Hz, 1H), 1.79 – 1.72 (m, 6H), 1.32 – 1.16 (m, 3H), 1.07 – 0.98(m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 151.9, 128.8, 123.1, 122.2, 62.6, 60.4, 50.8, 36.1, 30.9, 30.5, 29.1, 26.4, 25.9, 25.8.

IR (neat) 3382, 2924, 2358, 1617, 1446, 1217, 1058, 770, 695 cm^{-1}.

HRMS (EI+) calcd for $C_{17}H_{25}N_2OS$ $[M+H]^+$: 305.1688, found 305.1692.



3j

(*Z*)-*N*-(3-Benzyl-4-(hydroxymethyl)-4-phenylthiazolidin-2-ylidene)benzamide (3j) was prepared as colorless oil according to the General Procedure C (purification by flash column chromatography: hexanes/EtOAc = 3:1, 108.5 mg, 90% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 7.7 Hz, 2H), 7.67 – 7.32 (m, 11H), 7.29 (d, J = 6.2 Hz, 2H), 5.89 (d, J = 15.3 Hz, 1H), 4.09 – 3.99 (m, 3H), 3.88 (d, J = 11.3 Hz, 1H), 3.13 (d, J = 11.3 Hz, 1H), 1.71 (br s, 1H).

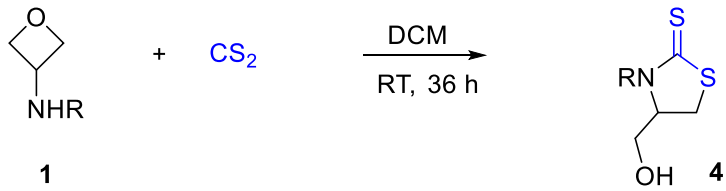
^{13}C NMR (100 MHz, $CDCl_3$) δ 176.1, 174.9, 139.3, 138.0, 136.6, 132.0, 129.7, 129.3 (2C), 128.6, 128.2, 128.1, 127.6, 125.9, 73.0, 63.5, 49.2, 37.8.

IR (neat) 3442, 2361, 1632, 1507, 1391, 1070, 783 cm^{-1}.

HRMS (EI+) calcd for $C_{24}H_{23}N_2O_2S$ $[M+H]^+$: 403.1480, found 403.1480.

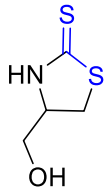
IV. [3+2] Annulation with Carbon Disulfide

General Procedure D



1 **4**

To a stirred solution of the 3-aminooxetane (0.4 mmol) in DCM (2 mL) was added CS_2 (0.6 mmol) at room temperature. The reaction mixture was continued to stir for 36 h at room temperature and it was concentrated under reduced pressure and purified by silica gel chromatography to afford the desired product.



4a

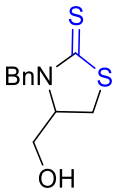
4-(Hydroxymethyl)thiazolidine-2-thione (4a) was prepared as colorless oil according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 57.4 mg, 97% yield).

^{1}H NMR (400 MHz, MeOD) δ 4.35 – 4.28 (m, 1H), 3.73 – 3.59 (m, 3H), 3.42 (dd, J = 11.3, 6.1 Hz, 1H).

^{13}C NMR (100 MHz, MeOD) δ 202.3, 66.8, 62.9, 35.6.

IR (neat) 3419, 1633, 1498, 1294, 1048, 982, 782 cm^{-1}.

HRMS (EI+) calcd for $C_4H_8NOS_2$ $[M+H]^+$: 150.0047, found 150.0040.



4b

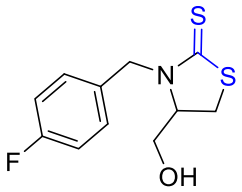
3-Benzyl-4-(hydroxymethyl)thiazolidine-2-thione (4b) was prepared as colorless oil according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 94.2 mg, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.02 (m, 5H), 5.66 (d, J = 15.1 Hz, 1H), 4.49 (d, J = 15.1 Hz, 1H), 4.23 – 4.17 (m, 1H), 3.88 – 3.83 (m, 1H), 3.74 – 3.70 (m, 1H), 3.37 – 3.32 (m, 1H), 3.27 – 3.23 (m, 1H), 2.76 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 135.1, 128.9, 128.1, 127.7, 67.5, 60.48, 50.9, 29.9.

IR (neat) 3337, 2941, 1450, 1302, 1225, 1029, 913, 700 cm^{-1}.

HRMS (EI+) calcd for $C_{11}H_{14}NOS_2$ $[M+H]^+$: 240.0517, found 240.0515.



4c

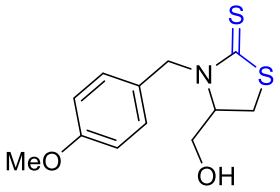
3-(4-Fluorobenzyl)-4-(hydroxymethyl)thiazolidine-2-thione (4c) was prepared as white solid according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 63.6 mg, 83% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, J = 8.0, 5.5 Hz, 2H), 7.03 (t, J = 8.5 Hz, 2H), 5.63 (d, J = 15.0 Hz, 1H), 4.49 (d, J = 15.0 Hz, 1H), 4.21 (dd, J = 8.6, 4.5 Hz, 1H), 3.87 (dd, J = 11.5, 5.5 Hz, 1H), 3.76 (dd, J = 11.5, 4.2 Hz, 1H), 3.46 – 3.31 (m, 1H), 3.25 (dd, J = 11.3, 4.4 Hz, 1H), 2.43 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.14, 162.4 (d, $J_{C\text{-}F}$ = 245.7 Hz), 131.0 (d, $J_{C\text{-}F}$ = 3.2 Hz), 129.7 (d, $J_{C\text{-}F}$ = 8.1 Hz), 115.8 (d, $J_{C\text{-}F}$ = 21.5 Hz), 67.44, 60.77, 50.29, 29.93.

IR (neat) 3393, 2933, 1604, 1509, 1462, 1223, 1160, 1037, 833 cm^{-1}.

HRMS (EI+) calcd for $C_{11}H_{13}FNOS_2$ $[M+H]^+$: 258.0423, found 258.0418.



4d

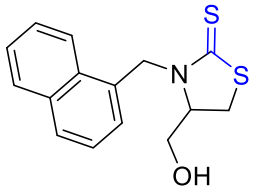
4-(Hydroxymethyl)-3-(4-methoxybenzyl)thiazolidine-2-thione (4d) was prepared as white solid according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 77.2 mg, 89% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, J = 8.1 Hz, 2H), 6.87 (d, J = 8.2 Hz, 2H), 5.60 (d, J = 14.8 Hz, 1H), 4.44 (d, J = 14.8 Hz, 1H), 4.23 – 4.20 (m, 1H), 3.88 (dd, J = 11.5, 5.5 Hz, 1H), 3.79 (s, 3H), 3.74 (dd, J = 11.6, 3.6 Hz, 1H), 3.40 – 3.30 (m, 1H), 3.26 (dd, J = 11.2, 4.3 Hz, 1H), 2.72 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 159.3, 129.2, 127.1, 114.2, 67.4, 60.4, 55.2, 50.4, 29.8.

IR (neat) 3419, 2933, 1612, 1522, 1462, 1299, 1248, 1176, 1030, 921, 733 cm^{-1}.

HRMS (EI+) calcd for $C_{12}H_{15}NO_2S_2$ $[M]^+$: 269.0544, found 269.0536.



4e

4-(Hydroxymethyl)-3-(naphthalen-1-ylmethyl)thiazolidine-2-thione (4e) was prepared as white solid according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 50.4 mg, 58% yield).

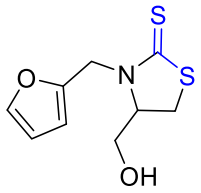
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.1 Hz, 1H), 7.93 – 7.79 (m, 2H), 7.63 – 7.42 (m, 4H), 6.22 (d, J = 15.2 Hz, 1H), 4.76 (d, J = 15.2 Hz, 1H), 4.01 (dd, J = 6.8,

4.4 Hz, 1H), 3.93 – 3.69 (m, 2H), 3.26 (dd, *J* = 11.3, 8.4 Hz, 1H), 3.11 (dd, *J* = 11.4, 2.1 Hz, 1H), 1.98 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 133.9, 131.4, 130.8, 129.3, 128.8, 127.4, 127.2, 126.4, 125.3, 123.5, 66.8, 60.8, 50.1, 30.0.

IR (neat) 3684, 1845, 1693, 1456, 1296, 1178, 1052, 782 cm^{-1}.

HRMS (EI+) calcd for $C_{15}H_{15}NOS_2$ $[M]^+$: 289.0595, found 289.0604.



4f

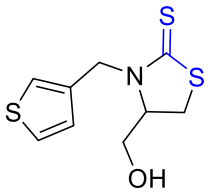
3-(Furan-2-ylmethyl)-4-(hydroxymethyl)thiazolidine-2-thione (4f) was prepared as white solid according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 81.3 mg, 85% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 1.0 Hz, 1H), 6.39 (d, *J* = 3.1 Hz, 1H), 6.37 – 6.24 (m, 1H), 5.47 (d, *J* = 15.5 Hz, 1H), 4.57 (d, *J* = 15.5 Hz, 1H), 4.32 – 4.27 (m, 1H), 3.94 (dd, *J* = 11.7, 5.5 Hz, 1H), 3.78 (dd, *J* = 11.7, 4.1 Hz, 1H), 3.37 (dd, *J* = 11.2, 8.6 Hz, 1H), 3.26 (dd, *J* = 11.2, 4.7 Hz, 1H), 2.81 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 148.2, 142.6, 110.6, 109.9, 68.0, 60.5, 43.9, 29.8.

IR (neat) 3420, 2944, 1632, 1501, 1168, 1015, 736 cm^{-1}.

HRMS (EI+) calcd for $C_9H_{11}NO_2S_2$ $[M]^+$: 229.0231, found 229.0229.



4g

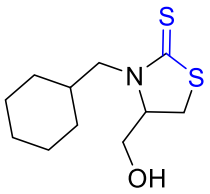
4-(Hydroxymethyl)-3-(thiophen-3-ylmethyl)thiazolidine-2-thione (4g) was prepared as white solid according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 95.3 mg, 98% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 2H), 7.10 (dd, J = 4.8, 1.0 Hz, 1H), 5.52 (d, J = 15.0 Hz, 1H), 4.61 (d, J = 15.0 Hz, 1H), 4.27 – 4.21 (m, 1H), 3.89 (dd, J = 11.6, 5.5 Hz, 1H), 3.75 (dd, J = 11.6, 4.2 Hz, 1H), 3.35 (dd, J = 11.2, 8.6 Hz, 1H), 3.25 (dd, J = 11.3, 4.9 Hz, 1H), 2.52 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 135.7, 127.2, 126.9, 123.8, 67.7, 60.7, 46.3, 29.9.

IR (neat) 3358, 2939, 1461, 1244, 1172, 1055, 910, 710 cm^{-1}.

HRMS (EI+) calcd for $C_9H_{11}NOS_3$ $[M]^+$: 245.0003, found 244.9995.



4h

3-(Cyclohexylmethyl)-4-(hydroxymethyl)thiazolidine-2-thione (4h) was prepared as white solid according to the General Procedure D (purification by flash column chromatography: hexanes/EtOAc = 2:1, 89.7 mg, 92% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.40-4.29 (m, 1H), 4.24 (dd, J = 13.6, 8.3 Hz, 1H), 3.84 (dd, J = 11.2, 6.6 Hz, 1H), 3.77 (dd, J = 11.3, 4.2 Hz, 1H), 3.47 (dd, J = 11.2, 8.4 Hz, 1H), 3.25 (dd, J = 11.3, 2.7 Hz, 1H), 3.03 (dd, J = 13.6, 6.8 Hz, 1H), 2.94 (br s, 1H), 1.95 – 1.77 (m, 1H), 1.65 (dd, J = 22.5, 15.0 Hz, 5H), 1.35–1.10 (m, 3H), 1.10–0.81 (m, 2H).

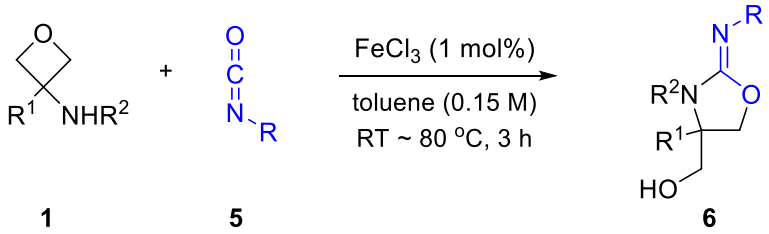
^{13}C NMR (100 MHz, $CDCl_3$) δ 196.7, 68.8, 59.9, 53.5, 36.0, 30.8, 30.2, 30.2, 26.1, 25.6, 25.5.

IR (neat) 3388, 2924, 1468, 1305, 1177, 954 cm^{-1}.

HRMS (EI+) calcd for $C_{11}H_{20}NOS_2$ $[M+H]^+$: 246.0986, found 246.0987.

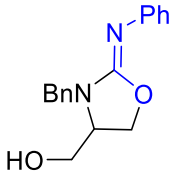
V. [3+2] Annulation with Isocyanates

General Procedure E



1 **5** **6**

At room temperature, a solution of 3-aminooxetane **1** (0.3 mmol) and isocyanate **5** (0.3 mmol) in toluene (2 mL) was stirred for about 30 min. Next, $FeCl_3$ (0.48 mg, 3 μmol) was added to the solution. The reaction mixture was then warmed to 80 °C and stirred at the same temperature for about 3 h. Upon completion, the reaction mixture was cooled to room temperature and concentrated under reduced pressure. The residue was purified by silica gel flash chromatography to afford the desired product.



6a

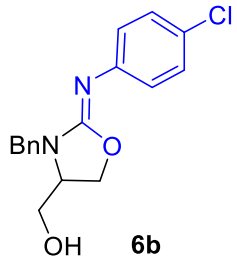
(*Z*)-(3-Benzyl-2-(phenylimino)oxazolidin-4-yl)methanol (6a) was prepared as white solid according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 2:1, 69 mg, 82% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.27 (m, 7H), 7.21 (s, 1H), 7.19 (s, 1H), 7.04 (t, J = 7.2 Hz, 1H), 5.01 (d, J = 15.4 Hz, 1H), 4.38 – 4.18 (m, 3H), 3.70 – 3.50 (m, 2H), 3.39 (d, J = 12.1 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 146.9, 136.6, 128.7, 128.6, 128.1, 127.7, 123.6, 122.4, 67.0, 59.6, 56.7, 46.5.

IR (neat) 3429, 2357, 1654, 1439, 1249, 1031, 699 cm^{-1}.

HRMS (EI+) calcd for $C_{17}H_{19}N_2O_2$ $[M+H]^+$: 283.1447, found 283.1437.



6b

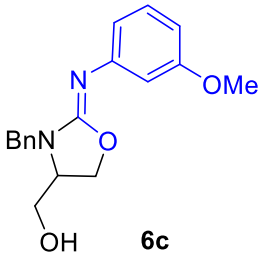
(*Z*)-(3-Benzyl-2-((4-chlorophenyl)imino)oxazolidin-4-yl)methanol (6b) was prepared as white solid according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 3:1→1 : 1, 79 mg, 83% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.31 (m, 5H), 7.27 (d, J = 8.5 Hz, 2H), 7.16 (d, J = 8.4 Hz, 2H), 4.99 (d, J = 15.3 Hz, 1H), 4.49 – 4.27 (m, 2H), 4.21 (d, J = 15.3 Hz, 1H), 3.95 (br s, 1H), 3.75 – 3.54 (m, 2H), 3.41 (d, J = 10.5 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 145.6, 136.3, 128.8, 128.5, 128.0, 127.8, 127.3, 124.9, 67.1, 59.6, 56.7, 46.5.

IR (neat) 3415, 2357, 2074, 1658, 1484, 1246, 1088, 706 cm^{-1}.

HRMS (EI+) calcd for $C_{17}H_{18}ClN_2O_2$ $[M+H]^+$: 317.1057, found 317.1069.



6c

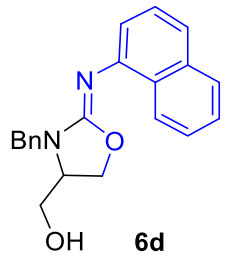
(*Z*)-(3-Benzyl-2-((3-methoxyphenyl)imino)oxazolidin-4-yl)methanol (6c) was prepared as colorless oil according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 2:1→1 : 1 , 85 mg, 91% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.27 (m, 5H), 7.21 (t, J = 8.0 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 6.78 (s, 1H), 6.61 (d, J = 8.1 Hz, 1H), 5.00 (d, J = 15.4 Hz, 1H), 4.34 – 4.20 (m, 3H), 3.80 (br s, 1H), 3.80 (s, 3H), 3.64 – 3.57 (m, 2H), 3.39 (d, J = 12.1 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 154.8, 148.2, 136.4, 129.1, 128.7, 128.0, 127.7, 116.2, 109.4, 108.0, 67.1, 59.6, 56.6, 55.1, 46.4.

IR (neat) 3422, 2357, 2076, 1661, 1480, 1259, 1037, 700 cm^{-1}.

HRMS (EI+) calcd for $C_{18}H_{21}N_2O_3$ $[M+H]^+$: 313.1552, found 313.1558.



6d

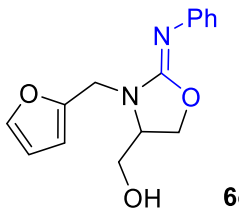
(*Z*)-(3-Benzyl-2-(naphthalen-1-ylimino)oxazolidin-4-yl)methanol (6d) was prepared as yellow solid according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 2:1→1:1, 91 mg, 91% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 7.6 Hz, 1H), 7.83 (d, J = 7.7 Hz, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.49 – 7.35 (m, 8H), 7.29 (d, J = 4.9 Hz, 1H), 5.06 (d, J = 15.4 Hz, 1H), 4.61 (d, J = 15.3 Hz, 1H), 4.30 – 4.28 (m, 2H), 3.71 – 3.68 (m, 2H), 3.49 (d, J = 10.9 Hz, 1H), 2.58 (br s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 143.4, 137.1, 134.4, 129.5, 128.9, 128.0, 127.8, 127.7, 125.8, 125.6, 124.9, 124.1, 122.4, 118.0, 67.0, 60.4, 57.3, 47.4.

IR (neat) 3430, 2357, 1652, 1261, 1018, 704 cm^{-1}.

HRMS (EI+) calcd for $C_{21}H_{21}N_2O_2$ $[M+H]^+$: 333.1603, found 333.1607.



6e

(*Z*)-(3-(Furan-2-ylmethyl)-2-(phenylimino)oxazolidin-4-yl)methanol (6e) was prepared as colorless oil according to the General Procedure E

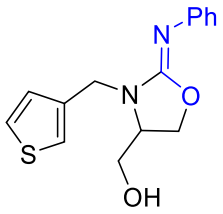
(purification by flash column chromatography: hexanes/EtOAc = 2:1→1:1, 59 mg, 73% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H), 7.30 (t, J = 7.7 Hz, 2H), 7.16 (d, J = 7.8 Hz, 2H), 7.03 (t, J = 7.3 Hz, 1H), 6.36 (s, 2H), 4.90 (d, J = 15.9 Hz, 1H), 4.45 – 4.24 (m, 3H), 3.84 (br s, 1H), 3.77 – 3.62 (m, 2H), 3.50 (d, J = 10.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 150.1, 146.7, 142.4, 128.6, 123.5, 122.5, 110.5, 109.0, 67.0, 59.6, 57.6, 39.9.

IR (neat) 3414, 2357, 2072, 1662, 1486, 1246, 1025, 749 cm^{-1}.

HRMS (EI+) calcd for $C_{15}H_{17}N_2O_3$ $[M+H]^+$: 273.1239, found 273.1240.



6f

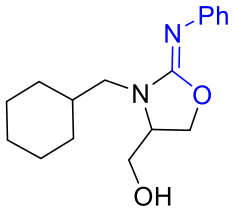
(*Z*)-(2-(Phenylimino)-3-(thiophen-3-ylmethyl)oxazolidin-4-yl)methanol (6f) was prepared as brown oil according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 2:1→1:1, 62 mg, 74% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 3H), 7.19 (s, 2H), 7.17 (s, 1H), 7.13 (d, J = 4.8 Hz, 1H), 7.03 (t, J = 7.2 Hz, 1H), 4.96 (d, J = 15.3 Hz, 1H), 4.40 – 4.14 (m, 3H), 3.75 (br s, 1H), 3.67 (dd, J = 12.3, 3.0 Hz, 1H), 3.61 (t, J = 7.6 Hz, 1H), 3.44 (dd, J = 12.3, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 146.5, 137.1, 128.6, 127.7, 126.6, 123.6, 123.5, 122.6, 67.1, 59.7, 56.9, 41.8.

IR (neat) 3420, 2356, 2075, 1655, 1245, 1032, 695 cm^{-1}.

HRMS (EI+) calcd for $C_{15}H_{17}N_2O_2S$ $[M+H]^+$: 289.1011, found 289.1010.



6g

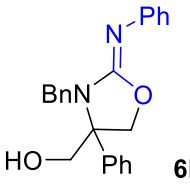
(*Z*)-(3-(Cyclohexylmethyl)-2-(phenylimino)oxazolidin-4-yl)methanol (6g) was prepared as colorless oil according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 3:1, 65.6 mg, 76% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 2H), 7.13 (d, J = 7.8 Hz, 2H), 7.00 (t, J = 7.3 Hz, 1H), 4.41 – 4.32 (m, 2H), 3.73 (d, J = 2.4 Hz, 1H), 3.68 – 3.52 (m, 2H), 3.45 (d, J = 12.2 Hz, 1H), 2.86 (dd, J = 14.3, 5.7 Hz, 1H), 1.77 – 1.68 (m, 6H), 1.28 – 1.21 (m, 3H), 1.03 (d, J = 10.1 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 146.9, 128.5, 123.7, 122.2, 67.1, 59.8, 57.8, 48.1, 35.6, 30.9, 30.4, 26.4, 25.8, 25.7.

IR (neat) 3424, 2925, 2075, 1655, 1253, 1034, 695 cm^{-1}.

HRMS (EI+) calcd for $C_{17}H_{25}N_2O_2$ $[M+H]^+$: 289.1916, found 289.1915.



6h

(*Z*)-(3-Benzyl-4-phenyl-2-(phenylimino)oxazolidin-4-yl)methanol (6h) was prepared as colorless oil according to the General Procedure E (purification by flash column chromatography: hexanes/EtOAc = 3:1, 76.3 mg, 71% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 4H), 7.43 – 7.25 (m, 10H), 7.06 (t, J = 7.2 Hz, 1H), 5.21 (d, J = 15.6 Hz, 1H), 4.65 (d, J = 8.2 Hz, 1H), 4.26 (d, J = 8.2 Hz, 1H), 3.92 (AB, J_{AB} = 12.4 Hz, 1H), 3.85 (BA, J_{BA} = 12.0 Hz, 1H), 3.79 (d, J = 15.6 Hz, 1H).

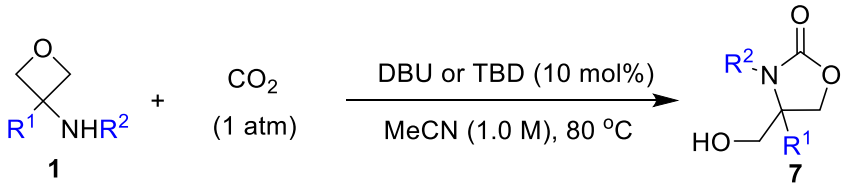
^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 147.3, 139.9, 139.1, 129.3, 129.1, 128.6, 128.5, 127.9, 127.9, 125.8, 123.6, 122.2, 74.5, 68.2, 62.2, 45.5.

IR (neat) 3393, 2358, 1664, 1486, 1242, 1056, 698 cm^{-1}.

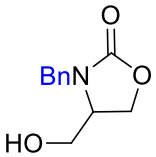
HRMS (EI+) calcd for $C_{23}H_{23}N_2O_2$ $[M+H]^+$: 359.1760, found 359.1763.

VI. [3+2] Annulation with CO_2

General Procedure F



A 10-mL Schlenk flask was purged by evacuating and refilling with CO_2 balloon for three times. A solution of 3-aminooxetane **1** (0.5 mmol) and DBU (7.5 μL, 0.05 mmol, 10 mol%) or TBD (14 mg, 0.05 mmol, 10 mol%) in MeCN (0.5 mL) was added to the flask. Then the reaction was stirred at 80 °C for 12 h, and the mixture was directly purified by silica gel column chromatography to afford the desired product **7**.



7a

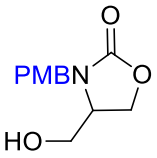
3-Benzyl-4-(hydroxymethyl)oxazolidin-2-one (7a) was prepared as white solid from **1b** (98 mg) according to the General Procedure F (purification by flash column chromatography: 5% MeOH in DCM) in 85% yield (106 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.21 (m, 5H), 4.72 (d, J = 15.3 Hz, 1H), 4.39 – 4.20 (m, 3H), 3.83 – 3.60 (m, 2H), 3.51 (d, J = 11.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 135.9, 128.9, 128.0 (2C), 64.5, 60.2, 55.7, 46.2.

IR (thin film) 3398, 3059, 2928, 1722, 1430, 1253, 1091 cm^{-1}.

HRMS (CI+) Calcd for $C_{11}H_{14}NO_3$ $[M+H]^+$: 208.0974, Found: 208.0978.



7b

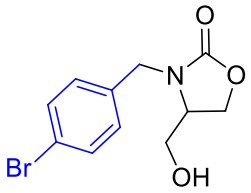
4-(Hydroxymethyl)-3-(4-methoxybenzyl)oxazolidin-2-one (7b) was prepared as colorless oil from **1d** (116 mg) according to the General Procedure F (purification by flash column chromatography: 3% MeOH in DCM) in 86% yield (122 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, J = 8.5 Hz, 2H), 6.86 (d, J = 8.5 Hz, 2H), 4.63 (d, J = 15.1 Hz, 1H), 4.33 – 4.22 (m, 2H), 4.19 (d, J = 15.1 Hz, 1H), 3.78 (s, 3H), 3.74 (dd, J = 11.9, 3.6 Hz, 1H), 3.71 – 3.63 (m, 1H), 3.51 (dd, J = 11.9, 2.7 Hz, 1H), 2.69 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 159.1, 129.4, 127.9, 114.2, 64.5, 60.3, 55.7, 55.2, 45.7.

IR (thin film) 3415, 3056, 2930, 1723, 1437, 1243, 1032, 729 cm^{-1}.

HRMS (CI+) Calcd For $C_{12}H_{16}NO_4$ $[M+H]^+$: 238.1077, Found: 238.1079.



7c

3-(4-Bromobenzyl)-4-(hydroxymethyl)oxazolidin-2-one (7c) was prepared as colorless oil from **1j** (128 mg) according to the General Procedure F (purification by flash column chromatography: 2% MeOH in DCM) in 99% yield (146 mg).

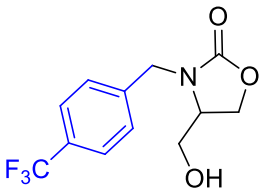
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.3 Hz, 2H), 7.18 (d, J = 8.3 Hz, 2H), 4.65 (d, J = 15.4 Hz, 1H), 4.31 (t, J = 8.8 Hz, 1H), 4.27 – 4.14 (m, 2H), 3.83 – 3.64 (m, 2H), 3.63 – 3.45 (m, 1H), 2.90 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 135.0, 132.0, 129.8, 122.0, 64.5, 60.6, 55.8,

45.7.

IR (thin film) 3406, 3056, 2924, 1723, 1436, 1254, 1078, 728 cm^{-1}.

HRMS (CI+) Calcd for $C_{11}H_{13}BrNO_3$ $[M+H]^+$: 286.0079, Found: 286.0084.



7d

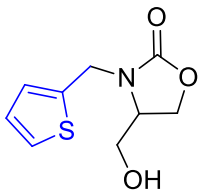
4-(Hydroxymethyl)-3-(4-(trifluoromethyl)benzyl)oxazolidin-2-one (7d) was prepared as colorless oil from **1k** (116 mg) according to the General Procedure F (purification by flash column chromatography: 3% MeOH in DCM) in 92% yield (127 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.1 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 4.77 (d, J = 15.6 Hz, 1H), 4.40 – 4.18 (m, 3H), 3.82 – 3.65 (m, 2H), 3.56 (dd, J = 11.7, 3.2 Hz, 1H), 2.84 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 140.1, 130.3 (q, J = 32.0 Hz), 128.3, 125.8 (q, J = 4.0 Hz), 123.9 (q, J = 271.0 Hz), 64.6, 60.6, 55.8, 45.8.

IR (thin film) 3417, 3058, 2927, 1727, 1323, 1118, 730 cm^{-1}.

HRMS (CI+) Calcd for $C_{12}H_{13}F_3NO_3$ $[M+H]^+$: 276.0848, Found: 276.0851.



7e

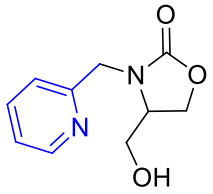
4-(Hydroxymethyl)-3-(thiophen-2-ylmethyl)oxazolidin-2-one (7e) was prepared as colorless oil from **1l** (101 mg) according to the General Procedure F (purification by flash column chromatography: 3% MeOH in DCM) in 88% yield (112 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, J = 5.9 Hz, 1H), 7.04 (d, J = 3.2 Hz, 1H), 6.98 (dd, J = 5.0, 3.6 Hz, 1H), 4.88 (d, J = 15.7 Hz, 1H), 4.49 (d, J = 15.7 Hz, 1H), 4.38 – 4.13 (m, 2H), 3.89 – 3.75 (m, 2H), 3.61 (dd, J = 13.0, 4.2 Hz, 1H), 2.77 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 138.1, 127.2, 127.1, 125.9, 64.6, 60.5, 55.6, 40.9.

IR (thin film) 3431, 3058, 2926, 1729, 1433, 1260, 733 cm^{-1}.

HRMS (CI+) Calcd for $C_9H_{12}NO_3S$ $[M]^+$: 214.0538, Found: 214.0537.



7f

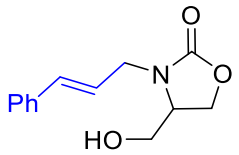
4-(Hydroxymethyl)-3-(pyridin-2-ylmethyl)oxazolidin-2-one (7f) was prepared as colorless oil from **1m** (99 mg) according to the General Procedure F (purification by flash column chromatography: 3% MeOH in DCM) in 91% yield (114 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 4.8 Hz, 1H), 7.71 (t, J = 7.7 Hz, 1H), 7.37 (d, J = 7.8 Hz, 1H), 7.30 – 7.19 (m, 1H), 6.91 (s, 1H), 4.73 (d, J = 16.0 Hz, 1H), 4.39 (t, J = 8.9 Hz, 1H), 4.30 (t, J = 7.9 Hz, 1H), 4.23 (d, J = 16.0 Hz, 1H), 4.01 – 3.89 (m, 1H), 3.82 (d, J = 13.1 Hz, 1H), 3.54 (dd, J = 13.1, 3.1 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 156.2, 148.7, 137.7, 123.3, 123.0, 64.2, 60.5, 59.7, 47.9.

IR (thin film) 3415, 3059, 2921, 1734, 1434, 1264, 1087, 910, 727 cm^{-1}.

HRMS (CI+) Calcd for $C_{10}H_{13}N_2O_3$ $[M+H]^+$: 209.0926, Found: 209.0927.



7g

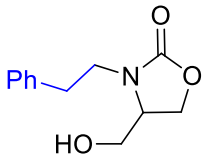
3-Cinnamyl-4-(hydroxymethyl)oxazolidin-2-one (7g) was prepared as colorless oil from **1n** (95 mg) according to the General Procedure F (purification by flash column chromatography: 5% MeOH in DCM) in 90% yield (105 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 7.2 Hz, 2H), 7.31 (t, J = 7.4 Hz, 2H), 7.28 – 7.20 (m, 1H), 6.58 (d, J = 15.9 Hz, 1H), 6.29 – 5.97 (m, 1H), 4.35 (t, J = 8.8 Hz, 1H), 4.31 – 4.21 (m, 2H), 3.98 – 3.76 (m, 3H), 3.62 (d, J = 11.6 Hz, 1H), 3.18 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 136.0, 134.0, 128.6, 128.0, 126.5, 123.2, 64.6, 60.6, 56.0, 44.5.

IR (thin film) 3396, 3056, 2924, 1724, 1437, 1256, 1090 cm^{-1}.

HRMS (CI+) Calcd for $C_{13}H_{16}NO_3$ $[M+H]^+$: 234.1130, Found: 234.1127.



7h

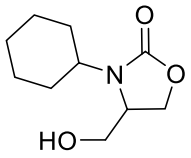
4-(Hydroxymethyl)-3-phenethyloxazolidin-2-one (7h) was prepared as colorless oil from **1o** (106 mg) according to the General Procedure F (TBD as base, purification by flash column chromatography: 3% MeOH in DCM) in 95% yield (126 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.26 (m, 2H), 7.22 (t, J = 6.4 Hz, 3H), 4.30 – 4.18 (m, 1H), 4.18 – 4.09 (m, 1H), 3.73 – 3.56 (m, 3H), 3.49 (dd, J = 11.3, 2.8 Hz, 1H), 3.42 – 3.29 (m, 1H), 3.11 (s, 1H), 2.96 – 2.80 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 138.4, 128.7, 128.6, 126.6, 64.5, 60.8, 56.7, 43.7, 33.8.

IR (thin film) 3408, 3030, 2930, 1721, 1431, 1259, 1035 cm^{-1}.

HRMS (CI+) Calcd for: $C_{12}H_{16}NO_3$ $[M+H]^+$: 222.1130, Found: 222.1140.



7i

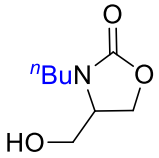
3-Cyclohexyl-4-(hydroxymethyl)oxazolidin-2-one (7i) was prepared as white solid from **1p** (93 mg) according to the General Procedure F (TBD as base, DMF as solvent at 100 °C (purification by flash column chromatography: 3% MeOH in DCM) in 89% yield (106 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.36 – 4.19 (m, 2H), 3.94 – 3.82 (m, 1H), 3.78 – 3.55 (m, 2H), 3.48 (tt, J = 12.1, 3.7 Hz, 1H), 3.18 (s, 1H), 1.89 (d, J = 11.9 Hz, 1H), 1.84 – 1.70 (m, 3H), 1.70 – 1.53 (m, 2H), 1.51 – 1.36 (m, 1H), 1.37 – 1.20 (m, 2H), 1.20 – 0.97 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 65.4, 62.7, 55.5, 54.0, 31.8, 30.0, 25.70, 25.69, 25.2.

IR (thin film) 3401, 2933, 2859, 1715, 1424, 1237, 1047 cm^{-1}.

HRMS (CI+) Calcd for $C_{10}H_{18}NO_3$ $[M+H]^+$: 200.1287, Found: 200.1291.



7j

3-Butyl-4-(hydroxymethyl)oxazolidin-2-one (7j) was prepared as colorless oil from **1s** (90 mg) according to the General Procedure F (TBD as base, purification by flash column chromatography: 3% MeOH in DCM) in 50% yield (61 mg).

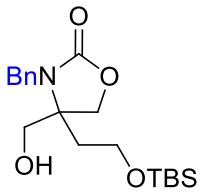
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.34 (t, J = 8.8 Hz, 1H), 4.25 (dd, J = 8.7, 5.6 Hz, 1H), 3.89 – 3.83 (m, 1H), 3.79 (dd, J = 11.8, 4.1 Hz, 1H), 3.64 (dd, J = 11.8, 3.2 Hz,

1H), 3.52 – 3.40 (m, 1H), 3.13 – 3.03 (m, 1H), 1.62 – 1.45 (m, 2H), 1.37 – 1.27 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 64.5, 60.8, 56.0, 41.8, 29.4, 19.9, 13.7.

IR (thin film) 3403, 2929, 2871, 1716, 1430, 1250, 1040 cm^{-1}.

HRMS (CI+) Calcd for $C_8H_{16}NO_3$ [M+H$^+$]: 174.1130, Found: 174.1133.



7k

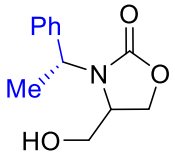
3-Benzyl-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-4-(hydroxymethyl)oxazolidin-2-one (7k) was prepared as white solid from **1q** (128 mg) according to the General Procedure (purification by flash column chromatography: 50% EtOAc in hexanes) in 78% yield (114 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 7.2 Hz, 2H), 7.36 – 7.23 (m, 3H), 4.58 (d, J = 15.7 Hz, 1H), 4.32 (d, J = 15.7 Hz, 1H), 4.22 (q, J = 8.8 Hz, 2H), 3.62 (t, J = 5.6 Hz, 2H), 3.55 – 3.42 (m, 2H), 2.53 (t, J = 6.5 Hz, 1H), 1.91 – 1.70 (m, 2H), 0.86 (s, 9H), 0.03 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 138.3, 128.9, 127.83, 127.79, 69.3, 65.0, 64.2, 58.3, 44.6, 36.0, 25.8, 18.1, -5.67.

IR (thin film) 3424, 3060, 2934, 1723, 1416, 1066, 729 cm^{-1}.

HRMS (CI+) Calcd for $C_{19}H_{32}NO_4Si$ [M+H]$^+$: 366.2101, Found: 366.2084.



7l

4-(Hydroxymethyl)-3-((*R*)-1-phenylethyl)oxazolidin-2-one (7l) was prepared as yellow oil from **1t** (89 mg) according to the General Procedure F with TBD

as catalyst and DMF as solvent at 100 °C. The product was obtained by flash column chromatography (5% MeOH in DCM) as an inseparable mixture of diastereomers in 83% yield (92 mg, 1.3:1 dr).

Major diastereomer:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 5H), 5.12 (q, J = 7.2 Hz, 1H), 4.24 – 4.13 (m, 2H), 3.61 – 3.45 (m, 2H), 3.18 – 3.17 (m, 1H), 2.84 (s, 1H), 1.67 (d, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 139.1, 128.8, 128.0, 127.2, 65.2, 62.4, 55.4, 52.7, 18.4.

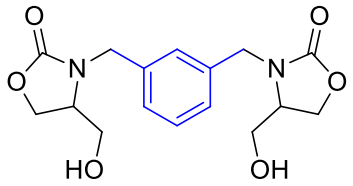
Minor diastereomer:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 4.42 (m, 2H), 7.37 – 7.28 (m, 3H), 5.18 (q, J = 7.2 Hz, 1H), 4.29 (t, J = 8.8 Hz, 1H), 4.24 – 4.13 (m, 1H), 3.97 – 3.87 (m, 1H), 3.61 – 3.56 (m, 1H), 3.18 – 3.17 (m, 1H), 1.75 (s, 1H), 1.64 (d, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 141.2, 128.8, 128.1, 126.7, 64.8, 61.2, 54.8, 51.1, 15.7.

IR (thin film) 3052, 2954, 2871, 1665, 1511, 1252 cm^{-1}.

HRMS (CI+) Calcd for $C_{12}H_{16}NO_3$ $[M+H]^+$: 222.1130, Found: 222.1129.



7m

3,3'-(1,3-Phenylenebis(methylene))bis(4-(hydroxymethyl)oxazolidin-2-one) (7m) was prepared as white solid from **1r** (74 mg) according to the General Procedure F (purification by flash column chromatography: 5% MeOH in DCM) as an inseparable mixture of diastereomers in 71% yield (71 mg, 1.2:1 dr).

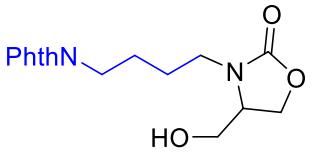
Major diastereomer:

^{1}H NMR (400 MHz, acetone-d_6) δ 7.44 – 7.36 (m, 2H), 7.32 (d, J = 7.8 Hz, 2H), 4.72 (dd, J = 15.5, 2.4 Hz, 2H), 4.43 – 4.32 (m, 3H), 4.30 (d, J = 3.5 Hz, 1H), 4.26 (s, 1H), 4.22 (dd, J = 8.6, 5.6 Hz, 2H), 3.89 – 3.71 (m, 4H), 3.61 (d, J = 9.9 Hz, 2H), 3.04 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 159.4, 138.5, 129.9, 128.4, 128.0, 65.3, 61.1, 56.7, 46.5.

IR (thin film) 3409, 3057, 2924, 1716, 1425, 1251, 1086, 727 cm^{-1}.

HRMS (CI+) Calcd for $C_{16}H_{21}N_2O_6$ [M+H]$^+$: 337.1400, Found: 337.1394.



7n

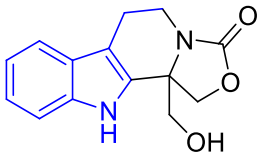
2-(4-(4-(Hydroxymethyl)-2-oxooxazolidin-3-yl)butyl)isoindoline-1,3-dione (7n) was prepared as white solid from **1u** (110 mg) according to the General Procedure F (with TBD as base). The product was obtained in 72% yield (92 mg) by direct filtration of the reaction mixture followed by washing with DCM.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 – 7.70 (m, 4H), 5.11 – 4.89 (m, 1H), 4.26 (t, J = 7.7 Hz, 1H), 4.17 – 3.98 (m, 1H), 3.85 – 3.70 (m, 1H), 3.64 – 3.53 (m, 3H), 3.34 – 3.21 (m, 1H), 3.15 – 3.01 (m, 1H), 1.72 – 1.30 (m, 4H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 168.5, 158.3, 134.8, 132.1, 123.5, 64.6, 60.0, 56.0, 41.3, 37.5, 25.7, 24.7.

IR (thin film) 3360, 2938, 2869, 1708, 1393 1261,1032 cm^{-1}.

HRMS (CI+) Calcd for $C_{16}H_{19}N_2O_5$ [M+H]$^+$: 319.1294, Found: 319.1292.



7o

11b-(Hydroxymethyl)-1,5,6,11b-tetrahydrooxazolo[3',4':1,2]pyrido[3,4-b]indol-3(11H)-one (7o) was prepared as pale yellow solid from **1v** (107 mg) according to the General Procedure F (TBD as base, DMF as solvent at 100 °C. Purification by flash column chromatography: 5% MeOH in DCM) in 85% yield (110 mg).

^{1}H NMR (400 MHz, CD_3OD) δ 7.37 (d, J = 7.9 Hz, 1H), 7.26 (d, J = 8.1 Hz, 1H), 7.06 (t, J = 7.6 Hz, 1H), 6.96 (t, J = 7.5 Hz, 1H), 4.68 (d, J = 8.4 Hz, 1H), 4.30 (d, J = 8.4 Hz, 1H), 4.04 (dd, J = 13.8, 6.2 Hz, 1H), 3.82 (d, J = 12.2 Hz, 1H), 3.73 (d, J = 12.2 Hz, 1H), 3.39 – 3.23 (m, 3H), 2.90 – 2.77 (m, 1H), 2.67 (dd, J = 15.6, 4.8 Hz, 1H).

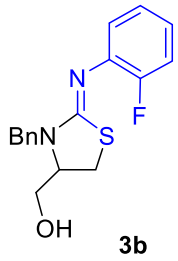
^{13}C NMR (100 MHz, CD_3OD) δ 160.8, 138.3, 132.8, 127.9, 123.3, 120.4, 119.3, 112.4, 109.5, 71.2, 64.6, 63.8, 38.6, 21.3.

IR (thin film) 3297, 3056, 2974, 2932, 1719, 1415, 1258, 1032 cm^{-1}.

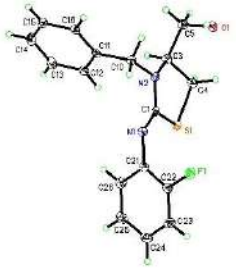
HRMS (CI+) Calcd for $C_{14}H_{15}N_2O_3$ $[M+H]^+$: 259.1083, Found: 259.1079.

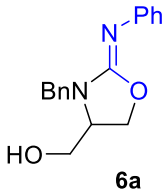
VII. Product Structure Determination

The structures of the products **3b** and **6a** were determined by X-ray crystallography. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 1987318 for **3b**; 1987319 for **6a**). The structures of other products were assumed by analogy.



3b





6a

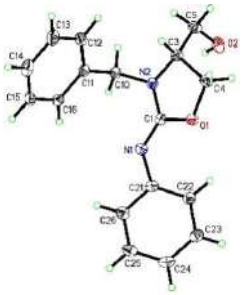


Table S1. Crystal data and structure refinement for 3b.

Identification code	**3b**
Empirical formula	$C_{17}H_{17}FN_2OS$
Formula weight	316.38
Temperature/K	100.15
Crystal system	triclinic
Space group	P-1
a/Å	9.7070(3)
b/Å	12.3991(6)
c/Å	13.7578(6)
α/°	110.620(4)
β/°	90.804(3)
γ/°	101.885(3)
Volume/Å^3	1509.77(12)
Z	4

ρ_{calc}g/cm^3	1.392
μ/mm^{-1}	2.029
F(000)	664.0
Crystal size/mm^3	0.25 ×0.22 ×0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.342 to 134.994
Index ranges	-11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -12 ≤ l ≤ 16
Reflections collected	8240
Independent reflections	5347 [R_{int} = 0.0147, R_{sigma} = 0.0198]
Data/restraints/parameters	5347/0/399
Goodness-of-fit on F^2	1.023
Final R indexes [I>=2σ (I)]	R_1 = 0.0276, wR_2 = 0.0695
Final R indexes [all data]	R_1 = 0.0287, wR_2 = 0.0705
Largest diff. peak/hole / e Å^{-3}	0.34/-0.21

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2 ×10^3) for 3b. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	7919.3(3)	7142.1(3)	4245.8(2)	17.77(8)
F1	4109.8(8)	5736.0(6)	2496.0(6)	24.28(17)
O1	7674.0(9)	4146.9(7)	5286.6(7)	19.63(18)
N1	5134.7(10)	6972.9(9)	4560.7(8)	16.6(2)
N2	6526.5(10)	6282.9(9)	5510.3(8)	15.2(2)
C1	6331.9(12)	6786.8(10)	4801.0(9)	14.7(2)
C3	8006.0(12)	6302.2(10)	5781.2(9)	16.7(2)
C4	8757.5(13)	6293.0(11)	4814.7(10)	19.2(2)
C5	8166.7(13)	5266.2(11)	6091.2(10)	18.6(2)
C10	5478.7(12)	6214.1(10)	6249.2(9)	15.5(2)
C11	5700.0(12)	7298.6(10)	7242.2(9)	15.2(2)
C12	6529.0(13)	8388.1(11)	7323.0(10)	18.5(2)
C13	6708.9(13)	9349.3(11)	8257.8(10)	21.7(3)
C14	6032.6(14)	9239.7(11)	9110.6(10)	22.8(3)
C15	5171.0(13)	8162.3(12)	9025.5(10)	20.9(3)
C16	5020.3(12)	7194.6(11)	8101.4(10)	17.5(2)
C21	5124.3(12)	7550.7(11)	3838.2(9)	16.7(2)
C22	4586.8(13)	6929.8(11)	2805.8(10)	18.2(2)
C23	4506.1(13)	7450.9(12)	2077.7(10)	22.8(3)
C24	4981.0(15)	8668.7(13)	2397.2(11)	26.8(3)
C25	5496.7(15)	9327.7(12)	3430.1(11)	26.5(3)

C26	5568.8(13)	8773.7(11)	4142.8(10)	22.0(3)
S1A	1895.9(3)	2853.1(3)	697.6(2)	18.76(8)
F1A	-1378.5(9)	4107.5(7)	2446.4(6)	25.95(17)
O1A	3046.9(9)	5835.1(7)	-364.6(7)	20.01(18)
N1A	-833.9(11)	2984.0(9)	420.9(8)	17.6(2)
N2A	825.8(10)	3679.7(9)	-563.4(8)	16.1(2)
C1A	437.8(13)	3180.3(10)	157.5(9)	15.5(2)
C3A	2281.0(13)	3678.9(11)	-850.7(9)	17.4(2)
C4A	3113.7(13)	3702.7(11)	105.4(10)	19.8(3)
C5A	2929.1(13)	4717.3(11)	-1170.5(9)	19.0(2)
C10A	-247.2(13)	3714.5(10)	-1301.8(9)	16.8(2)
C11A	-578.0(12)	2638.2(10)	-2308.2(9)	15.9(2)
C12A	-339.1(13)	1545.7(11)	-2376.7(10)	20.0(3)
C13A	-671.5(14)	583.7(11)	-3310.4(11)	23.7(3)
C14A	-1267.7(14)	690.4(12)	-4184.5(10)	24.3(3)
C15A	-1535.5(13)	1772.3(12)	-4116.8(10)	22.8(3)
C16A	-1179.0(12)	2739.5(11)	-3187.9(10)	18.6(2)
C21A	-1077.7(12)	2375.1(11)	1122.2(9)	17.7(2)
C22A	-1391.4(13)	2937.9(11)	2133.9(10)	19.0(2)
C23A	-1705.9(13)	2379.7(12)	2836.2(10)	23.4(3)
C24A	-1709.6(14)	1184.5(13)	2515.6(11)	27.3(3)
C25A	-1414.4(15)	583.2(12)	1509.8(12)	28.1(3)
C26A	-1098.8(14)	1172.8(12)	821.8(10)	22.9(3)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3b. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	14.74(14)	21.13(15)	20.96(15)	11.28(12)	5.19(11)	4.92(11)
F1	30.4(4)	19.0(4)	19.7(4)	5.3(3)	2.5(3)	0.5(3)
O1	15.3(4)	18.8(4)	24.9(4)	8.3(4)	3.2(3)	3.2(3)
N1	14.9(5)	17.8(5)	17.9(5)	7.8(4)	1.5(4)	3.2(4)
N2	13.2(5)	17.2(5)	15.6(5)	6.2(4)	1.7(4)	3.6(4)
C1	15.2(6)	12.2(5)	14.3(5)	2.8(4)	2.4(4)	1.4(4)
C3	12.2(5)	18.8(6)	18.5(6)	6.7(5)	0.1(4)	2.8(4)
C4	15.1(6)	22.6(6)	22.9(6)	11.0(5)	3.7(5)	5.9(5)
C5	15.4(6)	21.5(6)	20.2(6)	9.1(5)	-0.1(4)	4.1(5)
C10	13.4(5)	16.4(6)	17.0(6)	7.3(5)	2.0(4)	1.8(4)
C11	13.1(5)	17.6(6)	17.5(6)	7.7(5)	1.2(4)	6.6(4)
C12	17.6(6)	19.0(6)	20.7(6)	8.8(5)	3.7(5)	5.1(5)

C13	19.2(6)	16.6(6)	27.7(7)	5.8(5)	2.7(5)	4.2(5)
C14	20.6(6)	21.9(6)	22.0(6)	1.1(5)	2.5(5)	9.0(5)
C15	18.5(6)	28.1(7)	19.5(6)	9.4(5)	6.0(5)	10.7(5)
C16	14.6(6)	19.8(6)	21.2(6)	10.2(5)	2.8(5)	5.1(5)
C21	12.0(5)	21.1(6)	20.2(6)	10.0(5)	4.2(4)	5.5(5)
C22	14.4(6)	19.1(6)	21.9(6)	8.1(5)	4.7(5)	4.2(5)
C23	19.2(6)	33.0(7)	20.6(6)	13.3(5)	4.4(5)	9.0(5)
C24	27.1(7)	33.5(7)	31.9(7)	22.2(6)	11.1(6)	14.0(6)
C25	28.8(7)	20.6(6)	35.0(8)	14.5(6)	9.8(6)	7.6(5)
C26	19.8(6)	20.9(6)	24.4(6)	7.7(5)	3.6(5)	3.8(5)
S1A	15.59(15)	23.56(16)	21.51(15)	12.58(12)	1.25(11)	6.05(11)
F1A	34.1(4)	23.4(4)	21.2(4)	6.5(3)	1.9(3)	11.1(3)
O1A	17.8(4)	19.5(4)	23.4(4)	7.5(4)	0.8(3)	6.4(3)
N1A	17.0(5)	19.9(5)	18.4(5)	8.9(4)	2.8(4)	6.1(4)
N2A	14.6(5)	19.1(5)	16.4(5)	7.7(4)	2.2(4)	5.5(4)
C1A	17.6(6)	13.8(5)	14.6(5)	3.8(4)	-0.1(4)	5.1(4)
C3A	15.6(6)	19.0(6)	18.6(6)	6.7(5)	3.1(5)	6.1(5)
C4A	15.9(6)	23.7(6)	23.2(6)	12.0(5)	2.7(5)	5.3(5)
C5A	18.2(6)	21.3(6)	19.3(6)	8.3(5)	4.8(5)	6.3(5)
C10A	17.2(6)	18.5(6)	17.4(6)	8.2(5)	2.0(4)	7.1(5)
C11A	11.2(5)	18.8(6)	18.4(6)	8.2(5)	3.6(4)	2.3(4)
C12A	18.7(6)	20.6(6)	22.8(6)	10.3(5)	1.7(5)	4.4(5)
C13A	20.3(6)	17.4(6)	31.9(7)	7.8(5)	4.2(5)	3.3(5)
C14A	17.3(6)	24.0(6)	22.8(6)	0.7(5)	1.6(5)	-0.4(5)
C15A	16.8(6)	30.8(7)	19.4(6)	9.0(5)	0.5(5)	2.5(5)
C16A	14.5(6)	22.2(6)	21.6(6)	10.7(5)	3.4(5)	4.5(5)
C21A	12.0(5)	22.6(6)	20.6(6)	10.6(5)	0.6(4)	3.4(5)
C22A	15.1(6)	20.6(6)	21.4(6)	7.8(5)	-0.6(5)	4.5(5)
C23A	17.8(6)	34.6(7)	21.6(6)	14.3(5)	3.0(5)	6.6(5)
C24A	22.1(7)	34.3(7)	33.3(7)	23.0(6)	3.3(5)	3.9(6)
C25A	28.0(7)	22.4(7)	37.4(8)	15.8(6)	1.3(6)	4.3(5)
C26A	22.4(6)	22.0(6)	24.8(6)	8.5(5)	3.3(5)	5.8(5)

Table S4. Bond Lengths for 3b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C1	1.7727(12)	S1A	C1A	1.7718(12)
S1	C4	1.8163(12)	S1A	C4A	1.8137(12)
F1	C22	1.3619(14)	F1A	C22A	1.3569(15)
O1	C5	1.4177(15)	O1A	C5A	1.4184(15)

N1	C1	1.2910(16)	N1A	C1A	1.2904(16)
N1	C21	1.4162(15)	N1A	C21A	1.4153(16)
N2	C1	1.3604(15)	N2A	C1A	1.3624(16)
N2	C3	1.4719(15)	N2A	C3A	1.4722(15)
N2	C10	1.4594(15)	N2A	C10A	1.4624(15)
C3	C4	1.5232(16)	C3A	C4A	1.5223(17)
C3	C5	1.5240(16)	C3A	C5A	1.5233(17)
C10	C11	1.5164(16)	C10A	C11A	1.5201(16)
C11	C12	1.3888(17)	C11A	C12A	1.3921(17)
C11	C16	1.3941(17)	C11A	C16A	1.3921(17)
C12	C13	1.3905(18)	C12A	C13A	1.3884(19)
C13	C14	1.3869(19)	C13A	C14A	1.387(2)
C14	C15	1.3873(19)	C14A	C15A	1.390(2)
C15	C16	1.3876(18)	C15A	C16A	1.3887(18)
C21	C22	1.3878(18)	C21A	C22A	1.3900(18)
C21	C26	1.3925(18)	C21A	C26A	1.3953(18)
C22	C23	1.3789(18)	C22A	C23A	1.3777(18)
C23	C24	1.388(2)	C23A	C24A	1.389(2)
C24	C25	1.390(2)	C24A	C25A	1.388(2)
C25	C26	1.3895(19)	C25A	C26A	1.3883(19)

Table S5. Bond Angles for 3b.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	S1	C4	90.70(6)	C1A	S1A	C4A	90.78(6)
C1	N1	C21	116.85(10)	C1A	N1A	C21A	116.63(10)
C1	N2	C3	115.34(10)	C1A	N2A	C3A	115.10(10)
C1	N2	C10	119.91(10)	C1A	N2A	C10A	120.09(10)
C10	N2	C3	119.75(9)	C10A	N2A	C3A	119.58(10)
N1	C1	S1	124.50(9)	N1A	C1A	S1A	124.36(9)
N1	C1	N2	123.92(11)	N1A	C1A	N2A	123.95(11)
N2	C1	S1	111.58(8)	N2A	C1A	S1A	111.69(9)
N2	C3	C4	105.19(9)	N2A	C3A	C4A	105.44(9)
N2	C3	C5	113.29(10)	N2A	C3A	C5A	113.05(10)
C4	C3	C5	111.39(10)	C4A	C3A	C5A	111.47(10)
C3	C4	S1	105.90(8)	C3A	C4A	S1A	105.97(8)
O1	C5	C3	113.66(10)	O1A	C5A	C3A	113.50(10)
N2	C10	C11	114.48(10)	N2A	C10A	C11A	114.41(10)
C12	C11	C10	122.79(11)	C12A	C11A	C10A	122.50(11)
C12	C11	C16	118.99(11)	C12A	C11A	C16A	118.68(11)

C16	C11	C10	118.21(11)	C16A	C11A	C10A	118.79(11)
C11	C12	C13	120.30(12)	C13A	C12A	C11A	120.48(12)
C14	C13	C12	120.42(12)	C14A	C13A	C12A	120.57(12)
C13	C14	C15	119.53(12)	C13A	C14A	C15A	119.29(12)
C14	C15	C16	120.07(12)	C16A	C15A	C14A	120.08(12)
C15	C16	C11	120.65(11)	C15A	C16A	C11A	120.87(12)
C22	C21	N1	121.34(11)	C22A	C21A	N1A	121.11(11)
C22	C21	C26	116.85(11)	C22A	C21A	C26A	116.62(11)
C26	C21	N1	121.69(11)	C26A	C21A	N1A	122.17(11)
F1	C22	C21	117.95(11)	F1A	C22A	C21A	117.84(11)
F1	C22	C23	118.20(11)	F1A	C22A	C23A	118.30(11)
C23	C22	C21	123.85(12)	C23A	C22A	C21A	123.86(12)
C22	C23	C24	118.12(12)	C22A	C23A	C24A	118.13(12)
C23	C24	C25	119.90(12)	C25A	C24A	C23A	120.05(12)
C26	C25	C24	120.48(12)	C24A	C25A	C26A	120.37(13)
C25	C26	C21	120.77(12)	C25A	C26A	C21A	120.97(12)

Table S6. Hydrogen Bonds for 3b.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/ °
O1	H1	N1[1]	0.84	2.01	2.8403(13)	172.7
O1A	H1A	N1A[2]	0.84	2.02	2.8522(13)	169.5

[1]1-X,1-Y,1-Z; [2]-X,1-Y,-Z

Table S7. Torsion Angles for 3b.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
F1	C22	C23	C24	179.43(11)	F1A	C22A	C23A	C24A	-179.61(11)
N1	C21	C22	F1	-2.16(17)	N1A	C21A	C22A	F1A	-3.62(17)
N1	C21	C22	C23	177.74(11)	N1A	C21A	C22A	C23A	176.74(11)
N1	C21	C26	C25	-177.39(11)	N1A	C21A	C26A	C25A	-176.56(12)
N2	C3	C4	S1	34.46(11)	N2A	C3A	C4A	S1A	34.10(11)
N2	C3	C5	O1	61.62(13)	N2A	C3A	C5A	O1A	61.70(13)
N2	C10	C11	C12	18.72(16)	N2A	C10A	C11A	C12A	23.80(16)
N2	C10	C11	C16	-162.33(10)	N2A	C10A	C11A	C16A	-158.03(10)
C1	S1	C4	C3	-26.64(8)	C1A	S1A	C4A	C3A	-26.32(9)
C1	N1	C21	C22	103.47(13)	C1A	N1A	C21A	C22A	111.94(13)
C1	N1	C21	C26	-80.61(14)	C1A	N1A	C21A	C26A	-71.89(15)

C1	N2	C3	C4	-28.69(13)	C1A	N2A	C3A	C4A	-28.32(13)
C1	N2	C3	C5	-150.58(10)	C1A	N2A	C3A	C5A	-150.34(10)
C1	N2	C10	C11	-86.98(13)	C1A	N2A	C10A	C11A	-89.30(13)
C3	N2	C1	S1	8.74(12)	C3A	N2A	C1A	S1A	8.59(12)
C3	N2	C1	N1	-171.70(11)	C3A	N2A	C1A	N1A	-172.15(11)
C3	N2	C10	C11	66.85(13)	C3A	N2A	C10A	C11A	63.91(14)
C4	S1	C1	N1	-168.22(11)	C4A	S1A	C1A	N1A	-168.05(11)
C4	S1	C1	N2	11.33(9)	C4A	S1A	C1A	N2A	11.21(9)
C4	C3	C5	O1	-56.74(13)	C4A	C3A	C5A	O1A	-56.87(13)
C5	C3	C4	S1	157.57(8)	C5A	C3A	C4A	S1A	157.13(8)
C10	N2	C1	S1	163.68(8)	C10A	N2A	C1A	S1A	162.95(8)
C10	N2	C1	N1	-16.77(17)	C10A	N2A	C1A	N1A	-17.80(17)
C10	N2	C3	C4	176.33(10)	C10A	N2A	C3A	C4A	177.19(10)
C10	N2	C3	C5	54.44(14)	C10A	N2A	C3A	C5A	55.17(14)
C10	C11	C12	C13	-179.19(11)	C10A	C11A	C12A	C13A	179.33(11)
C10	C11	C16	C15	-179.18(11)	C10A	C11A	C16A	C15A	-178.22(11)
C11	C12	C13	C14	-1.75(19)	C11A	C12A	C13A	C14A	-1.07(19)
C12	C11	C16	C15	-0.19(18)	C12A	C11A	C16A	C15A	0.02(18)
C12	C13	C14	C15	-0.08(19)	C12A	C13A	C14A	C15A	-0.22(19)
C13	C14	C15	C16	1.76(19)	C13A	C14A	C15A	C16A	1.39(19)
C14	C15	C16	C11	-1.63(18)	C14A	C15A	C16A	C11A	-1.30(19)
C16	C11	C12	C13	1.87(18)	C16A	C11A	C12A	C13A	1.16(18)
C21	N1	C1	S1	-3.03(15)	C21A	N1A	C1A	S1A	-5.61(15)
C21	N1	C1	N2	177.47(10)	C21A	N1A	C1A	N2A	175.23(11)
C21	C22	C23	C24	-0.47(19)	C21A	C22A	C23A	C24A	0.02(19)
C22	C21	C26	C25	-1.30(18)	C22A	C21A	C26A	C25A	-0.22(19)
C22	C23	C24	C25	-1.05(19)	C22A	C23A	C24A	C25A	-0.6(2)
C23	C24	C25	C26	1.4(2)	C23A	C24A	C25A	C26A	0.7(2)
C24	C25	C26	C21	-0.1(2)	C24A	C25A	C26A	C21A	-0.3(2)
C26	C21	C22	F1	-178.27(10)	C26A	C21A	C22A	F1A	180.00(10)
C26	C21	C22	C23	1.63(18)	C26A	C21A	C22A	C23A	0.37(18)

Table S8. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3b.

Atom	*x*	*y*	*z*	U(eq)
H1	6826	3876	5348	29
H3	8422	7058	6372	20
H4A	8652	5473	4315	23
H4B	9778	6660	5007	23

H5A	9178	5360	6299	22
H5B	7639	5290	6706	22
H10A	5495	5516	6438	19
H10B	4529	6088	5900	19
H12	6975	8477	6737	22
H13	7299	10086	8313	26
H14	6158	9898	9749	27
H15	4684	8087	9600	25
H16	4448	6454	8054	21
H23	4136	6989	1377	27
H24	4954	9051	1911	32
H25	5802	10163	3651	32
H26	5926	9235	4846	26
H1A	2328	6095	-420	30
H3A	2279	2925	-1442	21
H4AA	3459	4526	599	24
H4AB	3936	3343	-99	24
H5AA	3882	4639	-1390	23
H5AB	2341	4682	-1779	23
H10C	78	4429	-1477	20
H10D	-1130	3790	-957	20
H12A	54	1458	-1780	24
H13A	-489	-154	-3351	28
H14A	-1491	31	-4823	29
H15A	-1963	1850	-4707	27
H16A	-1347	3480	-3152	22
H23A	-1914	2801	3521	28
H24A	-1914	778	2985	33
H25A	-1428	-237	1291	34
H26A	-894	751	136	28

Table S9. Crystal data and structure refinement for 6a.

Identification code	**6a**
Empirical formula	$C_{17}H_{18}N_2O_2$
Formula weight	282.33
Temperature/K	100.15
Crystal system	monoclinic

Space group	$P2_1/n$
a/Å	10.7941(3)
b/Å	9.6492(3)
c/Å	14.6149(4)
α/°	90
β/°	109.529(3)
γ/°	90
Volume/Å^3	1434.64(8)
Z	4
ρ_{calc}g/cm^3	1.307
μ/mm^{-1}	0.695
F(000)	600.0
Crystal size/mm^3	0.15 × 0.12 × 0.06
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.914 to 134.99
Index ranges	$-12 \le h \le 12$, $-11 \le k \le 8$, $-17 \le l \le 17$
Reflections collected	7689
Independent reflections	2573 [R_{int} = 0.0271, R_{sigma} = 0.0274]
Data/restraints/parameters	2573/0/191
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0336, wR_2 = 0.0844
Final R indexes [all data]	R_1 = 0.0420, wR_2 = 0.0902
Largest diff. peak/hole / e Å^{-3}	0.17/-0.19

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	1227.5(8)	5125.7(9)	2281.6(6)	22.7(2)
O2	935.4(10)	2060.9(10)	720.7(7)	30.2(2)
N1	325.3(10)	6850.3(11)	1130.2(7)	20.5(2)
N2	1621.2(10)	5038.4(11)	882.7(7)	20.6(2)
C1	1010.6(11)	5742.0(13)	1412.8(8)	19.1(3)
C3	2464.4(12)	3932.2(13)	1455.4(9)	22.0(3)
C4	2052.0(13)	3916.0(14)	2358.9(9)	25.8(3)
C5	2236.6(13)	2544.5(14)	932.1(9)	25.6(3)
C10	1835.7(12)	5630.2(13)	25.7(9)	21.4(3)
C11	2926.8(12)	6693.9(13)	278.1(8)	21.2(3)
C12	4239.2(13)	6285.3(14)	601.9(10)	27.6(3)
C13	5237.6(14)	7263.1(16)	875.7(10)	33.2(3)

C14	4937.2(15)	8662.3(16)	811.1(10)	33.1(3)
C15	3638.9(15)	9077.7(15)	469.6(10)	32.0(3)
C16	2636.6(14)	8103.0(14)	203.0(9)	25.4(3)
C21	-322.1(11)	7521.7(13)	1705.8(9)	21.1(3)
C22	-761.9(12)	6885.1(14)	2402.5(9)	24.3(3)
C23	-1388.4(13)	7657.6(15)	2920.9(10)	27.7(3)
C24	-1605.3(13)	9061.2(15)	2751.3(10)	28.8(3)
C25	-1192.4(13)	9700.2(15)	2053.5(10)	29.1(3)
C26	-560.9(13)	8940.1(14)	1532.8(9)	25.1(3)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 6a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	24.7(5)	25.0(5)	17.8(4)	1.9(3)	6.4(3)	5.8(4)
O2	35.4(5)	26.6(5)	23.5(5)	4.0(4)	2.9(4)	-3.1(4)
N1	19.7(5)	21.1(5)	19.6(5)	-0.8(4)	4.9(4)	0.3(4)
N2	22.9(5)	20.8(5)	18.5(5)	1.7(4)	7.4(4)	2.8(4)
C1	17.5(6)	21.7(6)	16.6(5)	-1.3(5)	3.6(5)	-3.4(5)
C3	20.0(6)	25.0(7)	19.1(6)	2.2(5)	4.0(5)	3.5(5)
C4	29.0(7)	25.8(7)	22.4(6)	3.1(5)	8.3(5)	8.1(5)
C5	28.3(7)	25.6(7)	21.2(6)	2.1(5)	6.0(5)	7.8(5)
C10	24.7(6)	22.3(6)	17.0(6)	0.7(5)	6.6(5)	1.3(5)
C11	26.2(6)	23.5(6)	15.1(5)	1.5(5)	8.7(5)	1.0(5)
C12	27.6(7)	26.0(7)	29.5(7)	6.5(5)	9.8(5)	2.0(5)
C13	25.5(7)	40.5(8)	31.6(7)	9.4(6)	6.9(6)	-2.5(6)
C14	39.2(8)	35.6(8)	26.0(7)	-2.5(6)	12.8(6)	-14.9(6)
C15	50.2(9)	22.0(7)	32.2(7)	-1.5(5)	25.0(7)	-3.4(6)
C16	31.2(7)	25.1(7)	24.5(6)	2.9(5)	15.3(5)	3.5(5)
C21	15.7(6)	25.4(7)	18.8(6)	-3.9(5)	1.3(5)	-0.3(5)
C22	19.4(6)	24.5(7)	28.2(7)	-2.9(5)	6.9(5)	-2.4(5)
C23	22.2(6)	34.0(7)	28.0(7)	-3.5(6)	9.9(5)	-2.5(5)
C24	22.5(6)	34.1(8)	27.8(7)	-8.6(6)	5.7(5)	4.3(5)
C25	28.3(7)	27.5(7)	26.4(7)	-2.7(5)	2.5(6)	8.0(5)
C26	25.2(6)	26.3(7)	20.2(6)	1.1(5)	3.0(5)	3.2(5)

Table S12. Bond Lengths for 6a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

O1	C1	1.3497(15)	C11	C16	1.3914(18)
O1	C4	1.4492(15)	C12	C13	1.387(2)
O2	C5	1.4127(17)	C13	C14	1.384(2)
N1	C1	1.2873(16)	C14	C15	1.381(2)
N1	C21	1.4173(16)	C15	C16	1.387(2)
N2	C1	1.3554(16)	C21	C22	1.4011(18)
N2	C3	1.4693(15)	C21	C26	1.4000(19)
N2	C10	1.4636(15)	C22	C23	1.3890(19)
C3	C4	1.5280(17)	C23	C24	1.383(2)
C3	C5	1.5207(18)	C24	C25	1.387(2)
C10	C11	1.5121(17)	C25	C26	1.3886(19)
C11	C12	1.3921(18)			

Table S13. Bond Angles for 6a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C4	109.70(9)	C16	C11	C10	120.51(11)
C1	N1	C21	122.26(11)	C16	C11	C12	118.70(12)
C1	N2	C3	111.42(10)	C13	C12	C11	120.64(13)
C1	N2	C10	122.69(10)	C14	C13	C12	120.14(13)
C10	N2	C3	121.73(10)	C15	C14	C13	119.62(13)
O1	C1	N2	110.64(10)	C14	C15	C16	120.44(13)
N1	C1	O1	124.62(11)	C15	C16	C11	120.42(13)
N1	C1	N2	124.74(11)	C22	C21	N1	125.81(12)
N2	C3	C4	101.29(10)	C26	C21	N1	115.93(11)
N2	C3	C5	112.82(10)	C26	C21	C22	118.24(12)
C5	C3	C4	112.38(11)	C23	C22	C21	120.41(13)
O1	C4	C3	105.85(10)	C24	C23	C22	120.80(13)
O2	C5	C3	112.50(11)	C23	C24	C25	119.38(12)
N2	C10	C11	112.91(10)	C24	C25	C26	120.36(13)
C12	C11	C10	120.79(12)	C25	C26	C21	120.79(13)

Table S14. Hydrogen Bonds for 6a.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O2	H2	N1[1]	0.84	1.97	2.7950(13)	166.5

[1]-X,1-Y,-Z

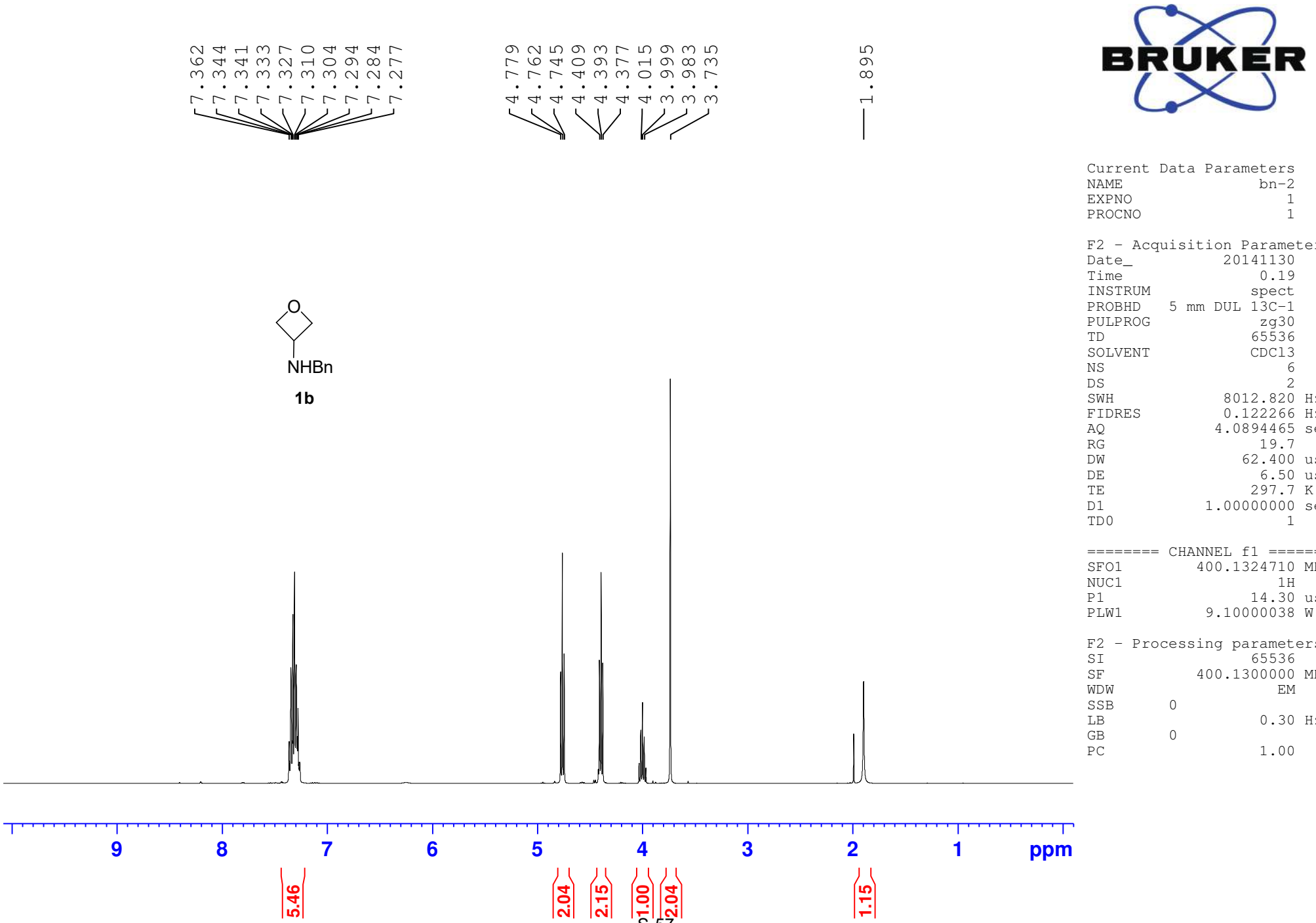
Table S15. Torsion Angles for 6a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C21	C22	C23	-179.87(11)	C10	N2	C1	N1	15.01(18)
N1	C21	C26	C25	179.82(11)	C10	N2	C3	C4	167.91(11)
N2	C3	C4	O1	-9.54(13)	C10	N2	C3	C5	-71.74(15)
N2	C3	C5	O2	-60.89(14)	C10	C11	C12	C13	-176.98(12)
N2	C10	C11	C12	77.85(15)	C10	C11	C16	C15	177.56(11)
N2	C10	C11	C16	-101.28(13)	C11	C12	C13	C14	-1.3(2)
C1	O1	C4	C3	6.18(13)	C12	C11	C16	C15	-1.59(18)
C1	N1	C21	C22	-26.87(18)	C12	C13	C14	C15	-0.2(2)
C1	N1	C21	C26	154.79(12)	C13	C14	C15	C16	0.8(2)
C1	N2	C3	C4	10.31(13)	C14	C15	C16	C11	0.1(2)
C1	N2	C3	C5	130.66(11)	C16	C11	C12	C13	2.17(19)
C1	N2	C10	C11	74.93(14)	C21	N1	C1	O1	-2.27(18)
C3	N2	C1	O1	-7.21(14)	C21	N1	C1	N2	178.22(11)
C3	N2	C1	N1	172.36(11)	C21	C22	C23	C24	0.86(19)
C3	N2	C10	C11	-80.14(14)	C22	C21	C26	C25	1.35(18)
C4	O1	C1	N1	-179.23(12)	C22	C23	C24	C25	0.1(2)
C4	O1	C1	N2	0.34(13)	C23	C24	C25	C26	-0.3(2)
C4	C3	C5	O2	52.88(14)	C24	C25	C26	C21	-0.4(2)
C5	C3	C4	O1	-130.20(11)	C26	C21	C22	C23	-1.56(18)
C10	N2	C1	O1	-164.56(11)					

Table S16. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6a.

Atom	*x*	*y*	*z*	U(eq)
H2	453	2415	198	45
H3	3410	4204	1635	26
H4A	1557	3059	2380	31
H4B	2833	3964	2955	31
H5A	2430	2638	319	31
H5B	2853	1852	1341	31
H10A	1011	6070	-390	26
H10B	2053	4874	-353	26
H12	4453	5327	636	33
H13	6130	6972	1108	40
H14	5620	9333	1001	40

H15	3430	10037	417	38
H16	1746	8400	-32	31
H22	-631	5919	2521	29
H23	-1671	7216	3398	33
H24	-2033	9583	3109	35
H25	-1342	10663	1931	35
H26	-288	9388	1054	30



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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 19.7
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

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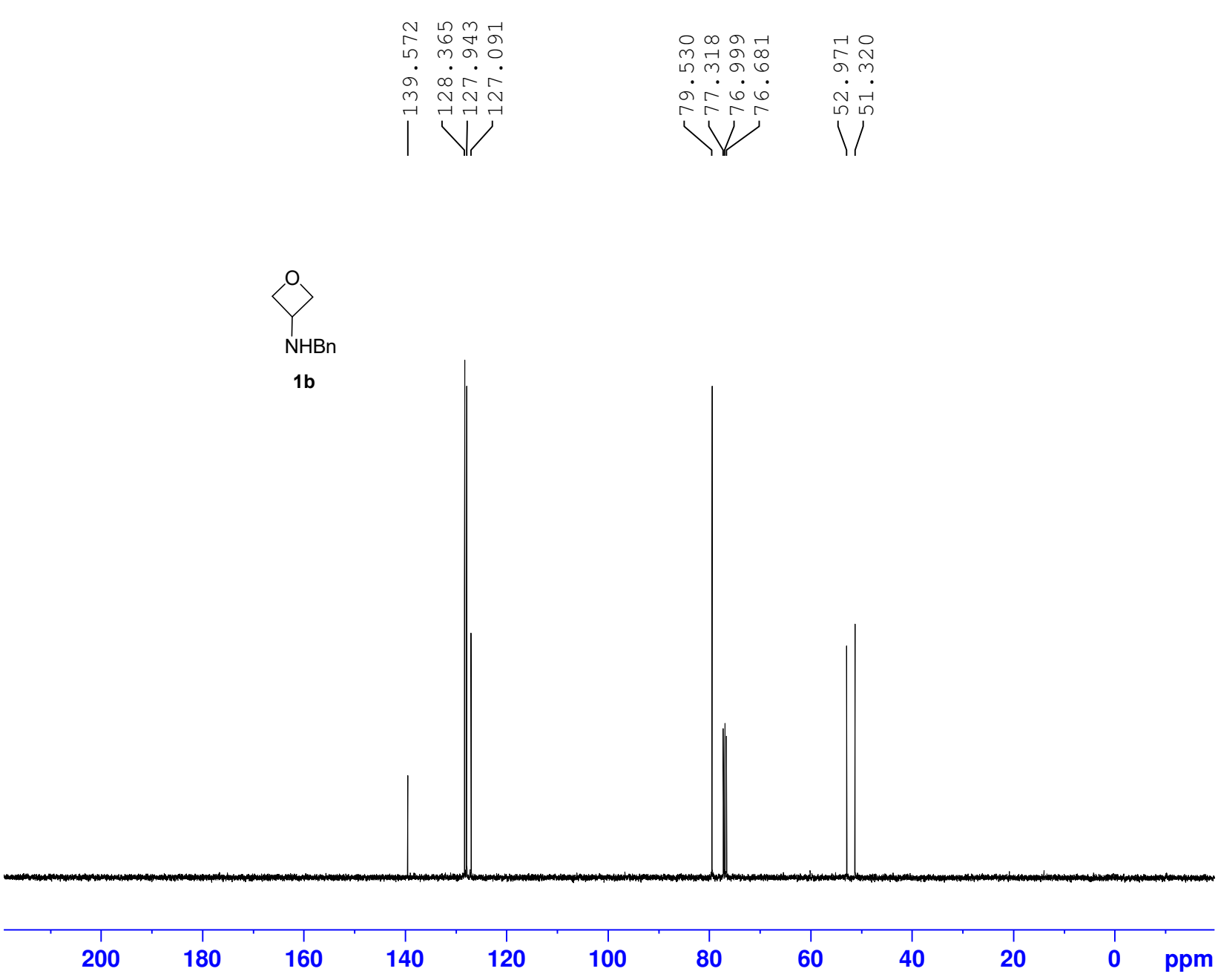
NUC1 1H
P1 14.30 usec
PLW1 9.10000038 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          25
DS                           2
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631488 sec
RG                      196.92
DW                      20.800 usec
DE                       6.50 usec
TE                      297.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                100.6228298 MHz
NUC1                        13C
P1                        9.70 usec
PLW1                46.98899841 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                11.99499989 W
PLW12                0.34213999 W
PLW13                0.27713001 W

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SF                  100.6127893 MHz
WDW                            EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
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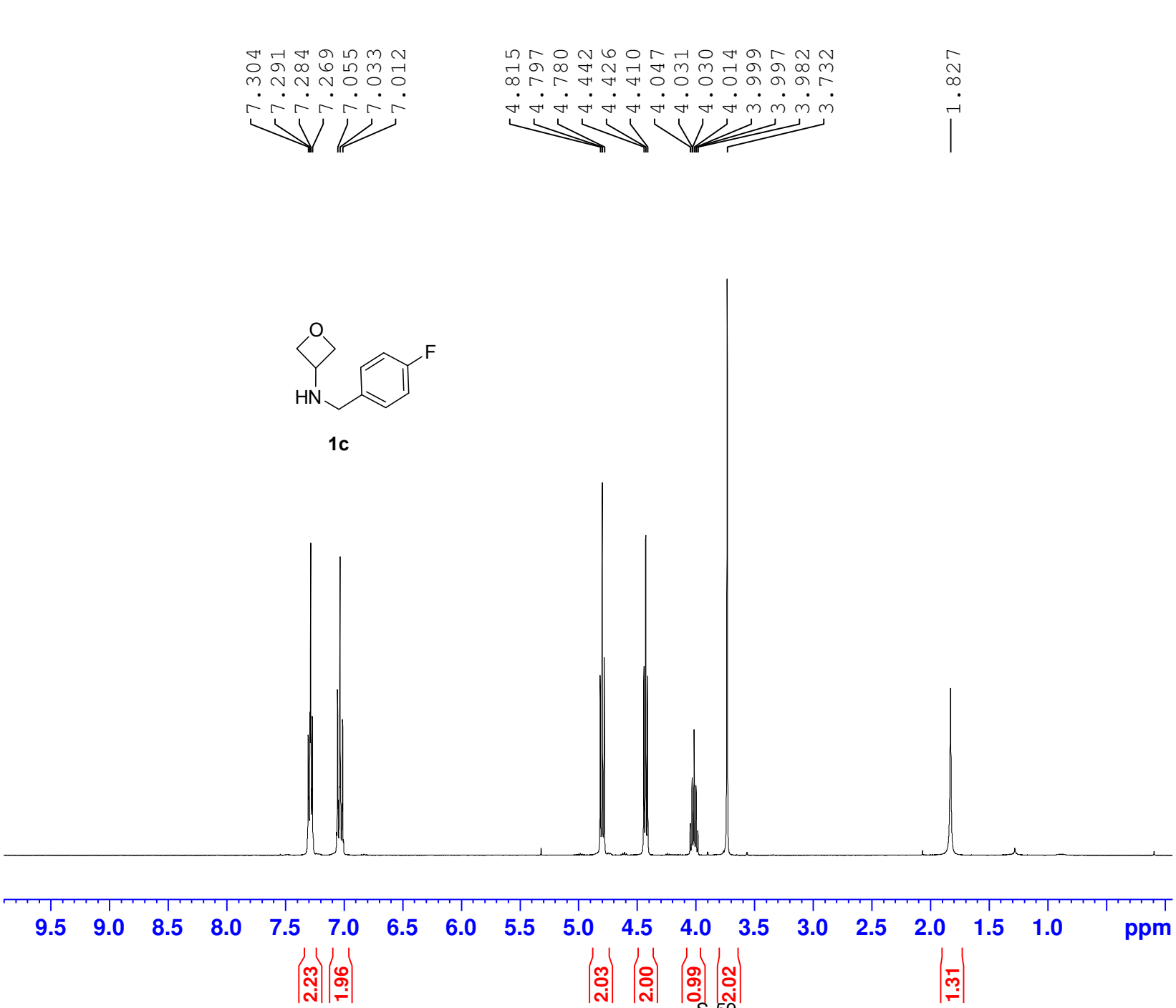


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PROCNO                     1

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PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         5
DS                         2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                     88.84
DW                    62.400 usec
DE                     6.50 usec
TE                    297.4 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            11.99499989 W

F2 - Processing parameters
SI                         65536
SF              400.1300000 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
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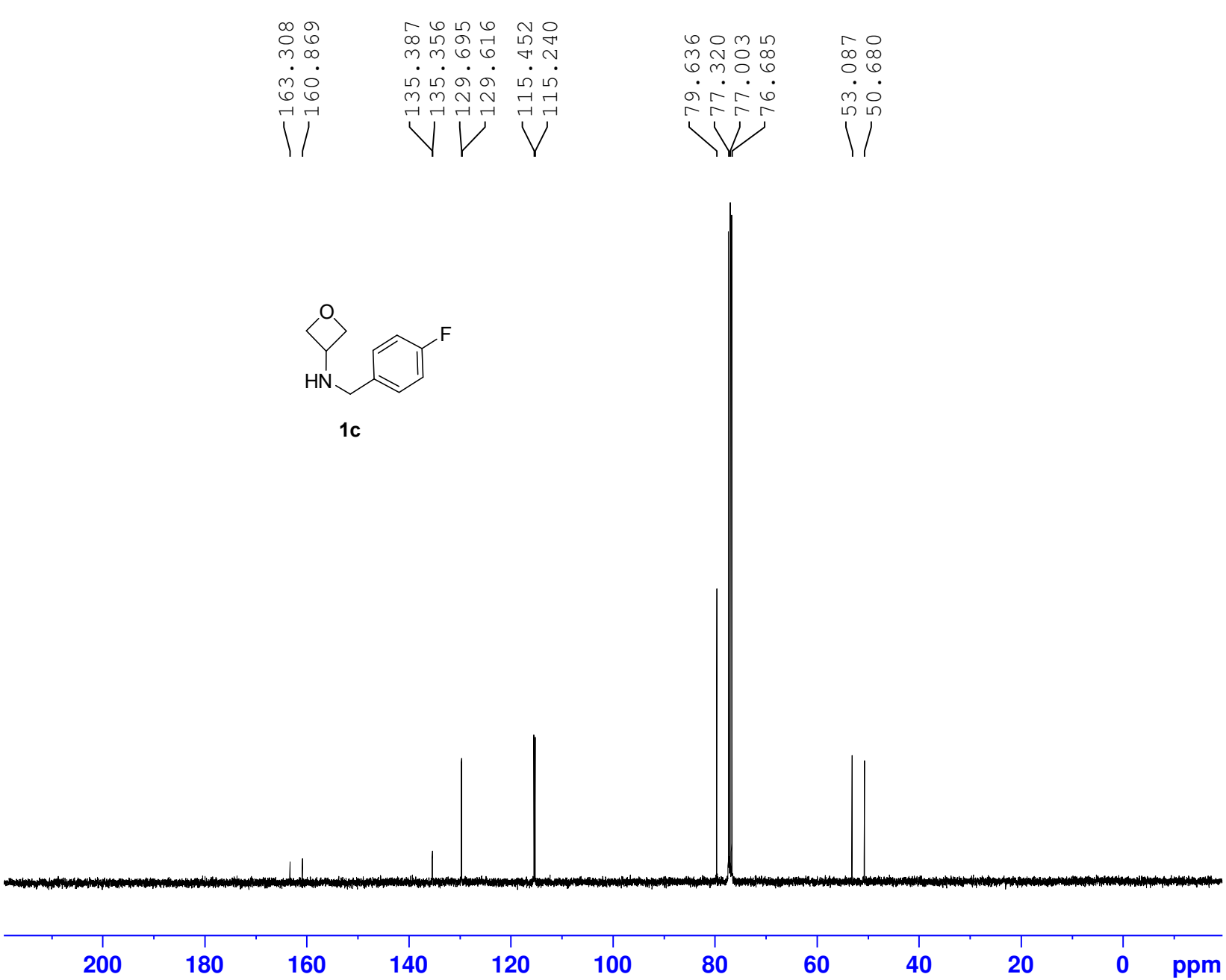


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PROCNO                 1

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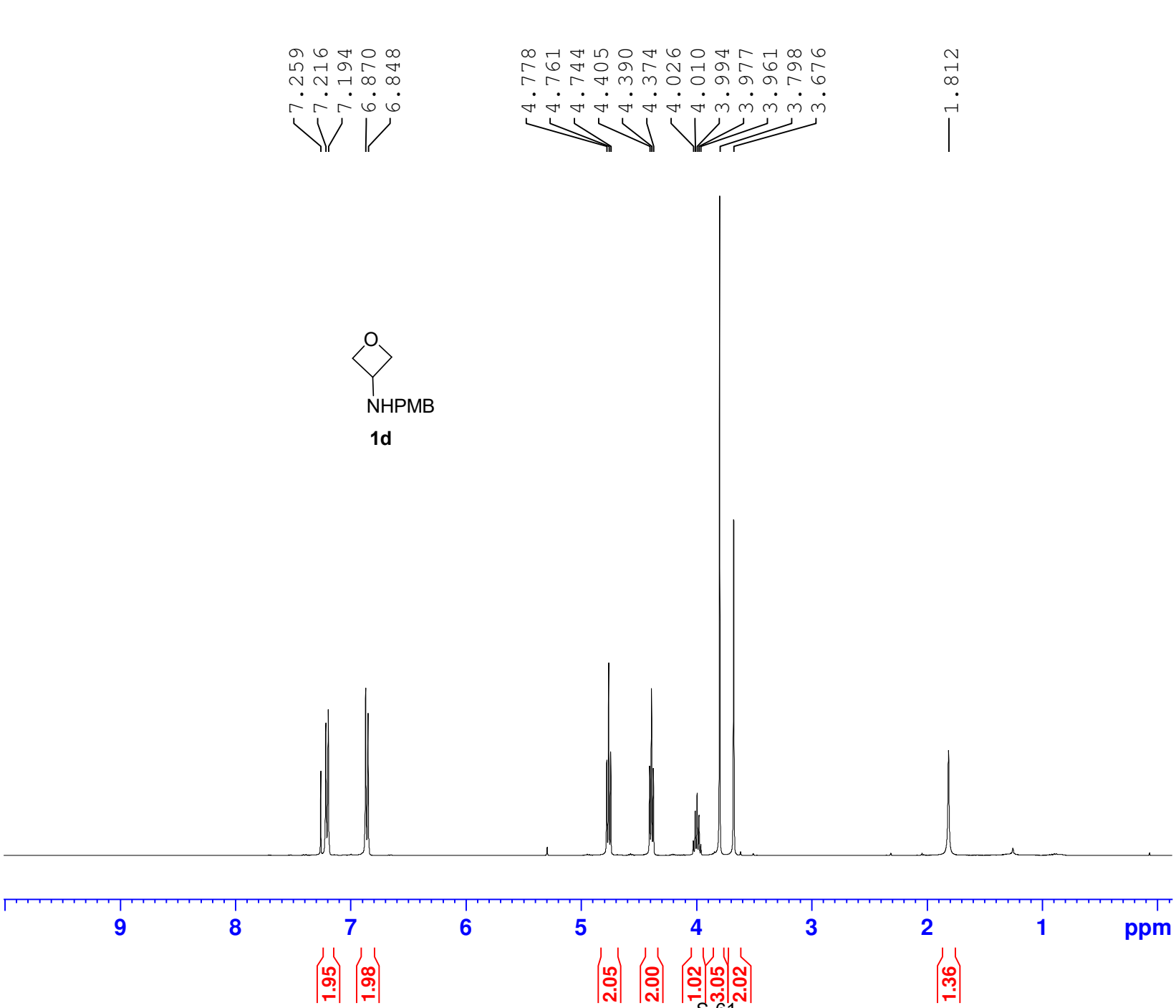
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   400
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127710 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

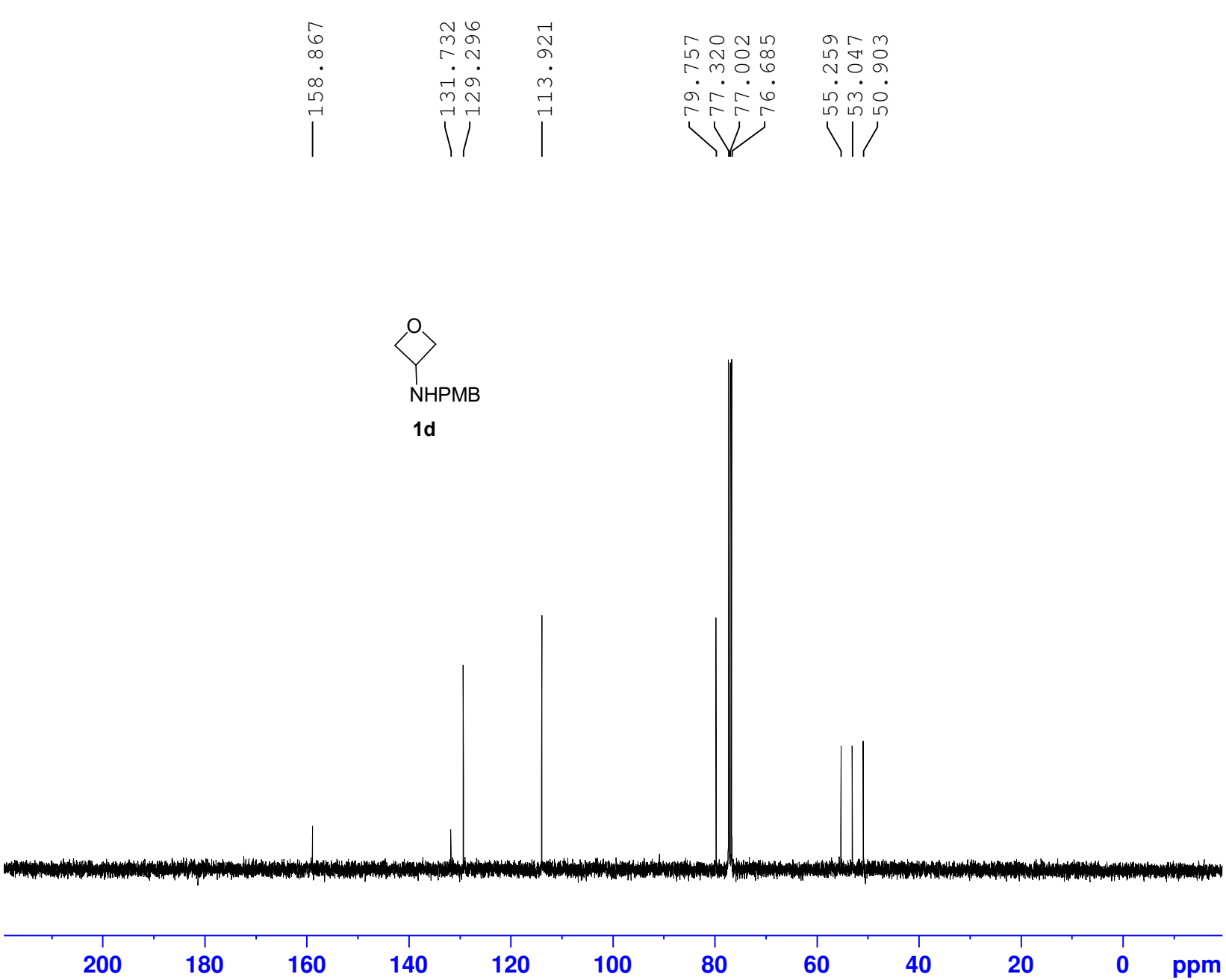


Current Data Parameters
NAME lzw2024A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150210
Time 17.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



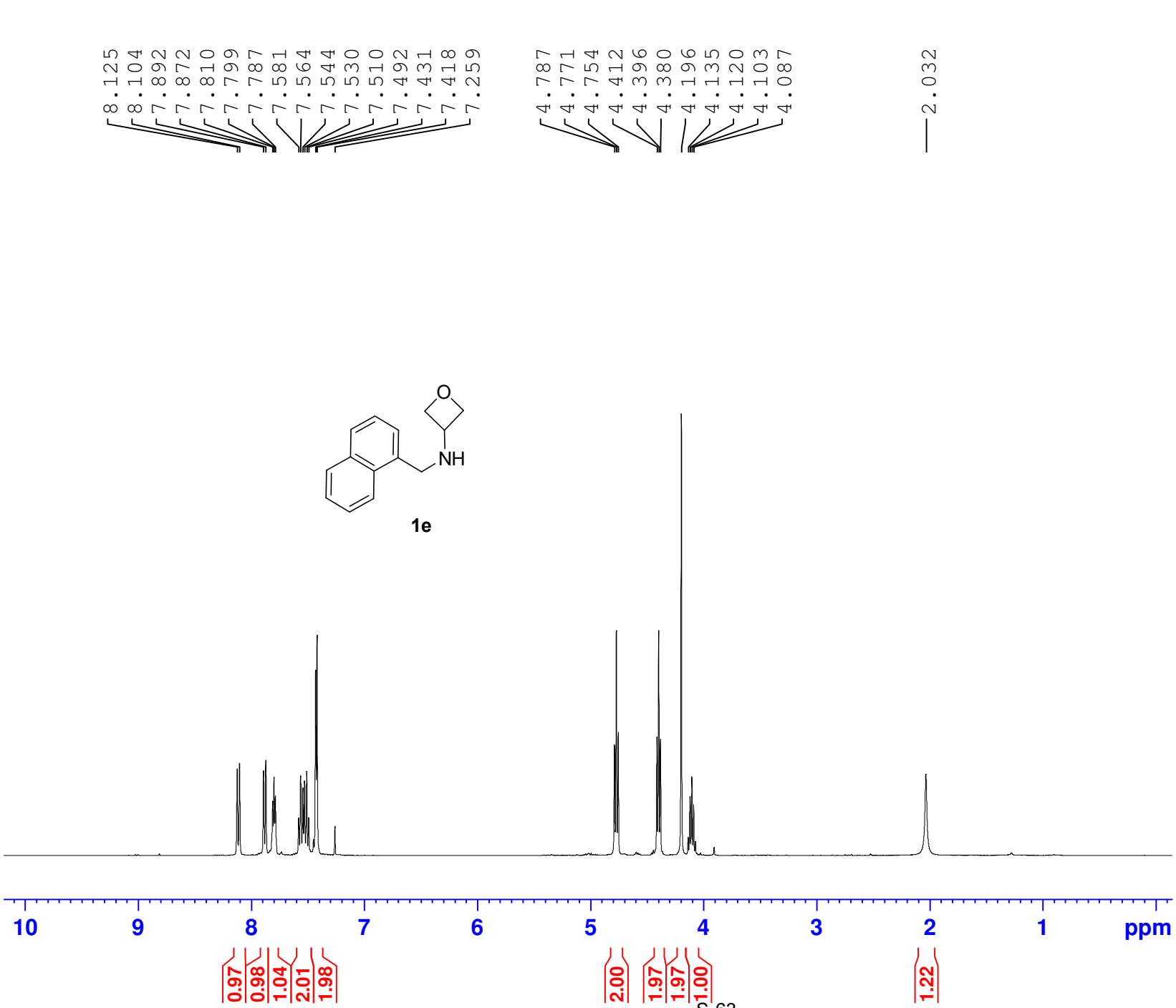

```
Current Data Parameters
NAME                 lzw2024A
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_               20150211
Time                   10.49
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         58
DS                          2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                       9.70 usec
PLW1               46.98899841 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   90.00 usec
PLW2               11.99499989 W
PLW12               0.34213999 W
PLW13               0.27713001 W

F2 - Processing parameters
SI                         32768
SF                 100.6127722 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```



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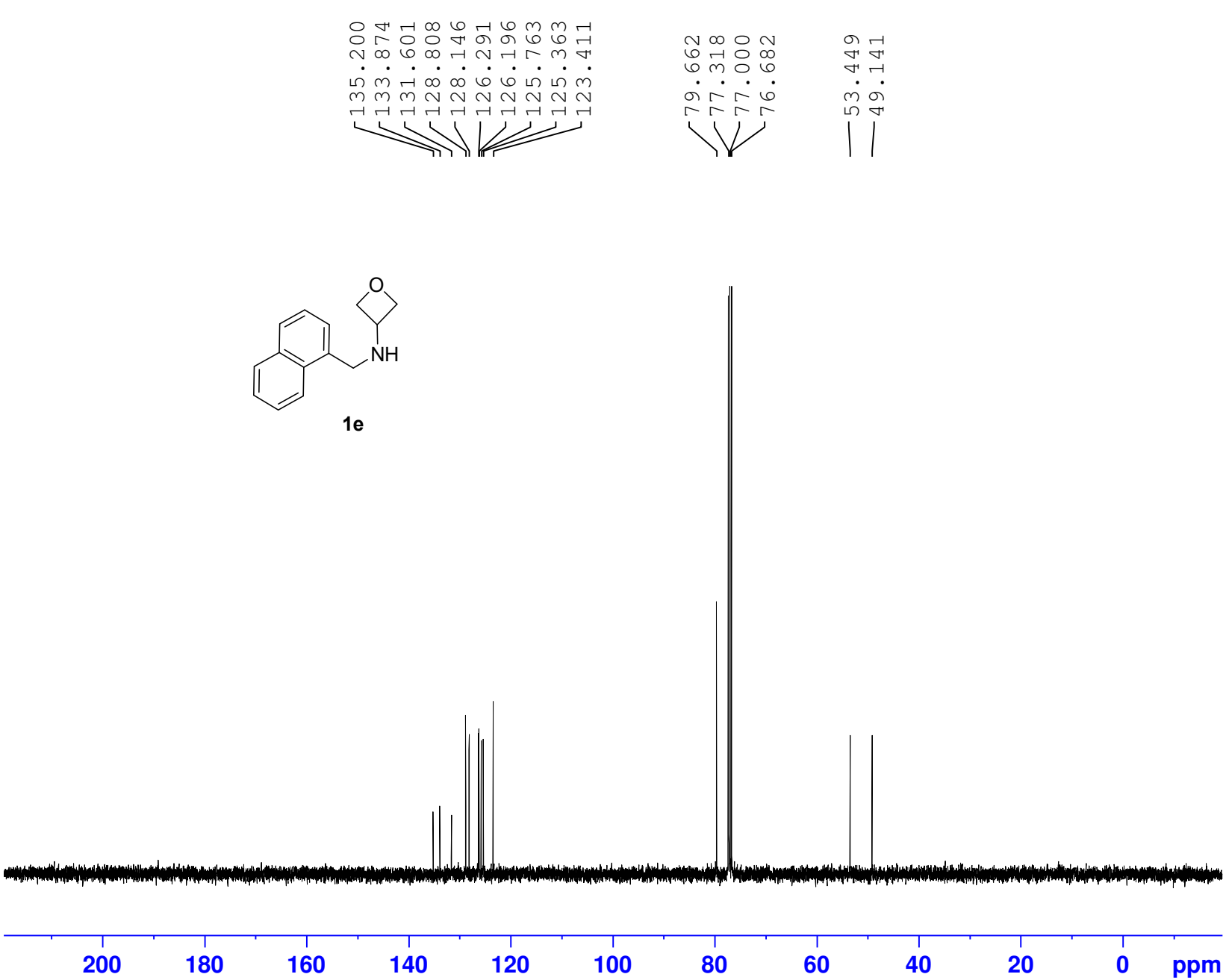
```
Current Data Parameters
NAME          lzw2002A-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150424
Time               19.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 70.97
DW                62.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300091 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



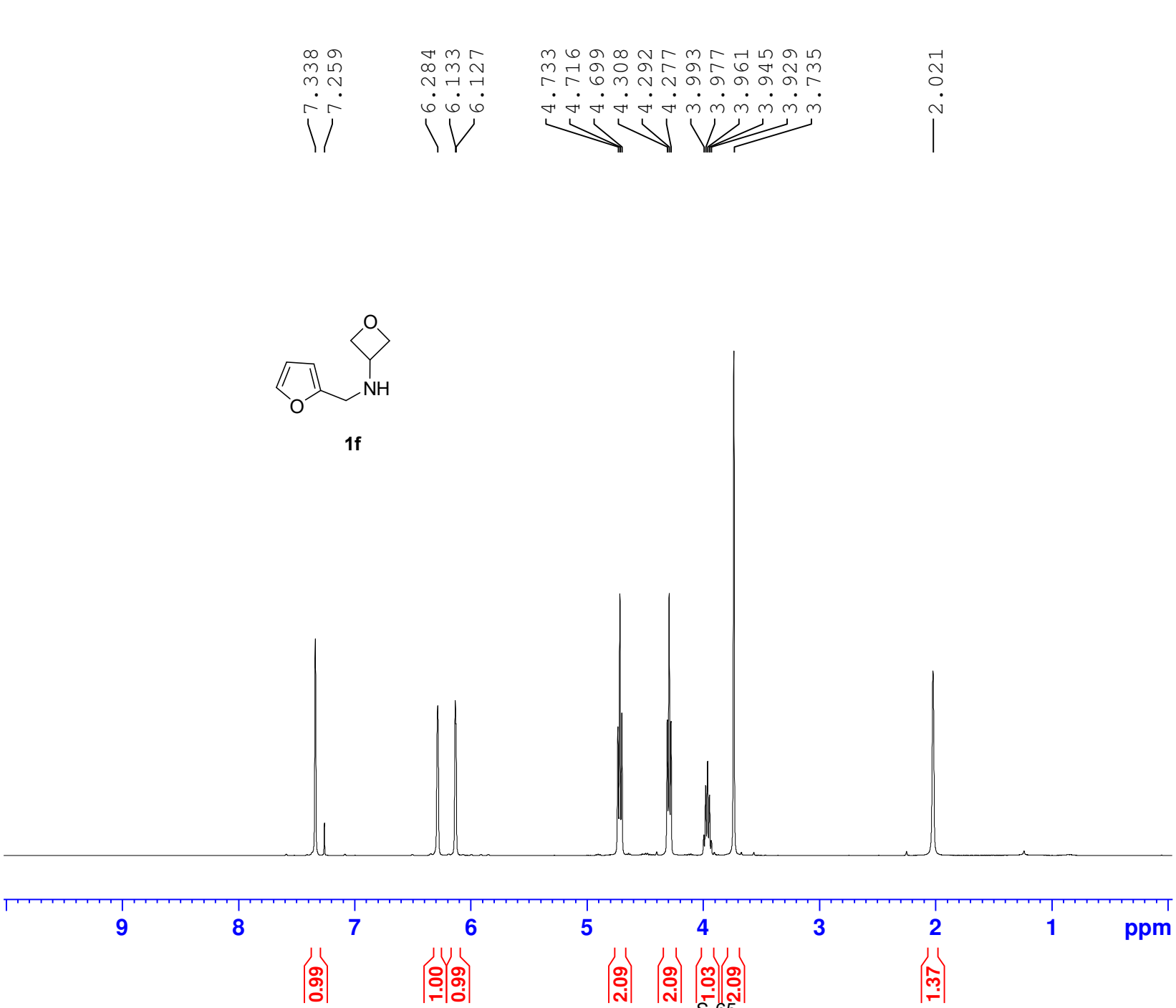

```
Current Data Parameters
NAME                  lzw2002A
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20150131
Time                     13.49
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          56
DS                           2
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631488 sec
RG                      196.92
DW                      20.800 usec
DE                       6.50 usec
TE                      297.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                100.6228298 MHz
NUC1                        13C
P1                        9.70 usec
PLW1                46.98899841 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                11.99499989 W
PLW12                0.34213999 W
PLW13                0.27713001 W

F2 - Processing parameters
SI                          32768
SF                  100.6127741 MHz
WDW                            EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```

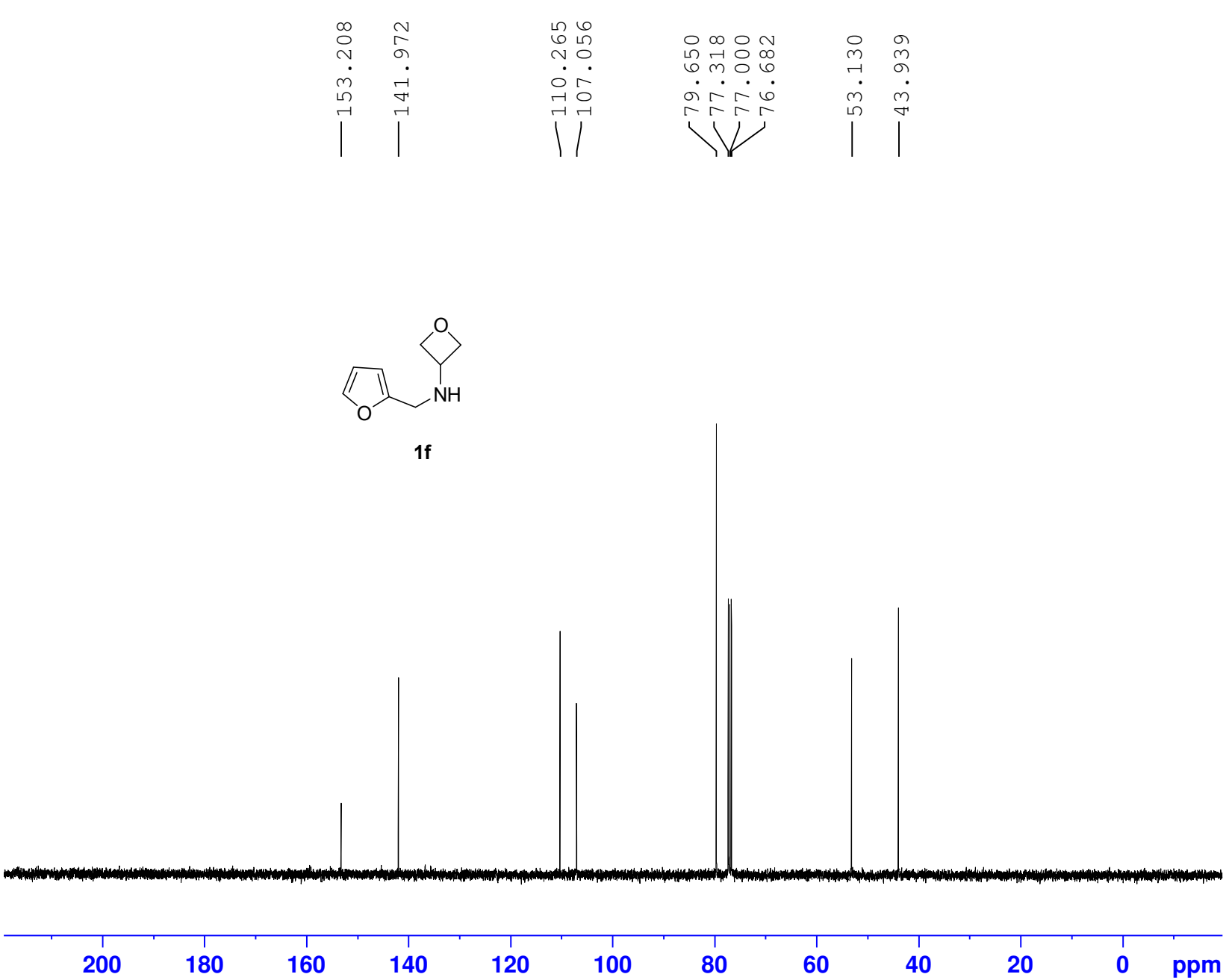


Current Data Parameters
NAME lzw2125A-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150417
Time 22.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 54.81
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



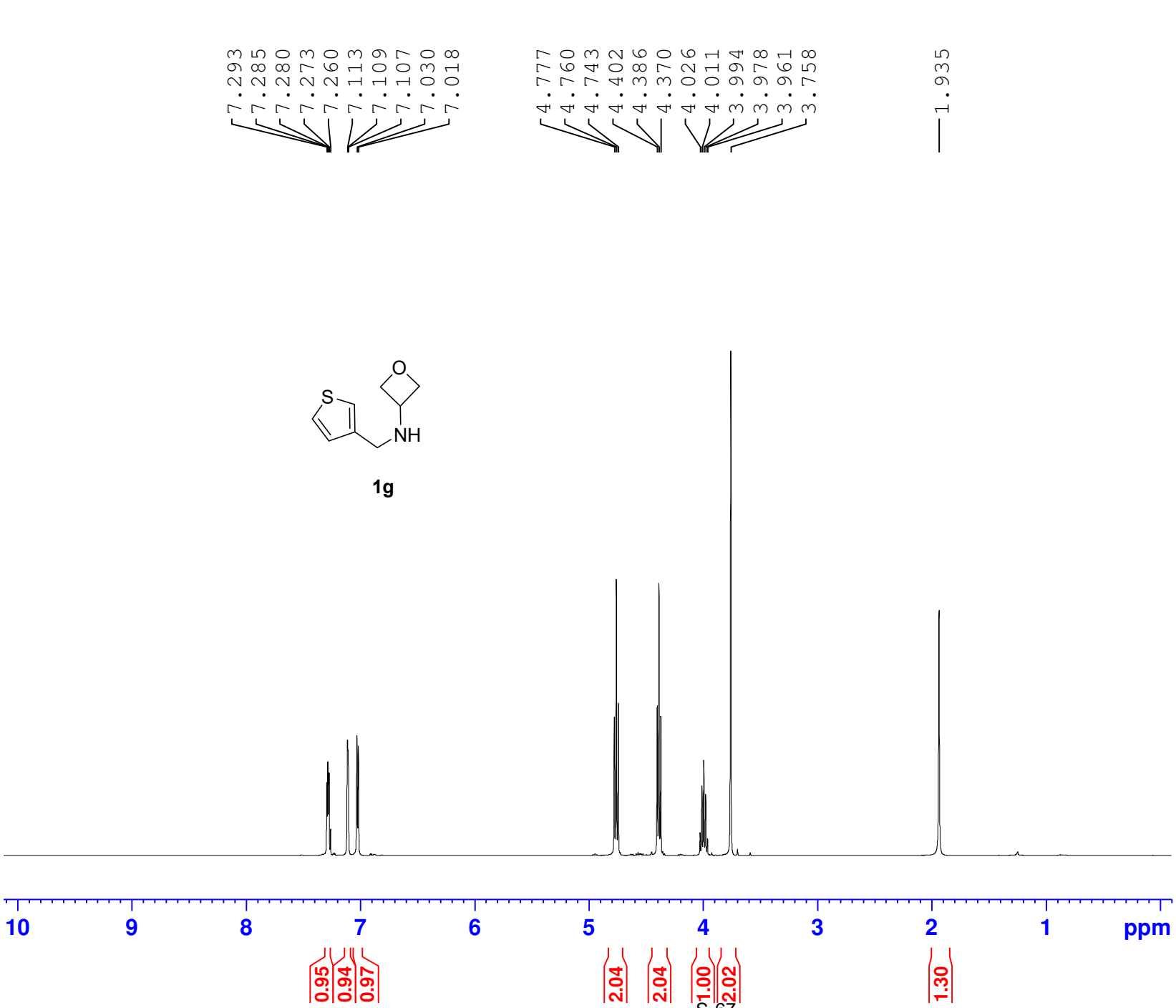

```
Current Data Parameters
NAME          lzw2125A-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150417
Time               22.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    49
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127769 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

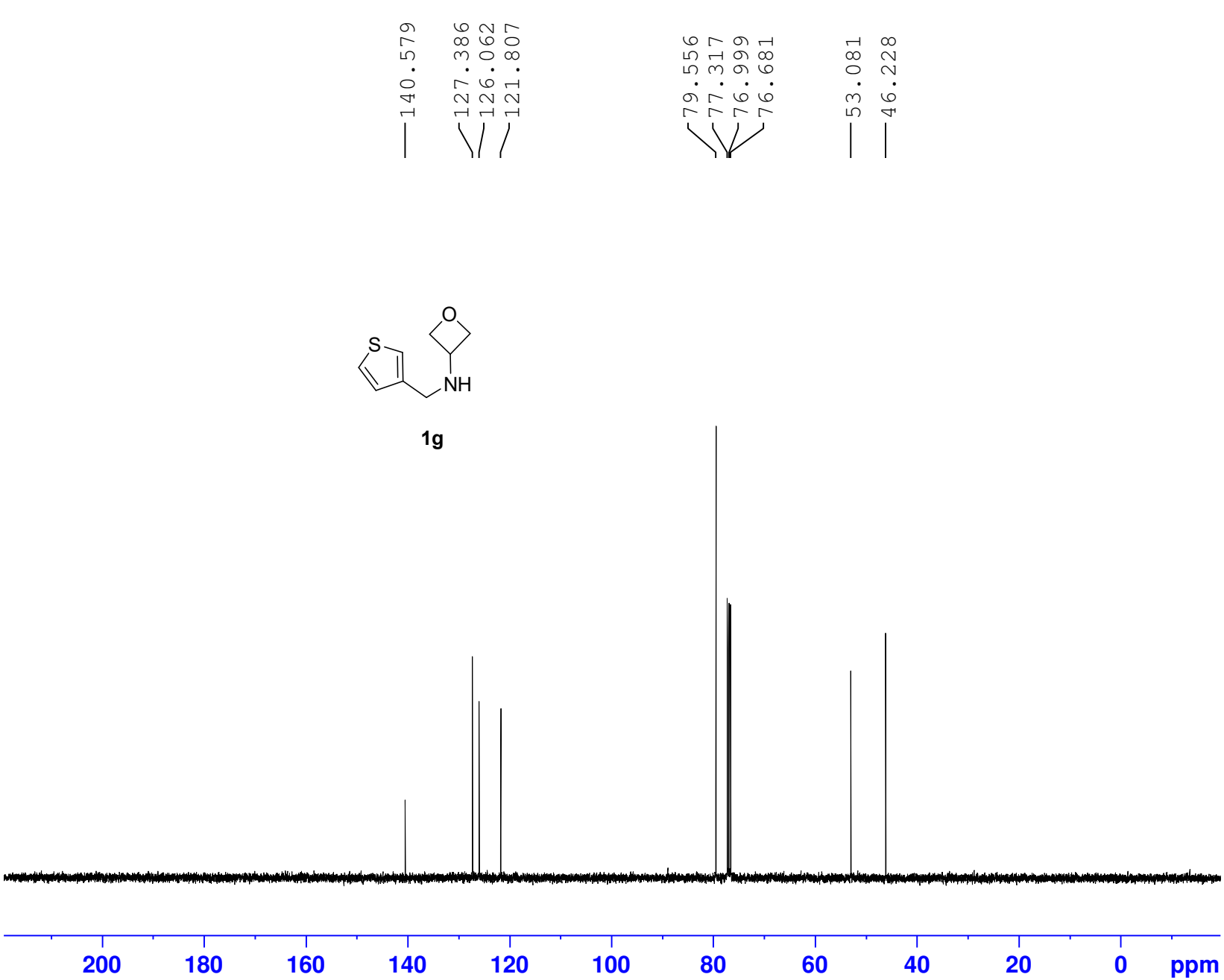


Current Data Parameters
NAME lzw2125B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150418
Time 14.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 49.32
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



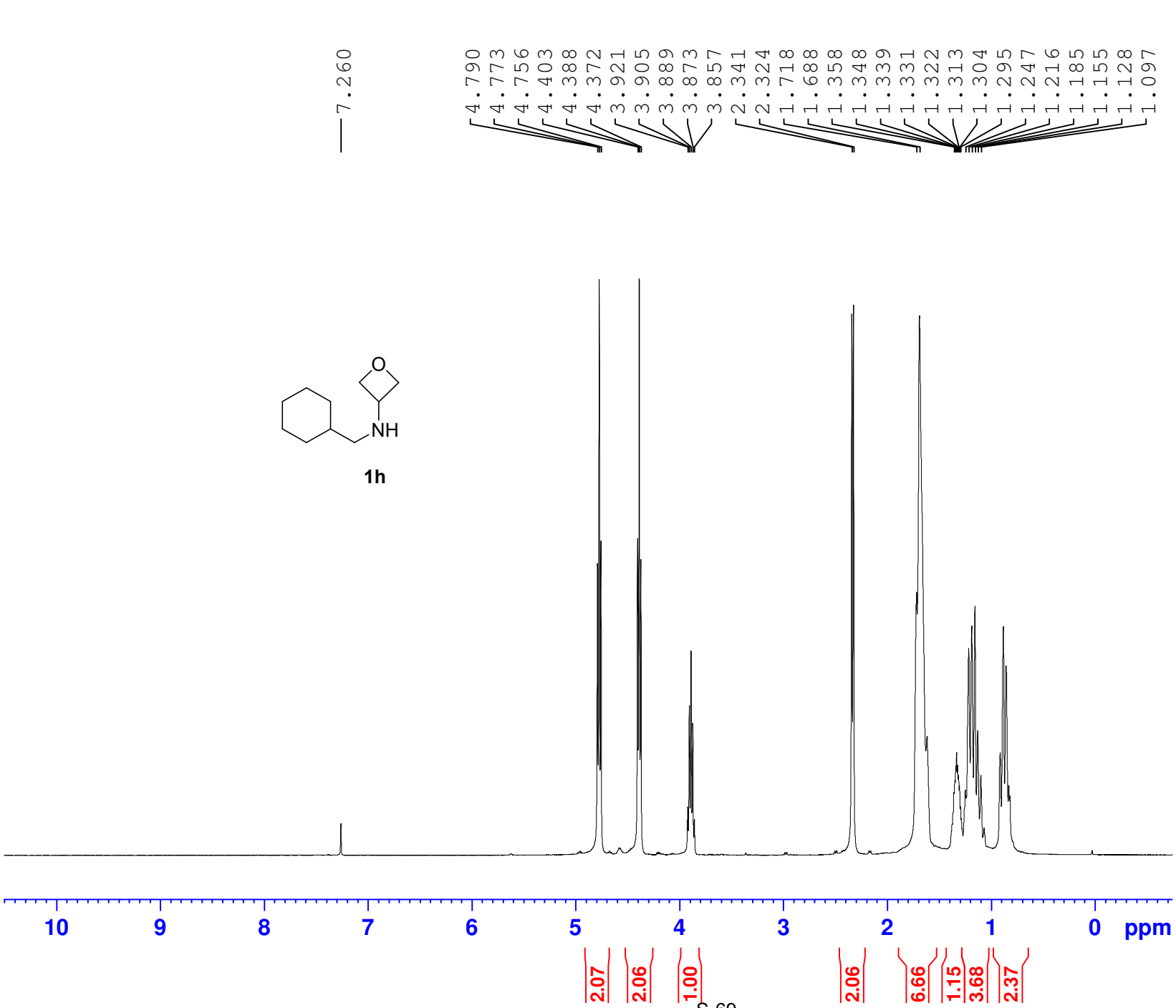

```
Current Data Parameters
NAME          lzw2125B-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150418
Time               14.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    35
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127791 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

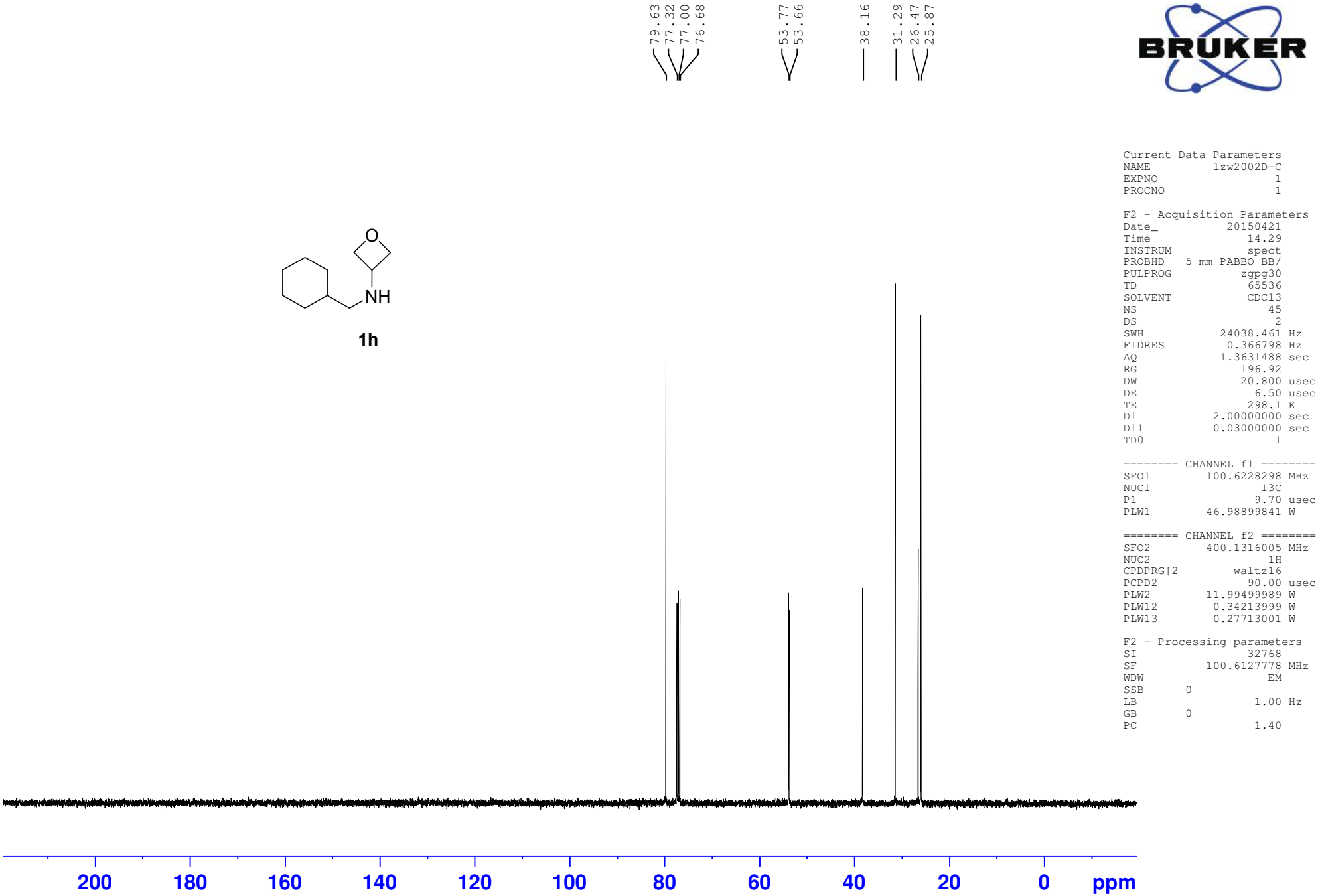


Current Data Parameters
NAME lzw2002D-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150421
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 3
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 25.32
DW 62.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



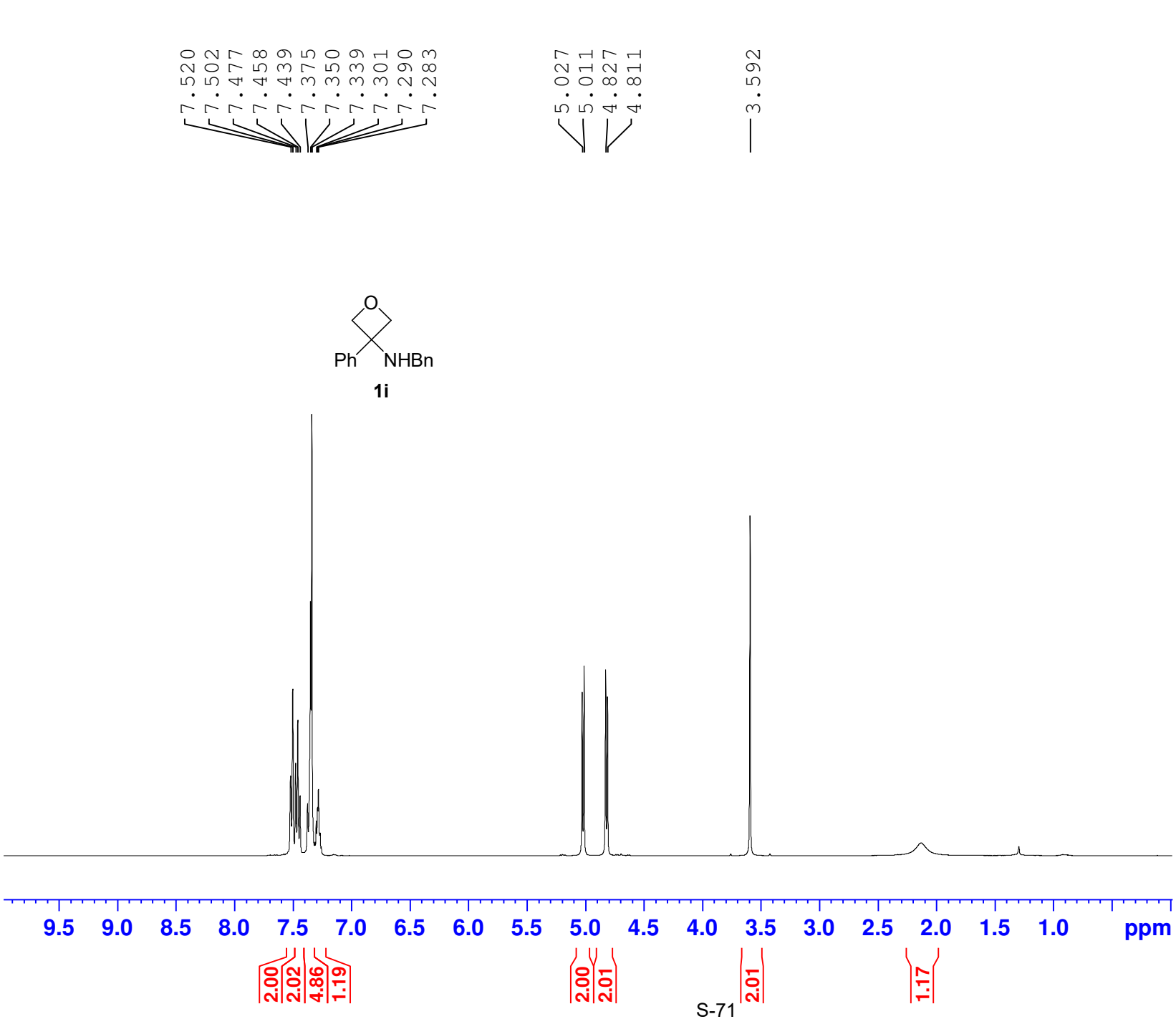

```
Current Data Parameters
NAME          lzw2002D-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150421
Time               14.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   45
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                  32768
SF           100.6127778 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

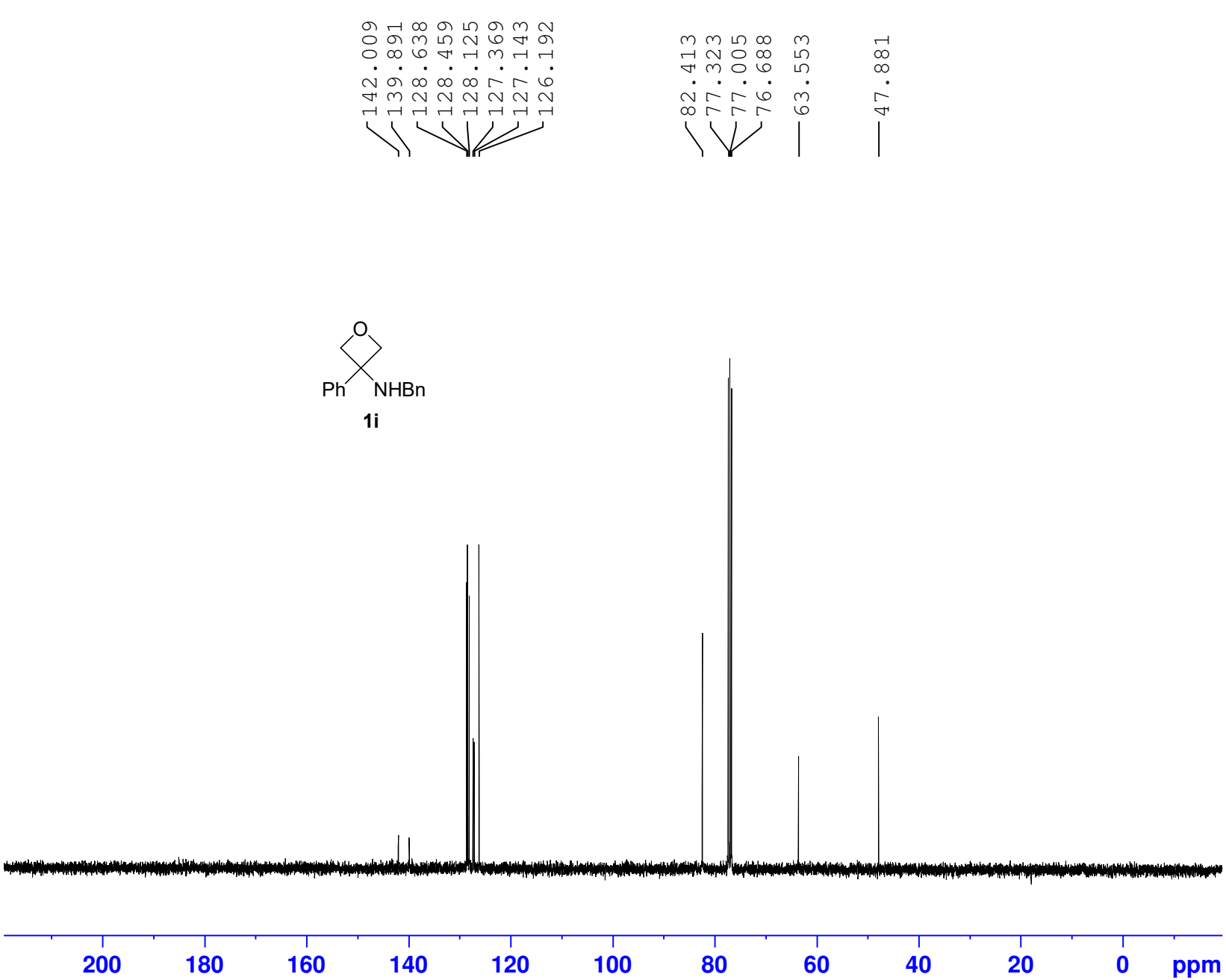



```
Current Data Parameters
NAME          lzw2138-H
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20150427
Time              22.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                62.93
DW               62.400 usec
DE                6.50 usec
TE                297.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                  1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



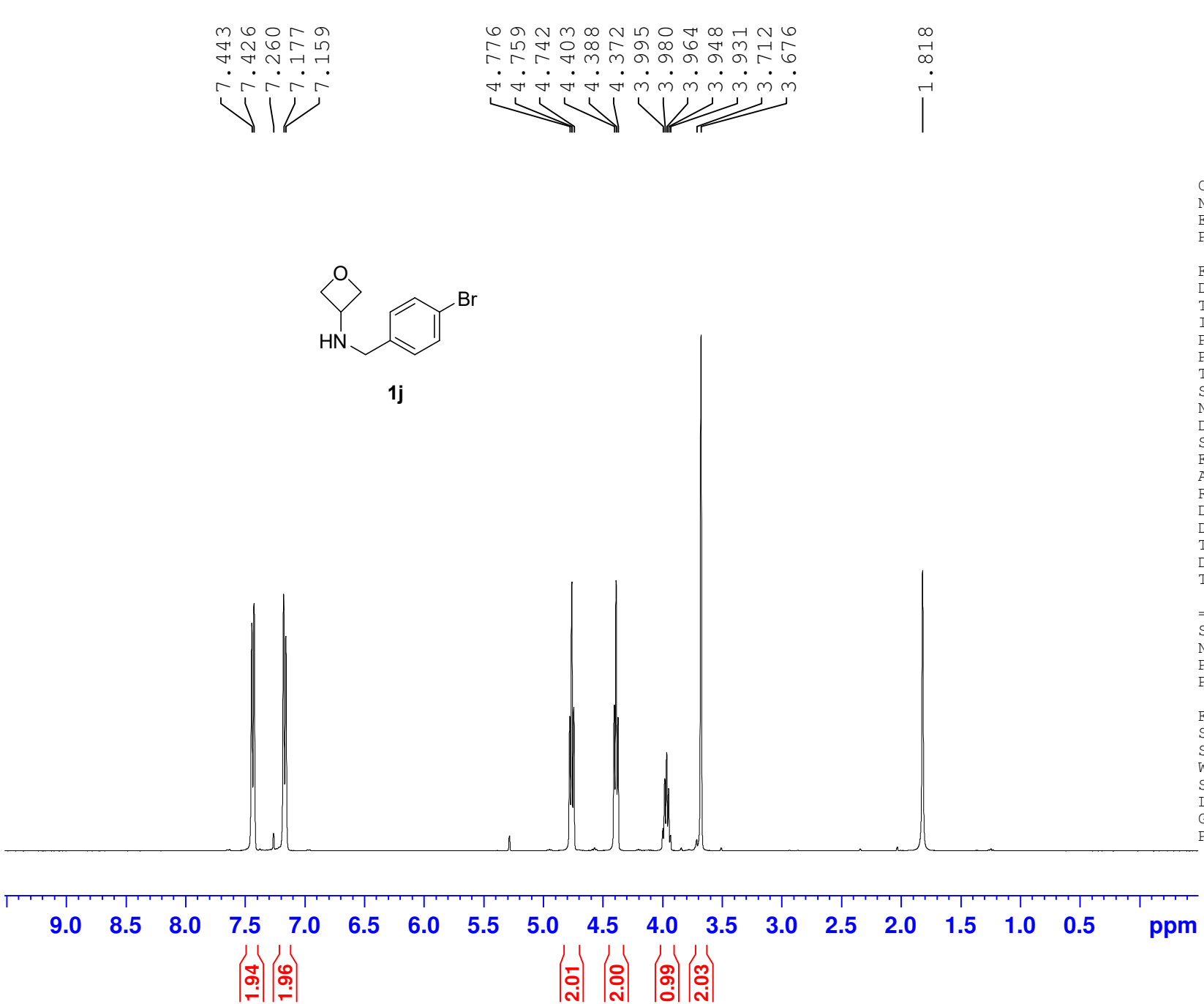

```
Current Data Parameters
NAME          lzw2138-C
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20150427
Time              22.38
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   63
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127739 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

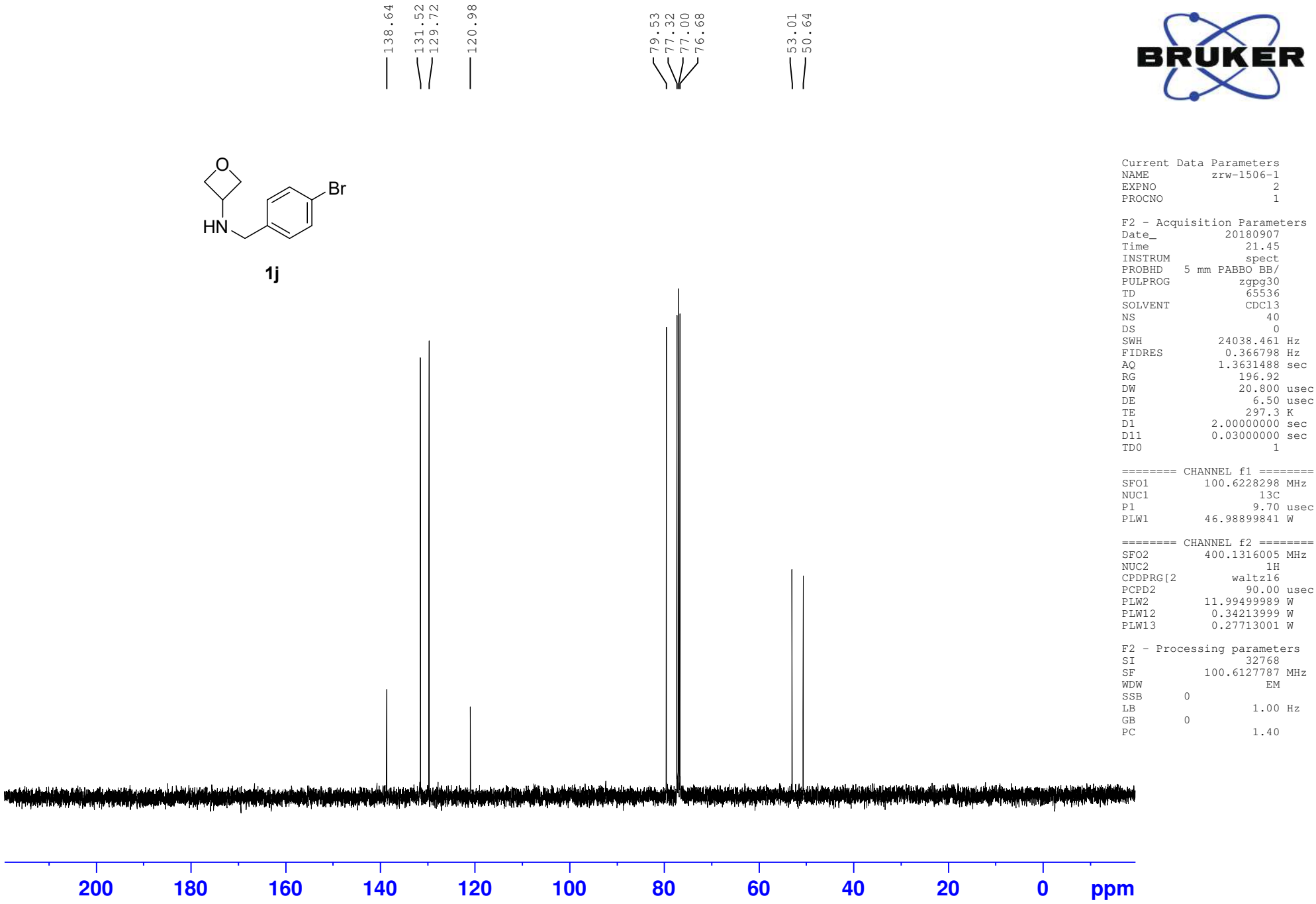



```
Current Data Parameters
NAME          zrw-1506-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180907
Time               21.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 82.92
DW                62.400 usec
DE                 6.50 usec
TE                296.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300104 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



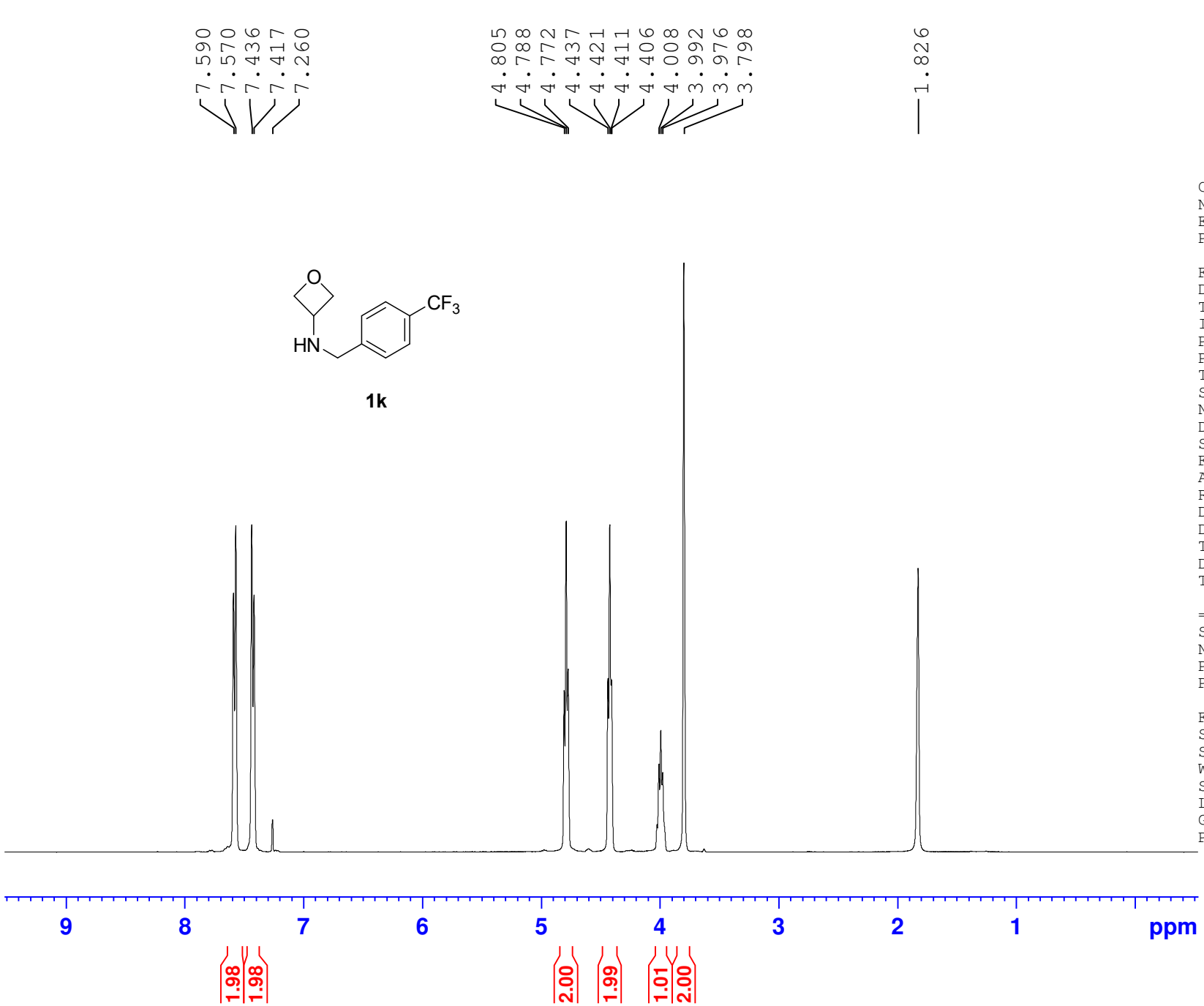

```
Current Data Parameters
NAME          zrw-1506-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180907
Time               21.45
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127787 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

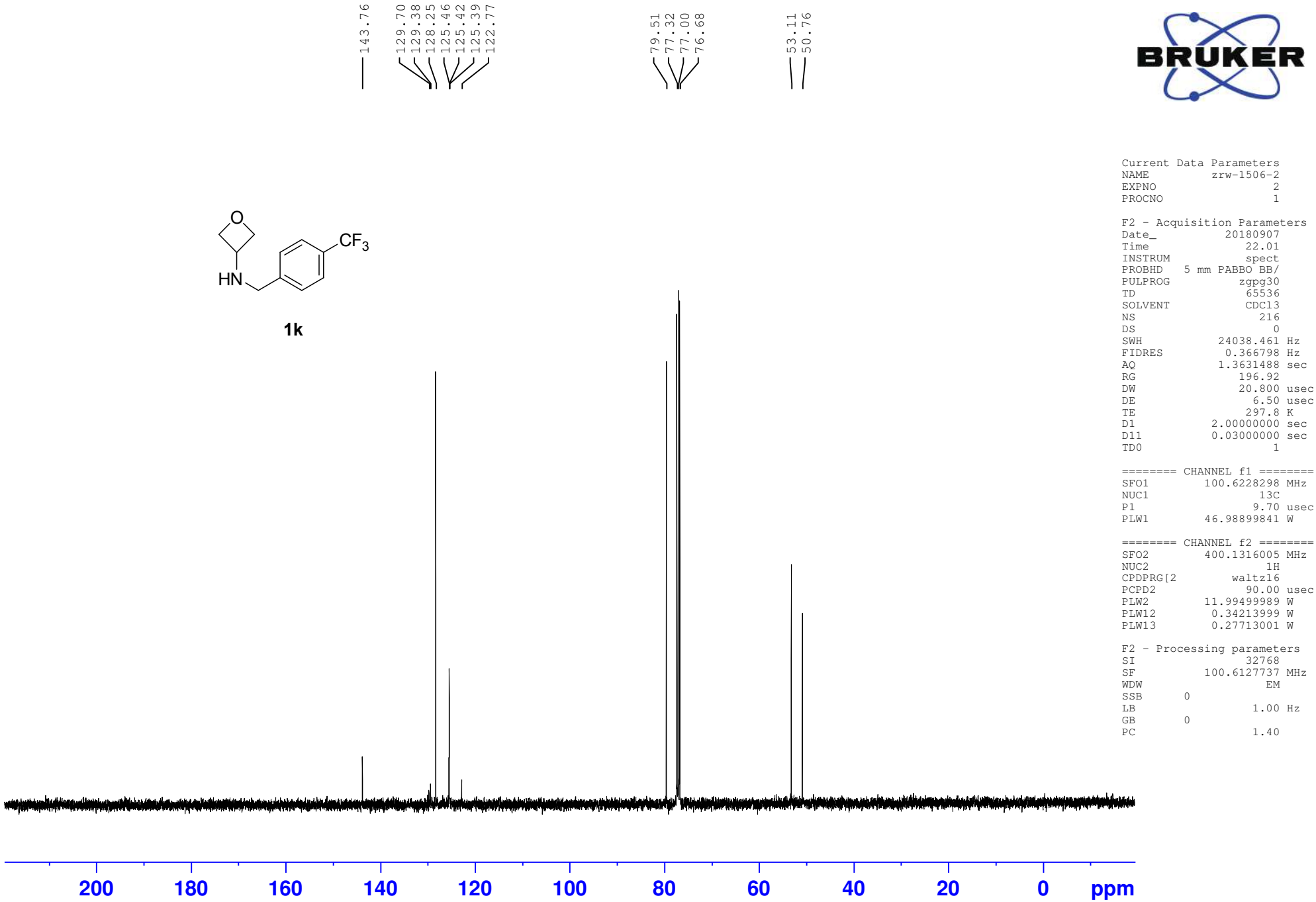



```
Current Data Parameters
NAME          zrw-1506-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180907
Time               21.48
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                103.52
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300106 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



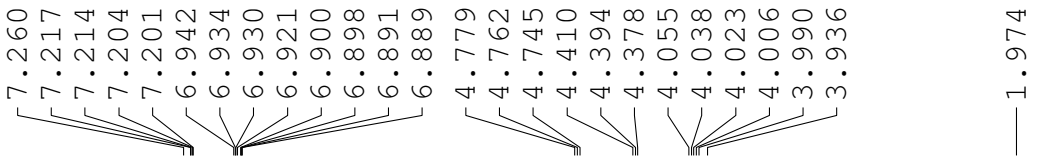

```
Current Data Parameters
NAME          zrw-1506-2
EXPNO                  2
PROCNO                 1

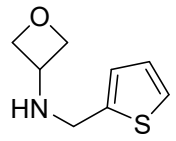
F2 - Acquisition Parameters
Date_           20180907
Time               22.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  216
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

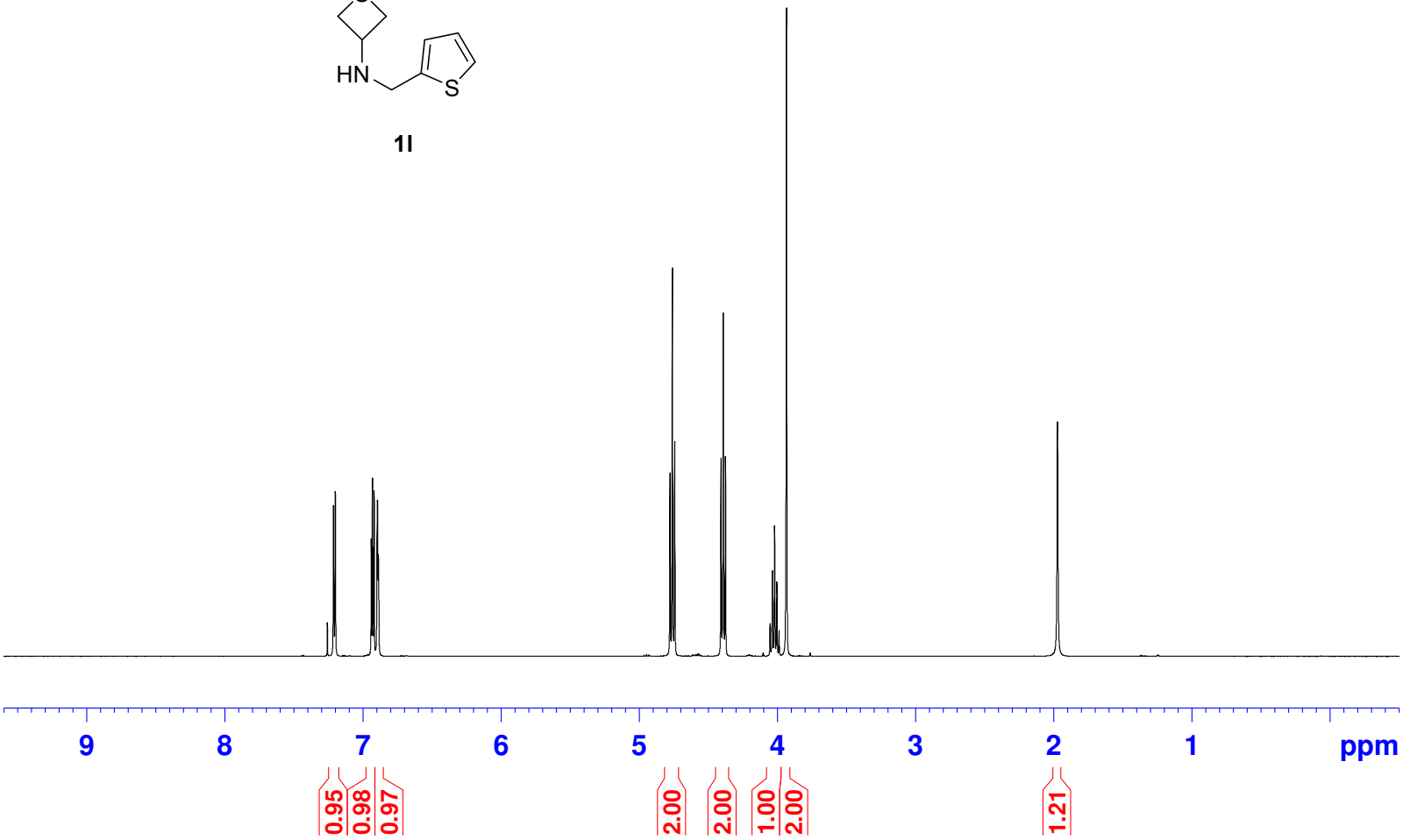
======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127737 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



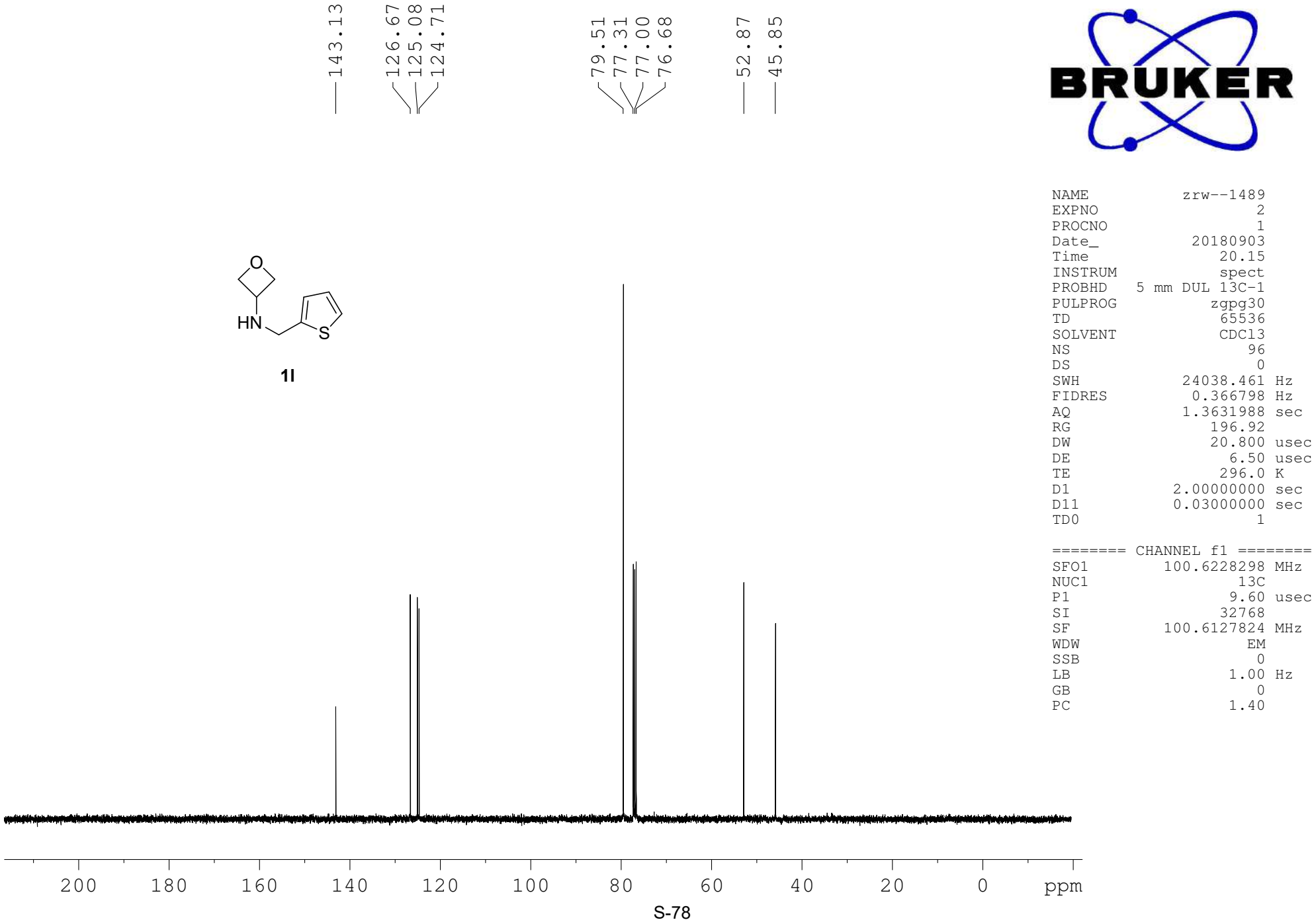


1l




```
NAME            zrw--1489
EXPNO                   1
PROCNO                  1
Date_            20180903
Time                20.09
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ              4.0894966 sec
RG                  54.81
DW                62.400 usec
DE                 6.50 usec
TE                295.5 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                  14.30 usec
SI                  65536
SF            400.1300096 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



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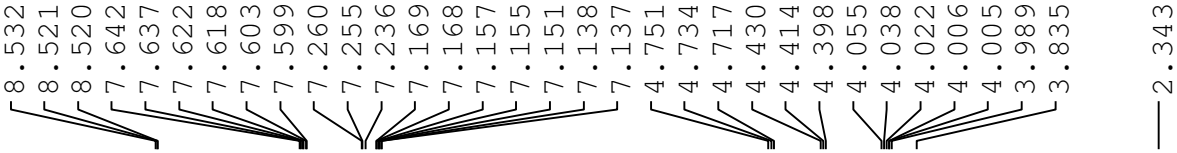
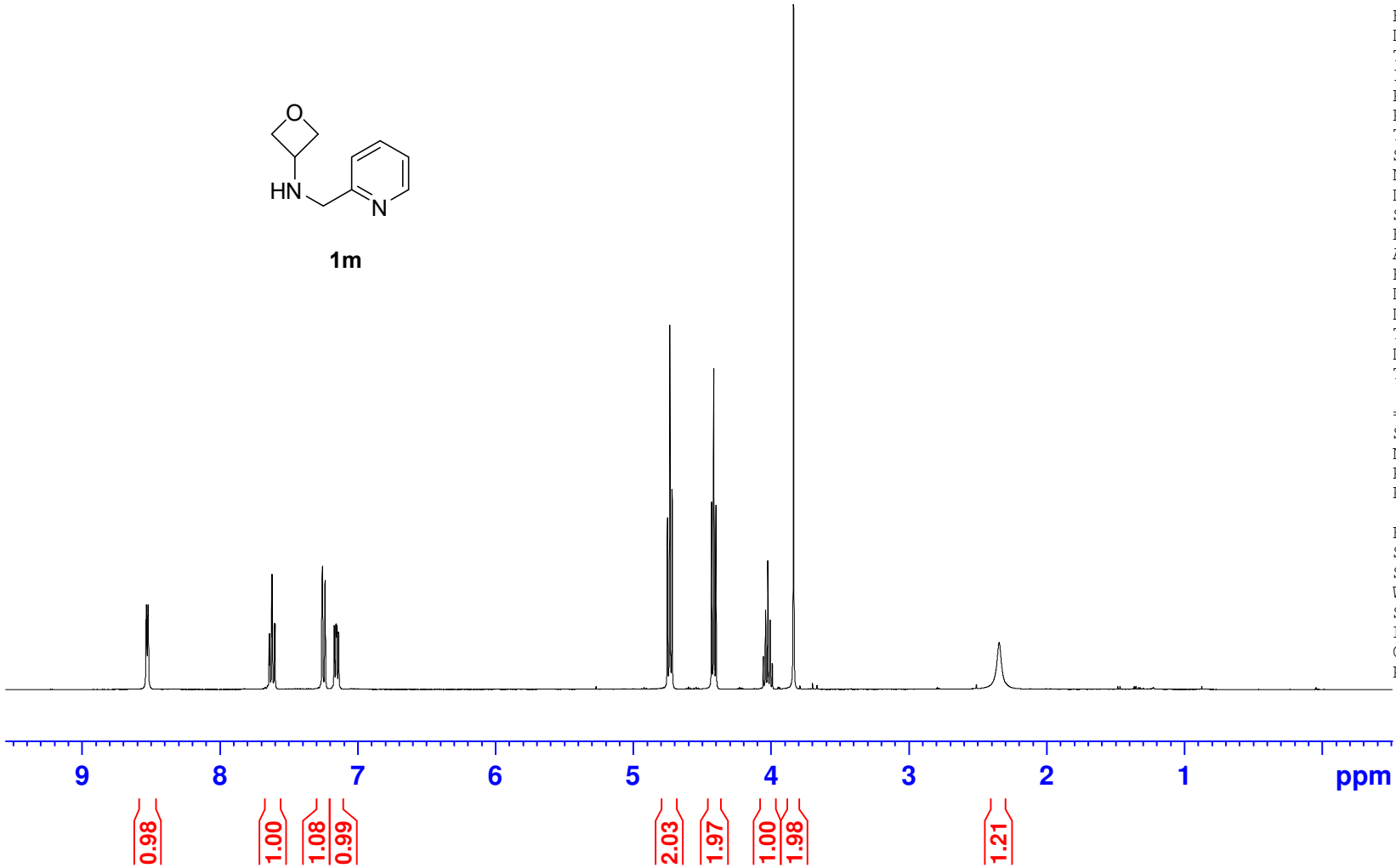
NAME	zrw--1489
EXPNO	2
PROCNO	1
Date_	20180903
Time	20.15
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	96
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.60 usec
SI	32768
SF	100.6127824 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



1m

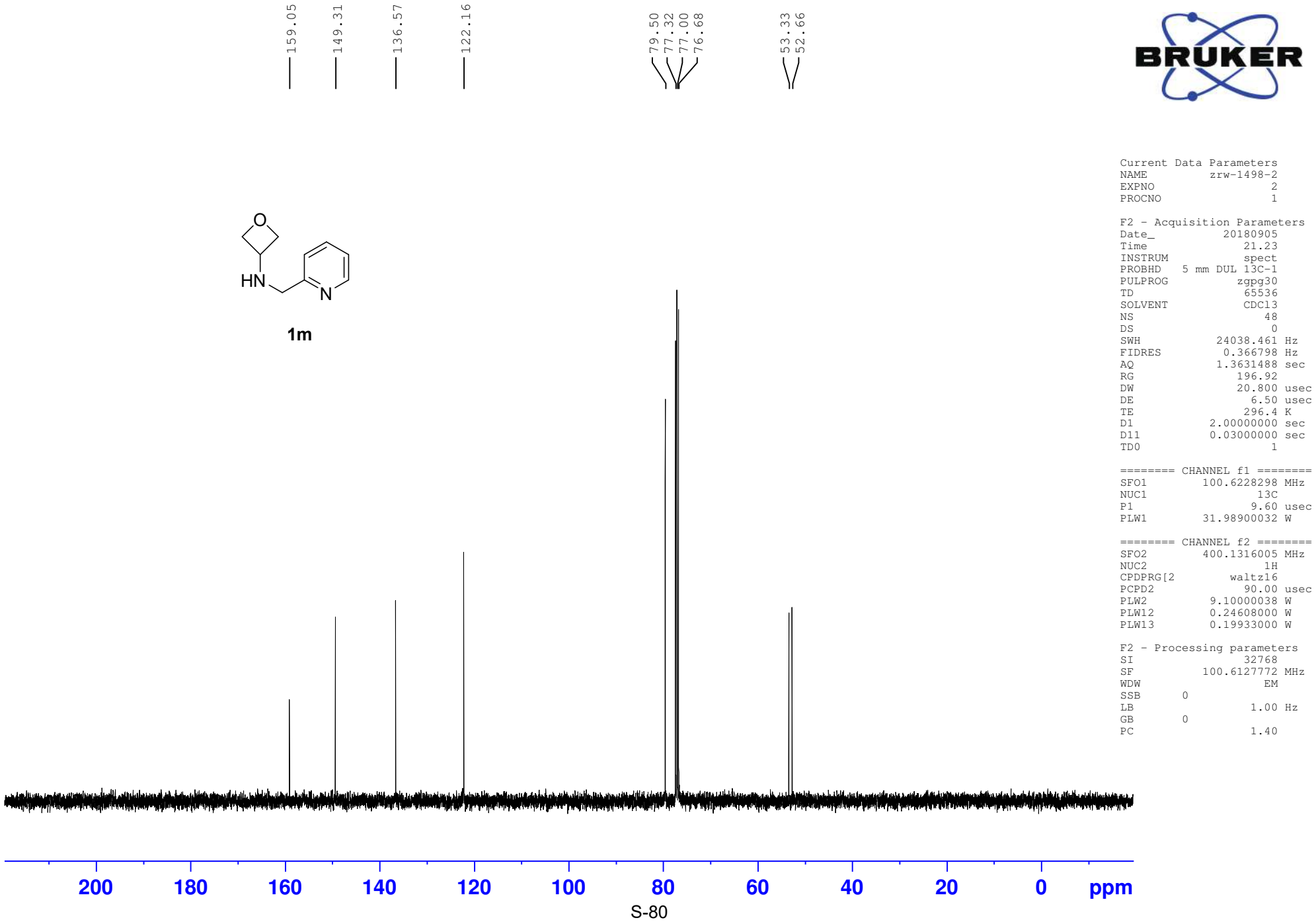


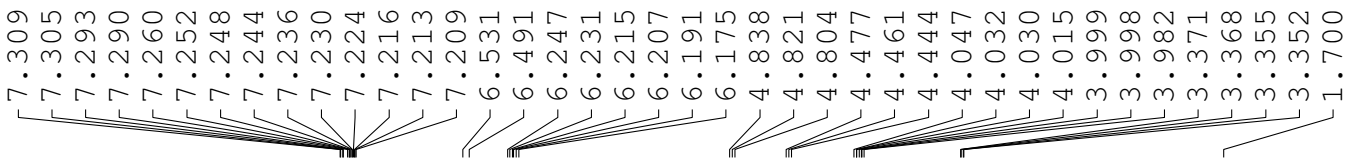

```
Current Data Parameters
NAME                  zrw-1498-2
EXPNO                          1
PROCNO                         1

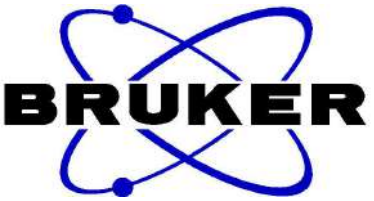
F2 - Acquisition Parameters
Date_                   20180905
Time                       21.20
INSTRUM                    spect
PROBHD    5 mm DUL 13C-1
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             8
DS                             0
SWH                     8012.820 Hz
FIDRES                  0.122266 Hz
AQ                      4.0894465 sec
RG                         82.92
DW                        62.400 usec
DE                         6.50 usec
TE                        295.8 K
D1                    1.00000000 sec
TD0                            1

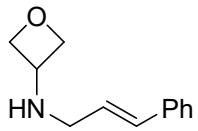
======== CHANNEL f1 ========
SFO1                 400.1324710 MHz
NUC1                         1H
P1                        14.30 usec
PLW1                  9.10000038 W

F2 - Processing parameters
SI                         65536
SF                   400.1300097 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```

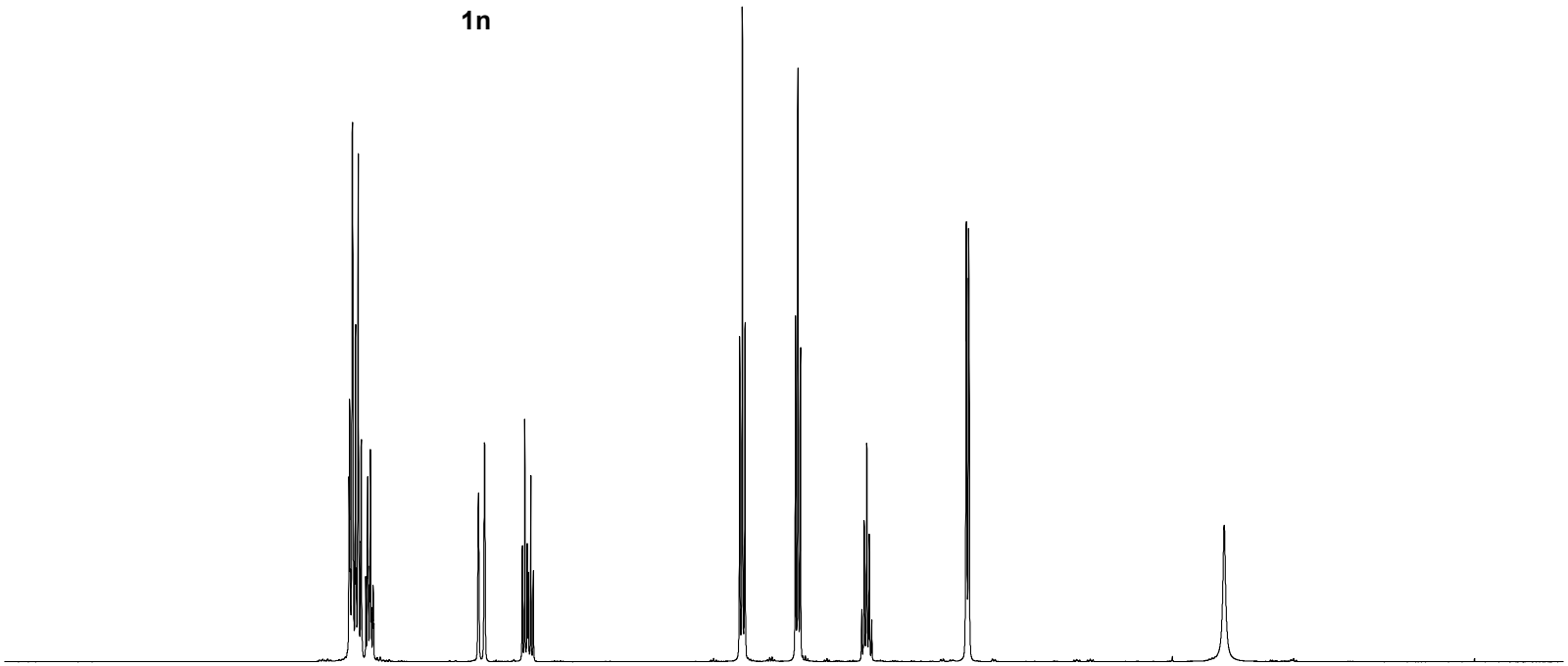

159.05
149.31
136.57
122.16
79.50
77.32
77.00
76.68
53.33
52.66
O
HN
N
1m
Current Data Parameters
NAME zrw-1498-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180905
Time 21.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.60 usec
PLW1 31.98900032 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 9.10000038 W
PLW12 0.24608000 W
PLW13 0.19933000 W
F2 - Processing parameters
SI 32768
SF 100.6127772 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

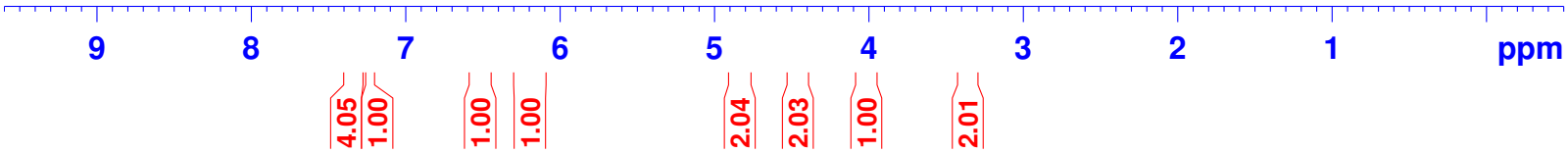




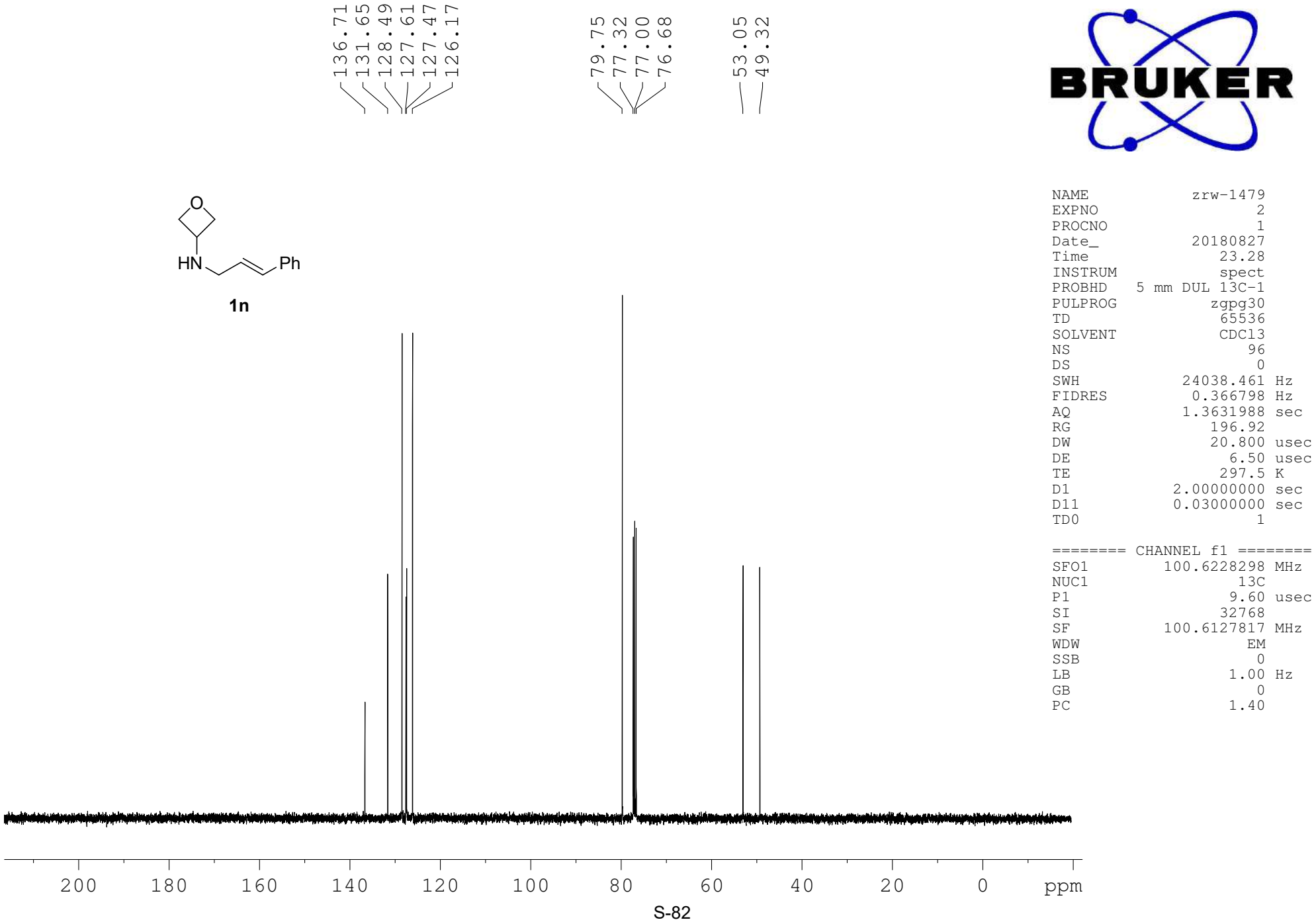


1n

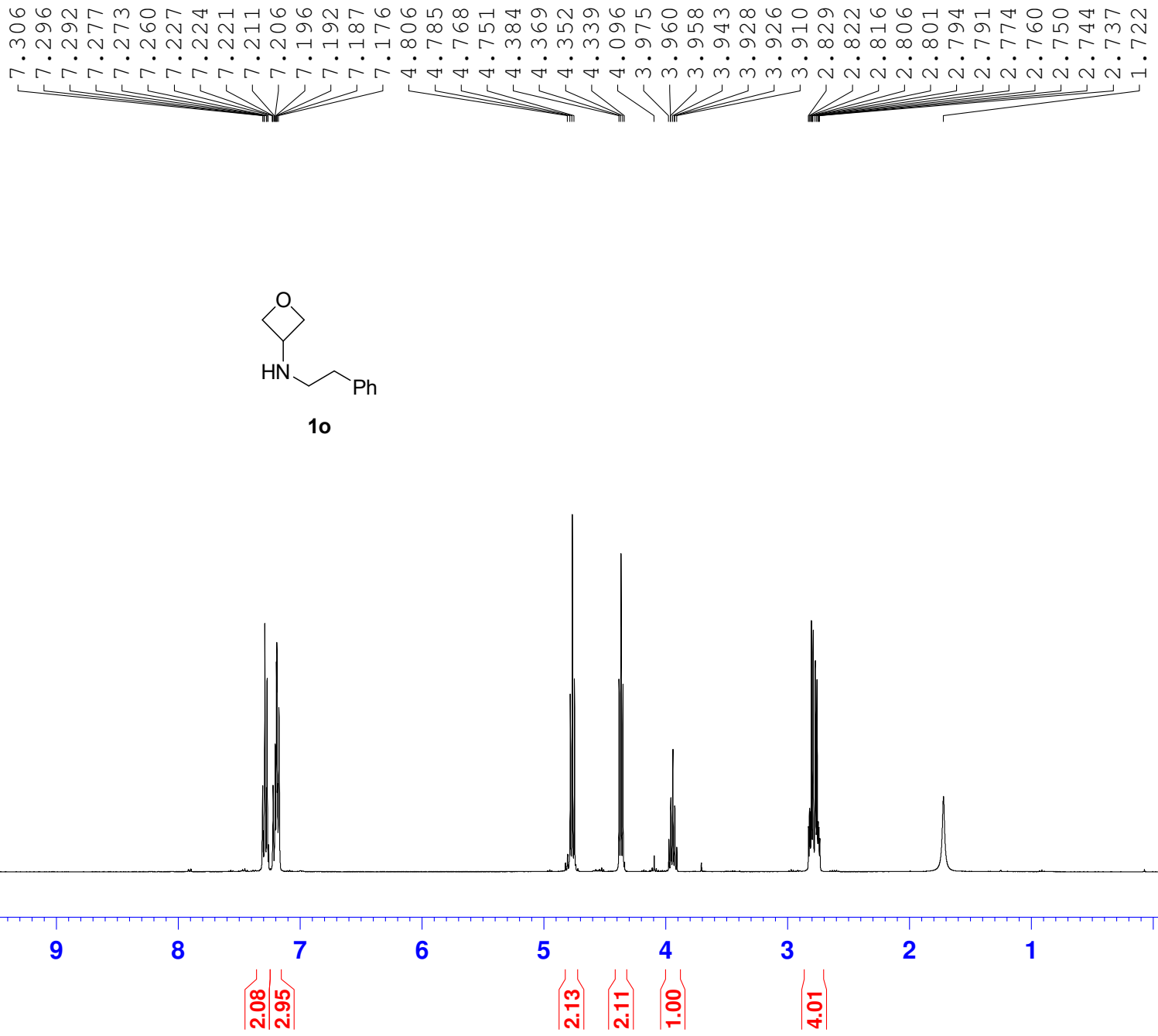




NAME	zrw-1479
EXPNO	1
PROCNO	1
Date_	20180827
Time	23.25
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	34.77
DW	62.400 usec
DE	6.50 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.30 usec
SI	65536
SF	400.1300097 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

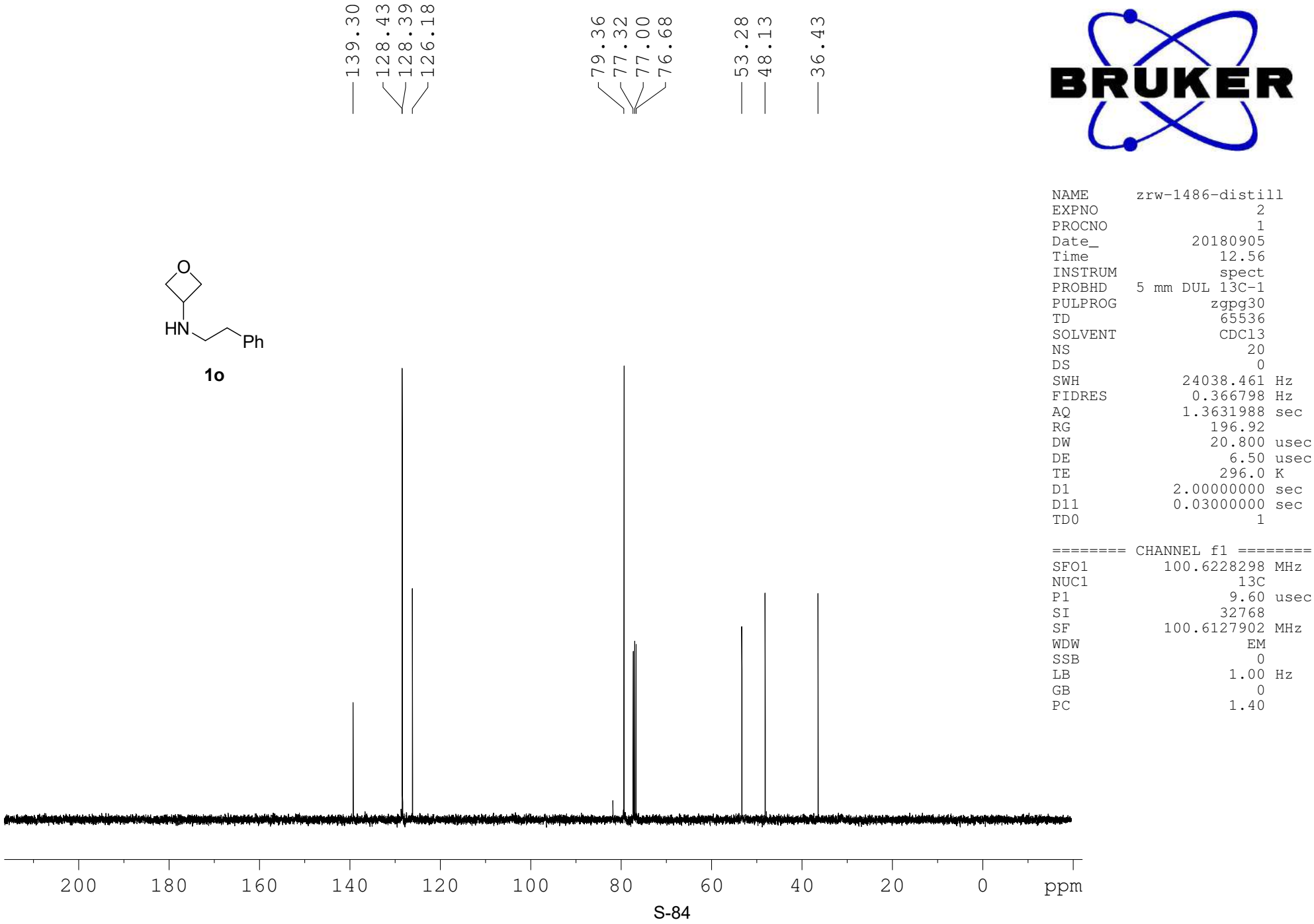


NAME	zrw-1479
EXPNO	2
PROCNO	1
Date_	20180827
Time	23.28
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	96
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.60 usec
SI	32768
SF	100.6127817 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



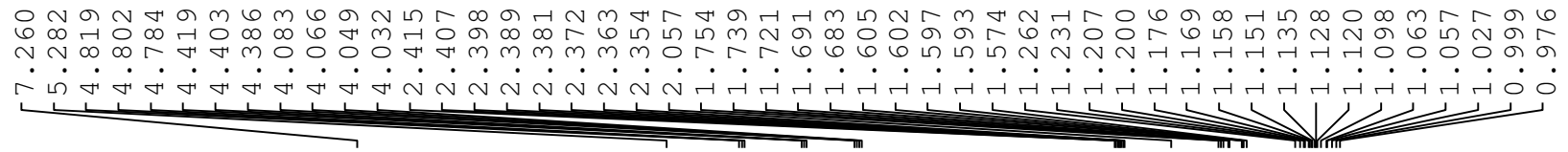
BRUKER

NAME	zrw-1486-distill
EXPNO	1
PROCNO	1
Date_	20180905
Time	12.55
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	2
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	22.47
DW	62.400 usec
DE	6.50 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.30 usec
SI	65536
SF	400.1300095 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

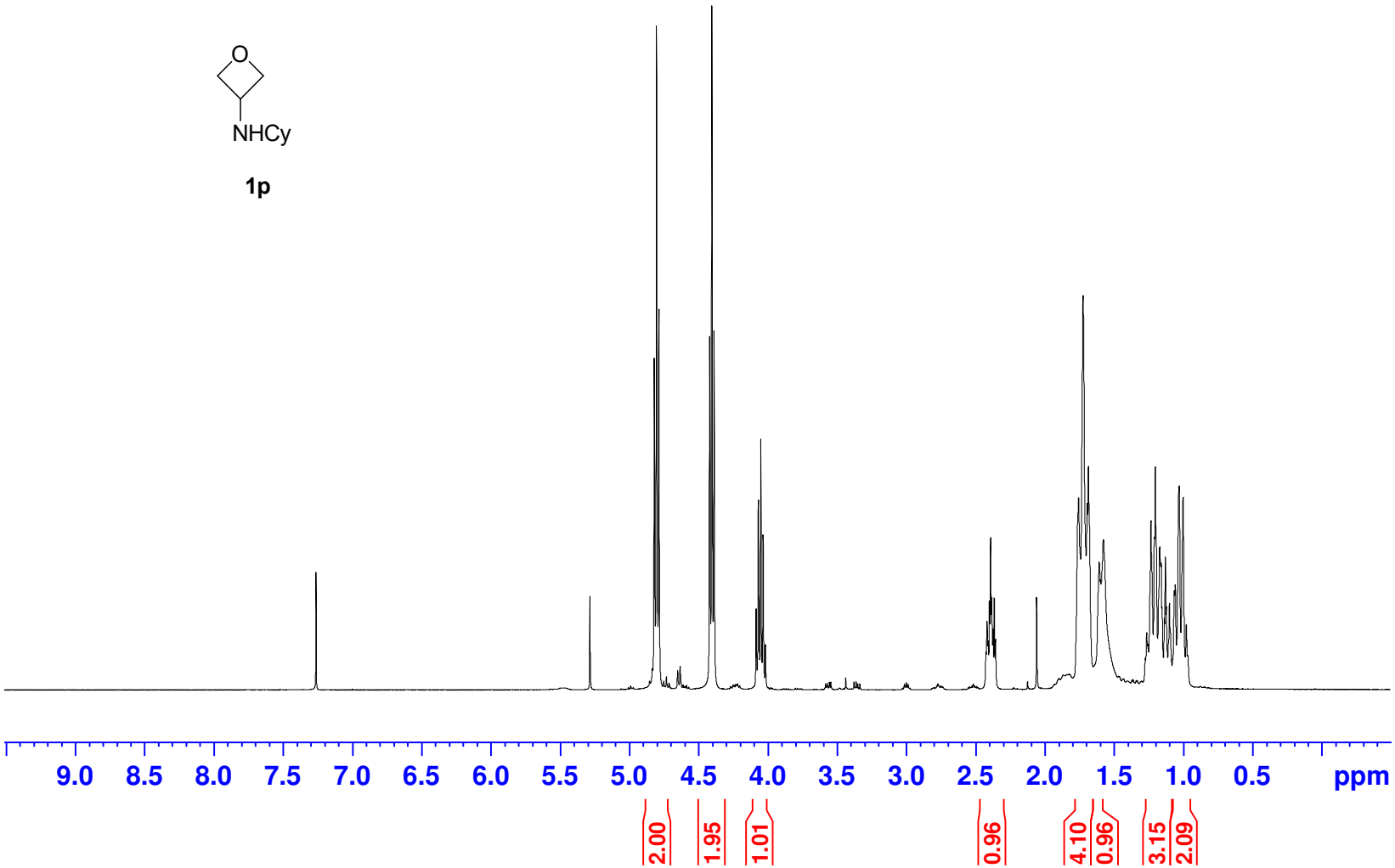



```
NAME      zrw-1486-distill
EXPNO                    2
PROCNO                   1
Date_             20180905
Time                 12.56
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     20
DS                      0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                 196.92
DW                 20.800 usec
DE                  6.50 usec
TE                 296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                   9.60 usec
SI                  32768
SF            100.6127902 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



1p

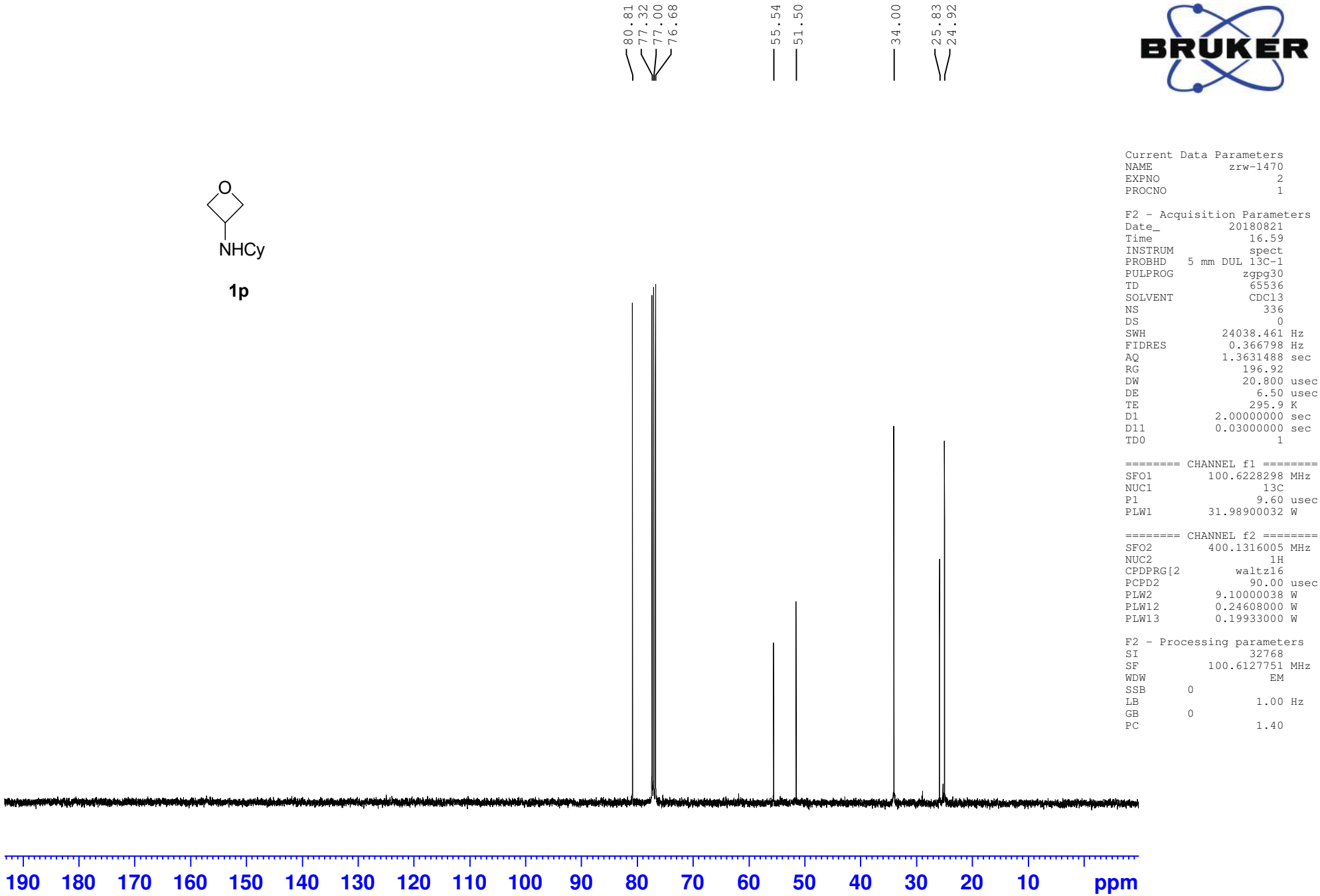



```
Current Data Parameters
NAME                  zrw-1470
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180821
Time                     16.54
INSTRUM                  spect
PROBHD    5 mm DUL 13C-1
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                       70.97
DW                      62.400 usec
DE                       6.50 usec
TE                      295.3 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                       14.30 usec
PLW1                 9.10000038 W

F2 - Processing parameters
SI                           65536
SF                  400.1300096 MHz
WDW                            EM
SSB                 0
LB                        0.30 Hz
GB                  0
PC                       1.00
```



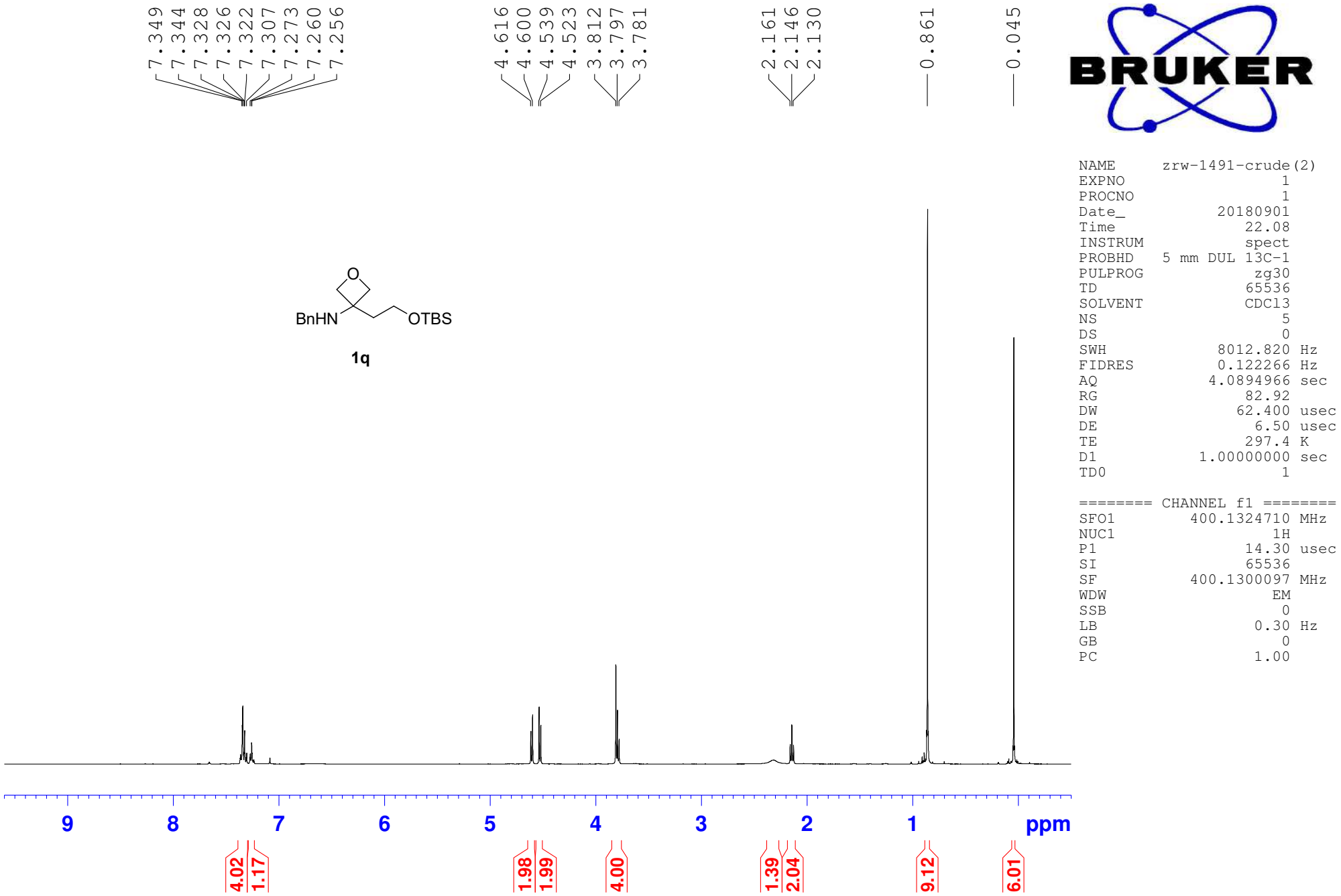

```
Current Data Parameters
NAME                 zrw-1470
EXPNO                       2
PROCNO                      1

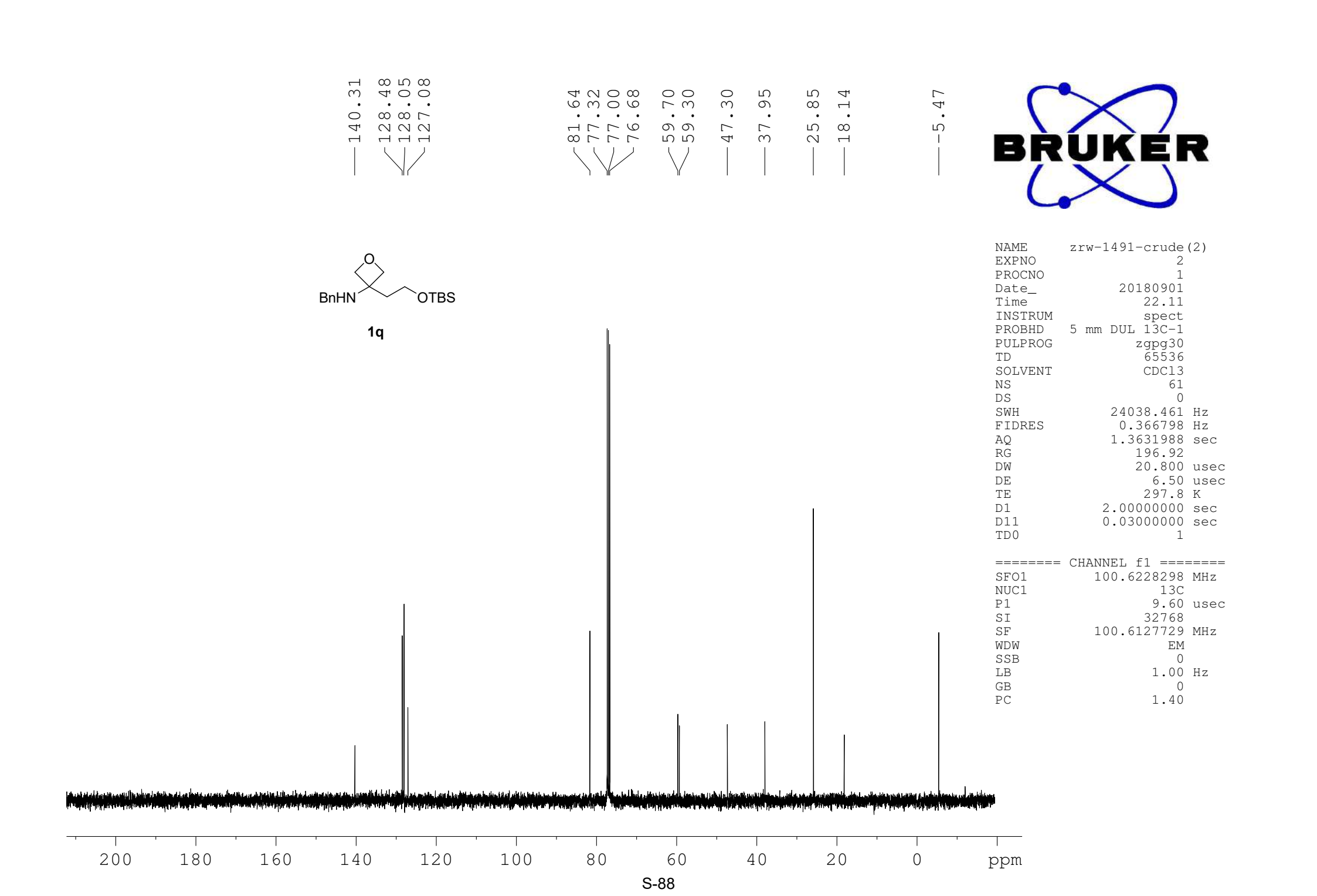
F2 - Acquisition Parameters
Date_               20180821
Time                   16.59
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       336
DS                         0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     295.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

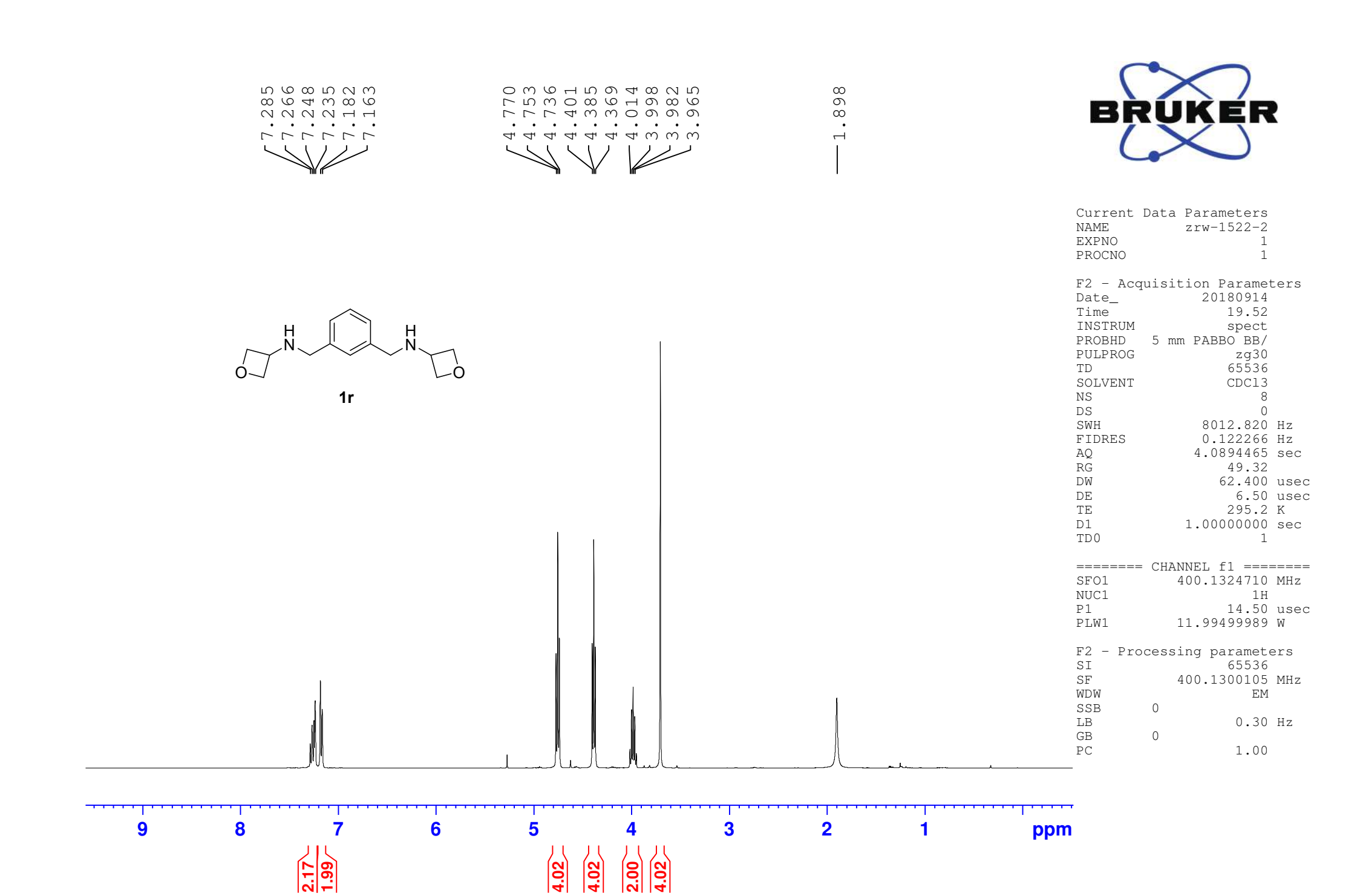
======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                      9.60 usec
PLW1               31.98900032 W

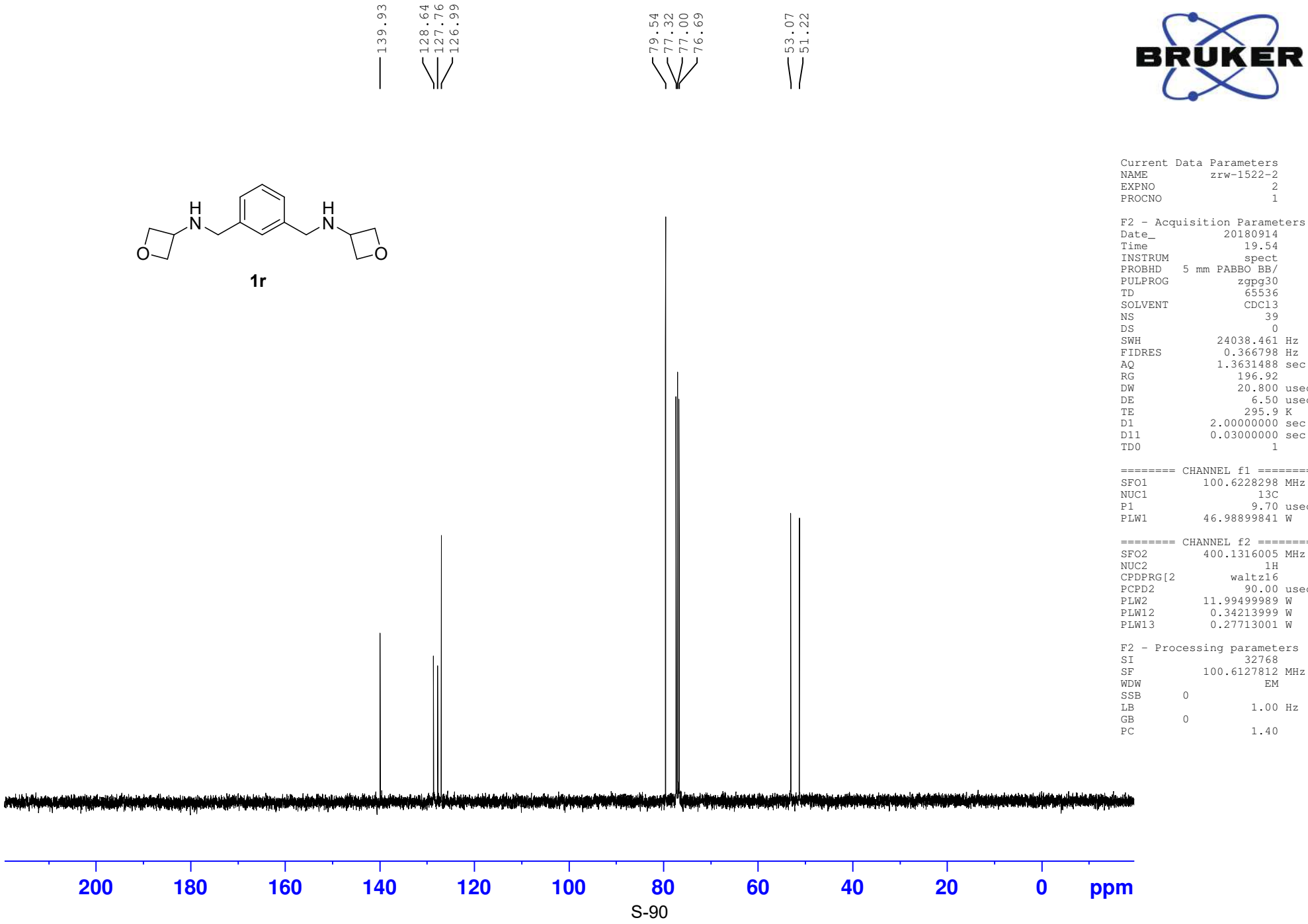
======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2                9.10000038 W
PLW12               0.24608000 W
PLW13               0.19933000 W

F2 - Processing parameters
SI                       32768
SF               100.6127751 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```


7.349
7.344
7.328
7.326
7.322
7.307
7.273
7.260
7.256
4.616
4.600
4.539
4.523
3.812
3.797
3.781
2.161
2.146
2.130
0.861
0.045
BRUKER
NAME zrw-1491-crude(2)
EXPNO 1
PROCNO 1
Date_ 20180901
Time 22.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 82.92
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.30 usec
SI 65536
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
BnHN
OTBS
1q
9
8
7
6
5
4
3
2
1
ppm
4.02
1.17
1.98
1.99
4.00
1.39
2.04
9.12
6.01


140.31
128.48
128.05
127.08
81.64
77.32
77.00
76.68
59.70
59.30
47.30
37.95
25.85
18.14
-5.47
BRUKER
O
BnHN
OTBS
1q
NAME zrw-1491-crude(2)
EXPNO 2
PROCNO 1
Date_ 20180901
Time 22.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 61
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.60 usec
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


7.285
7.266
7.248
7.235
7.182
7.163
4.770
4.753
4.736
4.401
4.385
4.369
4.014
3.998
3.982
3.965
1.898
BRUKER
H
N
H
N
O
O
1r
Current Data Parameters
NAME zrw-1522-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180914
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 49.32
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W
F2 - Processing parameters
SI 65536
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
2.17
1.99
4.02
4.02
2.00
4.02



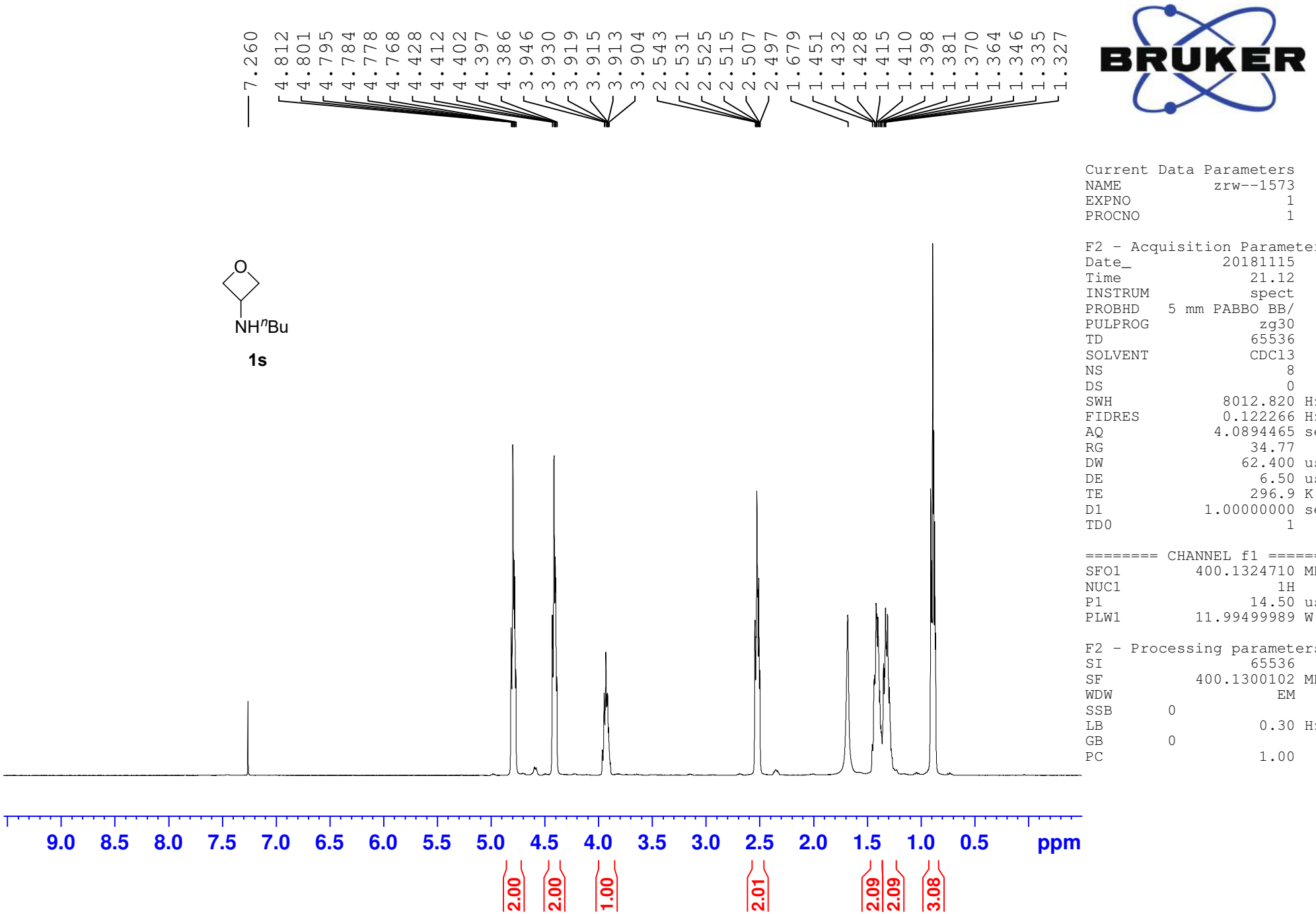

```
Current Data Parameters
NAME          zrw-1522-2
EXPNO                  2
PROCNO                 1

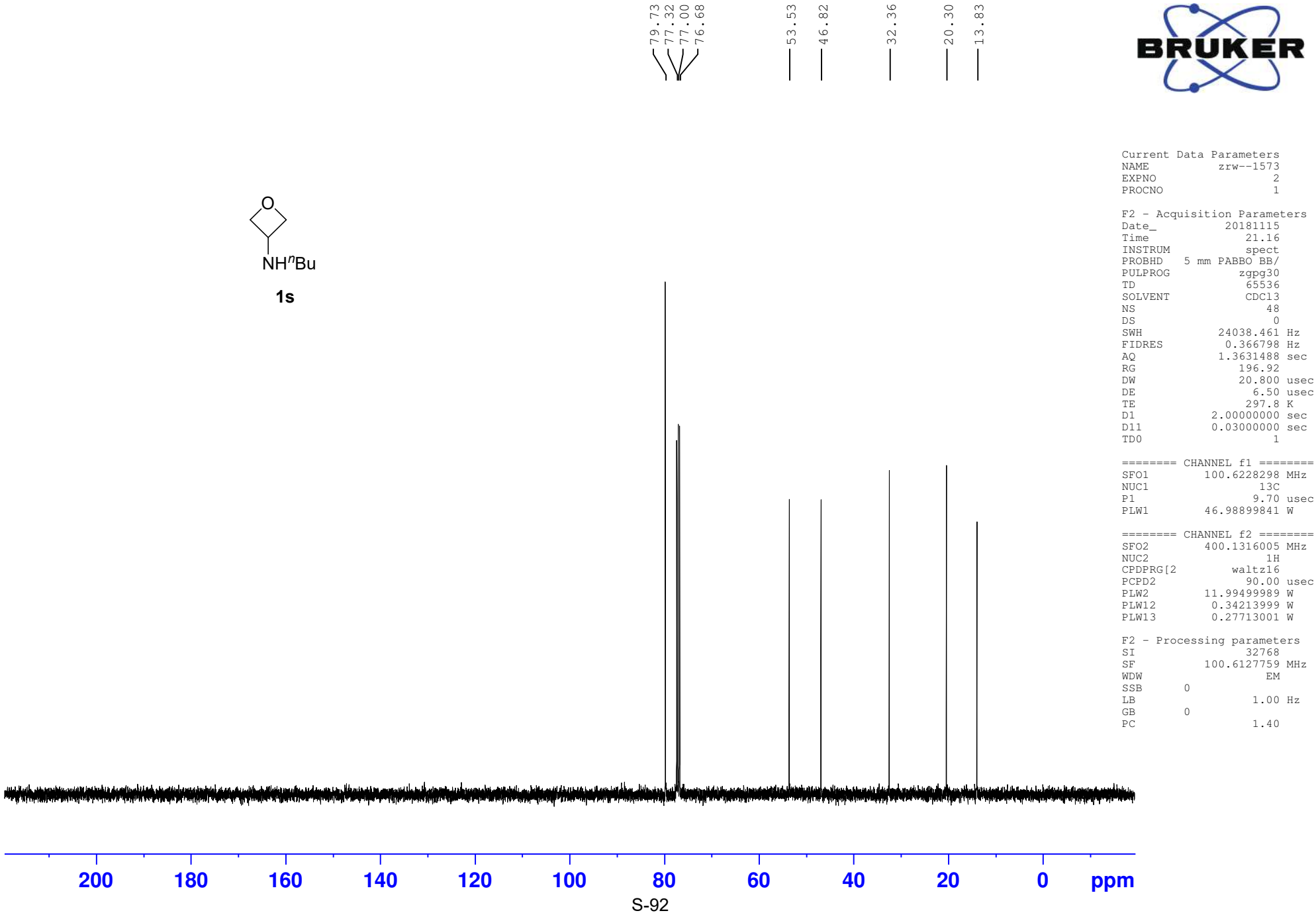
F2 - Acquisition Parameters
Date_           20180914
Time               19.54
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   39
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

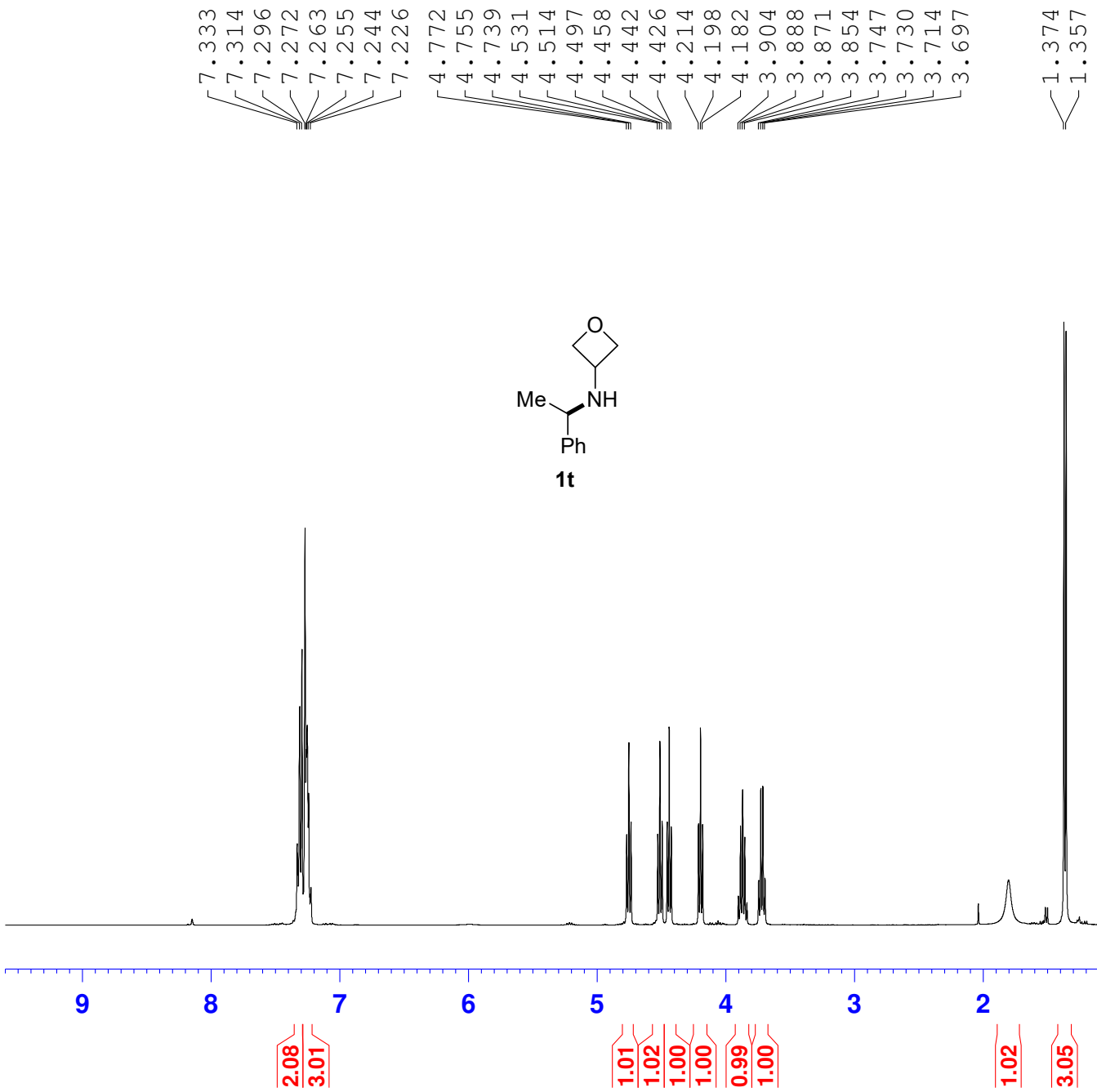
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

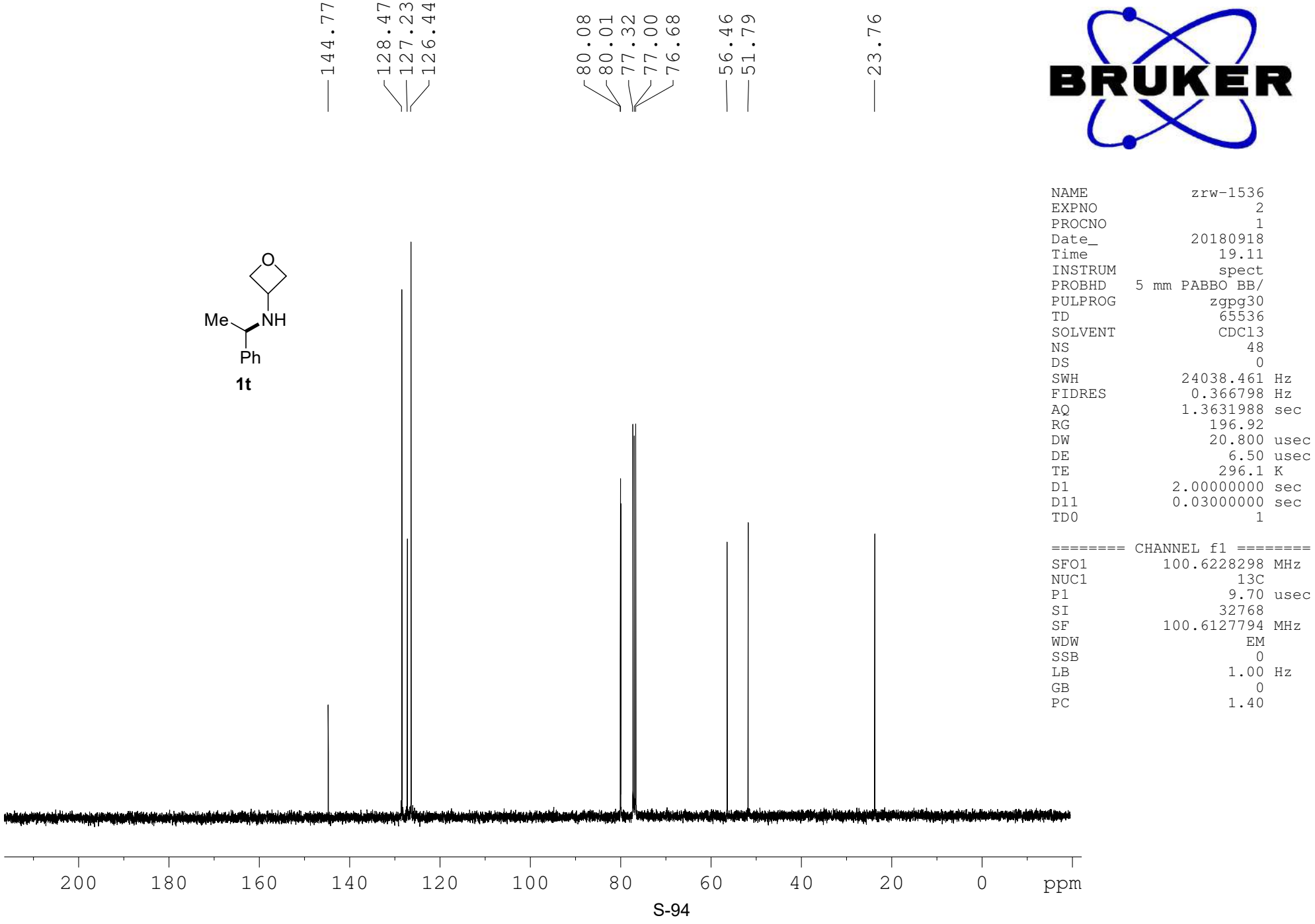
F2 - Processing parameters
SI                 32768
SF           100.6127812 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


7.260
4.812
4.801
4.795
4.784
4.778
4.768
4.428
4.412
4.402
4.397
4.386
3.946
3.930
3.919
3.915
3.913
3.904
2.543
2.531
2.525
2.515
2.507
2.497
1.679
1.451
1.432
1.428
1.415
1.410
1.398
1.381
1.370
1.364
1.346
1.335
1.327
O
NH^{n}Bu
1s
Current Data Parameters
NAME zrw--1573
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181115
Time 21.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 34.77
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W
F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.00
1.00
2.01
2.09
2.09
3.08


79.73
77.32
77.00
76.68
53.53
46.82
32.36
20.30
13.83
O
NH^{n}Bu
1s
Current Data Parameters
NAME zrw--1573
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181115
Time 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W
F2 - Processing parameters
SI 32768
SF 100.6127759 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

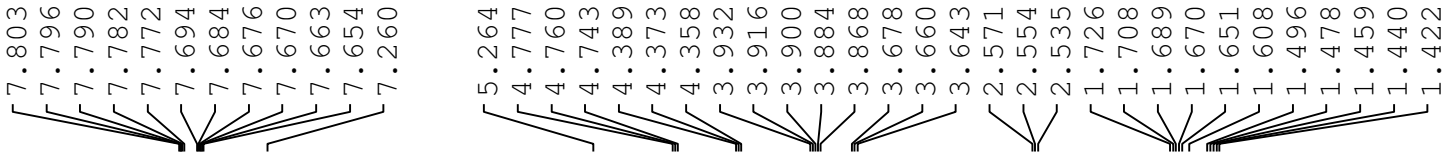


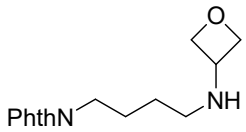
NAME	zrw-1536
EXPNO	1
PROCNO	1
Date_	20180918
Time	19.08
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	31.55
DW	62.400 usec
DE	6.50 usec
TE	295.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300106 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



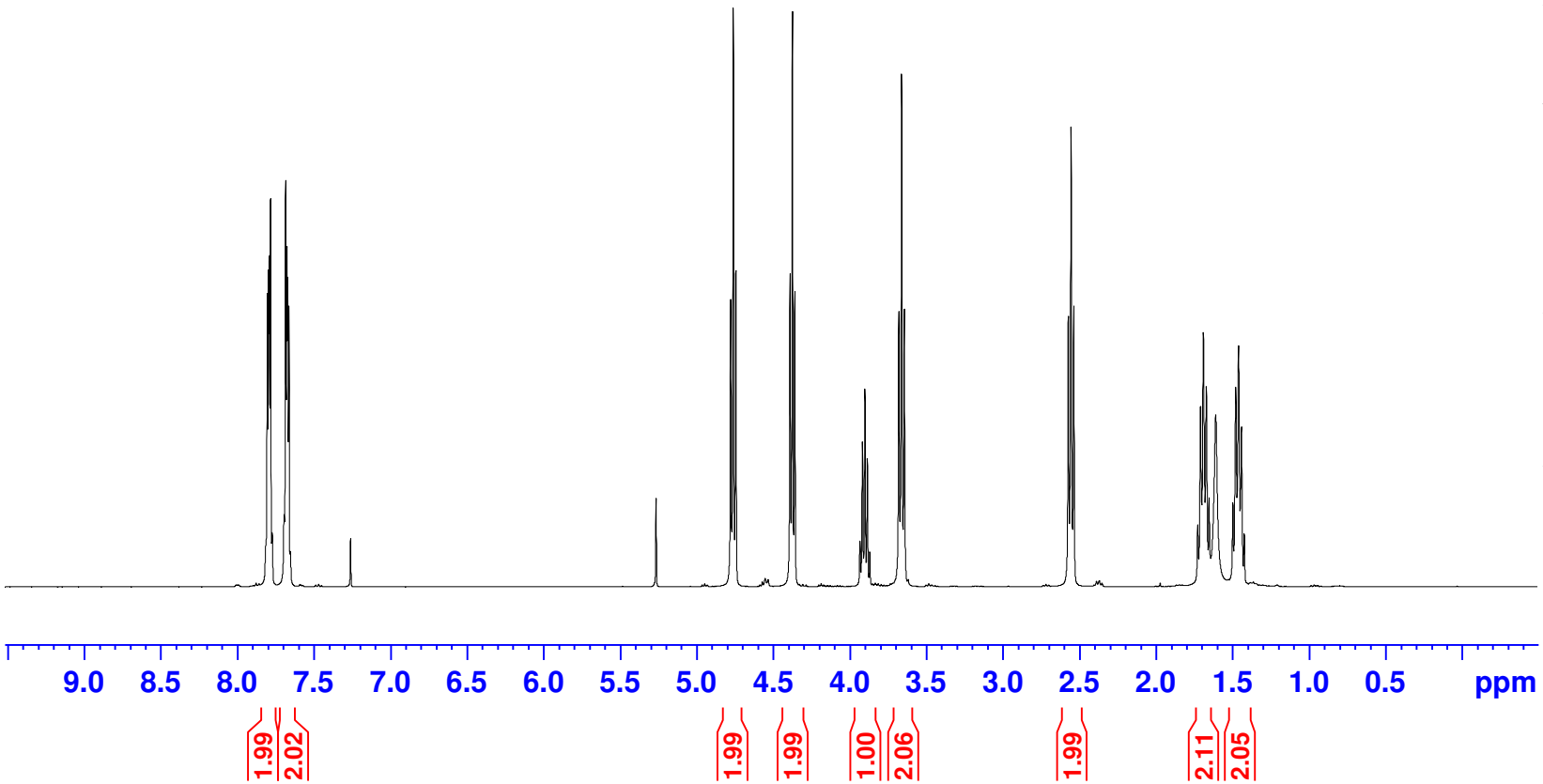
BRUKER

NAME	zrw-1536
EXPNO	2
PROCNO	1
Date_	20180918
Time	19.11
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127794 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





1u

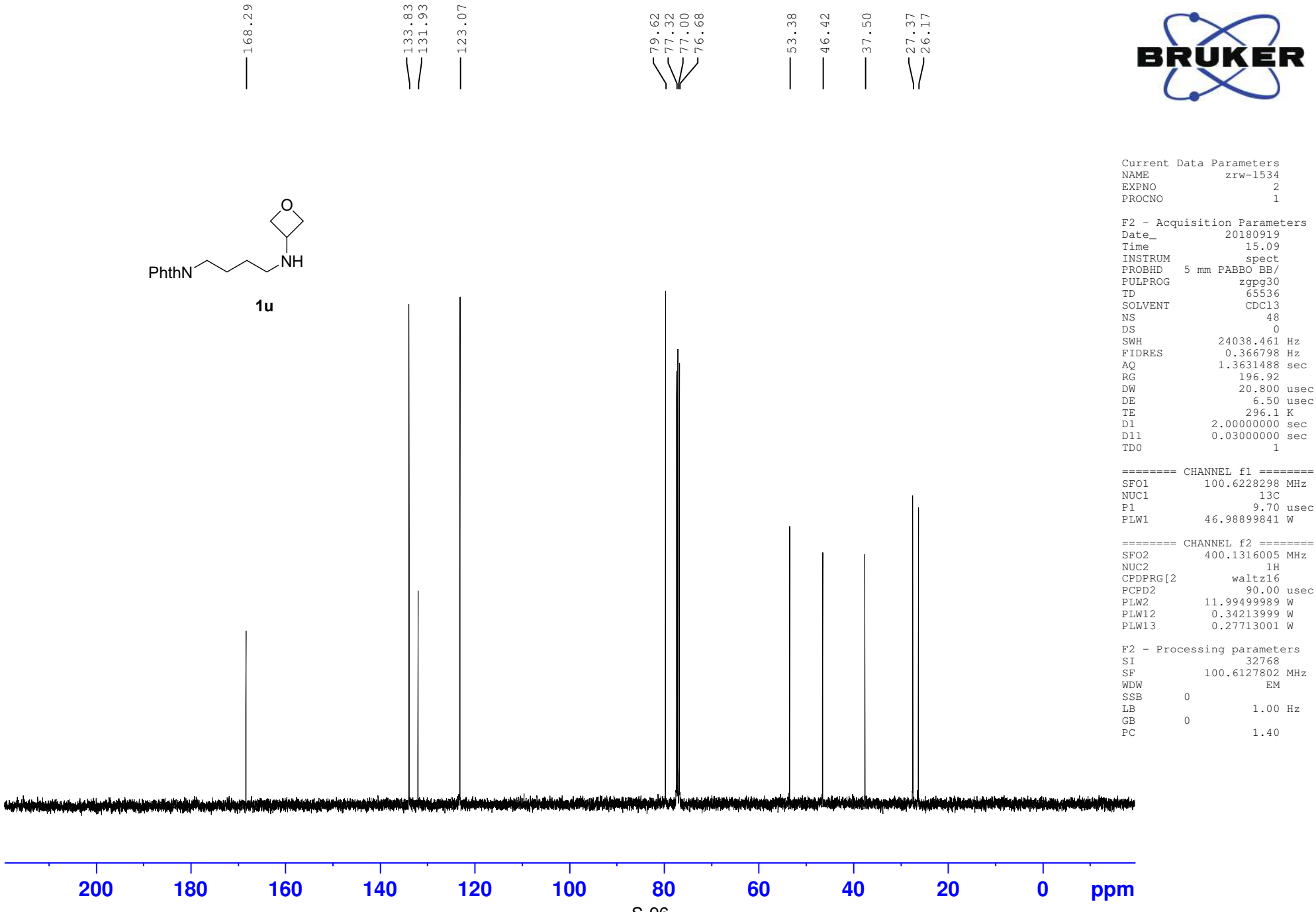



```
Current Data Parameters
NAME                 zrw-1534
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180919
Time                   15.06
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                     34.77
DW                    62.400 usec
DE                     6.50 usec
TE                    295.2 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                    14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                         65536
SF               400.1300104 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



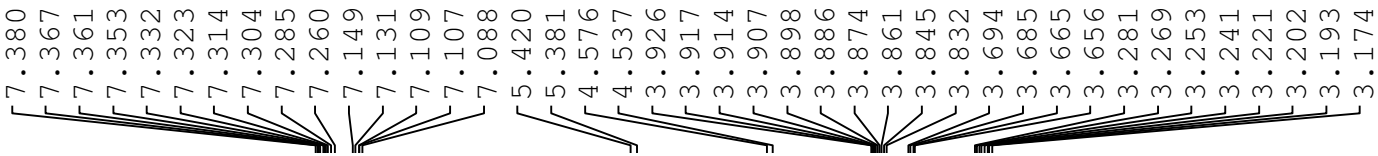

```
Current Data Parameters
NAME                 zrw-1534
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180919
Time                   15.09
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         48
DS                          0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     296.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

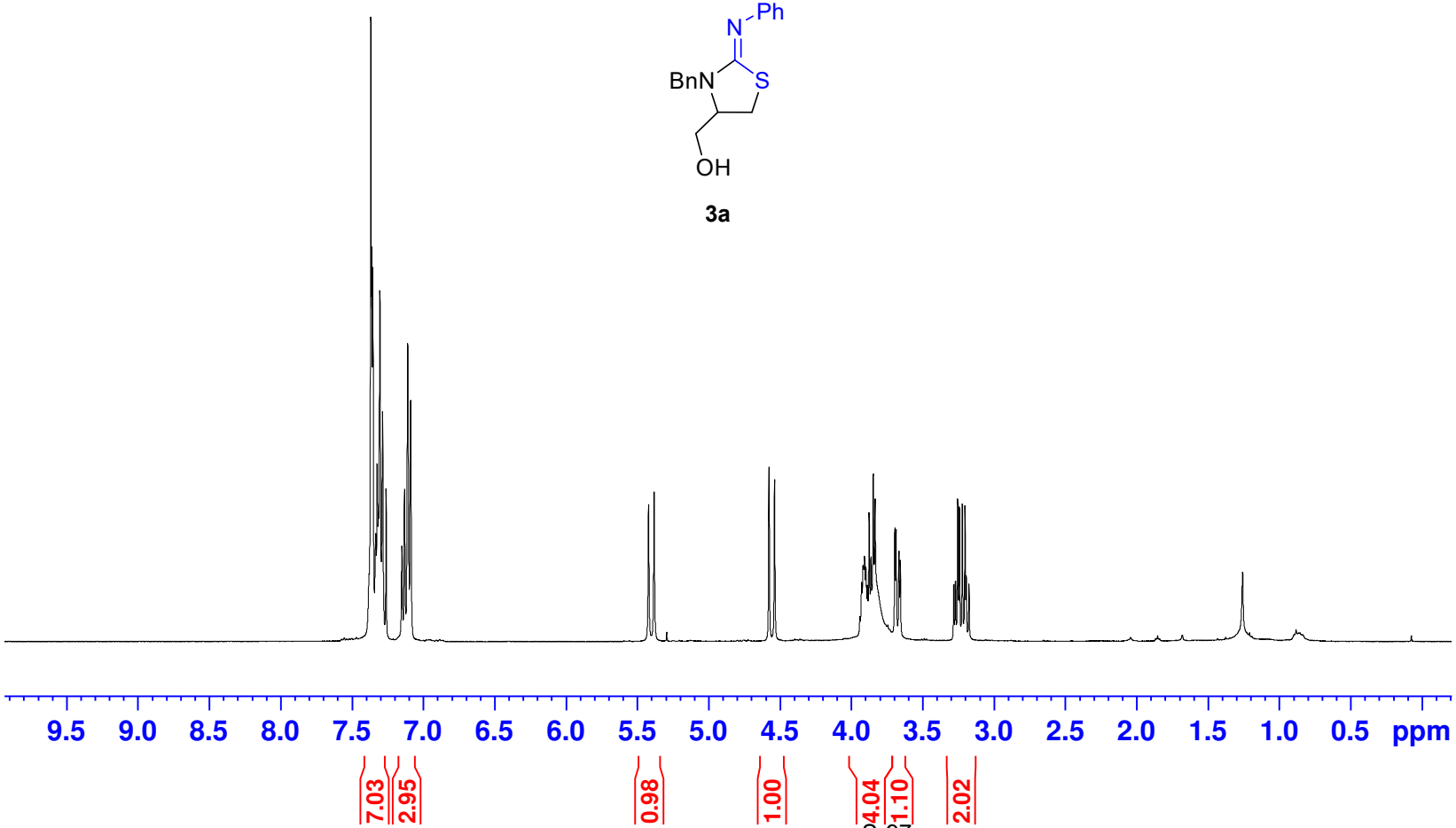
======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                        9.70 usec
PLW1               46.98899841 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2               11.99499989 W
PLW12               0.34213999 W
PLW13               0.27713001 W

F2 - Processing parameters
SI                         32768
SF                 100.6127802 MHz
WDW                        EM
SSB             0
LB                        1.00 Hz
GB              0
PC                        1.40
```



3a

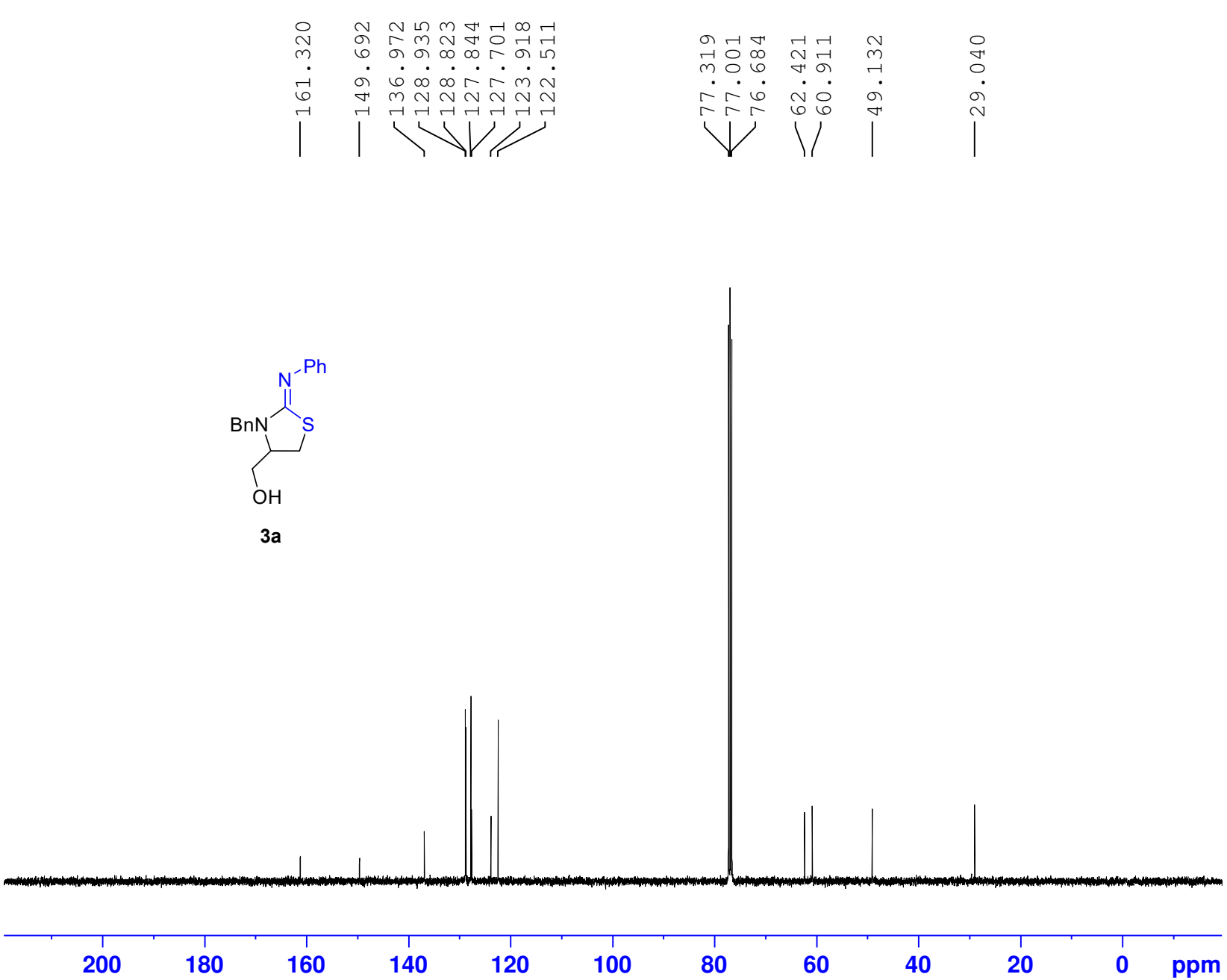



```
Current Data Parameters
NAME                  lzw1077A
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141105
Time                     19.34
INSTRUM                  spect
PROBHD    5 mm DUL 13C-1
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           6
DS                           2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       88.84
DW                     62.400 usec
DE                      6.50 usec
TE                      295.4 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                       1H
P1                      14.30 usec
PLW1                9.10000038 W

F2 - Processing parameters
SI                           65536
SF                 400.1300097 MHz
WDW                             EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



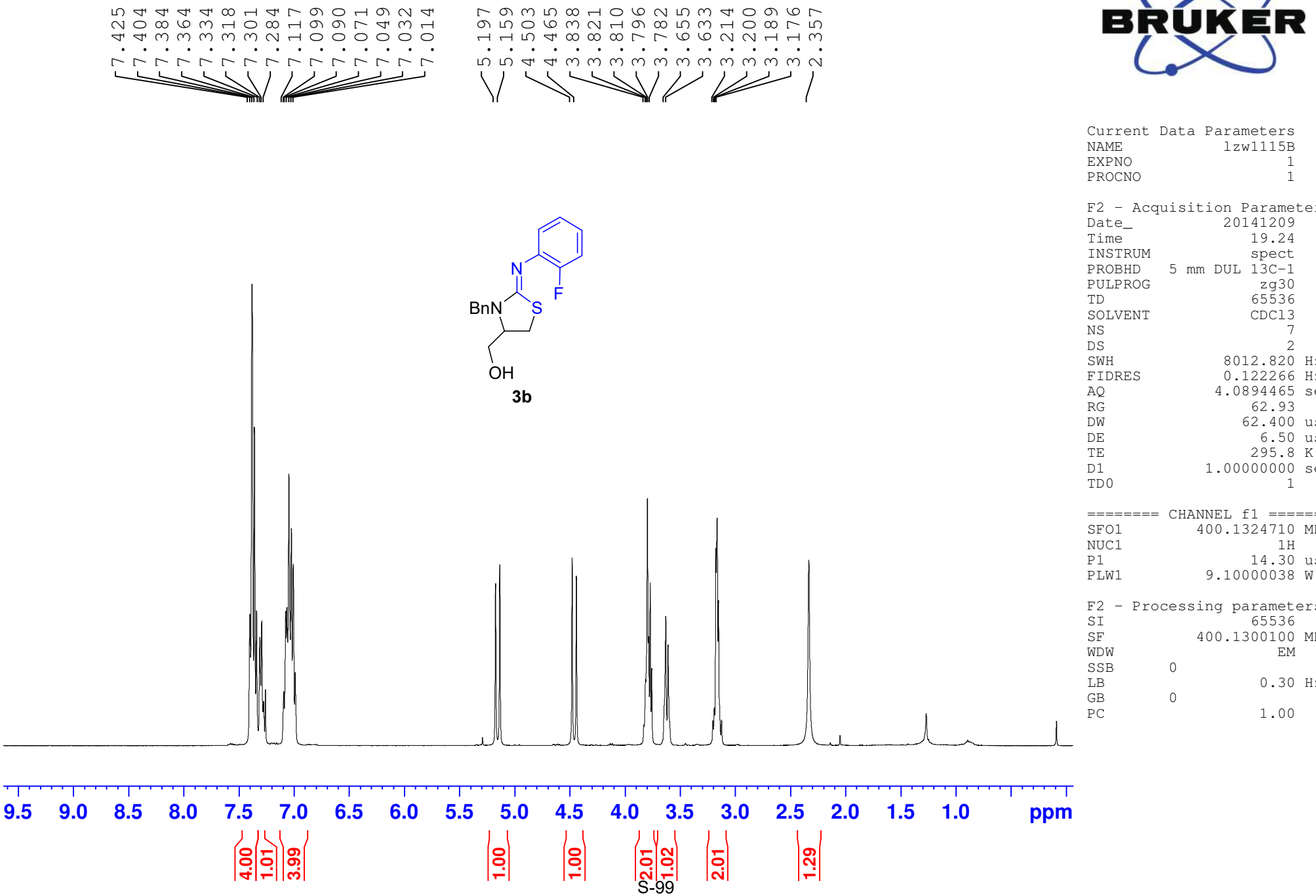

```
Current Data Parameters
NAME                 lzw1077A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20141105
Time                   16.26
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG              zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        273
DS                          2
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    196.92
DW                    20.800 usec
DE                     6.50 usec
TE                    297.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              100.6228298 MHz
NUC1                      13C
P1                      9.60 usec
PLW1              31.98900032 W

======== CHANNEL f2 ========
SFO2              400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                   90.00 usec
PLW2               9.10000038 W
PLW12              0.24608000 W
PLW13              0.19933000 W

F2 - Processing parameters
SI                        32768
SF                400.6127735 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

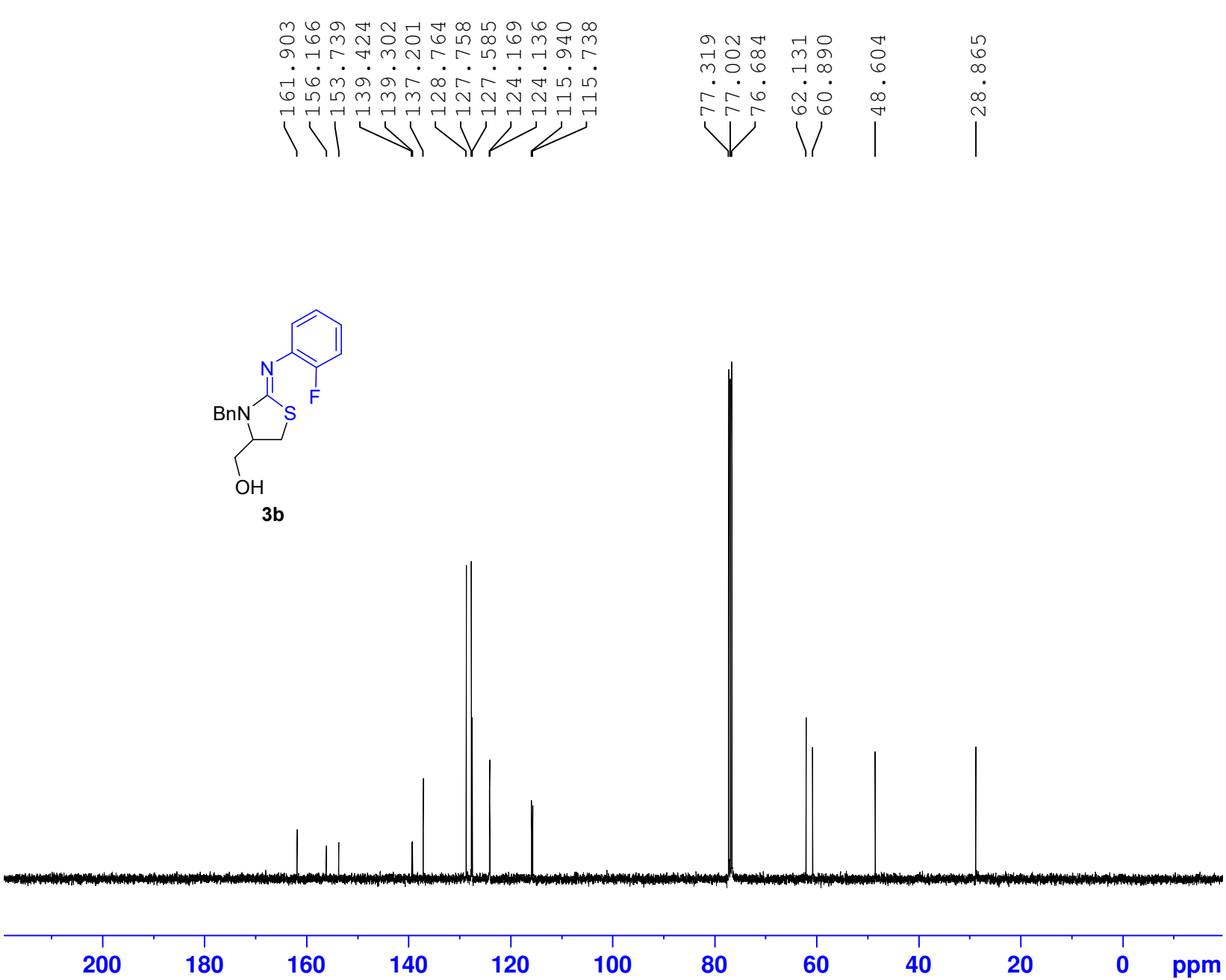


Current Data Parameters
NAME lzw1115B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141209
Time 19.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 62.93
DW 62.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.30 usec
PLW1 9.10000038 W

F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



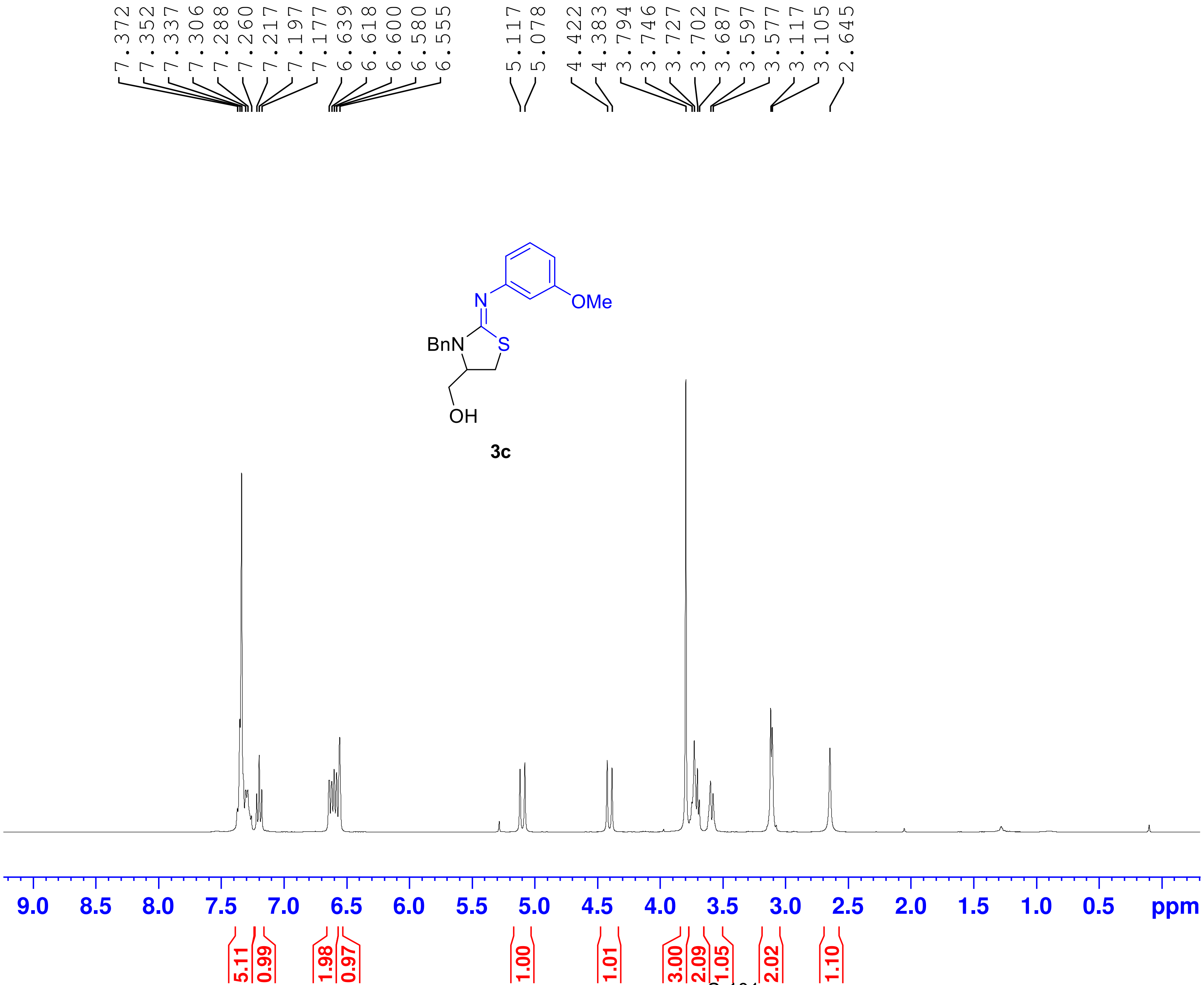

```
Current Data Parameters
NAME                  lzw1115B
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141209
Time                     19.33
INSTRUM                  spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         126
DS                           2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                      196.92
DW                      20.800 usec
DE                       6.50 usec
TE                      296.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                        9.60 usec
PLW1               31.98900032 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                9.10000038 W
PLW12               0.24608000 W
PLW13               0.19933000 W

F2 - Processing parameters
SI                         32768
SF                 100.6127768 MHz
WDW                           EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



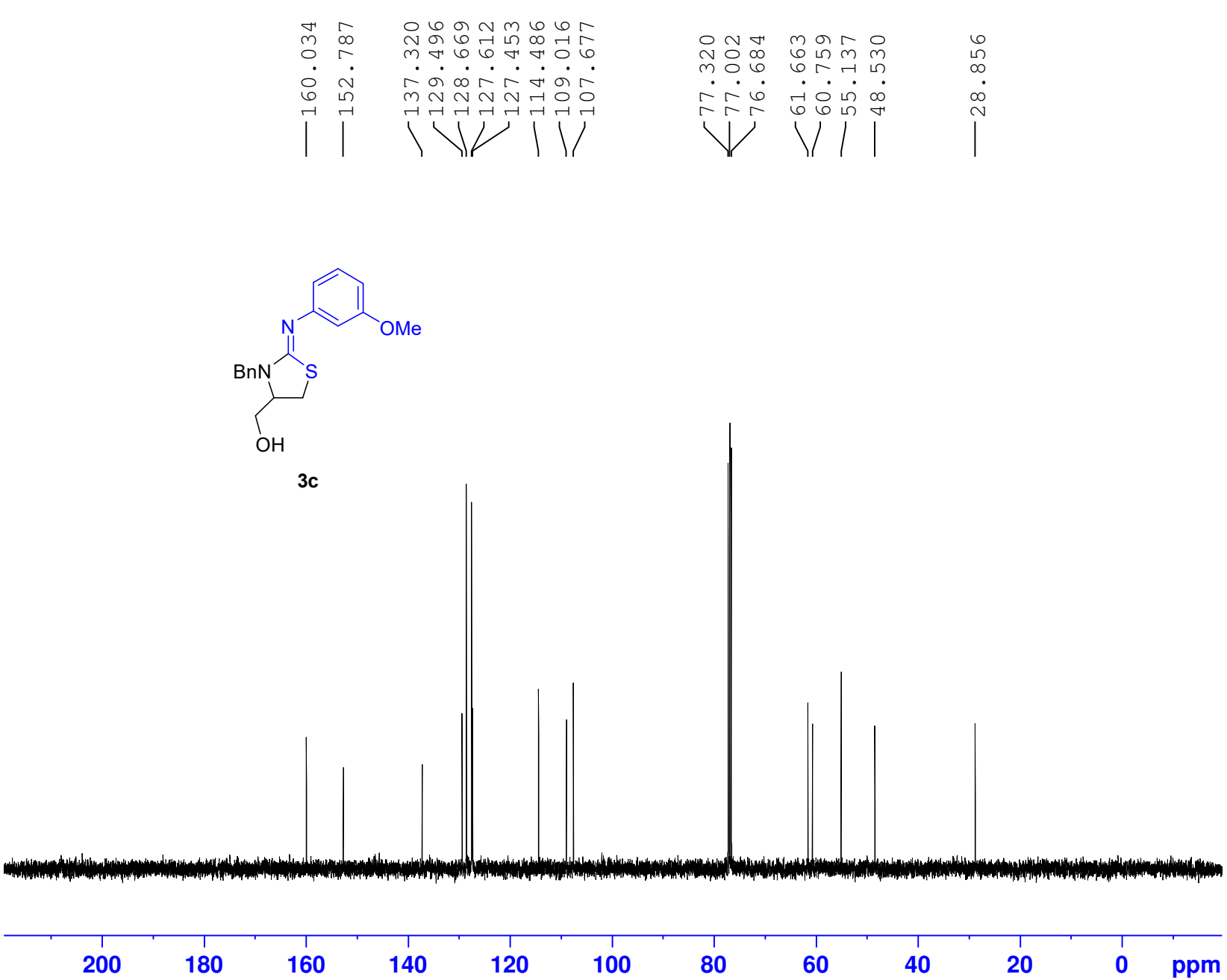
3c

Current Data Parameters
NAME lzw1120D
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141213
Time 19.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 27.78
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.30 usec
PLW1 9.10000038 W

F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



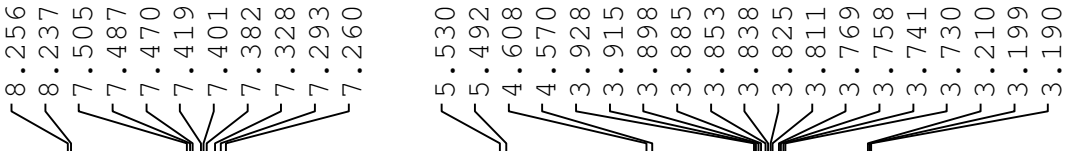

```
Current Data Parameters
NAME            lzw1120D
EXPNO                  4
PROCNO                 1

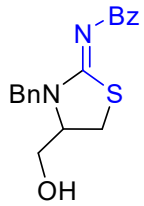
F2 - Acquisition Parameters
Date_           20141213
Time               19.45
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    26
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.60 usec
PLW1         31.98900032 W

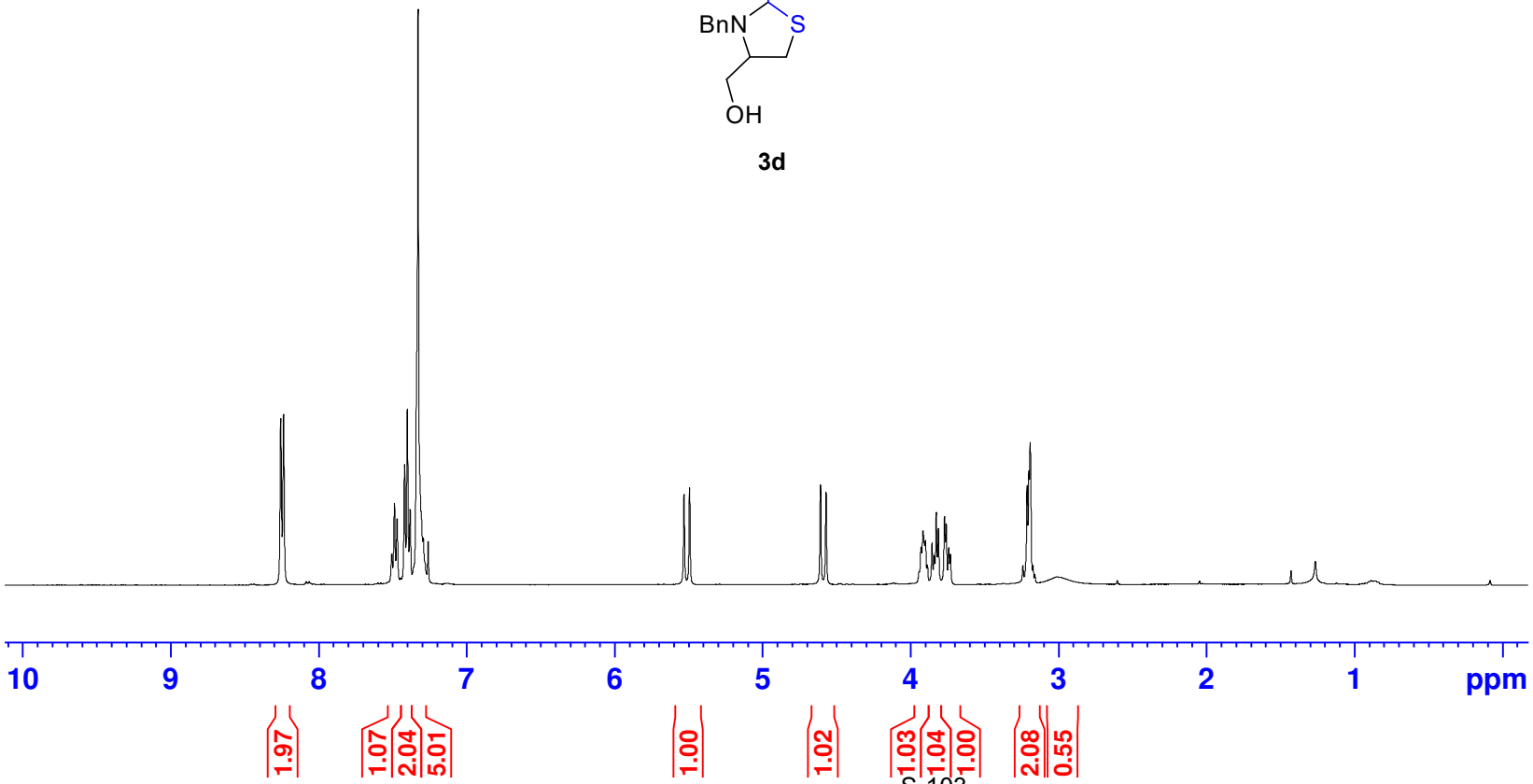
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2          9.10000038 W
PLW12         0.24608000 W
PLW13         0.19933000 W

F2 - Processing parameters
SI                 32768
SF           100.6127822 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





3d

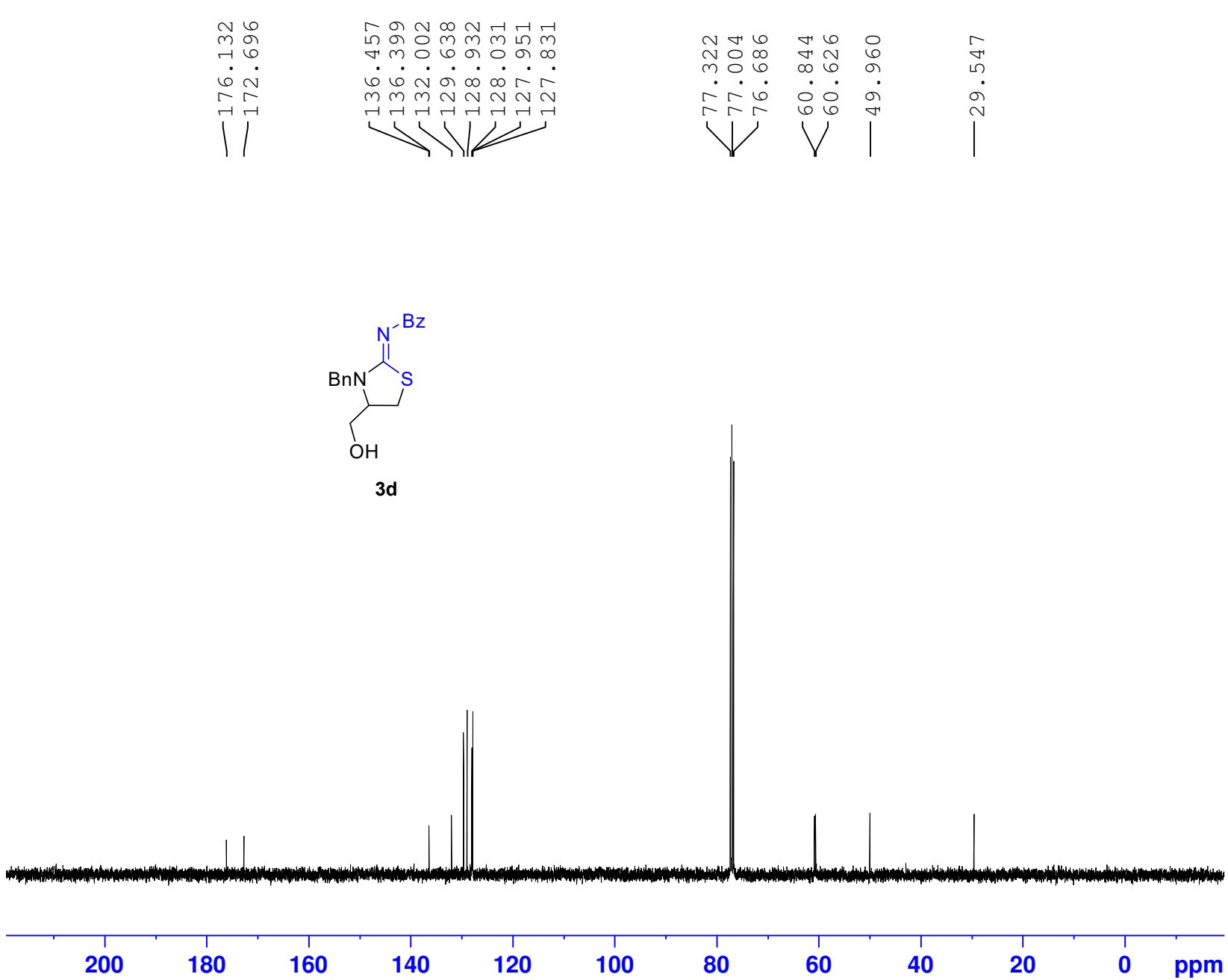



```
Current Data Parameters
NAME                  lzw1179
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20150122
Time                   21.29
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                          9
DS                          2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                     82.92
DW                    62.400 usec
DE                     6.50 usec
TE                     295.7 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                       1H
P1                      14.30 usec
PLW1             9.10000038 W

F2 - Processing parameters
SI                         65536
SF              400.1300097 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



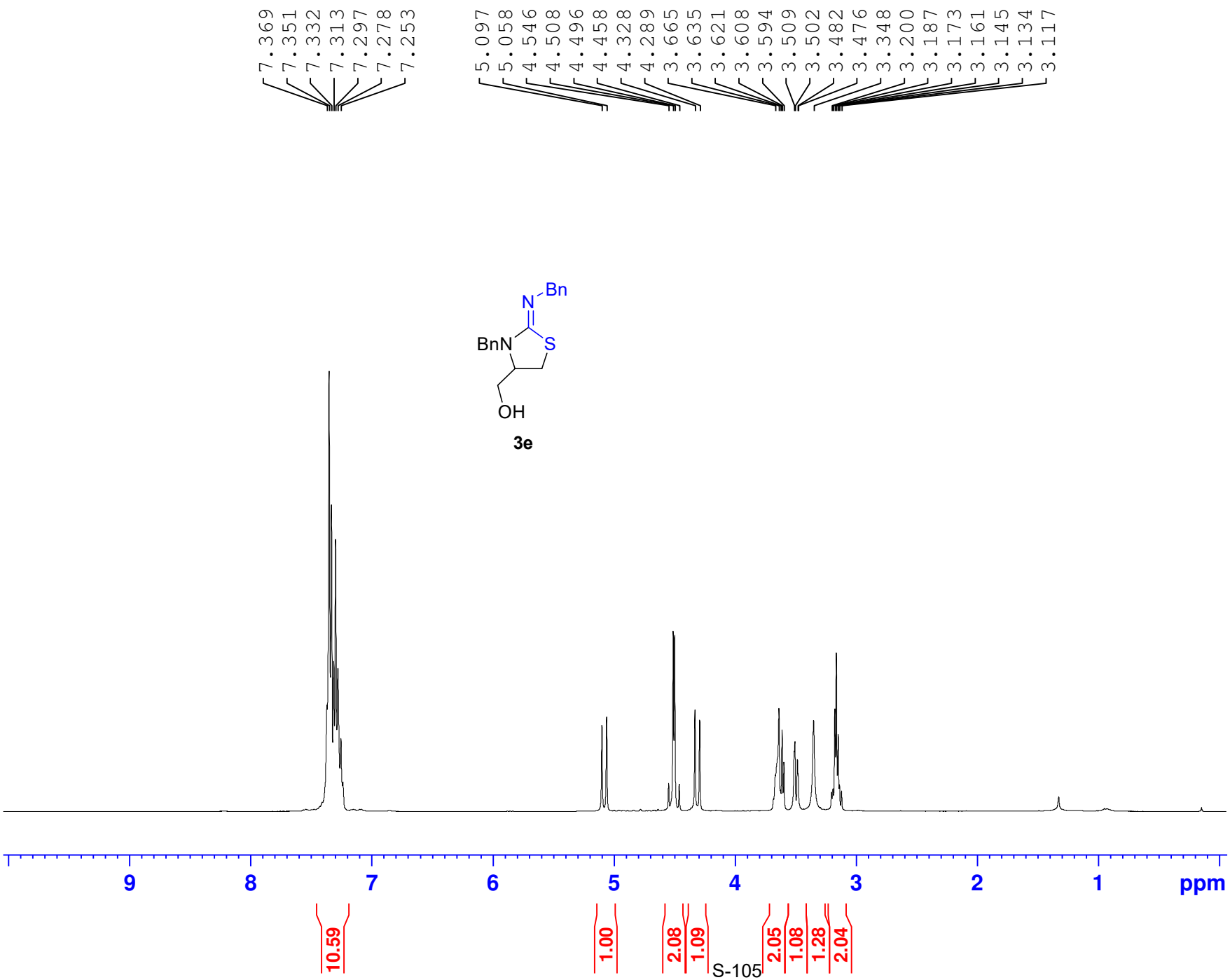
Current Data Parameters
NAME lzw1179
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150122
Time 11.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 49
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.60 usec
PLW1 31.98900032 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 9.10000038 W
PLW12 0.24608000 W
PLW13 0.19933000 W

F2 - Processing parameters
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

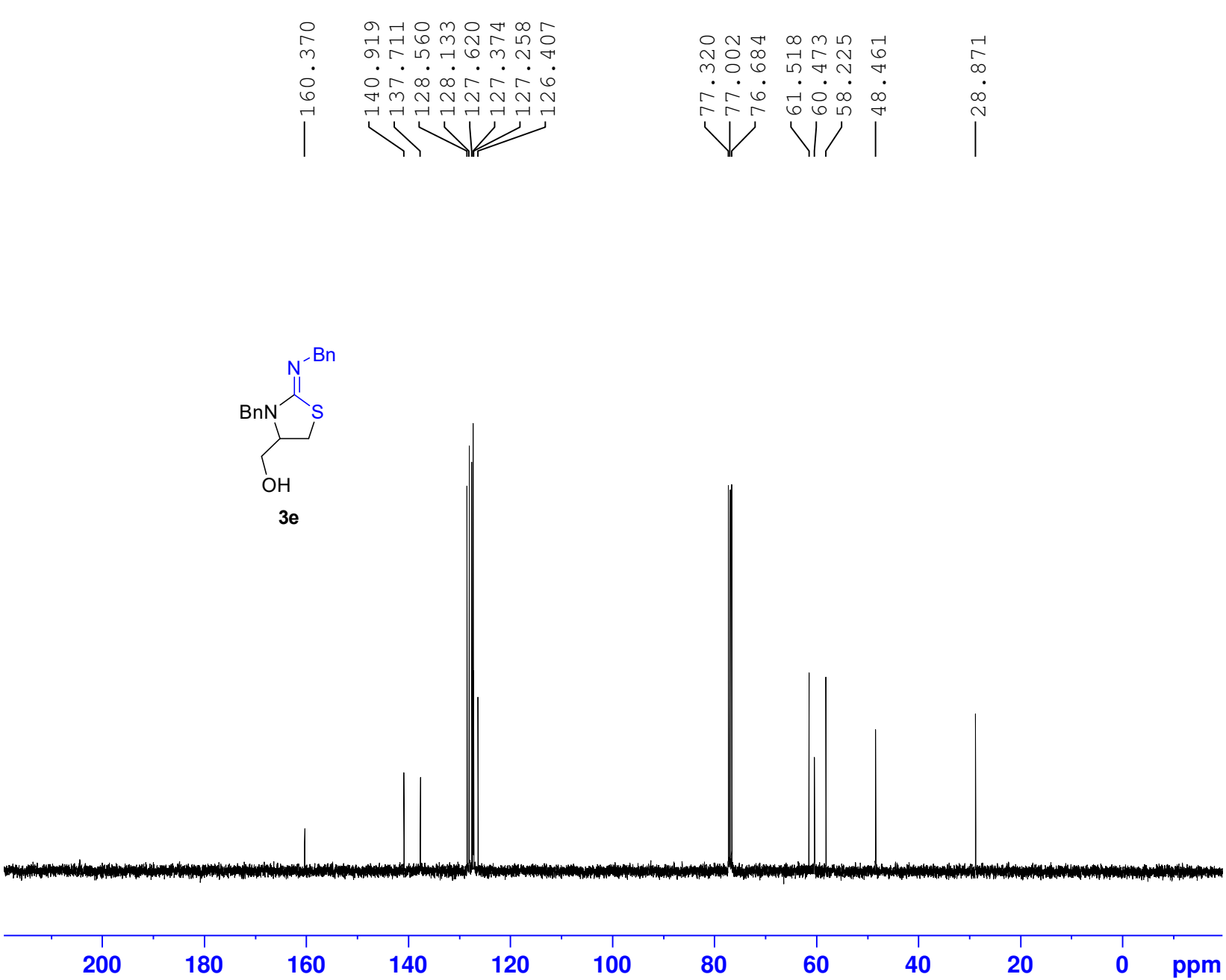


Current Data Parameters
NAME lzw2135B-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150423
Time 19.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 34.77
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



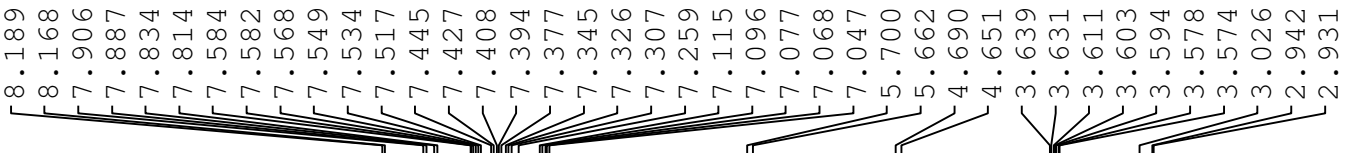

```
Current Data Parameters
NAME          lzw2135B-C
EXPNO                  1
PROCNO                 1

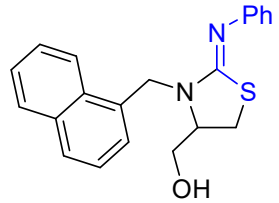
F2 - Acquisition Parameters
Date_           20150423
Time               14.03
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    28
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

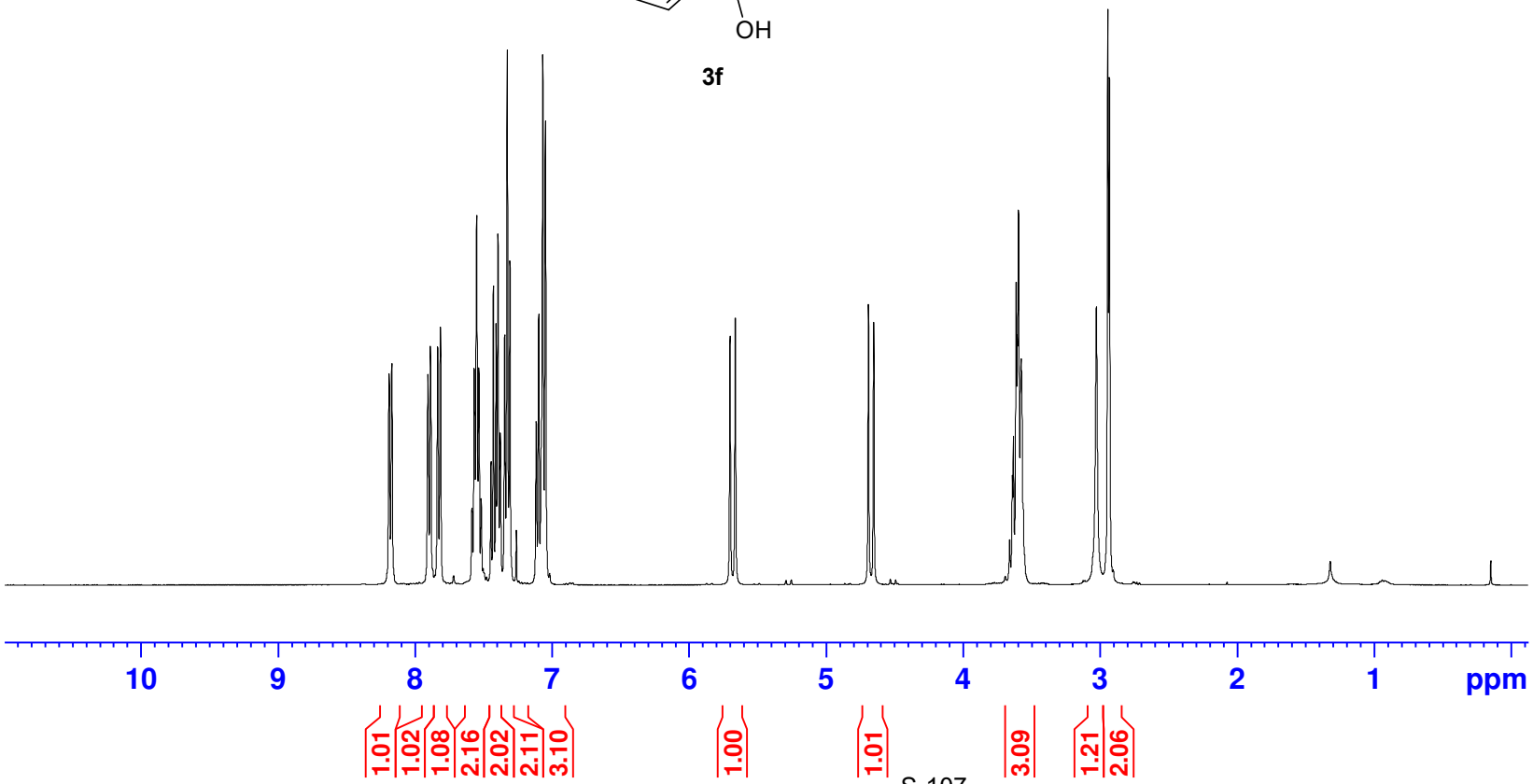
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127812 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





3f

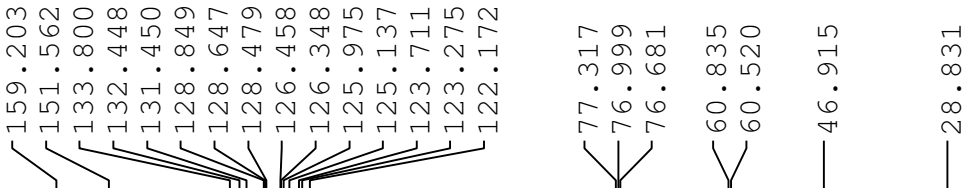


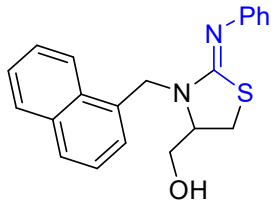

```
Current Data Parameters
NAME                  lzw2139-H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150425
Time                      13.38
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            0
SWH                    8012.820 Hz
FIDRES                 0.122266 Hz
AQ                     4.0894465 sec
RG                        27.78
DW                       62.400 usec
DE                        6.50 usec
TE                       296.7 K
D1                    1.00000000 sec
TD0                           1

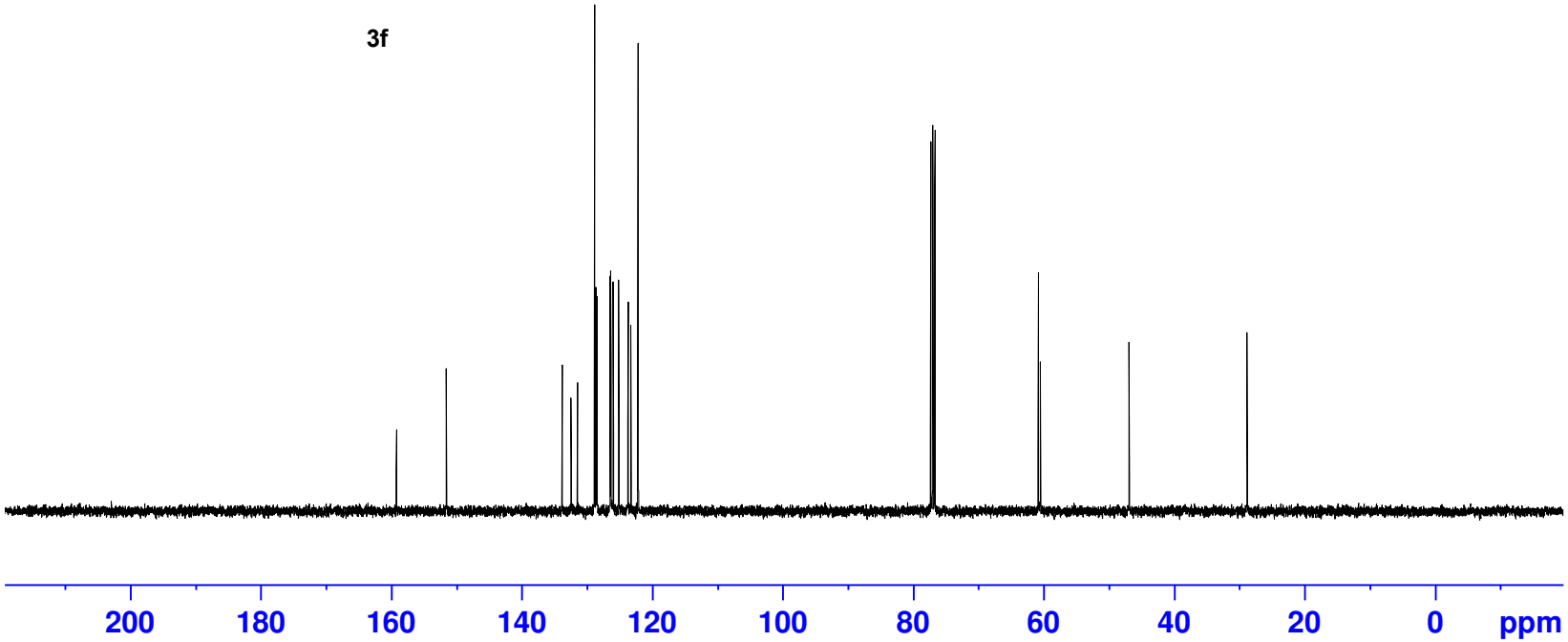
======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                       14.50 usec
PLW1                11.99499989 W

F2 - Processing parameters
SI                        65536
SF                  400.1300090 MHz
WDW                         EM
SSB                0
LB                        0.30 Hz
GB                 0
PC                        1.00
```





3f



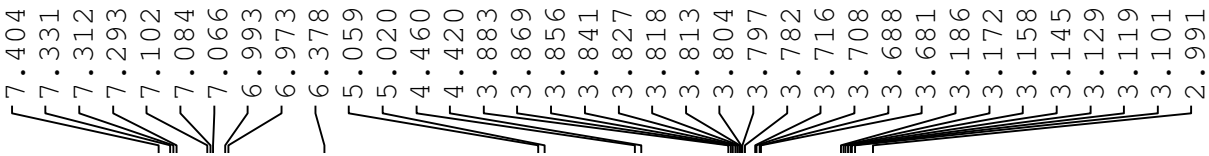

```
Current Data Parameters
NAME            lzw2139-C
EXPNO                   1
PROCNO                  1

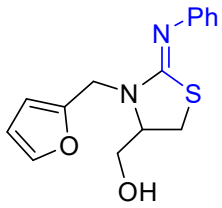
F2 - Acquisition Parameters
Date_           20150425
Time               13.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    42
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1         46.98899841 W

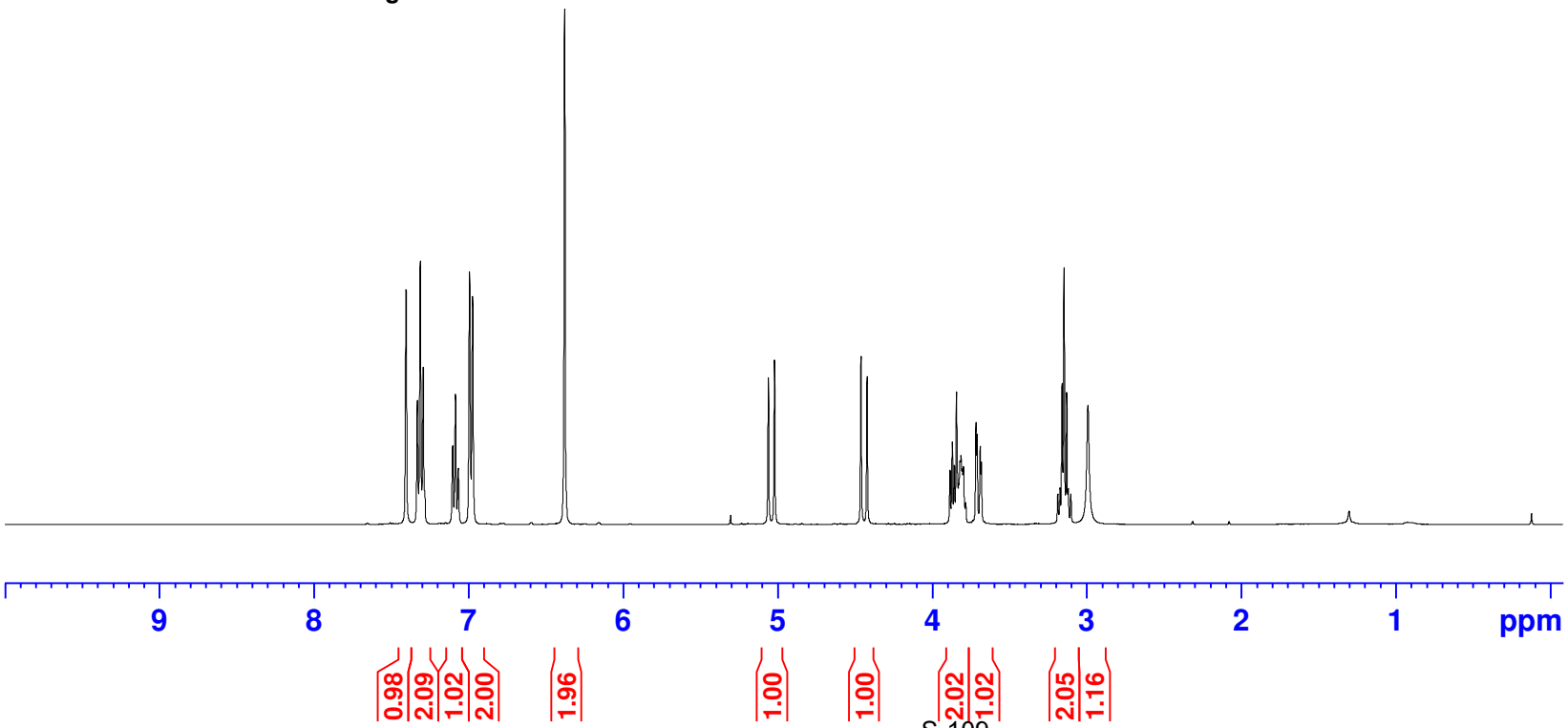
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127860 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





3g

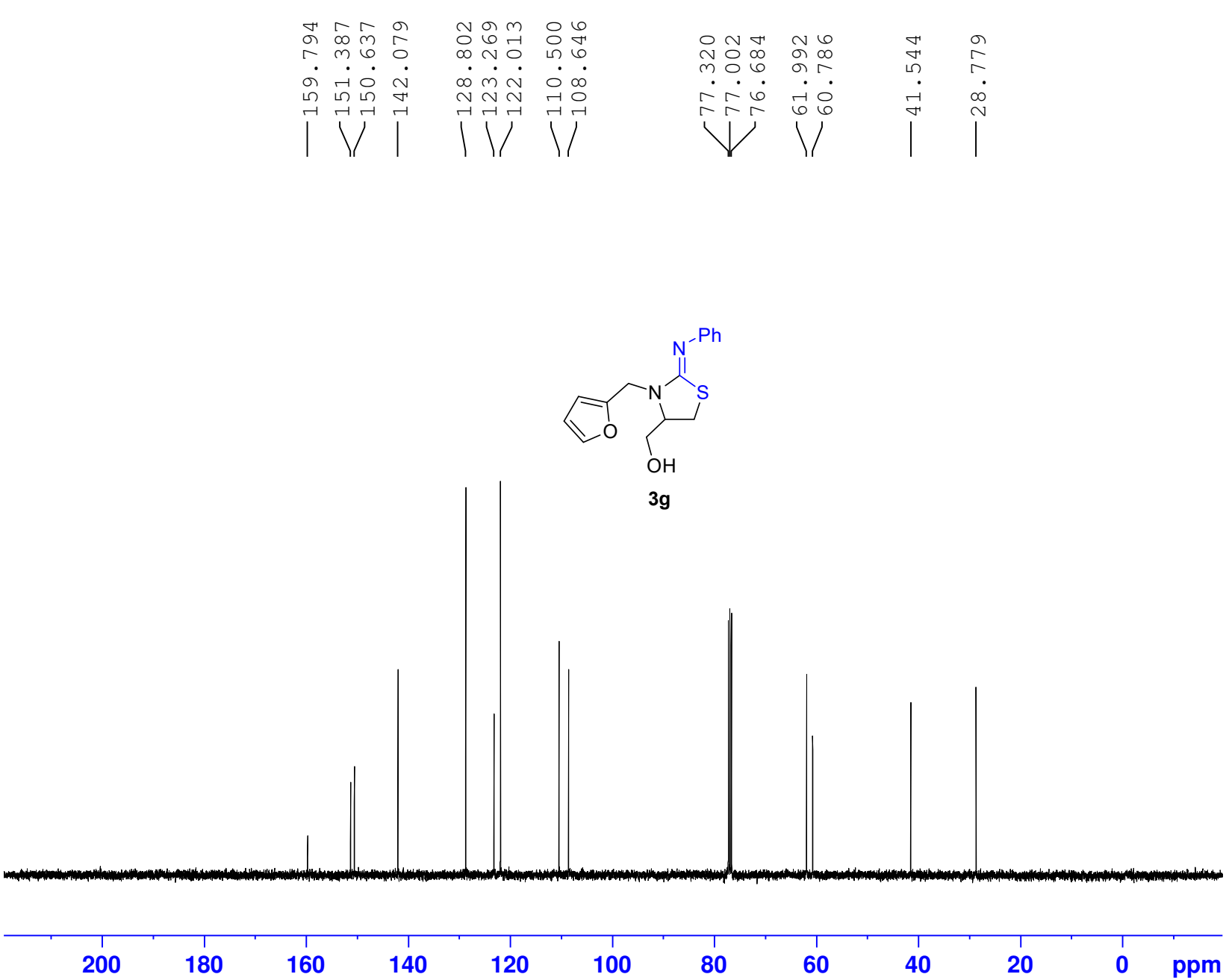



```
Current Data Parameters
NAME          lzw2137A-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150424
Time               13.49
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                296.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



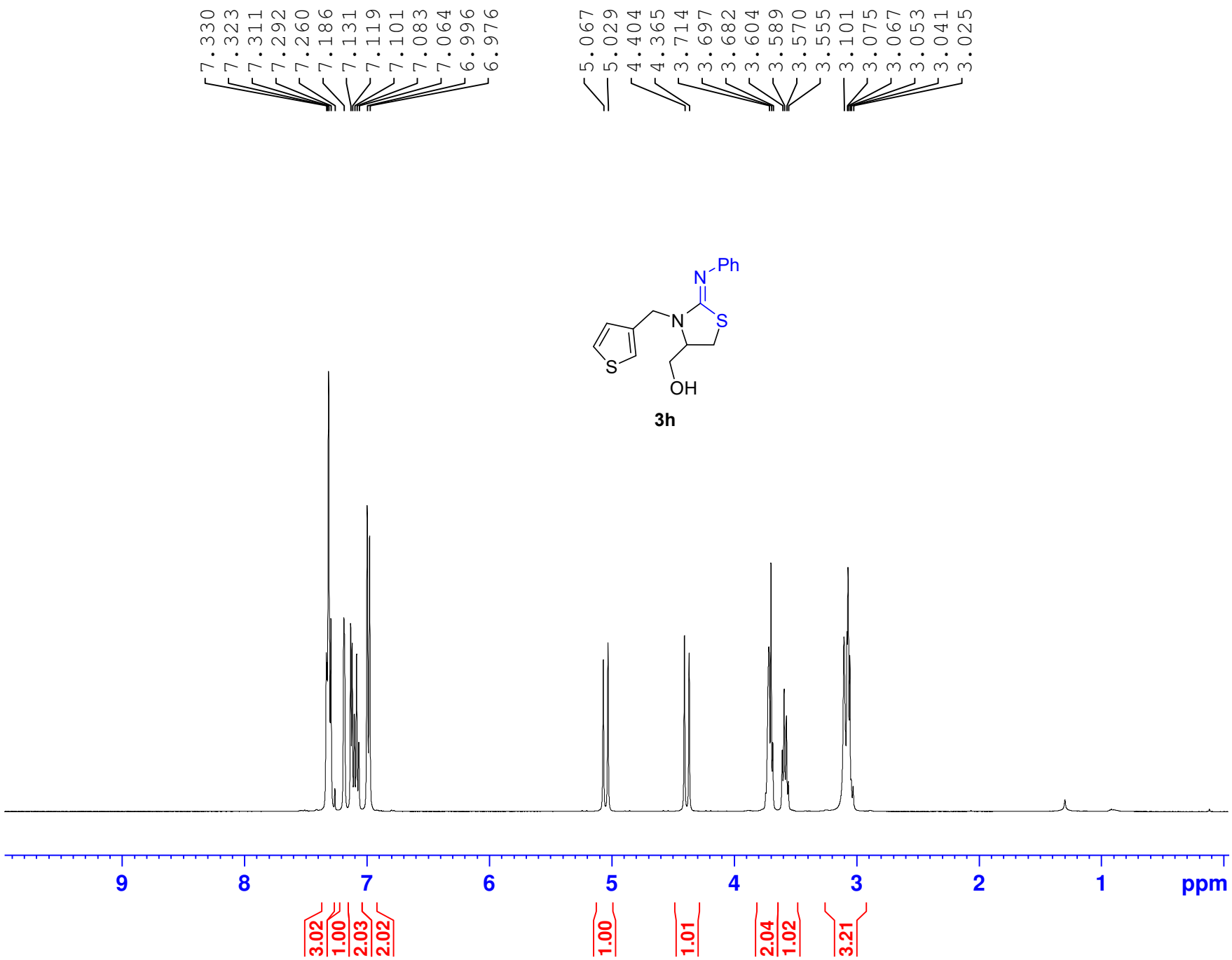

```
Current Data Parameters
NAME                 lzw2137A-C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150424
Time                      13.52
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           24
DS                            2
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                       196.92
DW                       20.800 usec
DE                        6.50 usec
TE                       296.9 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                100.6228298 MHz
NUC1                        13C
P1                        9.70 usec
PLW1                46.98899841 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                11.99499989 W
PLW12                0.34213999 W
PLW13                0.27713001 W

F2 - Processing parameters
SI                        32768
SF                  100.6127828 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
```

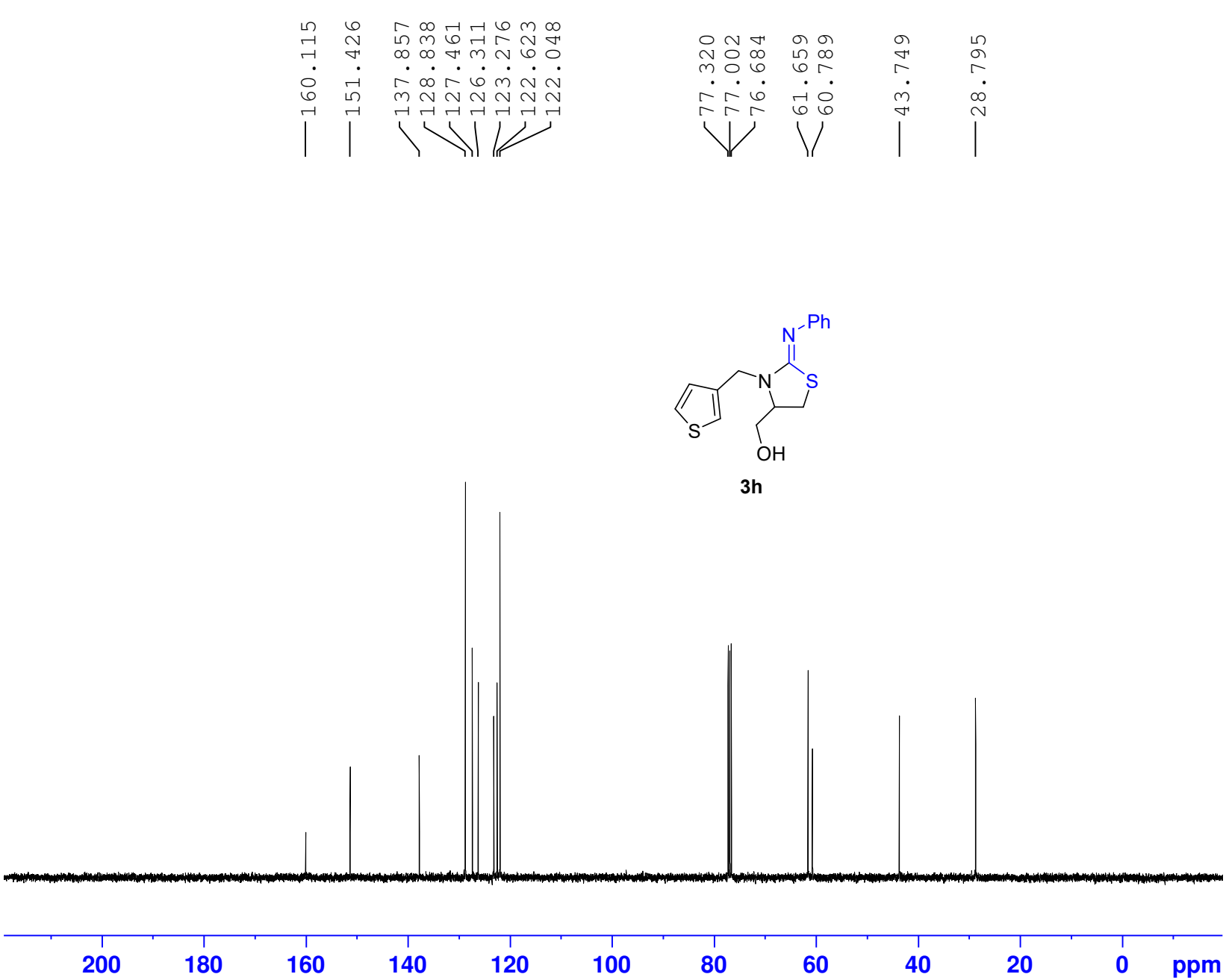



```
Current Data Parameters
NAME          lzw2137B-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150424
Time               13.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                 27.78
DW                 62.400 usec
DE                  6.50 usec
TE                 296.3 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1          11.99499989 W

F2 - Processing parameters
SI                 65536
SF            400.1300090 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



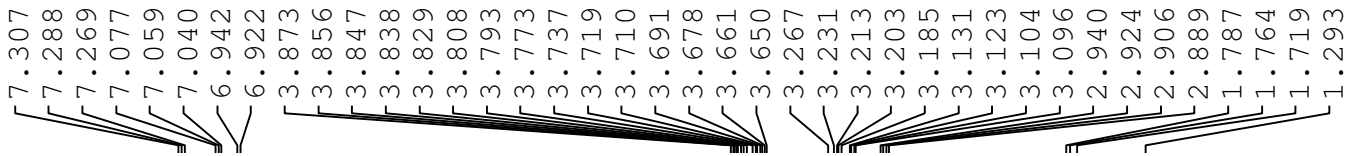

```
Current Data Parameters
NAME          lzw2137B-C
EXPNO                  1
PROCNO                 1

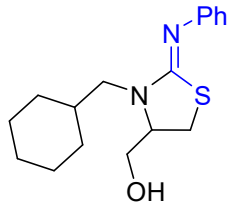
F2 - Acquisition Parameters
Date_           20150424
Time               13.58
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    26
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

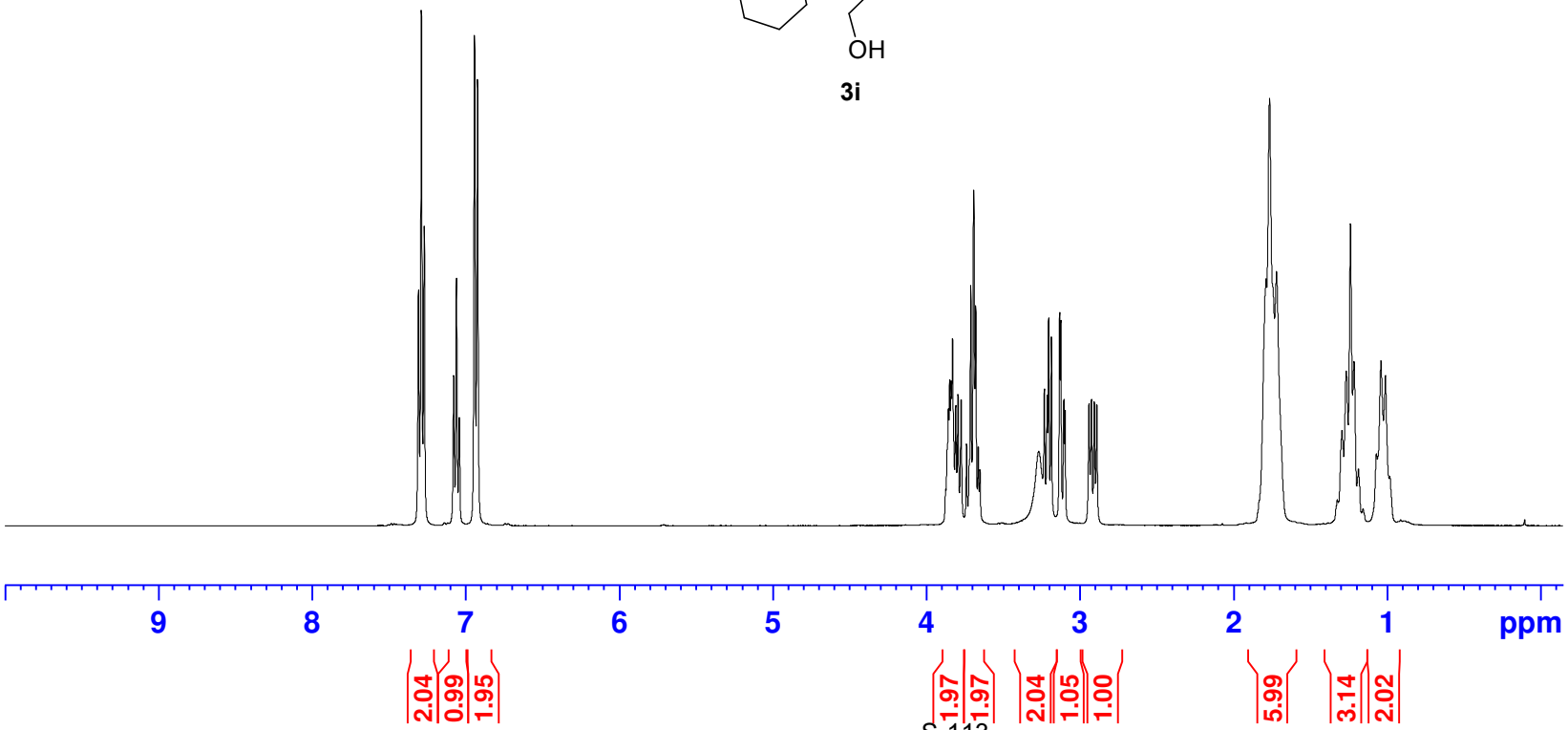
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127877 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





3i

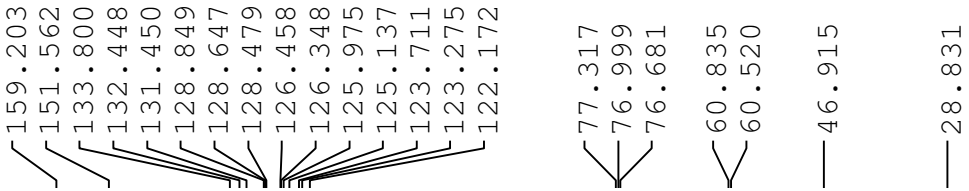


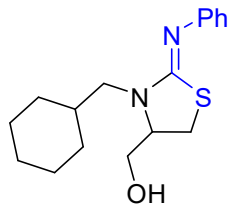
Current Data Parameters
NAME lzw2137C-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150424
Time 17.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 27.78
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

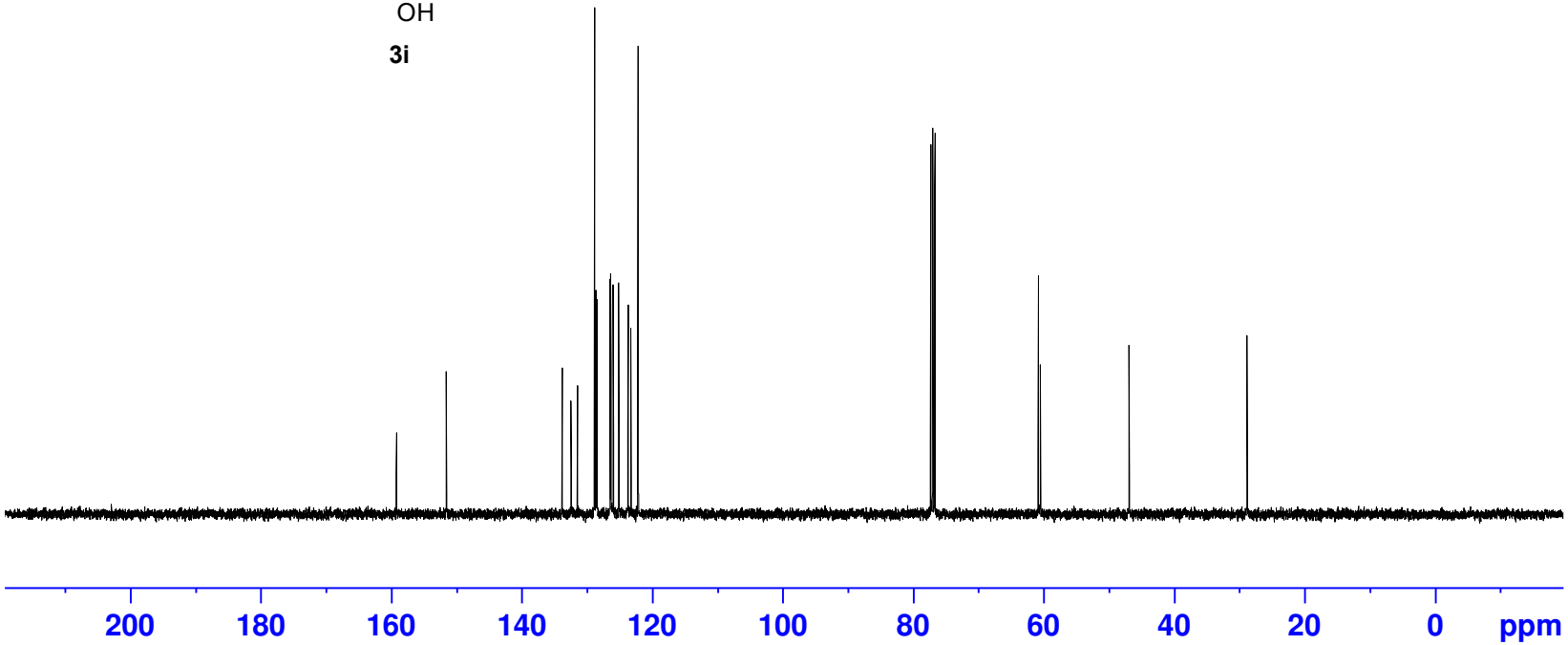
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





3i



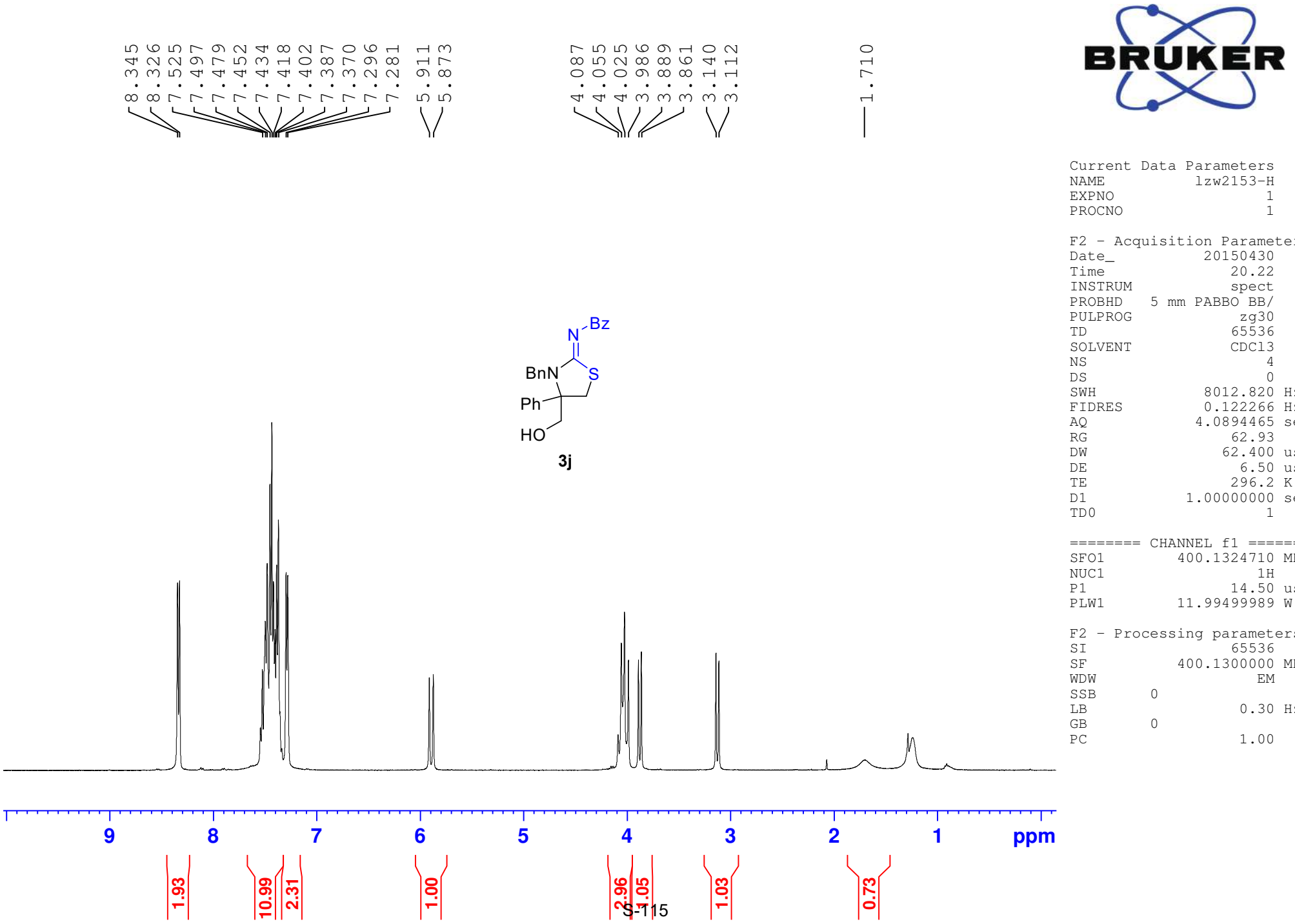

```
Current Data Parameters
NAME            lzw2139-C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150425
Time                13.42
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    42
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1          46.98899841 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          11.99499989 W
PLW12          0.34213999 W
PLW13          0.27713001 W

F2 - Processing parameters
SI                  32768
SF            100.6127860 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

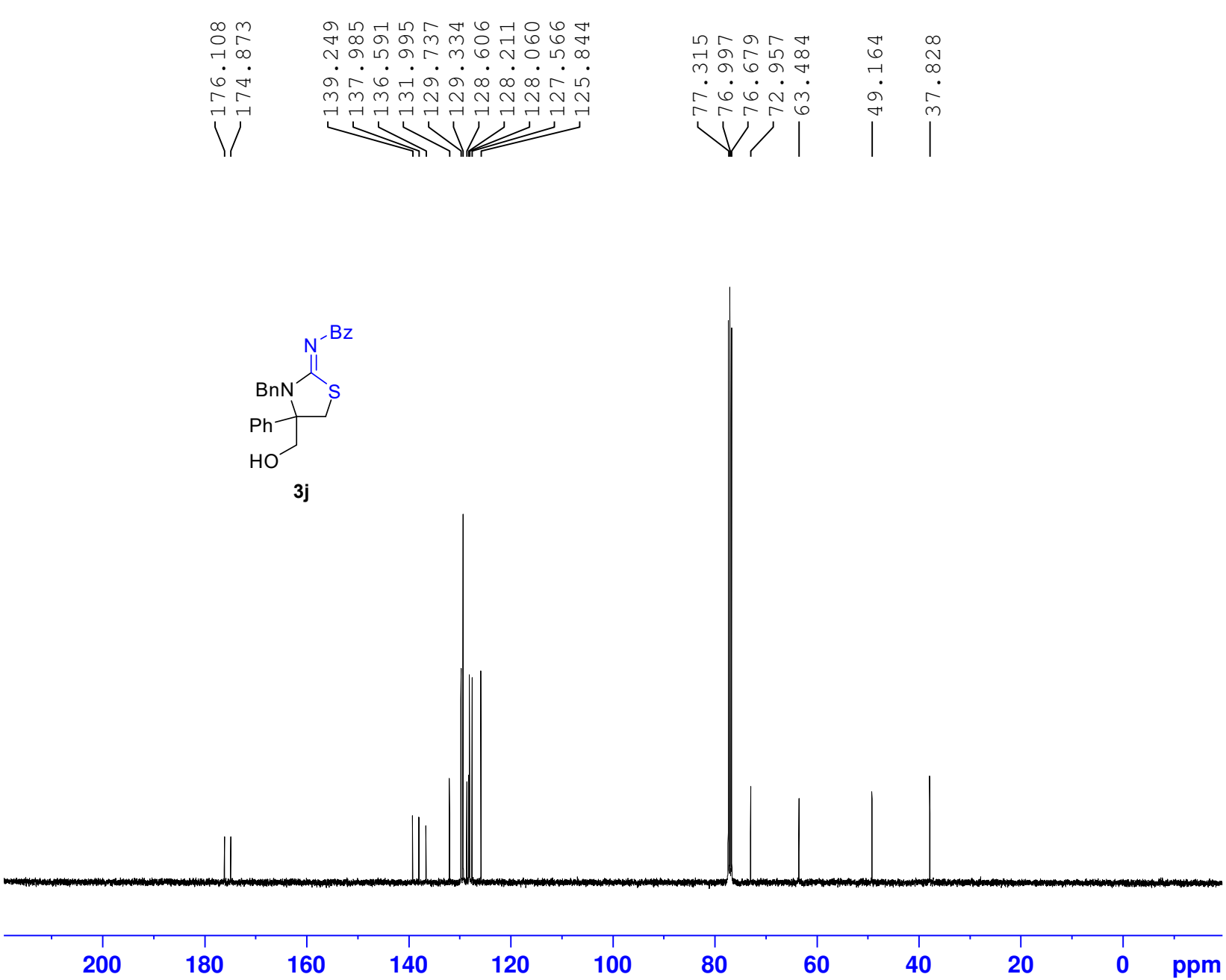


Current Data Parameters
NAME lzw2153-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150430
Time 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 62.93
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



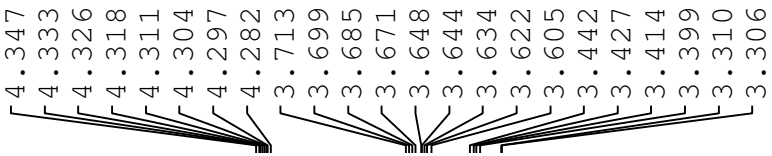

```
Current Data Parameters
NAME          lzw2153-C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20150430
Time              23.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  446
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

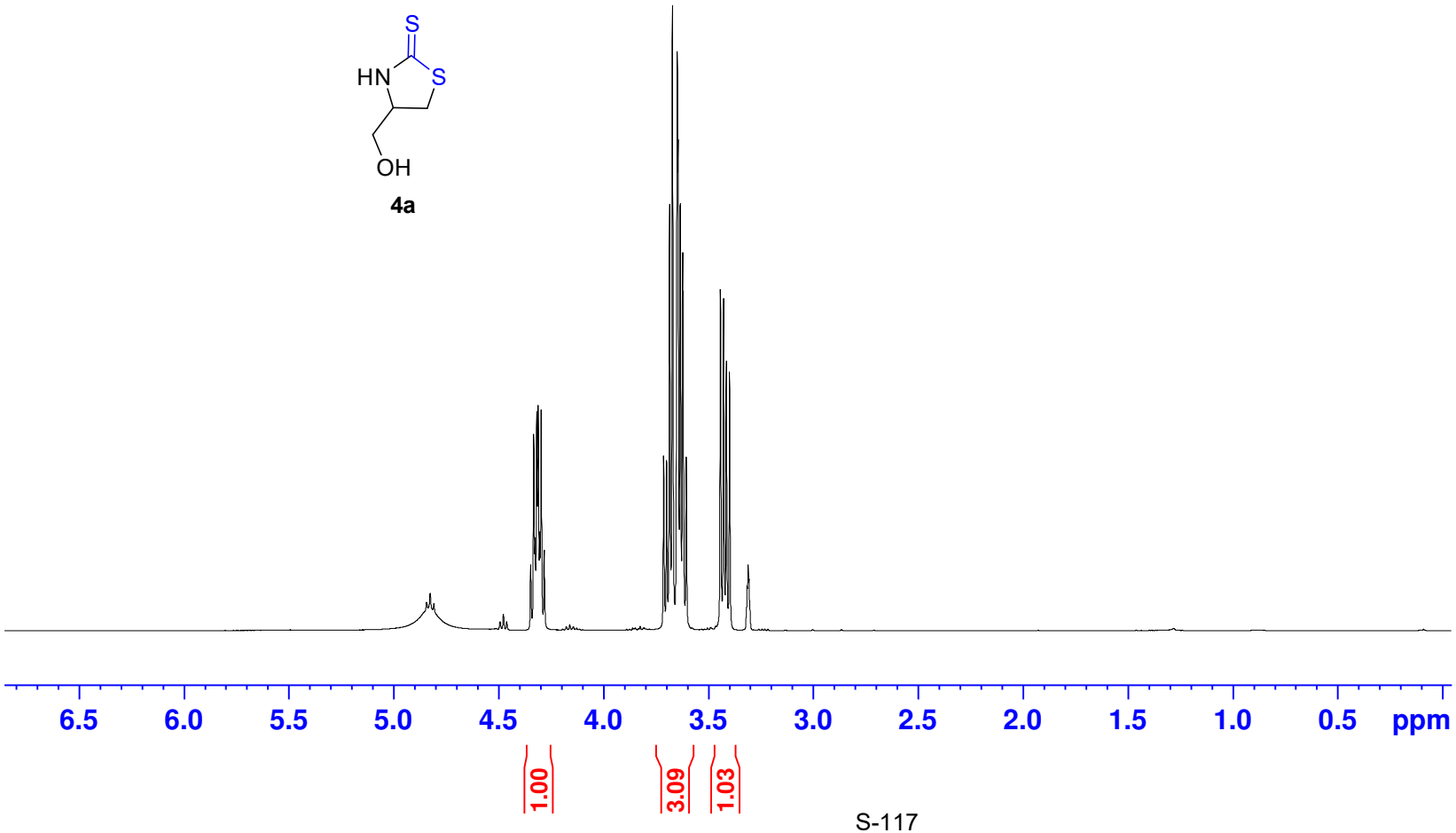
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127739 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



4a

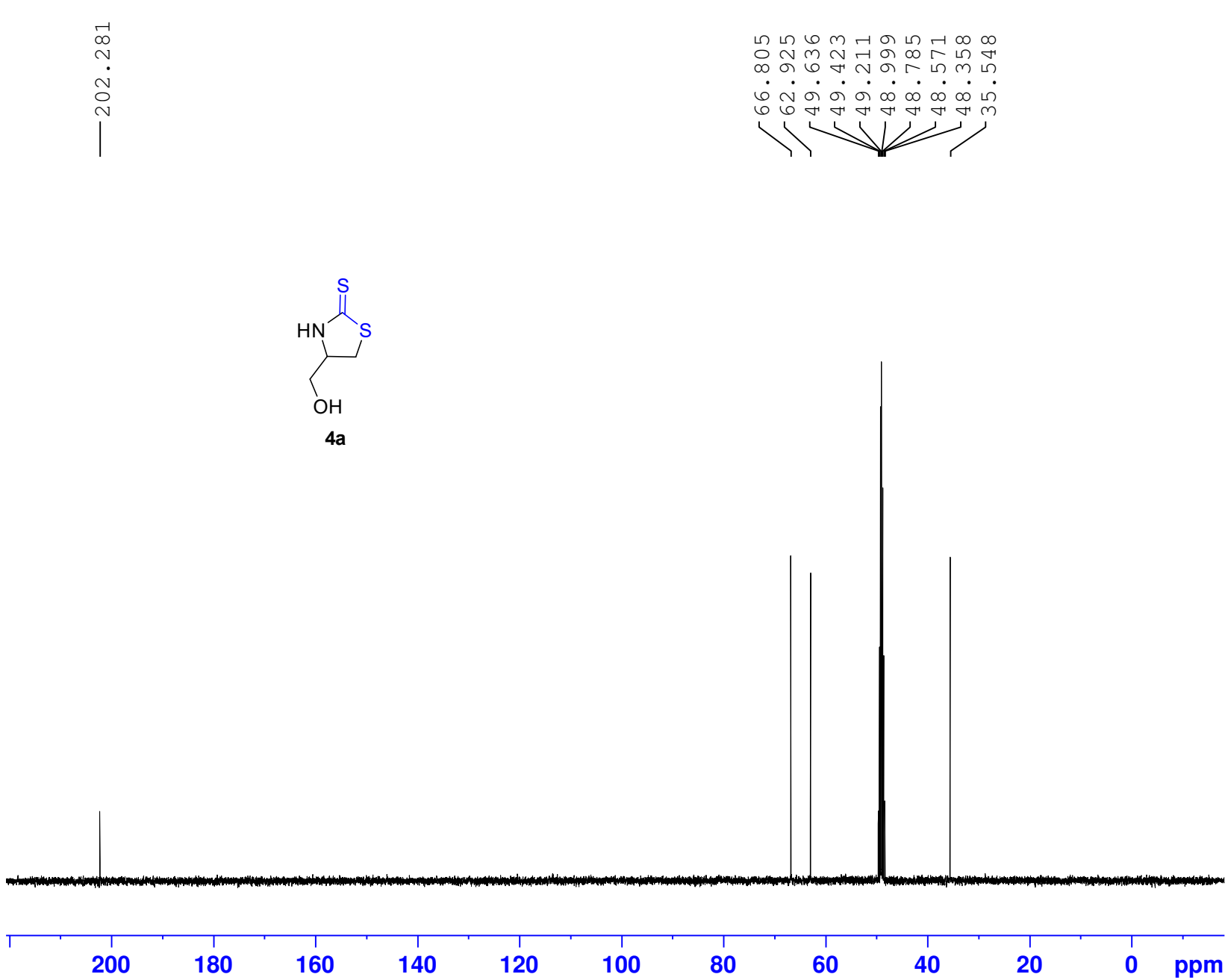



```
Current Data Parameters
NAME            lzw4105-H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151201
Time                20.52
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              MeOD
NS                      7
DS                      0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  45.67
DW                62.400 usec
DE                 6.50 usec
TE                 296.5 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                  65536
SF           400.1300076 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



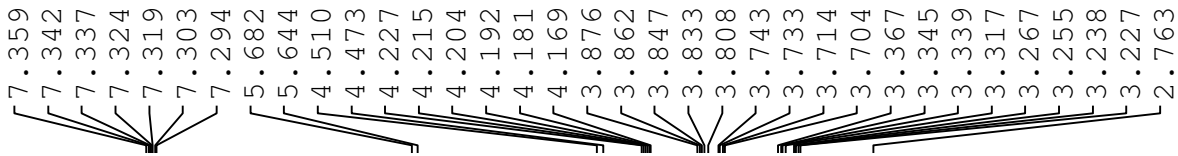
Current Data Parameters
NAME lzw4105-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151201
Time 20.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 30
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

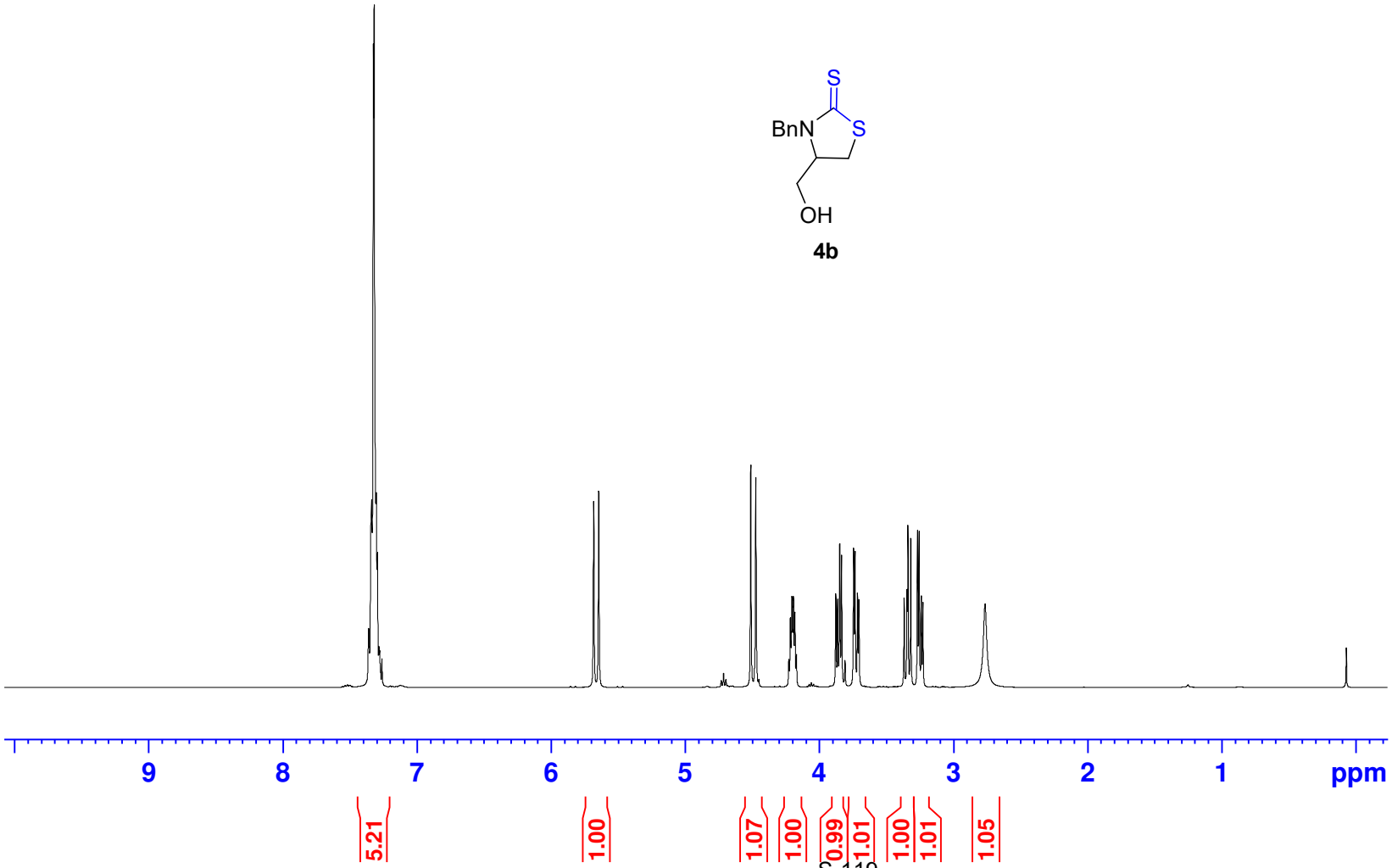
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6126418 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4b

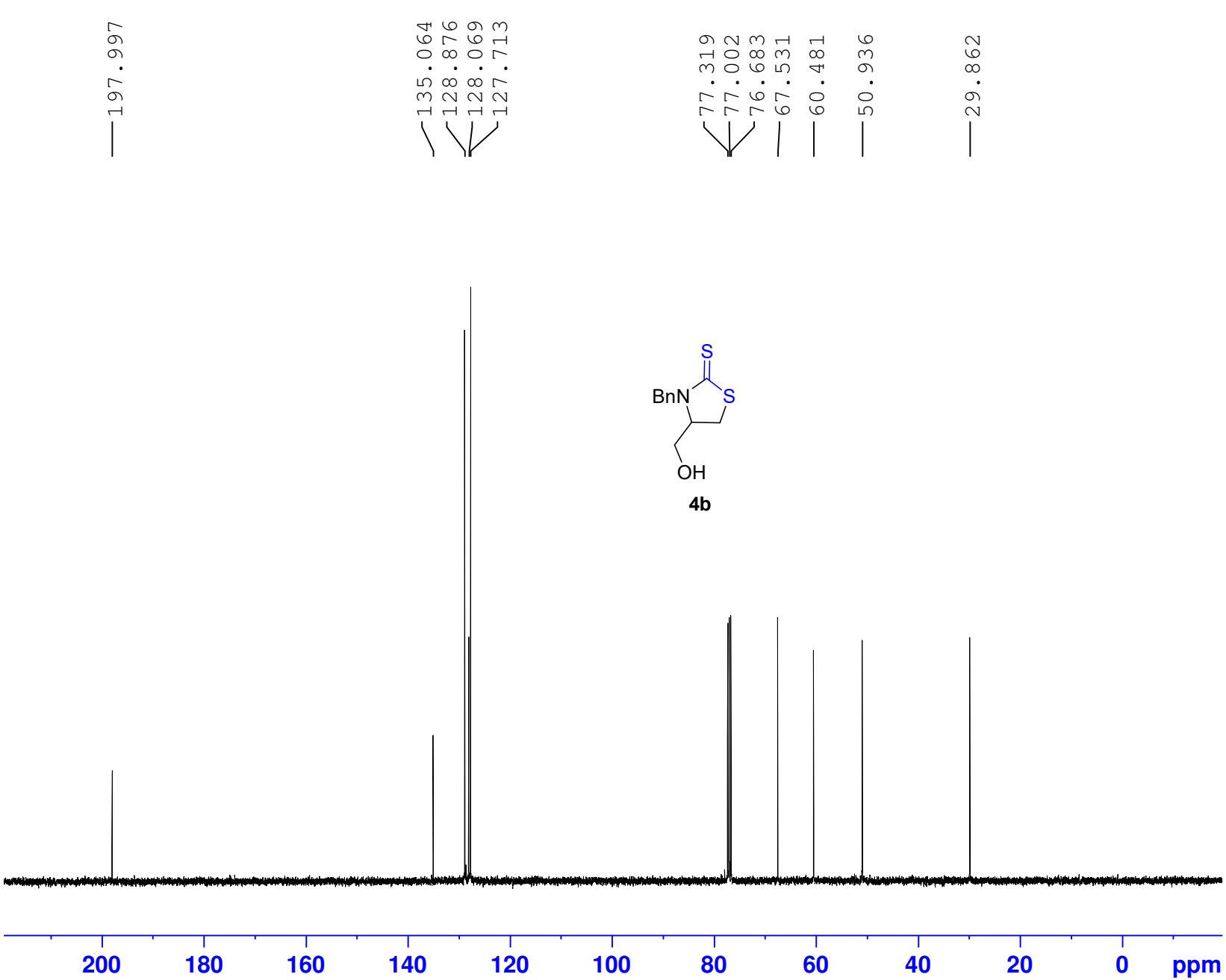



```
Current Data Parameters
NAME          lzw4110B-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151208
Time               20.32
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                299.6 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300095 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME          lzw4110B-C
EXPNO                  1
PROCNO                 1

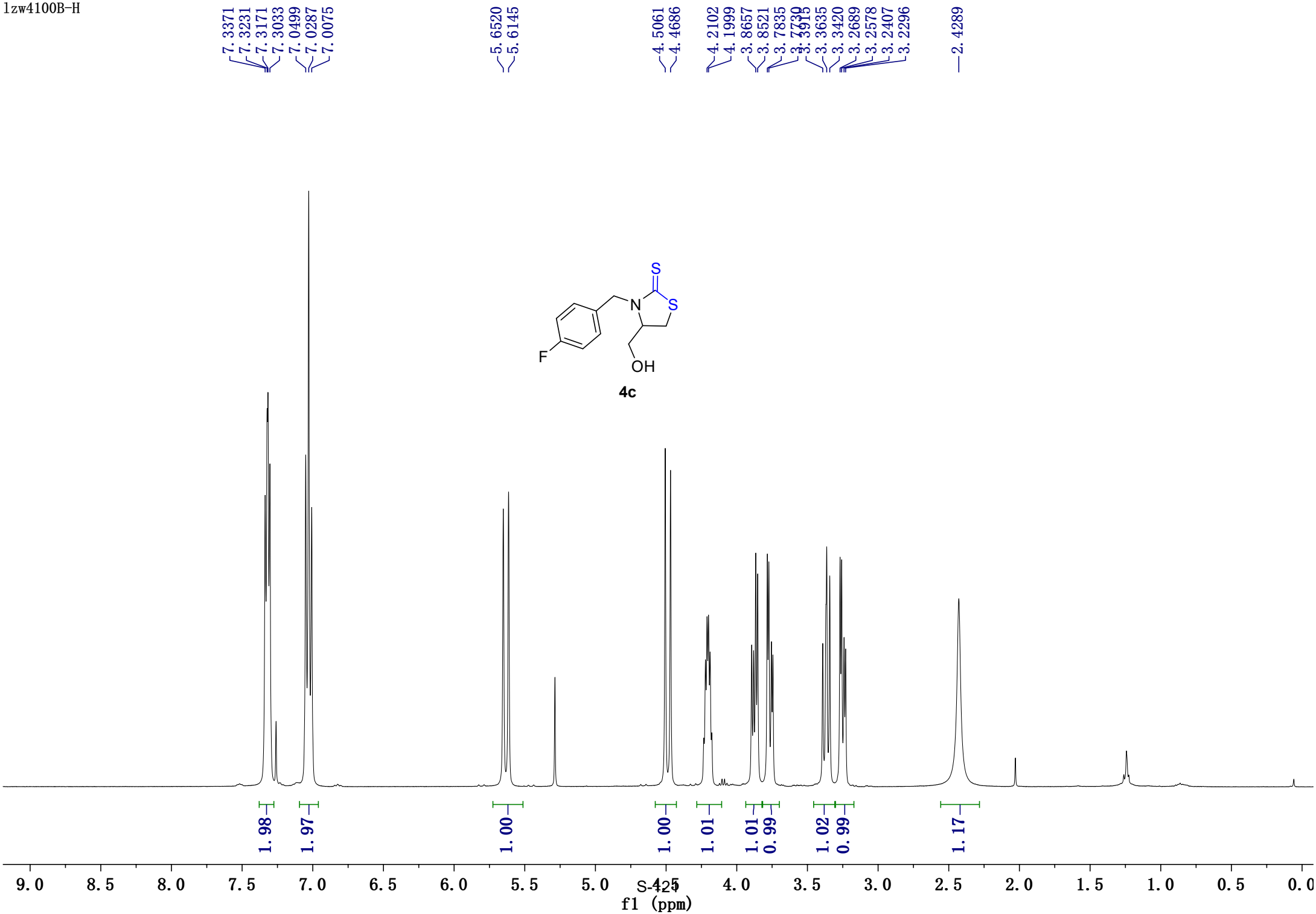
F2 - Acquisition Parameters
Date_           20151208
Time               20.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    45
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

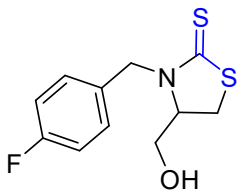
F2 - Processing parameters
SI                 32768
SF           100.6127872 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

1zw4100B-H


7.3371
7.3231
7.3171
7.3033
7.0499
7.0287
7.0075
5.6520
5.6145
4.5061
4.4686
4.2102
4.1999
3.8657
3.8521
3.7835
3.7730
3.7615
3.3635
3.3420
3.2689
3.2578
3.2407
3.2296
2.4289
S
N
S
F
OH
4c
1.98
1.97
1.00
1.00
1.01
1.01
0.99
1.02
0.99
1.17
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

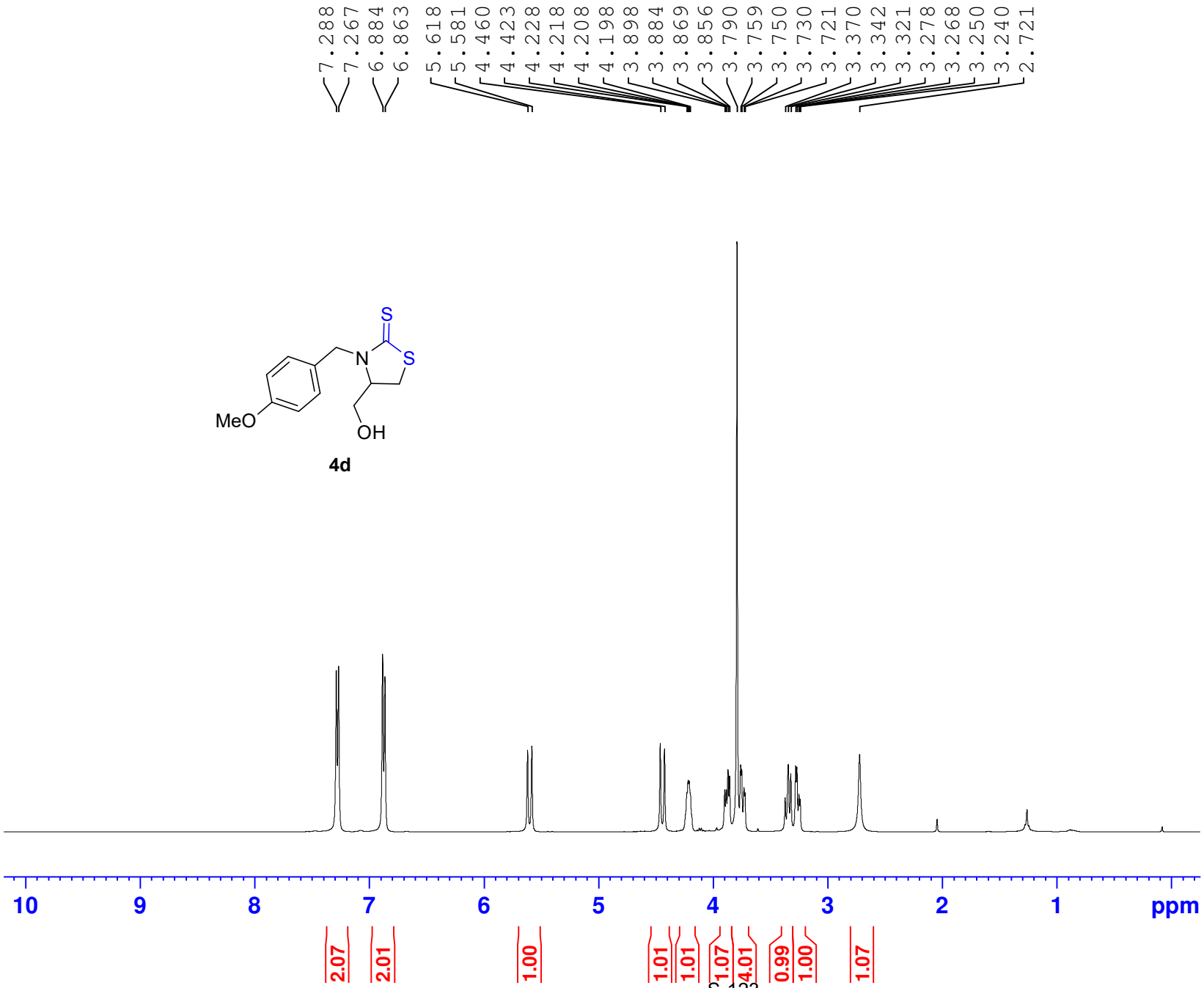
1zw4100B-C

198.1357
163.6489
161.1924
131.0052
129.7092
129.6285
115.9572
115.7426
77.3178
76.9998
76.6815
67.4410
60.7691
50.2877
29.9272



4c

f1 (ppm)

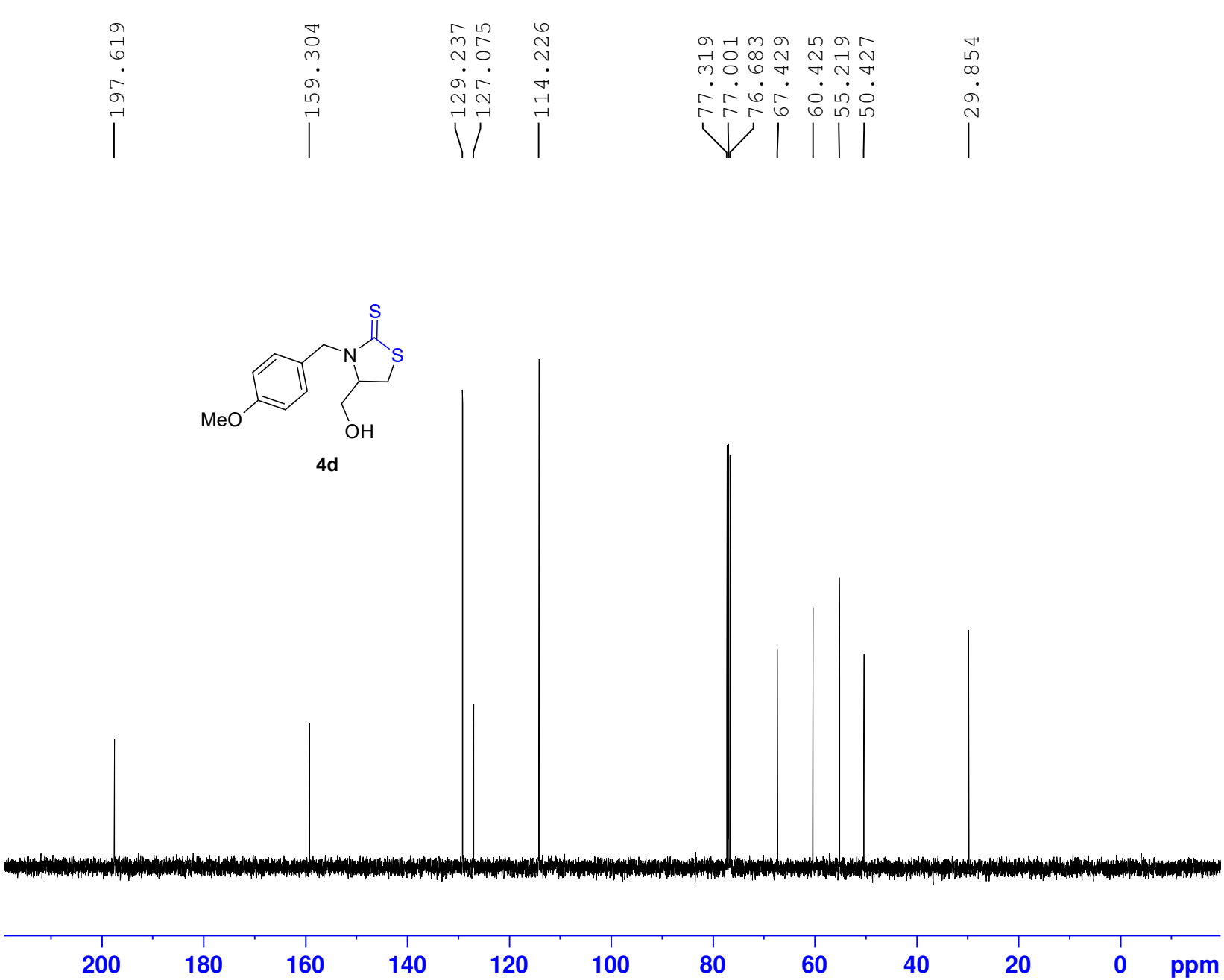


Current Data Parameters
NAME lzw4100C-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151126
Time 22.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 15
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.55
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



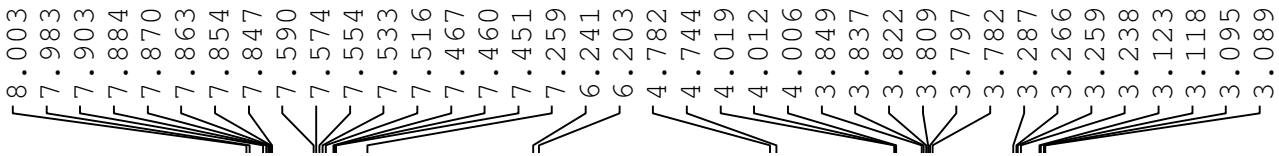

```
Current Data Parameters
NAME          lzw4100C-C
EXPNO                  1
PROCNO                 1

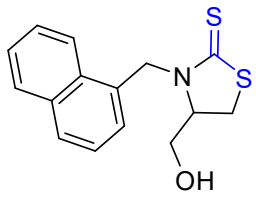
F2 - Acquisition Parameters
Date_           20151126
Time               22.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

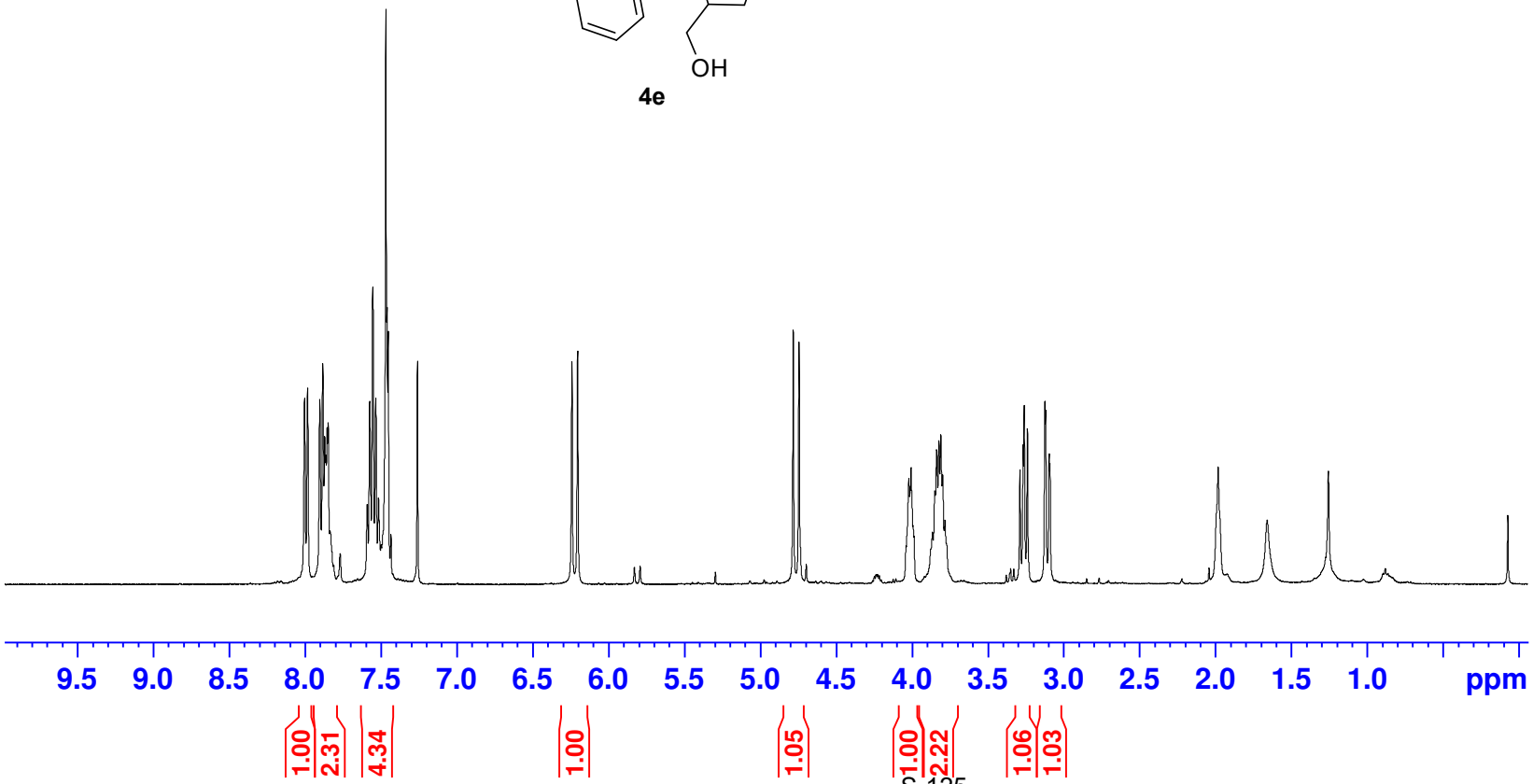
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127870 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





4e

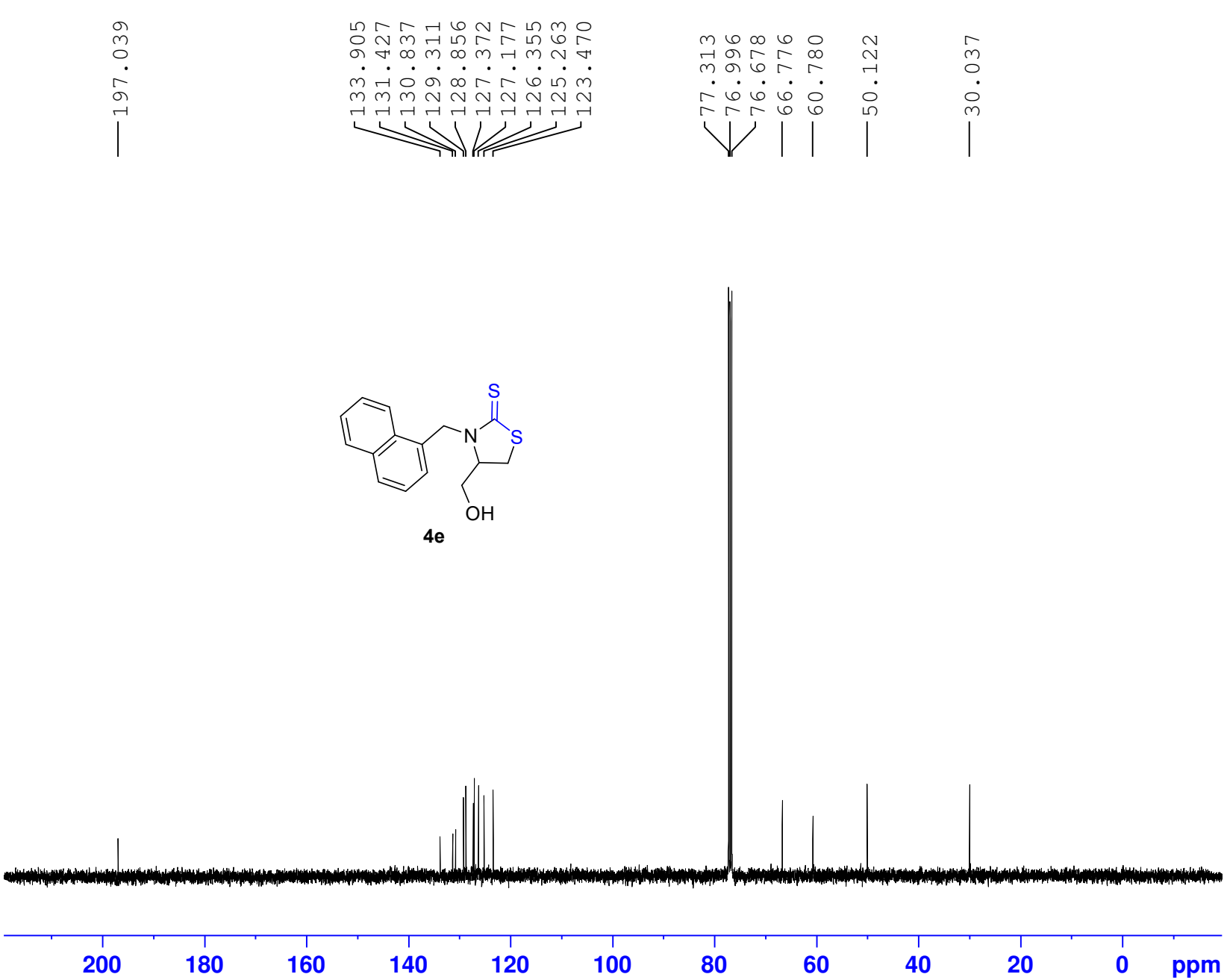



```
Current Data Parameters
NAME          lzw4100A-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151127
Time               19.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 88.84
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300098 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



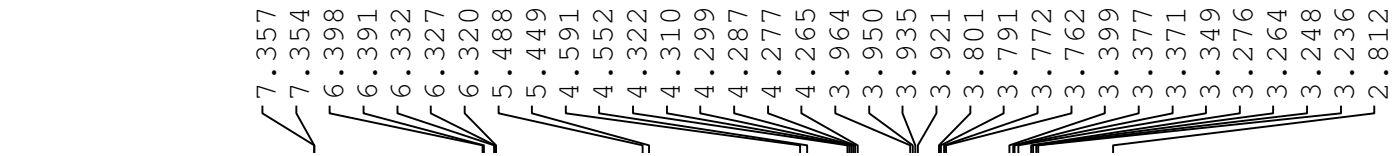

```
Current Data Parameters
NAME          lzw4100A-C
EXPNO                  1
PROCNO                 1

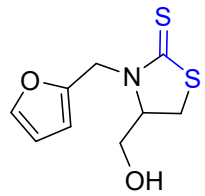
F2 - Acquisition Parameters
Date_           20151127
Time               19.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   104
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                297.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

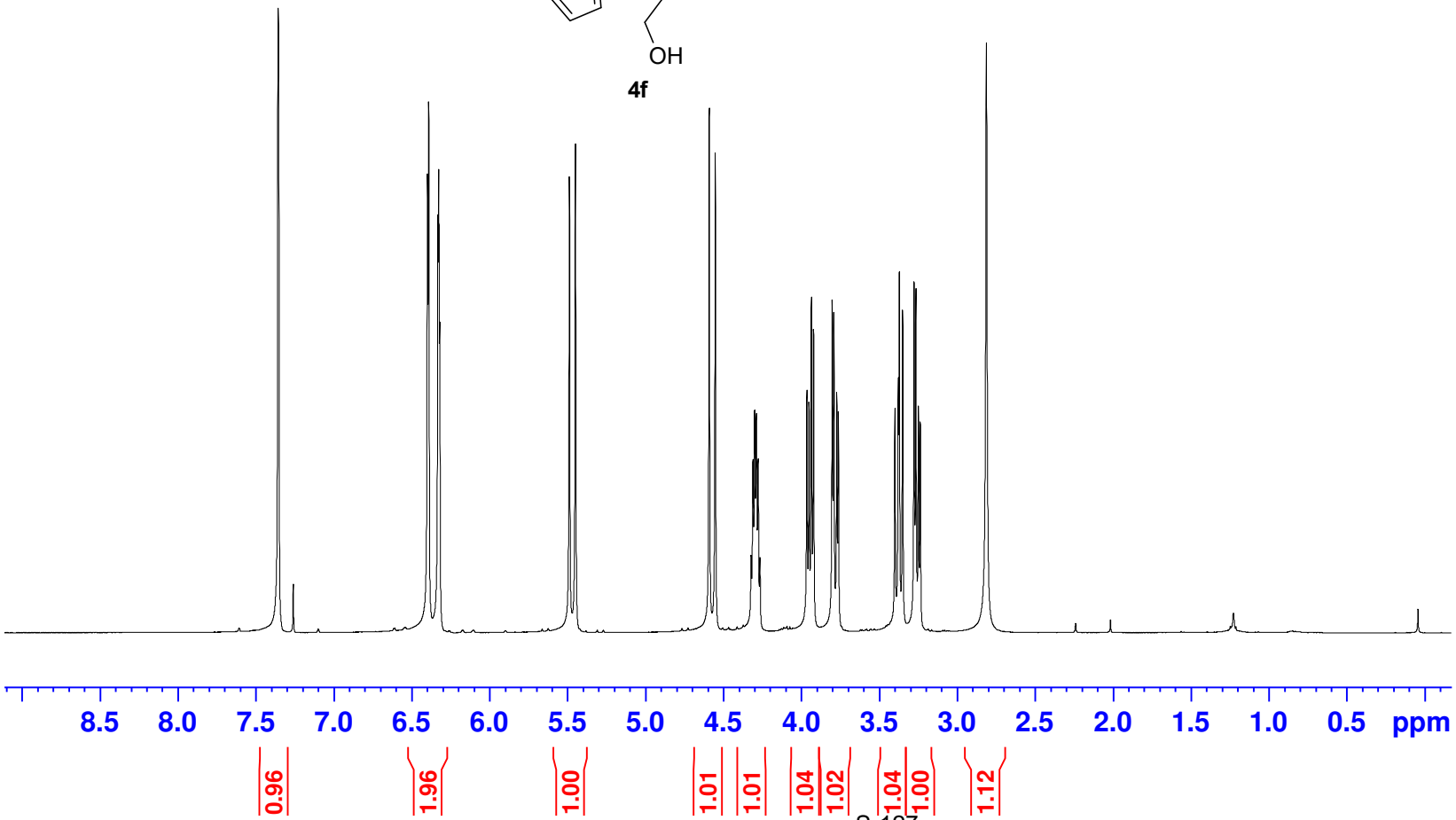
======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127737 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





4f

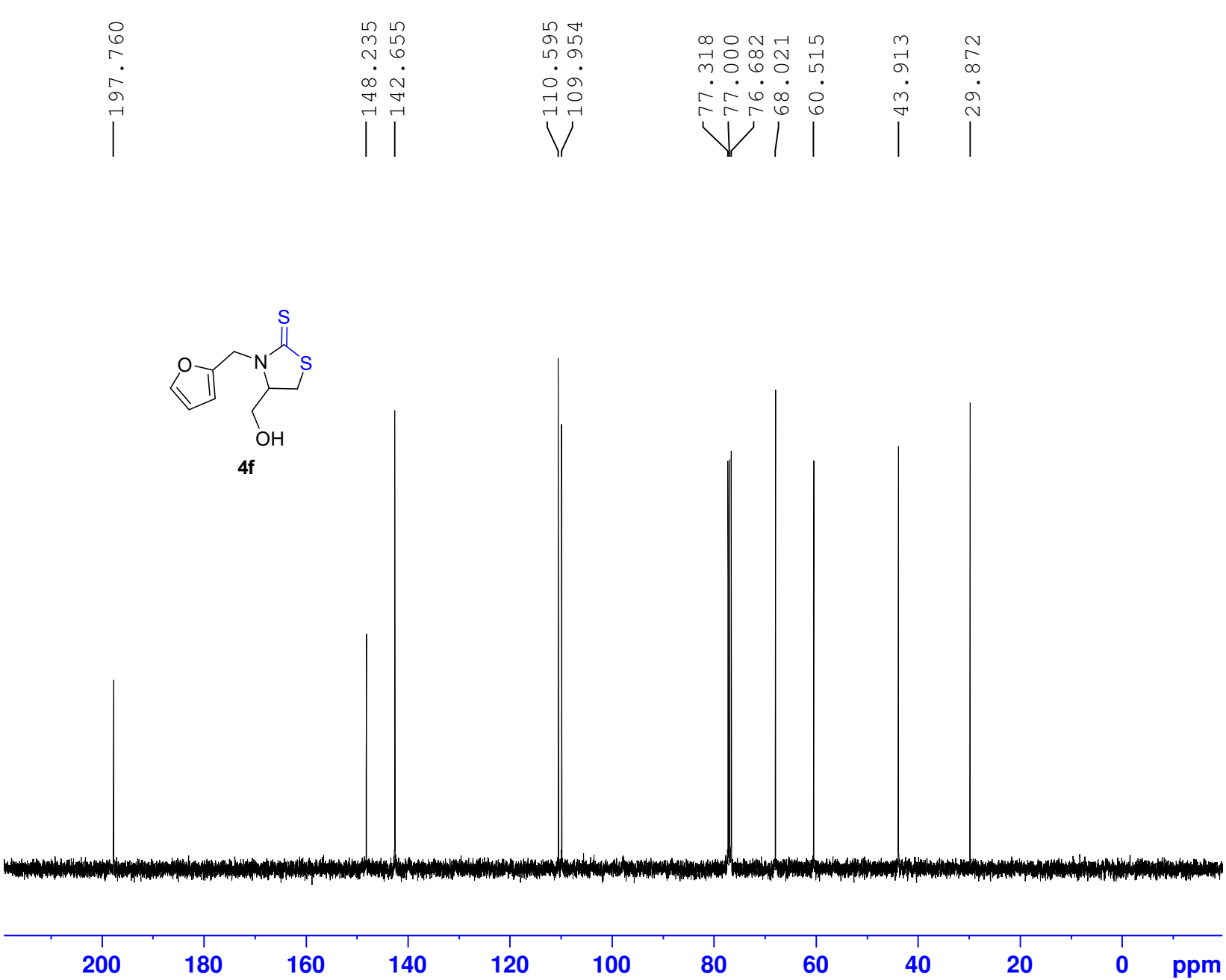



```
Current Data Parameters
NAME          lzw4110C-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151205
Time               22.00
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 34.77
DW                62.400 usec
DE                 6.50 usec
TE                297.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300097 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



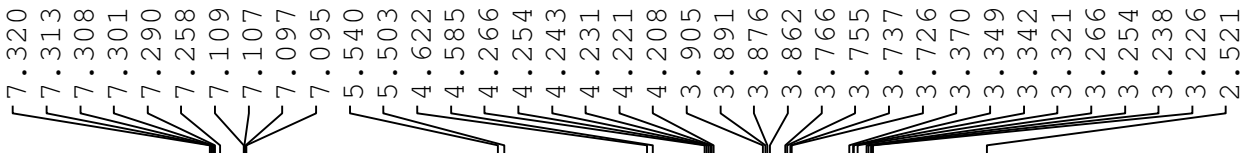
Current Data Parameters
NAME lzw4110C-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151205
Time 22.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 24
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

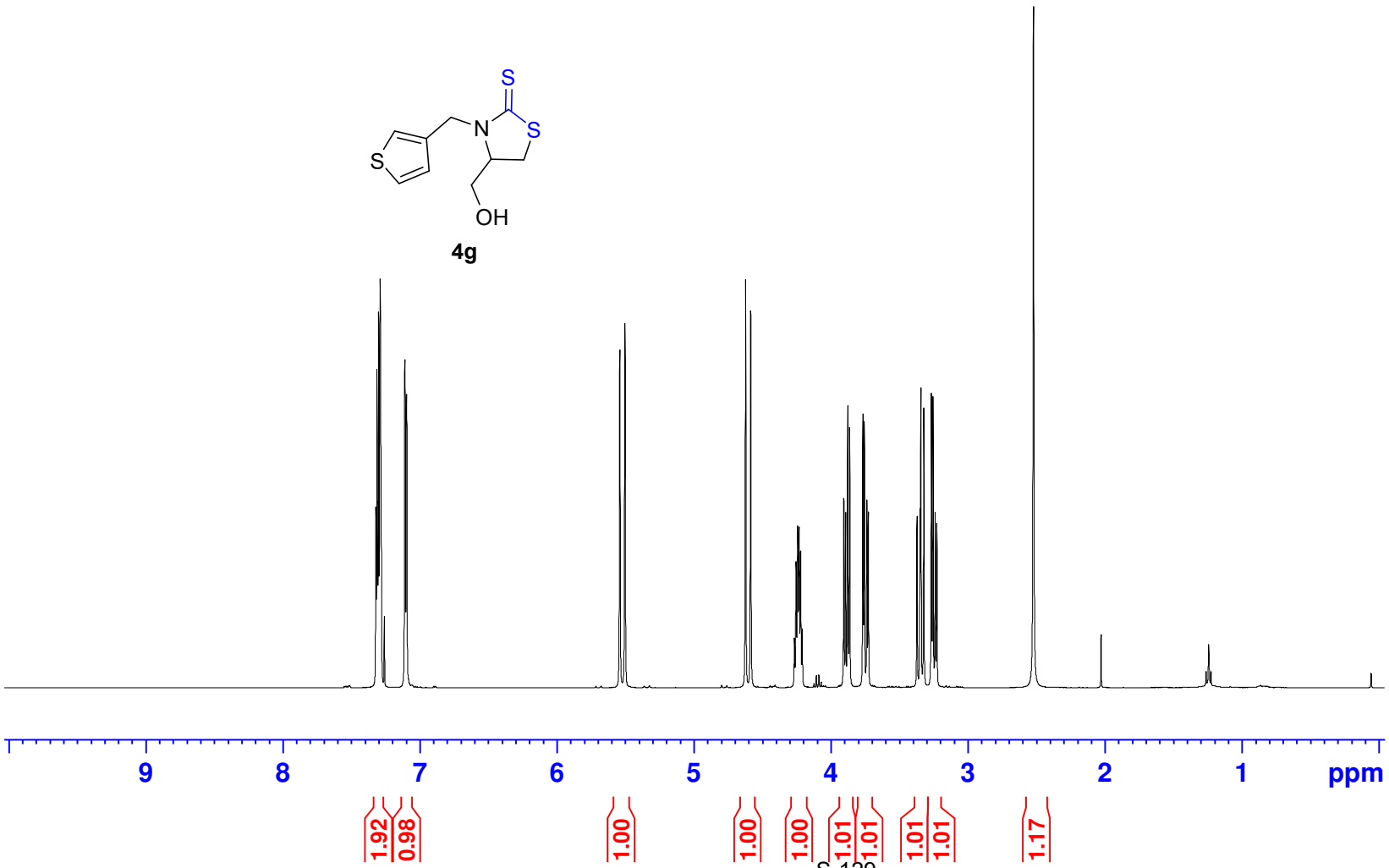
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127887 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4g

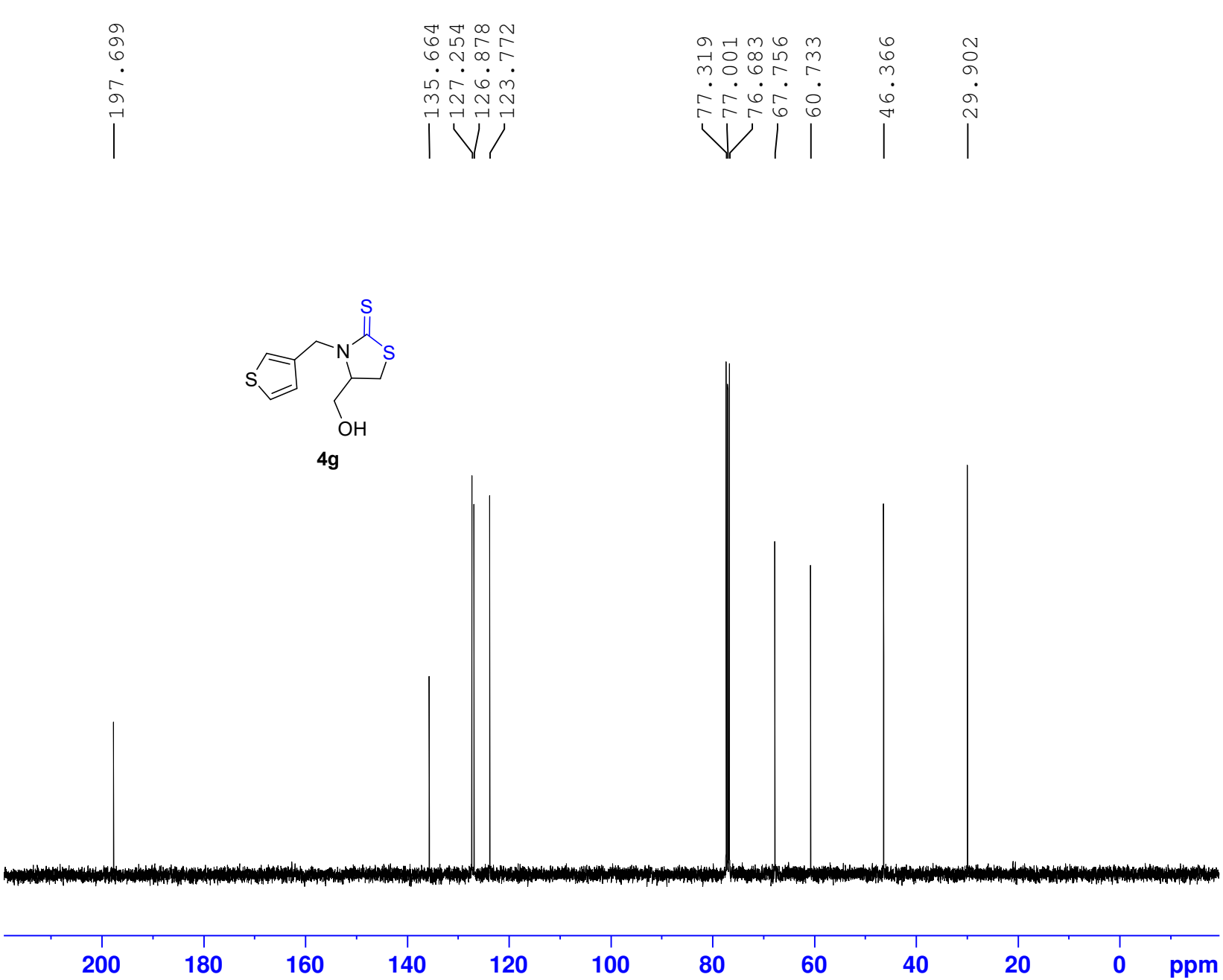



```
Current Data Parameters
NAME          lzw4110D-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151208
Time               20.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 45.67
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300101 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



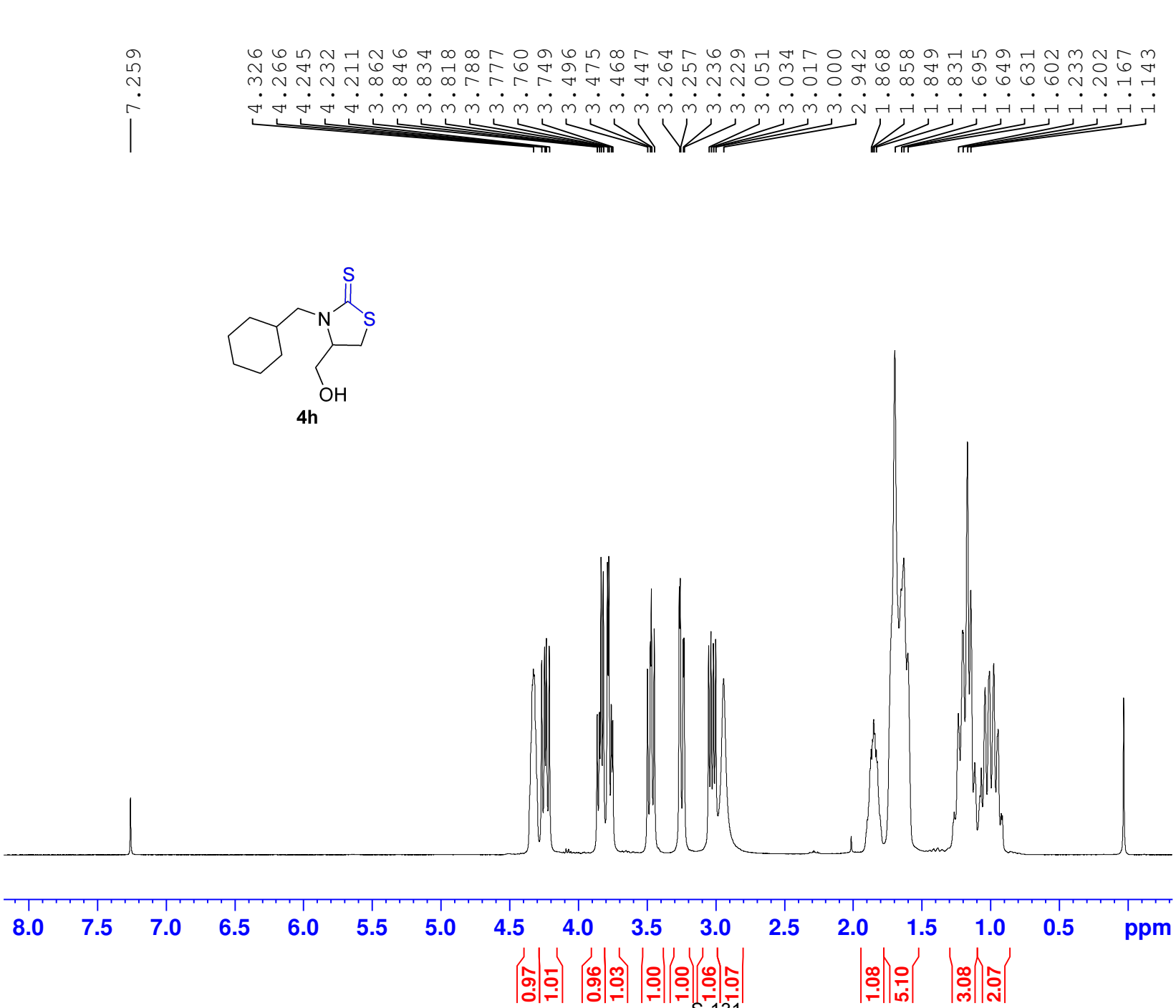

```
Current Data Parameters
NAME          lzw4110D-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151208
Time               20.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    39
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                299.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127827 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

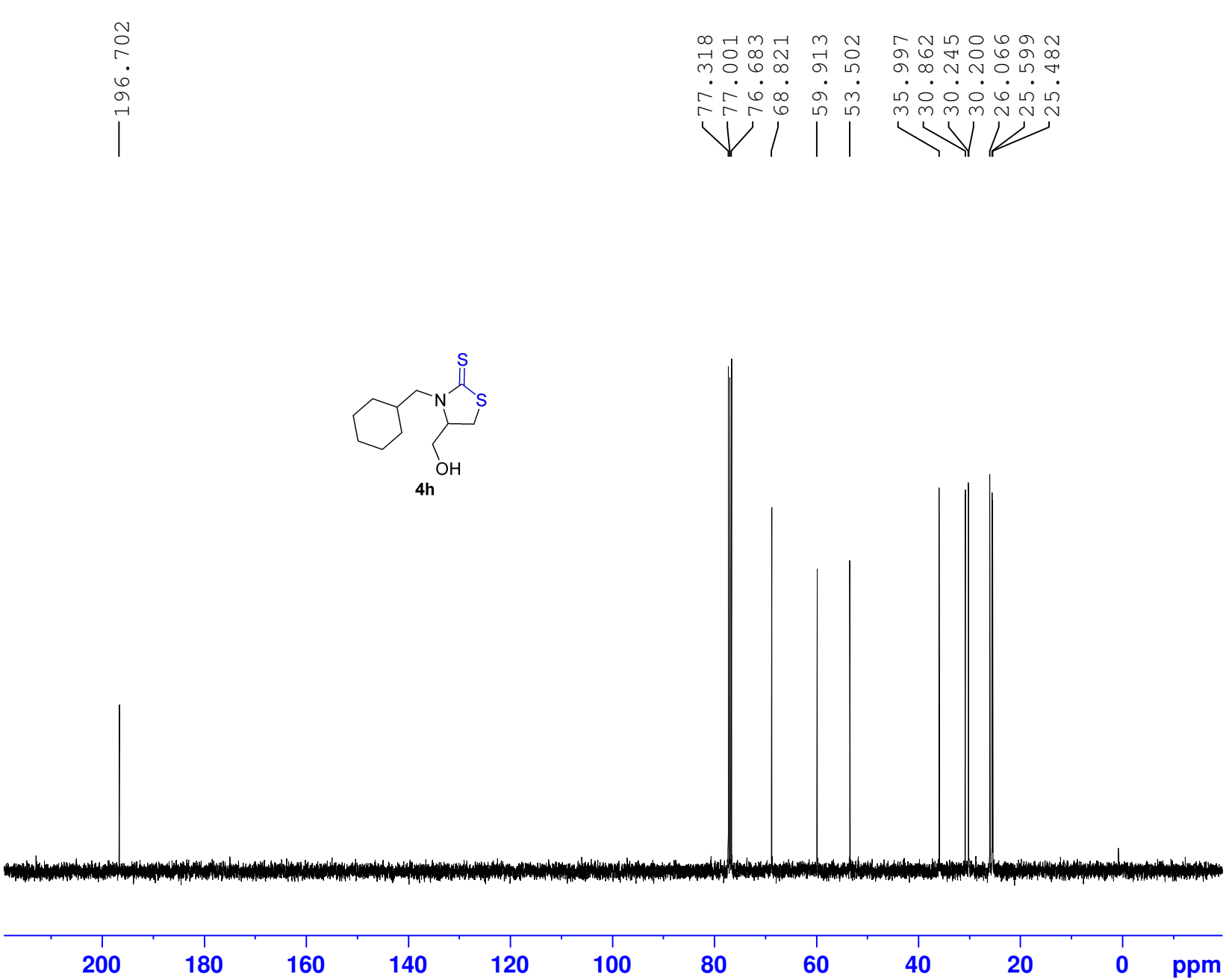


Current Data Parameters
NAME lzw4110A-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151205
Time 21.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 27.78
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



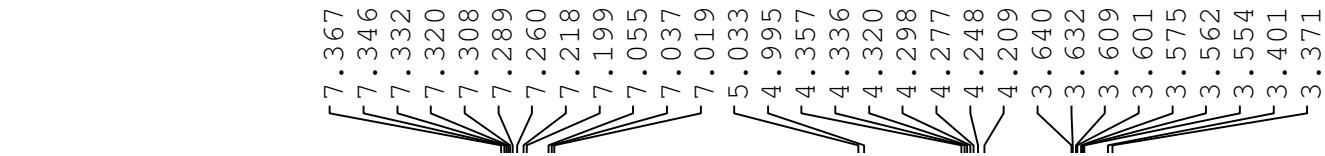

```
Current Data Parameters
NAME          lzw4110A-C
EXPNO                  1
PROCNO                 1

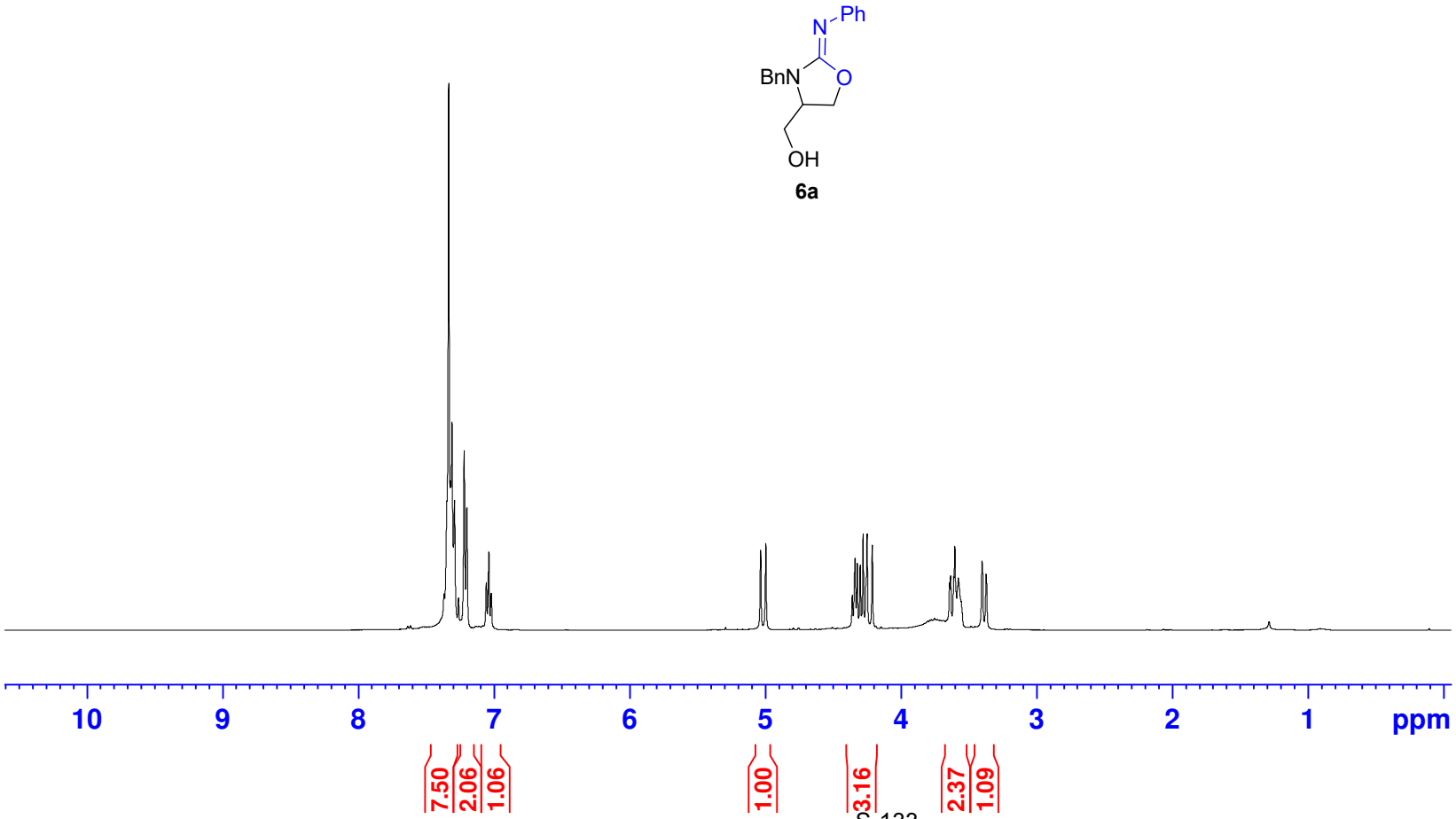
F2 - Acquisition Parameters
Date_           20151205
Time               21.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    35
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127836 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



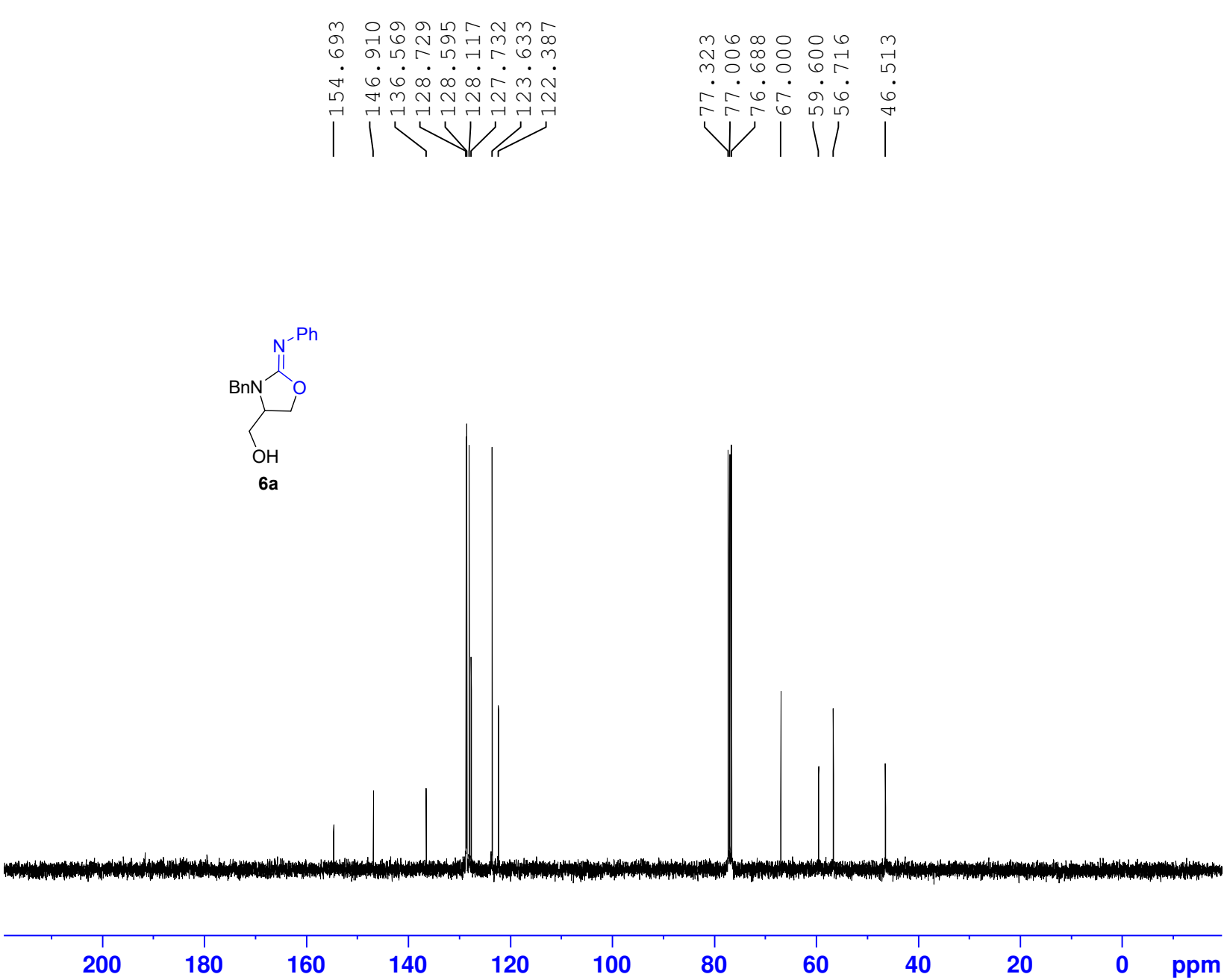



```
Current Data Parameters
NAME                 lzw2111
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150408
Time                  13.47
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       11
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                     45.67
DW                    62.400 usec
DE                     6.50 usec
TE                    296.2 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                      1H
P1                    14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                        65536
SF             400.1300092 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



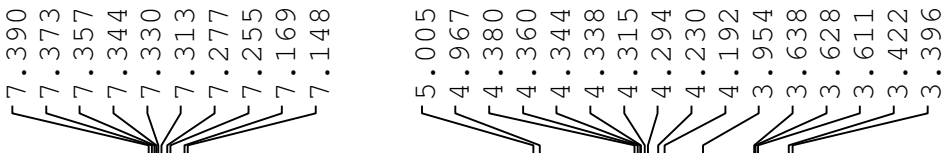

```
Current Data Parameters
NAME          lzw2111-C
EXPNO                 1
PROCNO                1

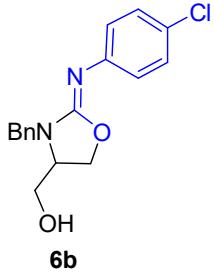
F2 - Acquisition Parameters
Date_          20150408
Time              23.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   33
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

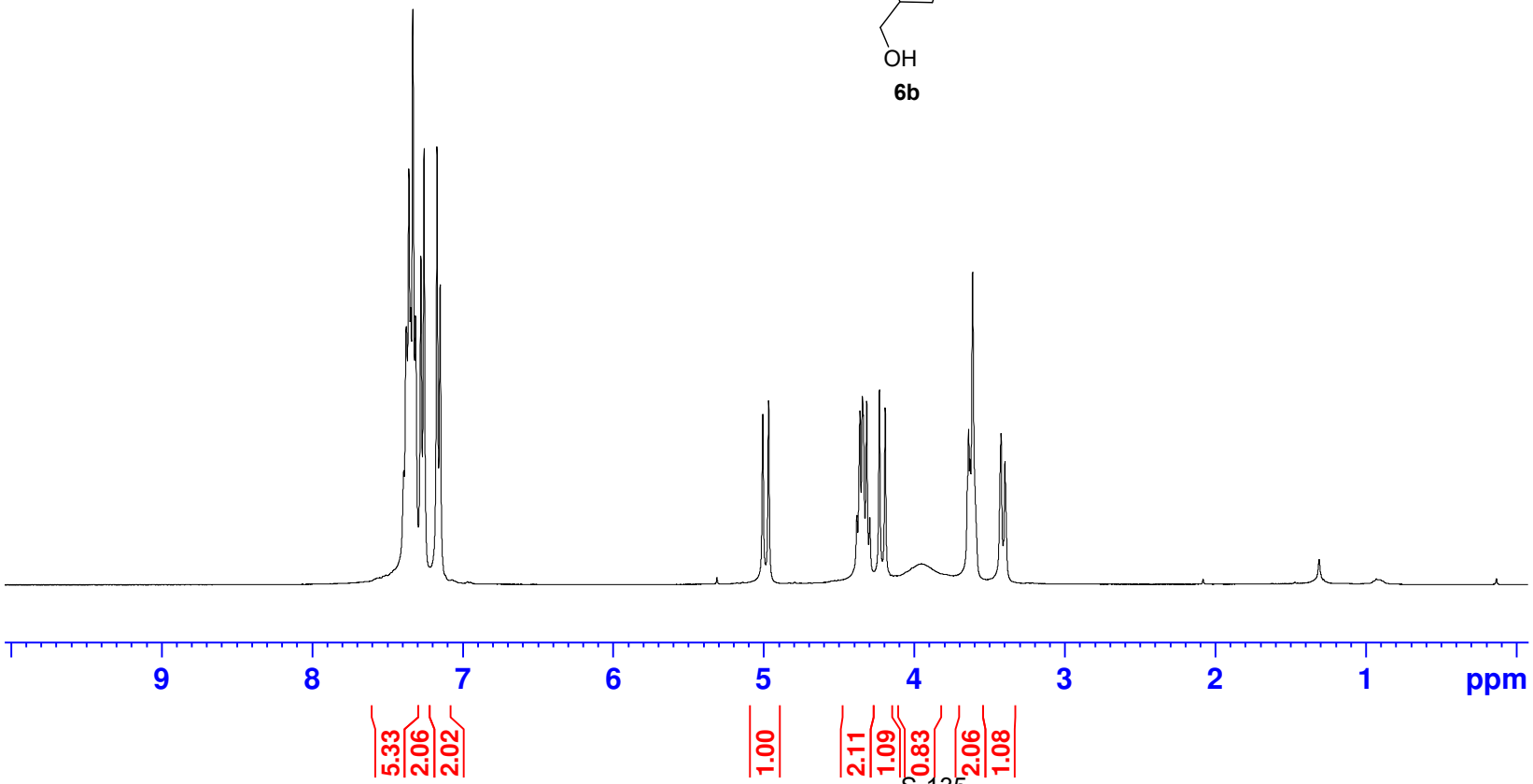
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127786 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





6b

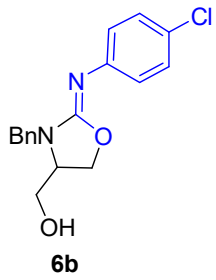



```
Current Data Parameters
NAME          lzw2124A-H
EXPNO                  1
PROCNO                 1

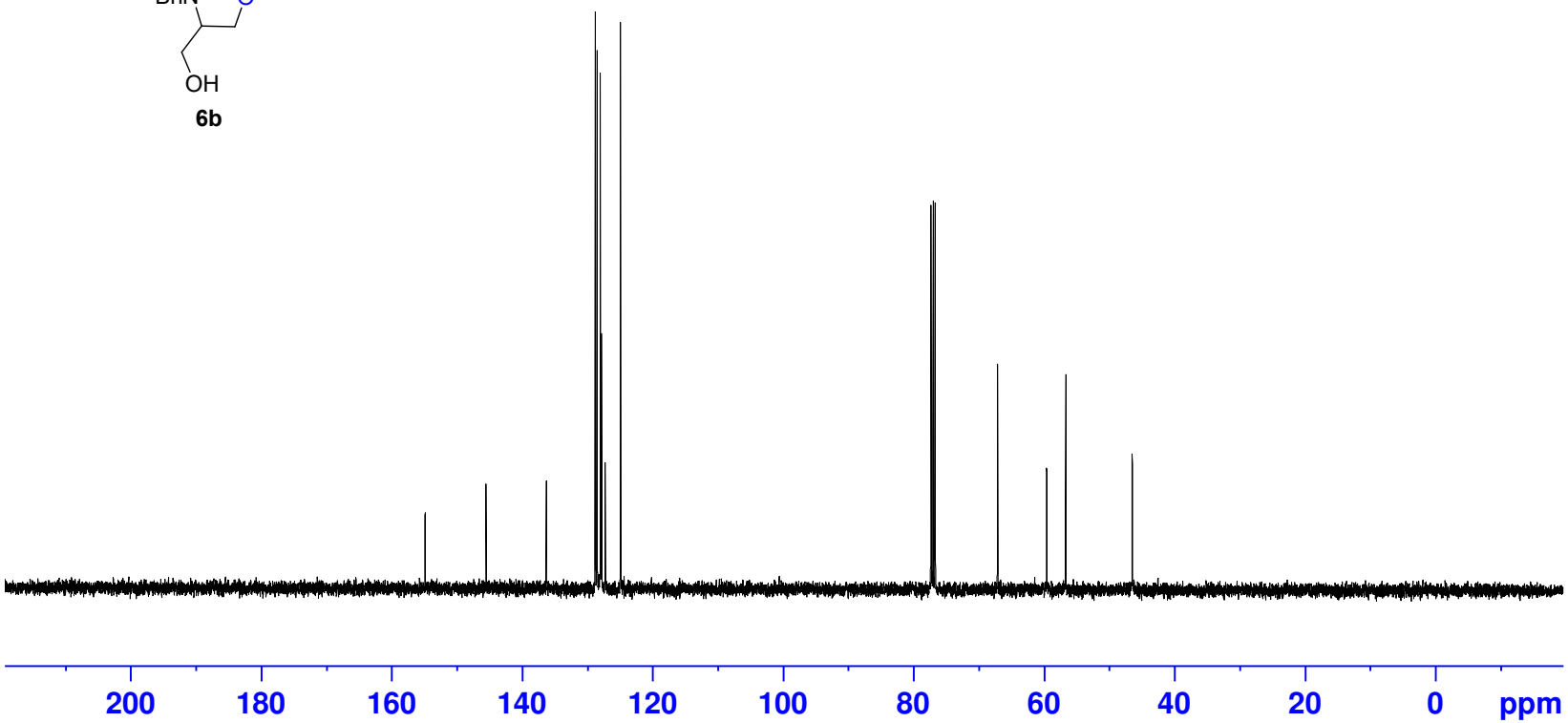
F2 - Acquisition Parameters
Date_           20150416
Time               22.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



6b



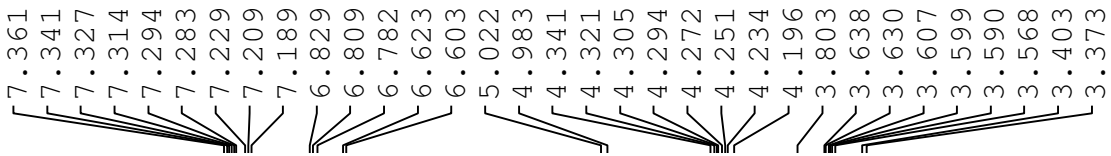

```
Current Data Parameters
NAME          lzw2124A-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150416
Time               22.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    30
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

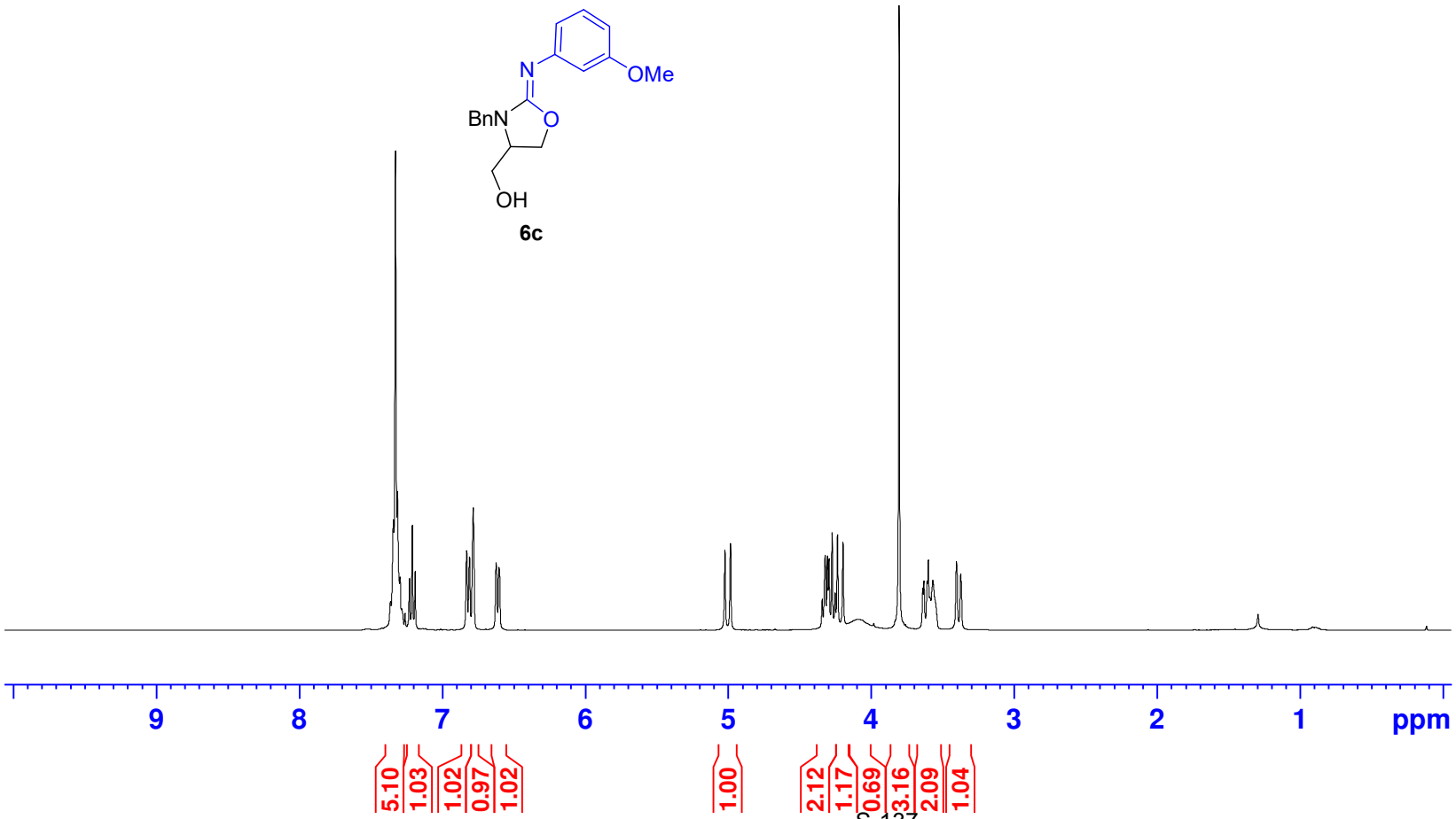
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127815 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



6c

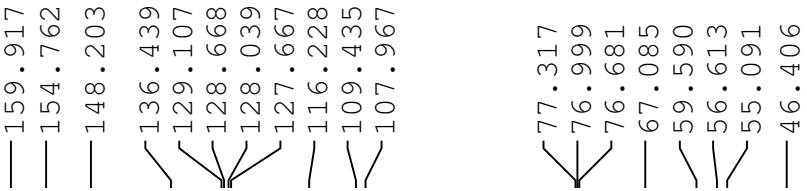


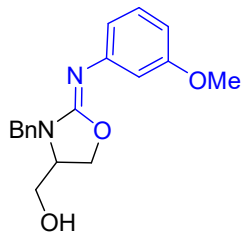

```
Current Data Parameters
NAME          lzw2124B-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150417
Time               15.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                296.2 K
D1             1.00000000 sec
TD0                    1

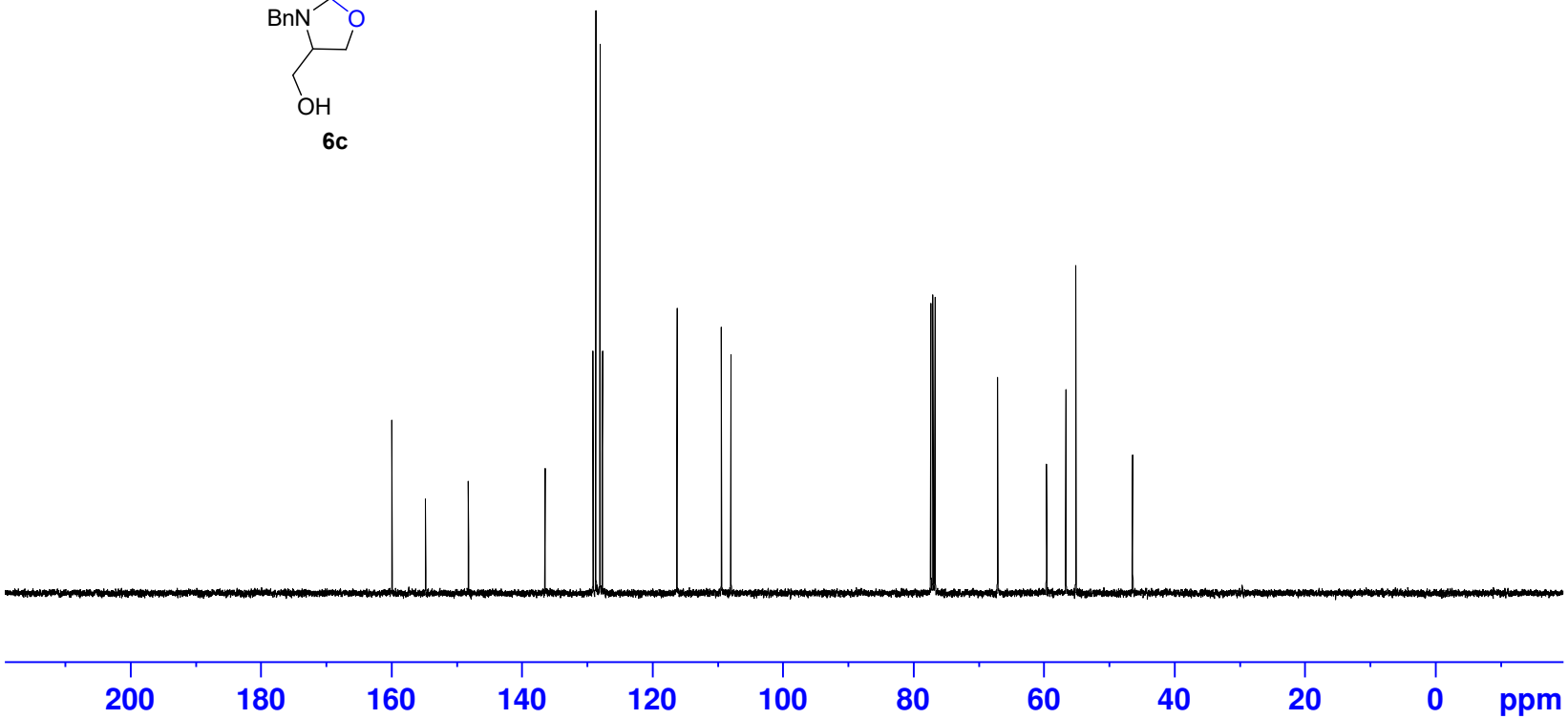
======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300089 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





6c



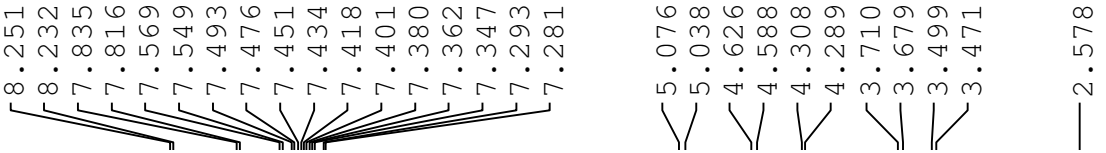

```
Current Data Parameters
NAME          lzw2124B-C
EXPNO                  1
PROCNO                 1

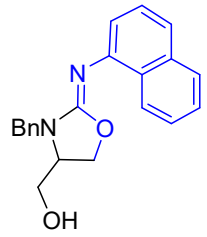
F2 - Acquisition Parameters
Date_           20150417
Time               16.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   101
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                  9.70 usec
PLW1          46.98899841 W

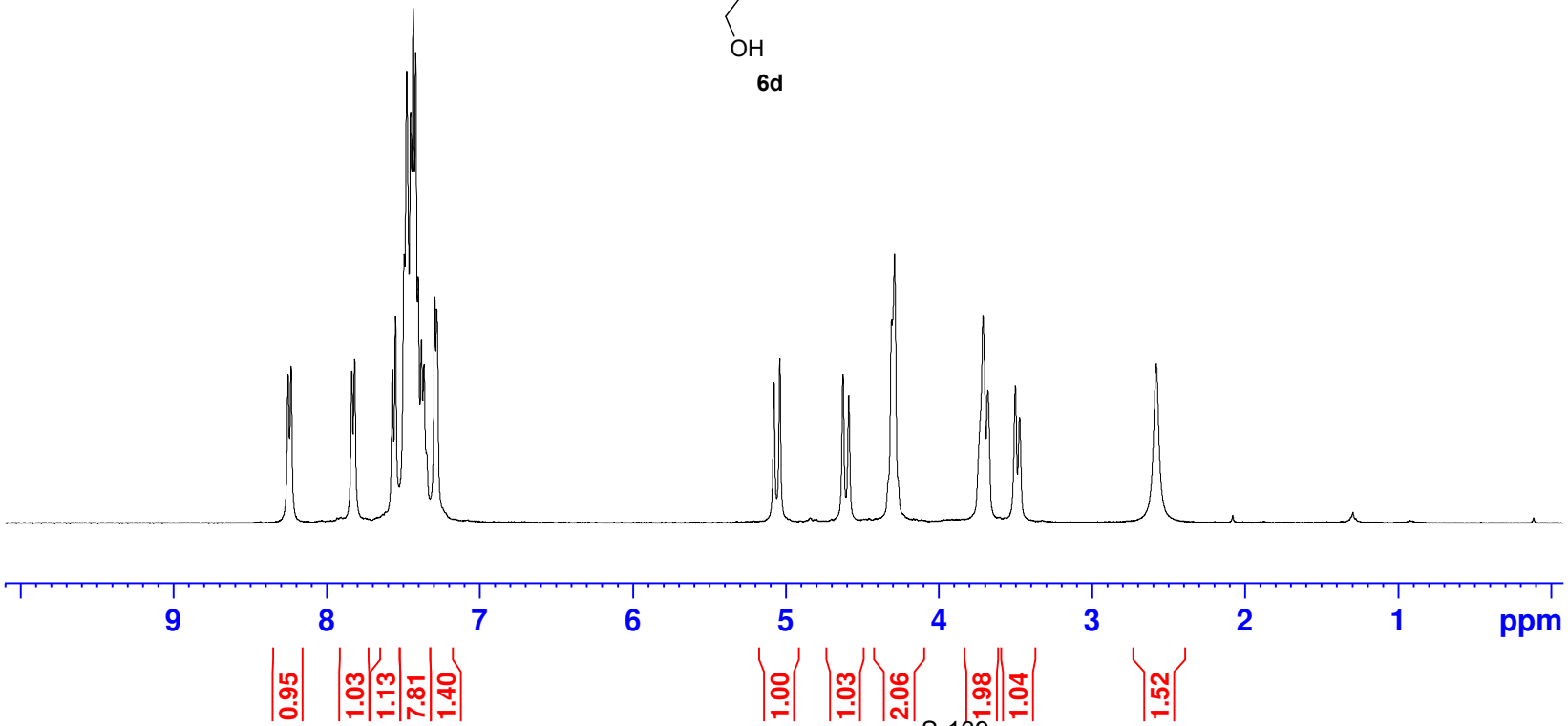
======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          11.99499989 W
PLW12          0.34213999 W
PLW13          0.27713001 W

F2 - Processing parameters
SI                 32768
SF            100.6127845 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





6d

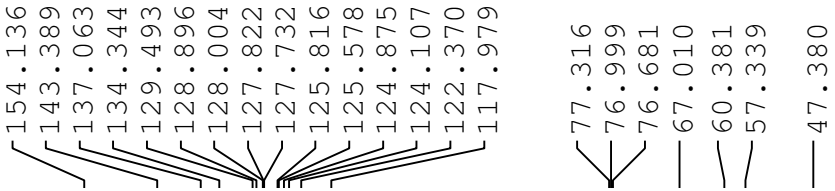


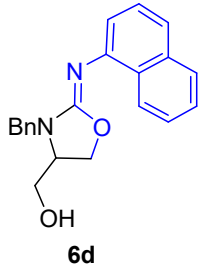

```
Current Data Parameters
NAME          lzw2121B-H
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150415
Time               17.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 103.52
DW                 62.400 usec
DE                  6.50 usec
TE                 296.1 K
D1             1.00000000 sec
TD0                    1

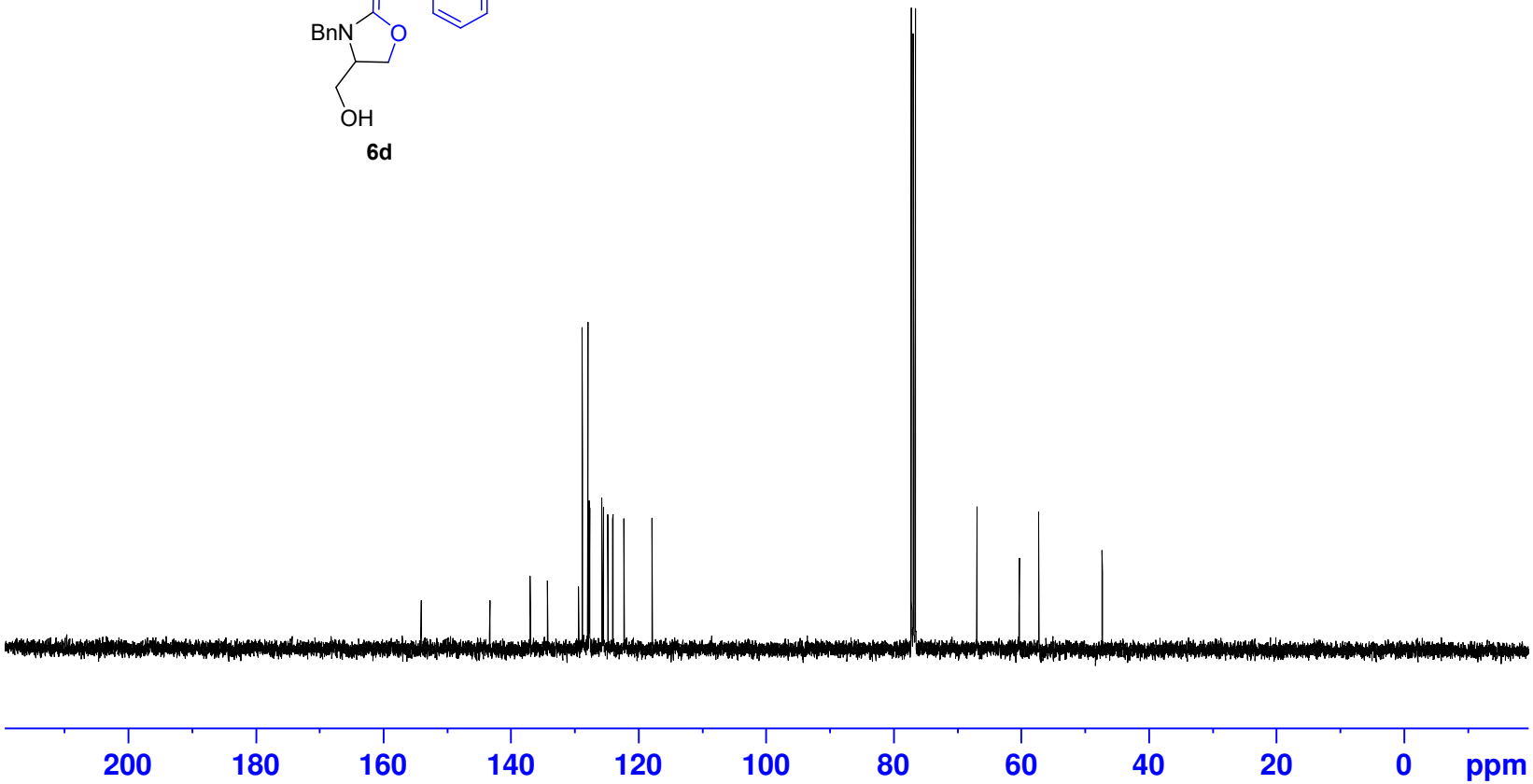
======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





6d



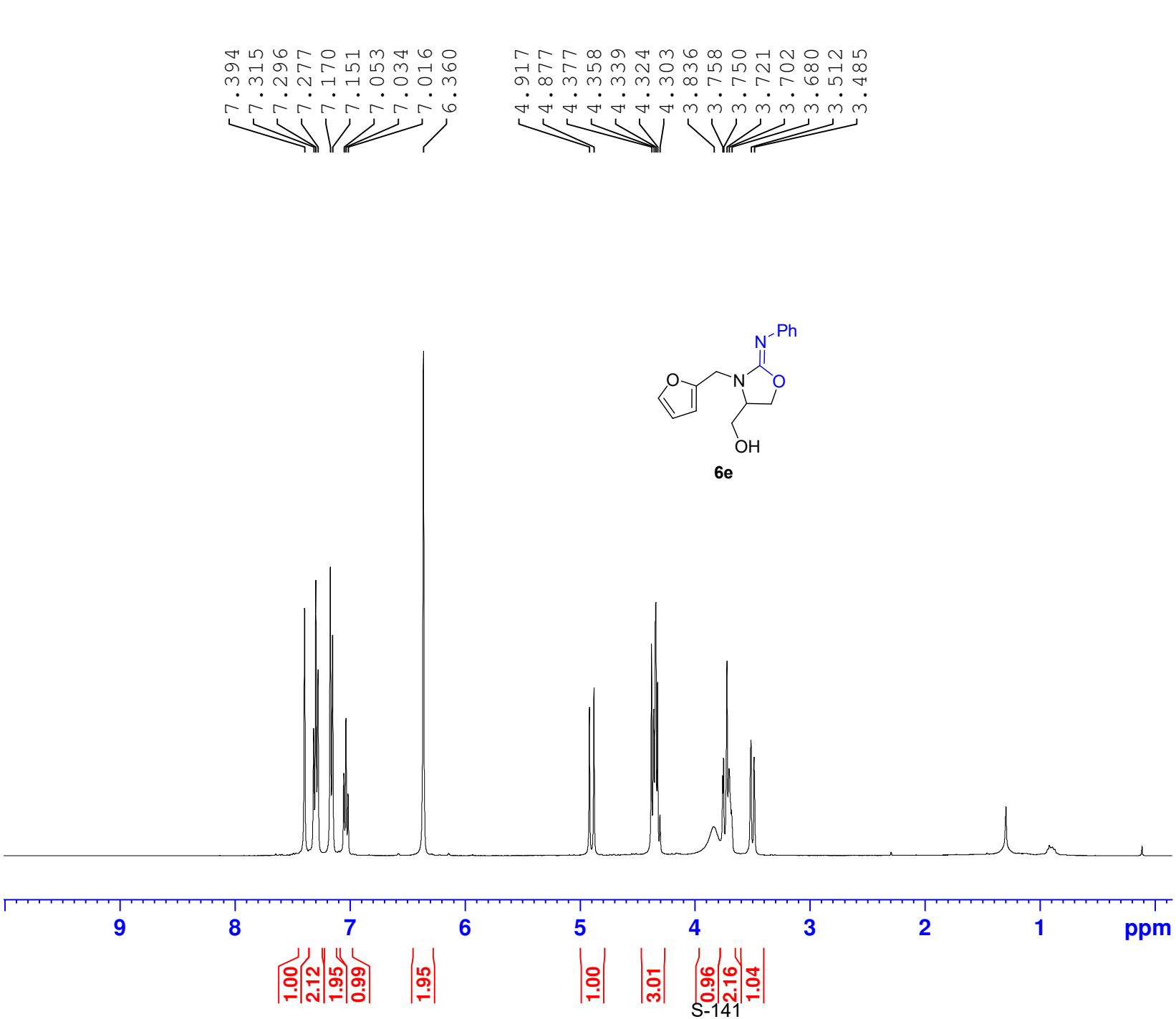

```
Current Data Parameters
NAME          lzw2121B-C
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150415
Time               14.49
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   123
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127748 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

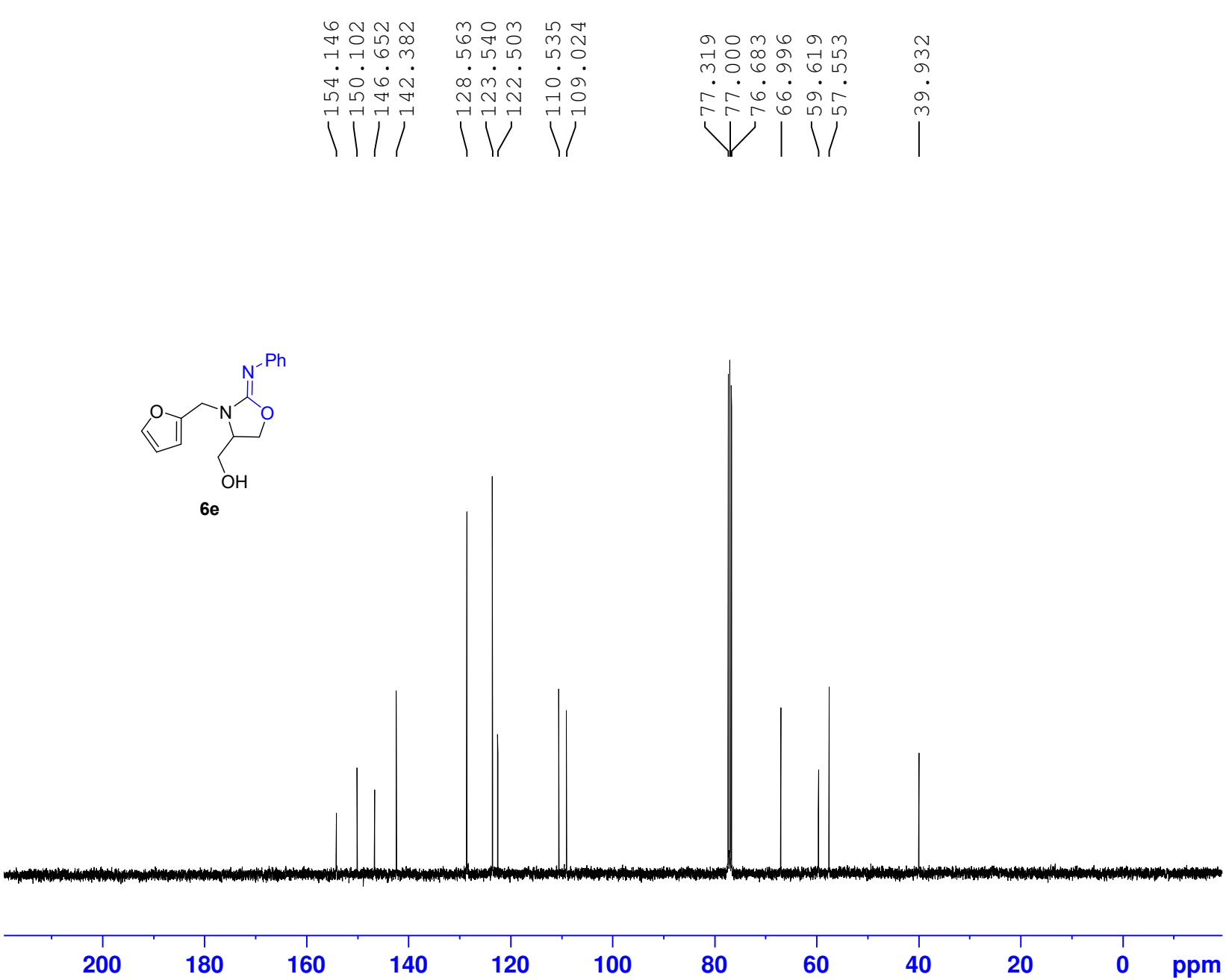



```
Current Data Parameters
NAME          lzw2130A-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150421
Time               23.49
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    13
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 54.81
DW                62.400 usec
DE                 6.50 usec
TE                297.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



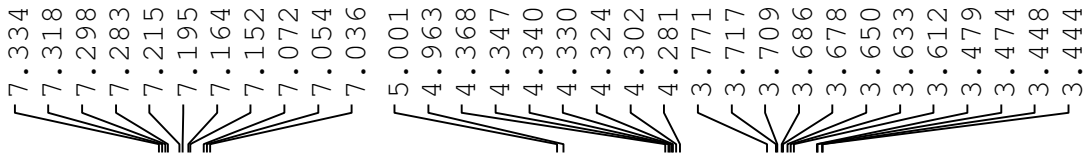

```
Current Data Parameters
NAME          lzw2130A-C
EXPNO                  1
PROCNO                 1

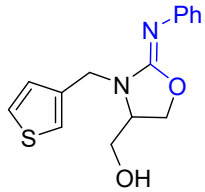
F2 - Acquisition Parameters
Date_           20150421
Time               23.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   113
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                  9.70 usec
PLW1          46.98899841 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          11.99499989 W
PLW12          0.34213999 W
PLW13          0.27713001 W

F2 - Processing parameters
SI                 32768
SF            100.6127766 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





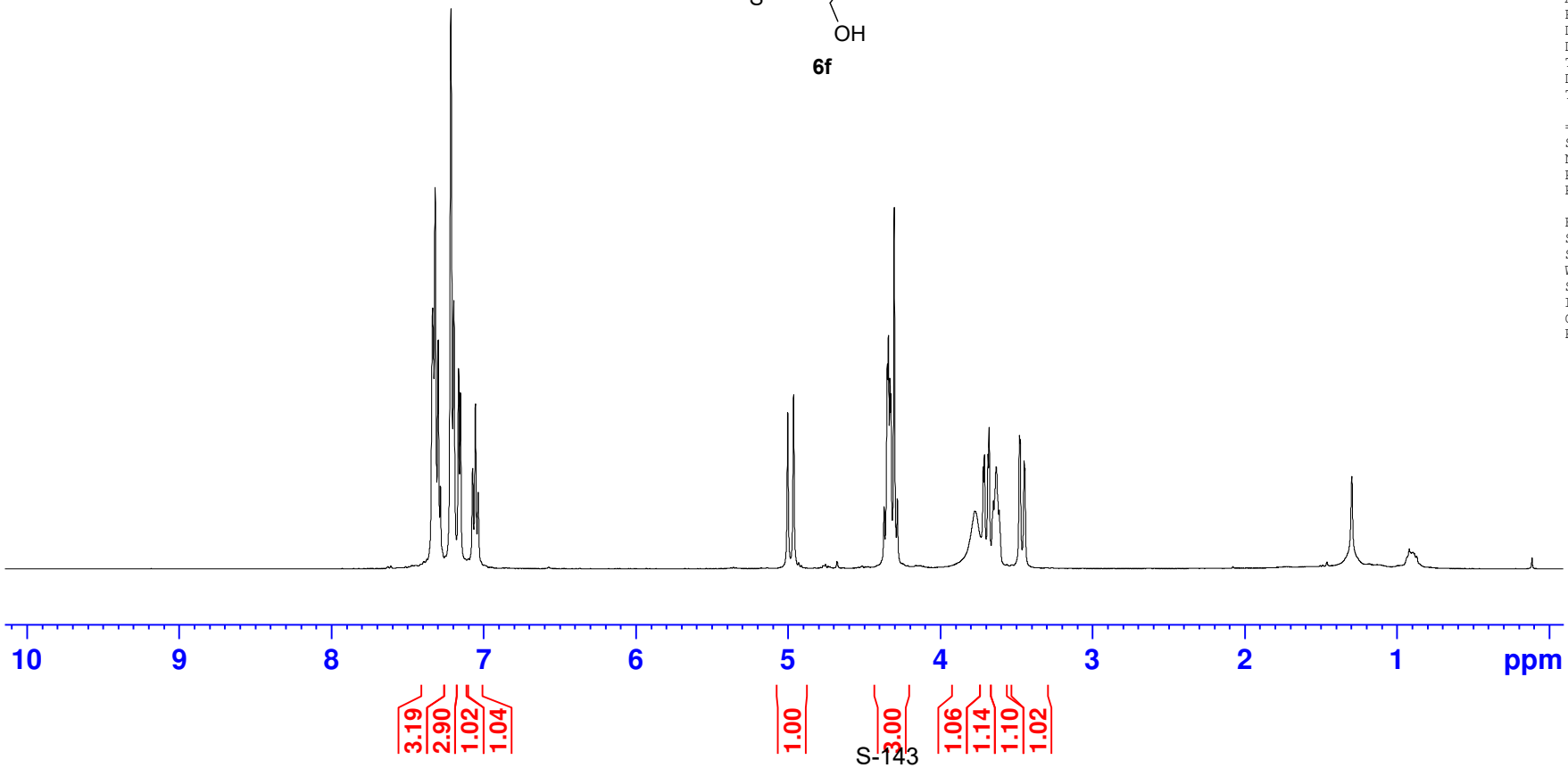
6f

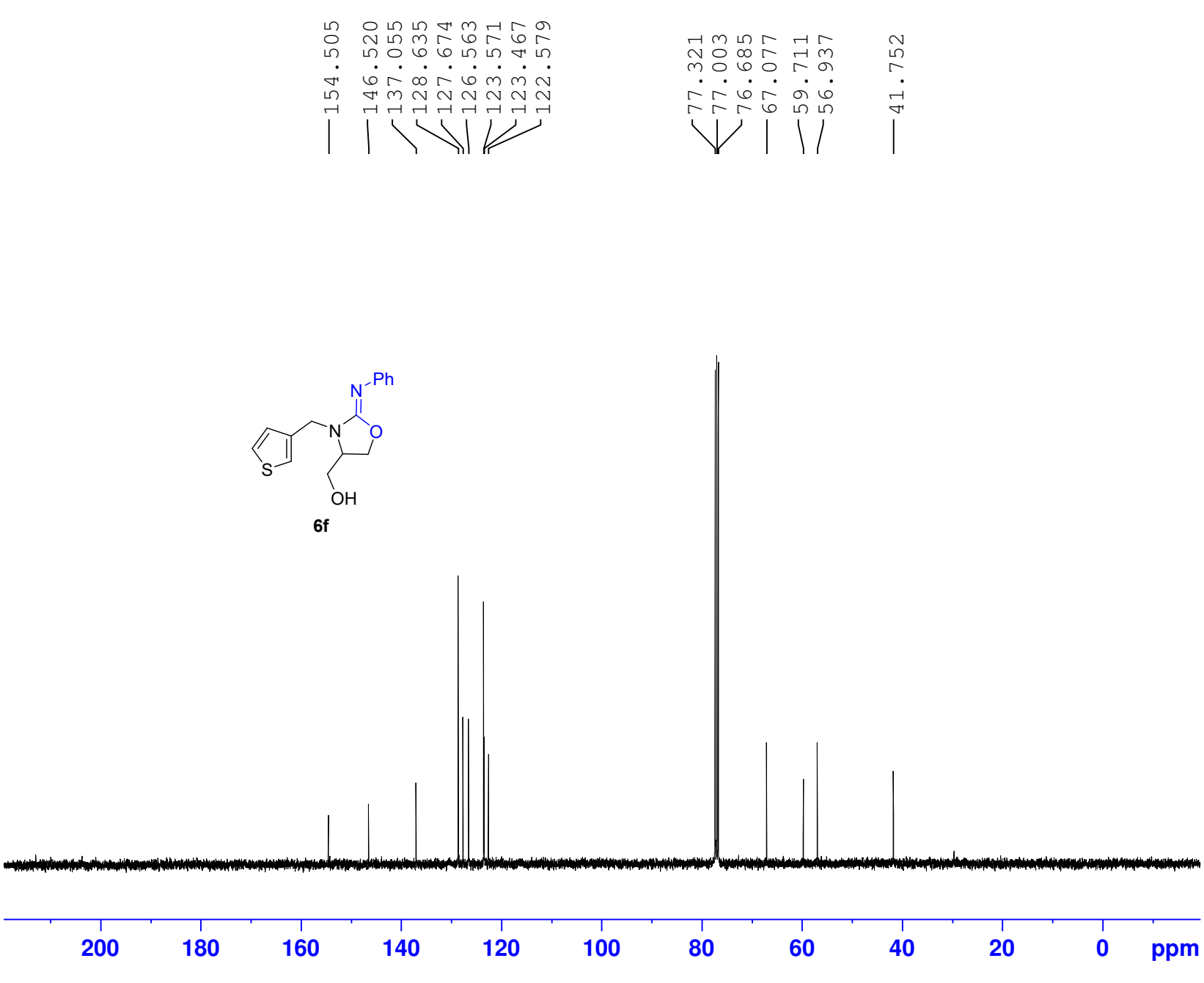
```
Current Data Parameters
NAME          lzw2130B-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150422
Time                0.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 54.81
DW                62.400 usec
DE                 6.50 usec
TE                297.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





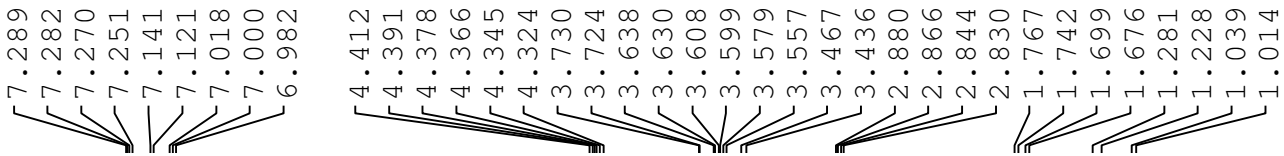
Current Data Parameters
NAME lzw2130B-C
EXPNO 1
PROCNO 1

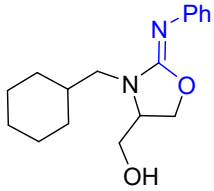
F2 - Acquisition Parameters
Date_ 20150422
Time 0.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 136
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W

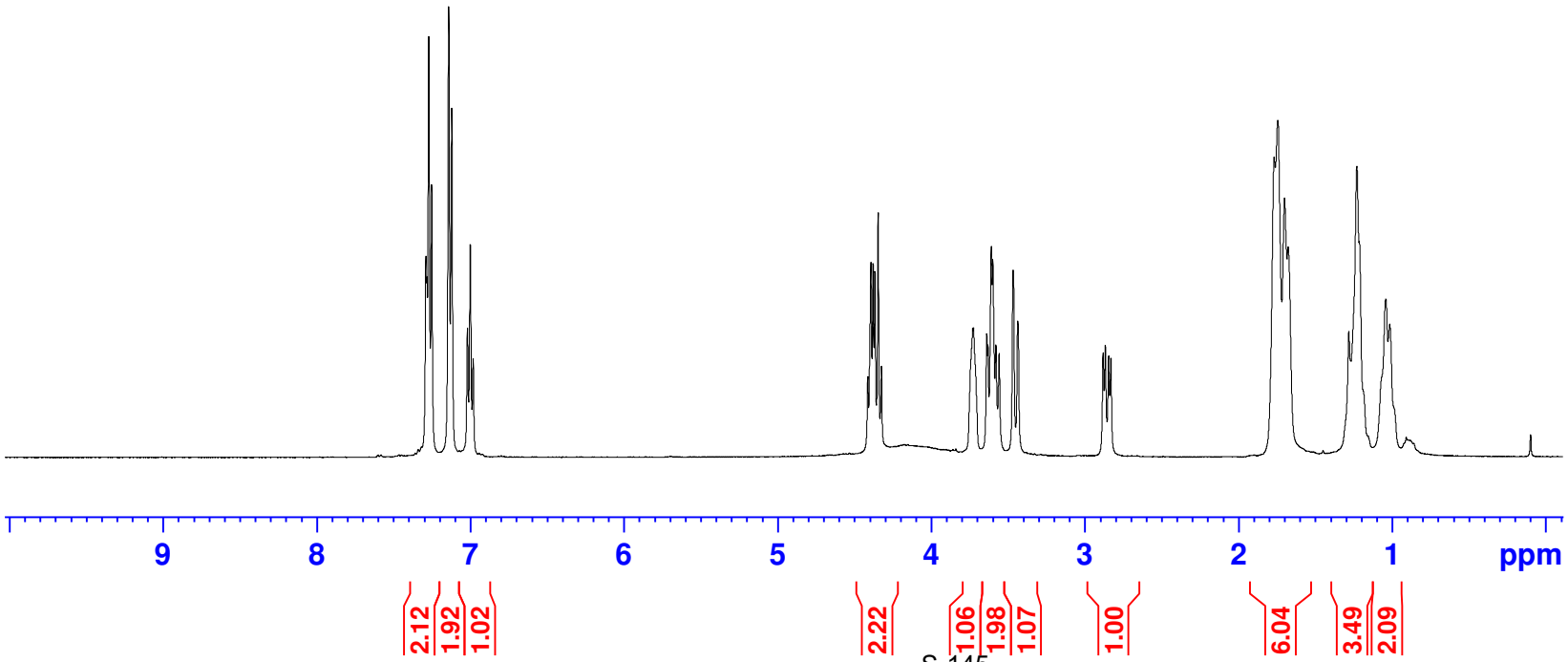
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W

F2 - Processing parameters
SI 32768
SF 100.6127761 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





6g

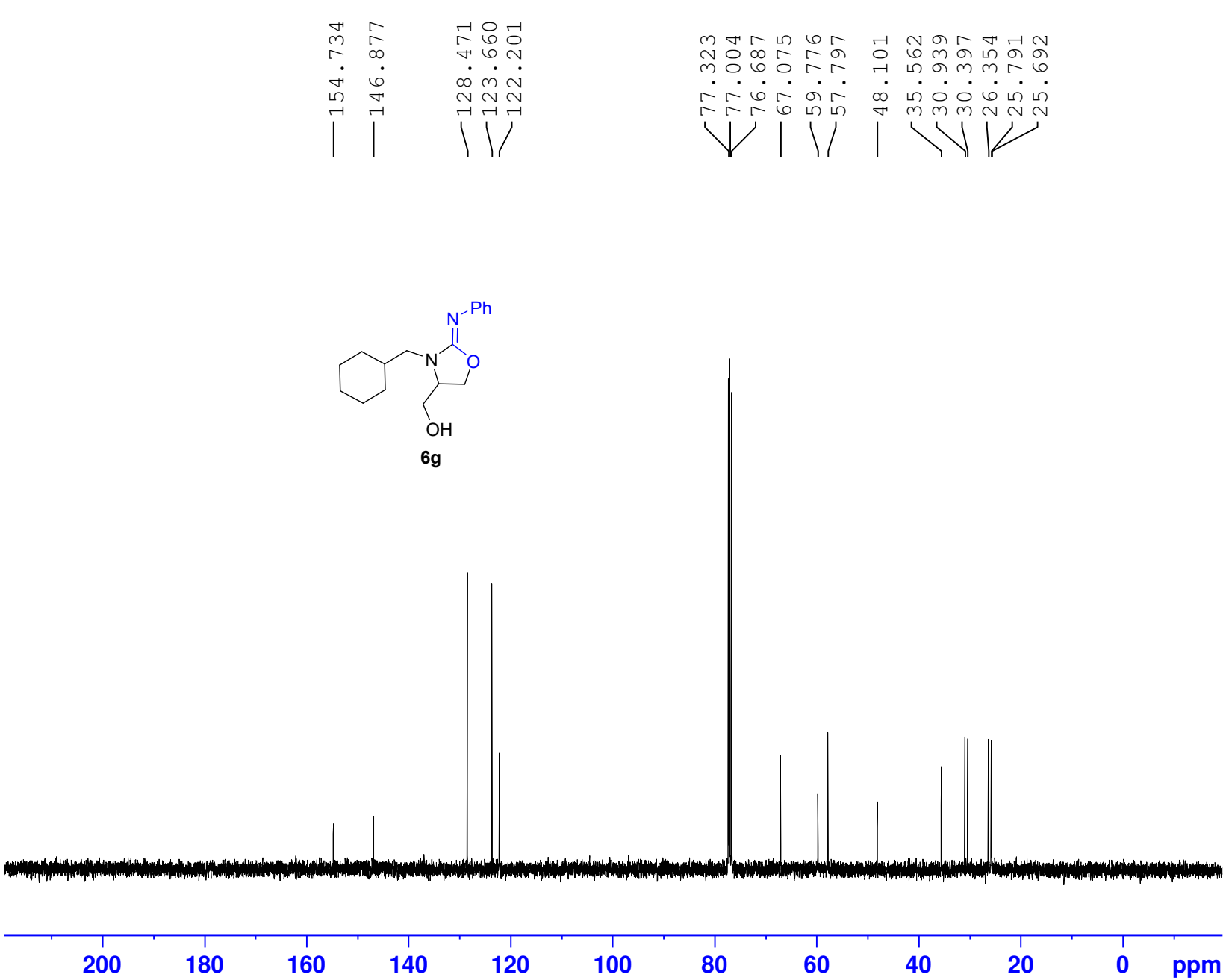



```
Current Data Parameters
NAME          lzw2131A-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150422
Time               16.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 45.67
DW                62.400 usec
DE                 6.50 usec
TE                296.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



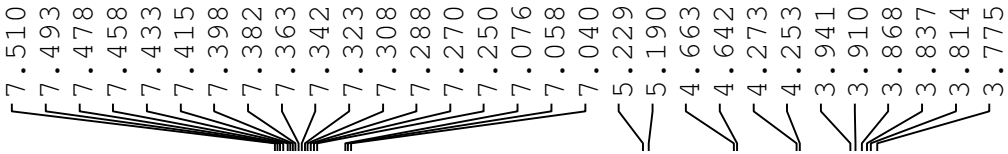

```
Current Data Parameters
NAME          lzw2131A-C
EXPNO                  1
PROCNO                 1

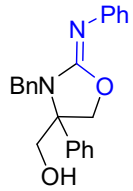
F2 - Acquisition Parameters
Date_           20150422
Time               16.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    36
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

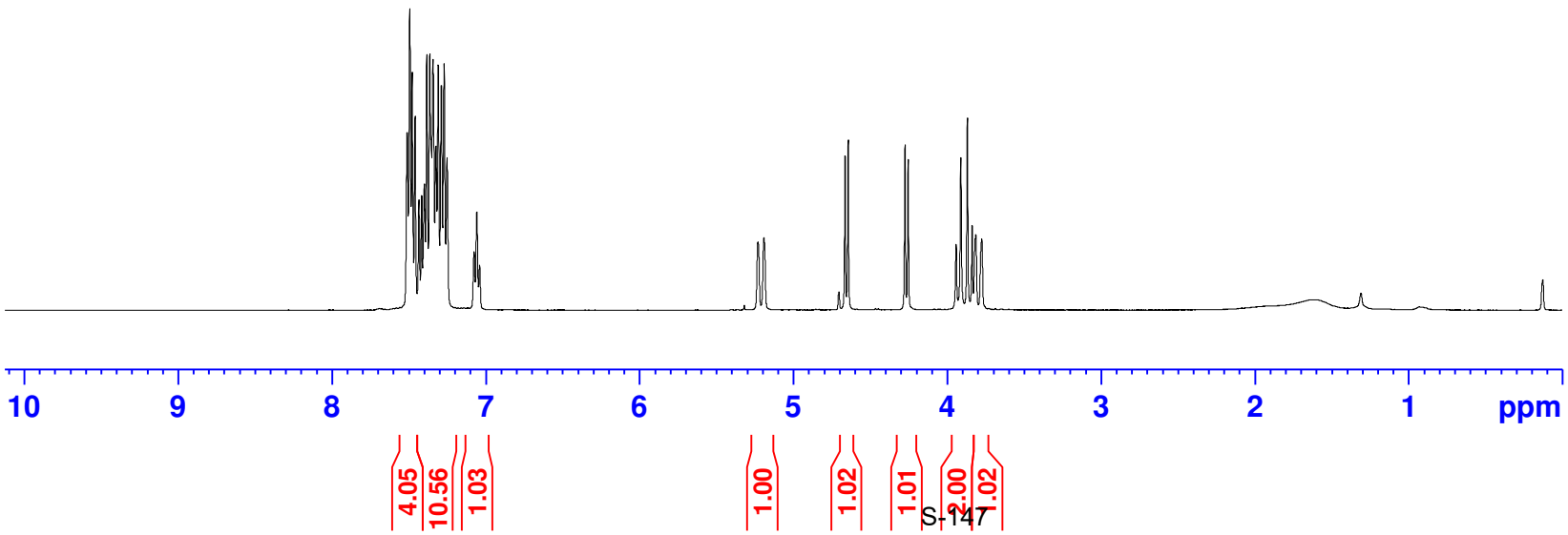
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127747 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





6h

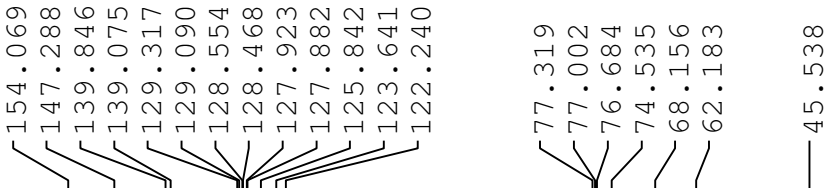


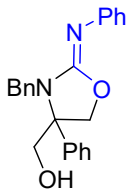

```
Current Data Parameters
NAME          lzw2131B-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150422
Time               17.10
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 49.32
DW                62.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

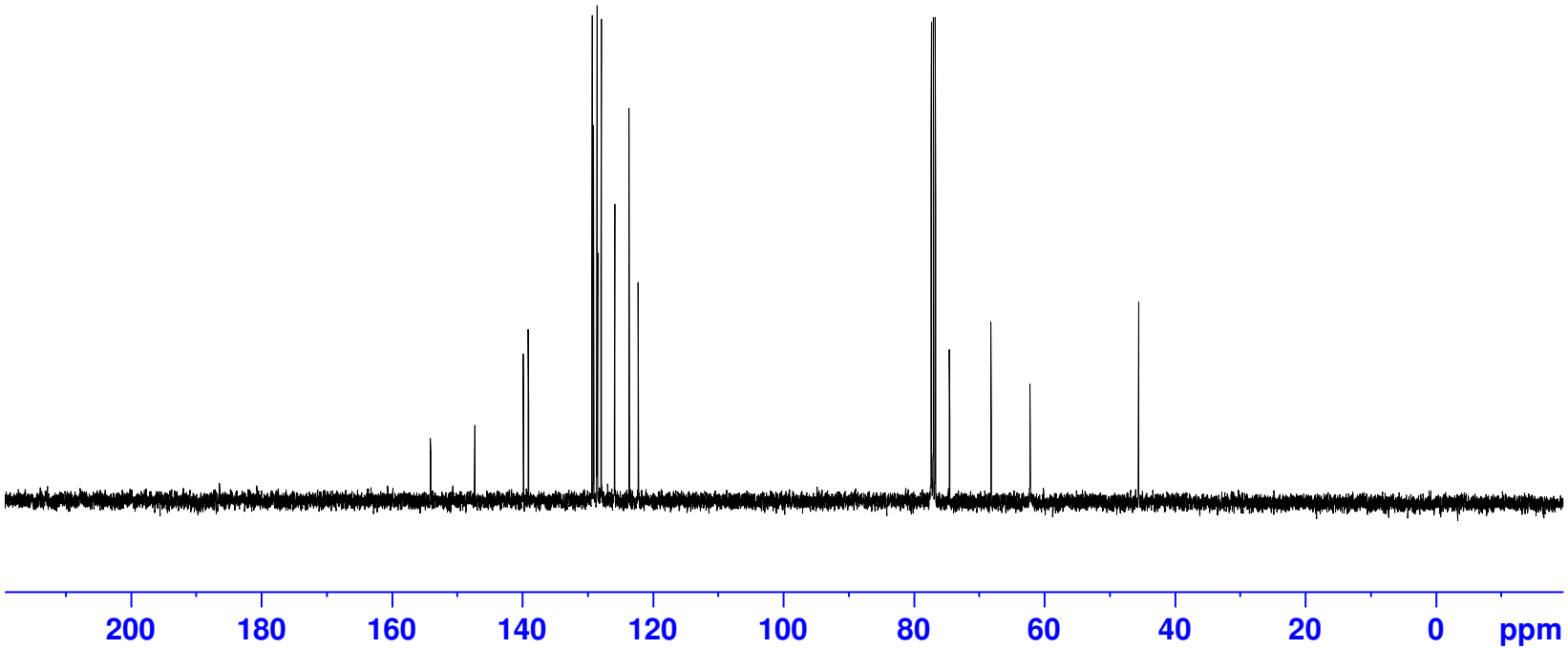
======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





6h



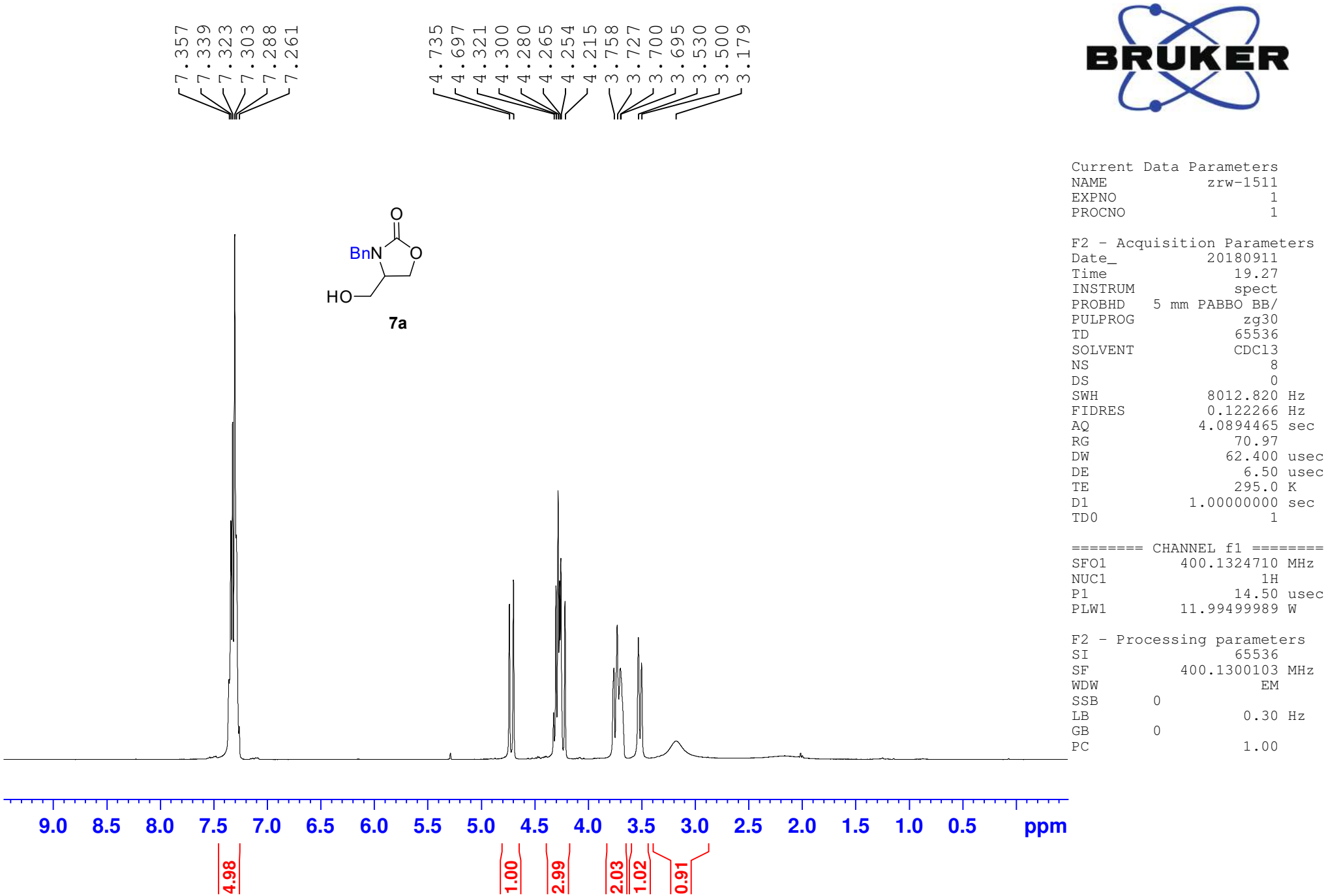

```
Current Data Parameters
NAME          lzw2131B-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150422
Time               17.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    71
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127777 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

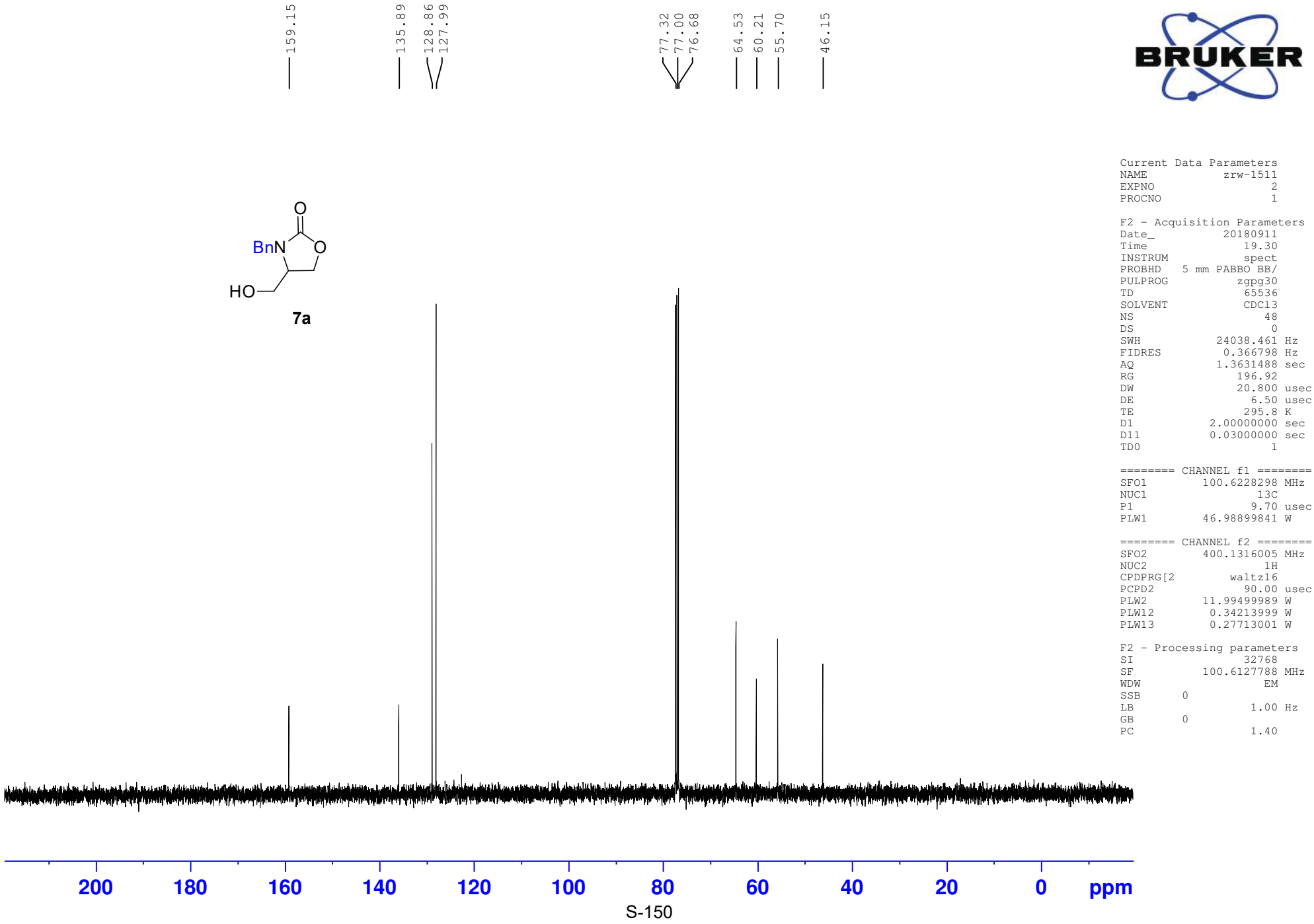



```
Current Data Parameters
NAME                  zrw-1511
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180911
Time                     19.27
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       70.97
DW                     62.400 usec
DE                      6.50 usec
TE                      295.0 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                           65536
SF                 400.1300103 MHz
WDW                             EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



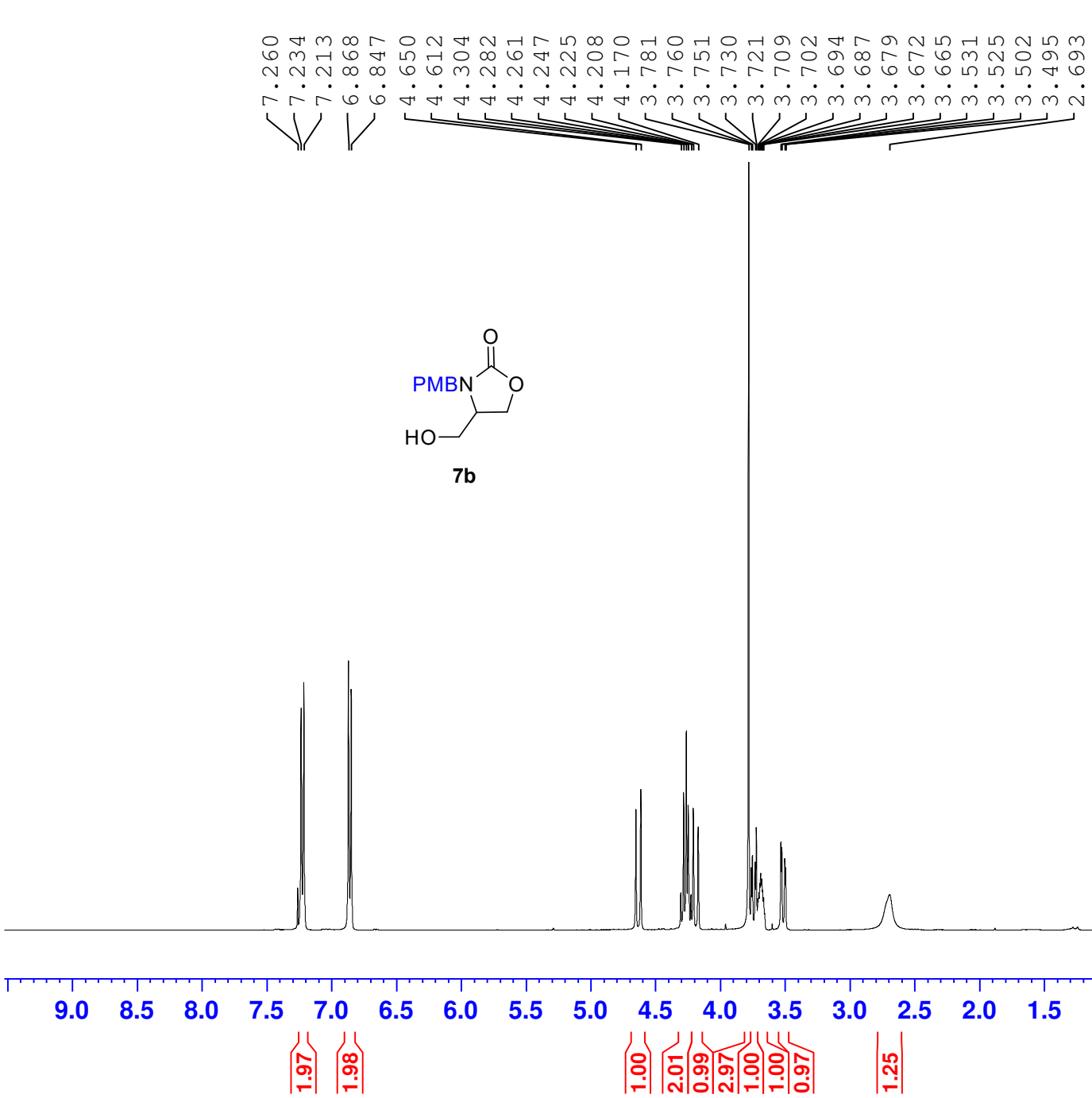

```
Current Data Parameters
NAME                 zrw-1511
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180911
Time                   19.30
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         48
DS                          0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     295.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                      9.70 usec
PLW1              46.98899841 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              11.99499989 W
PLW12              0.34213999 W
PLW13              0.27713001 W

F2 - Processing parameters
SI                      32768
SF               100.6127788 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

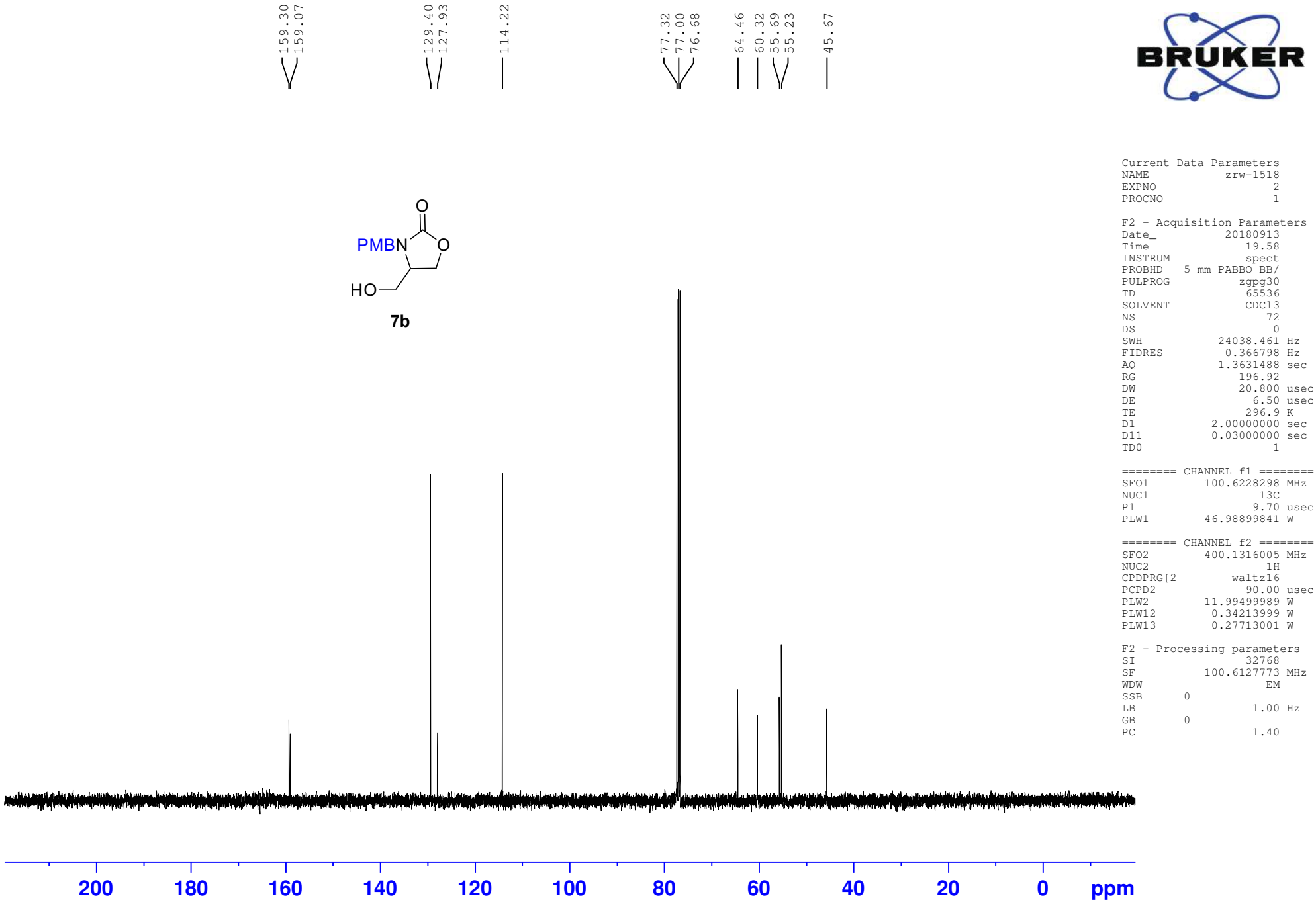


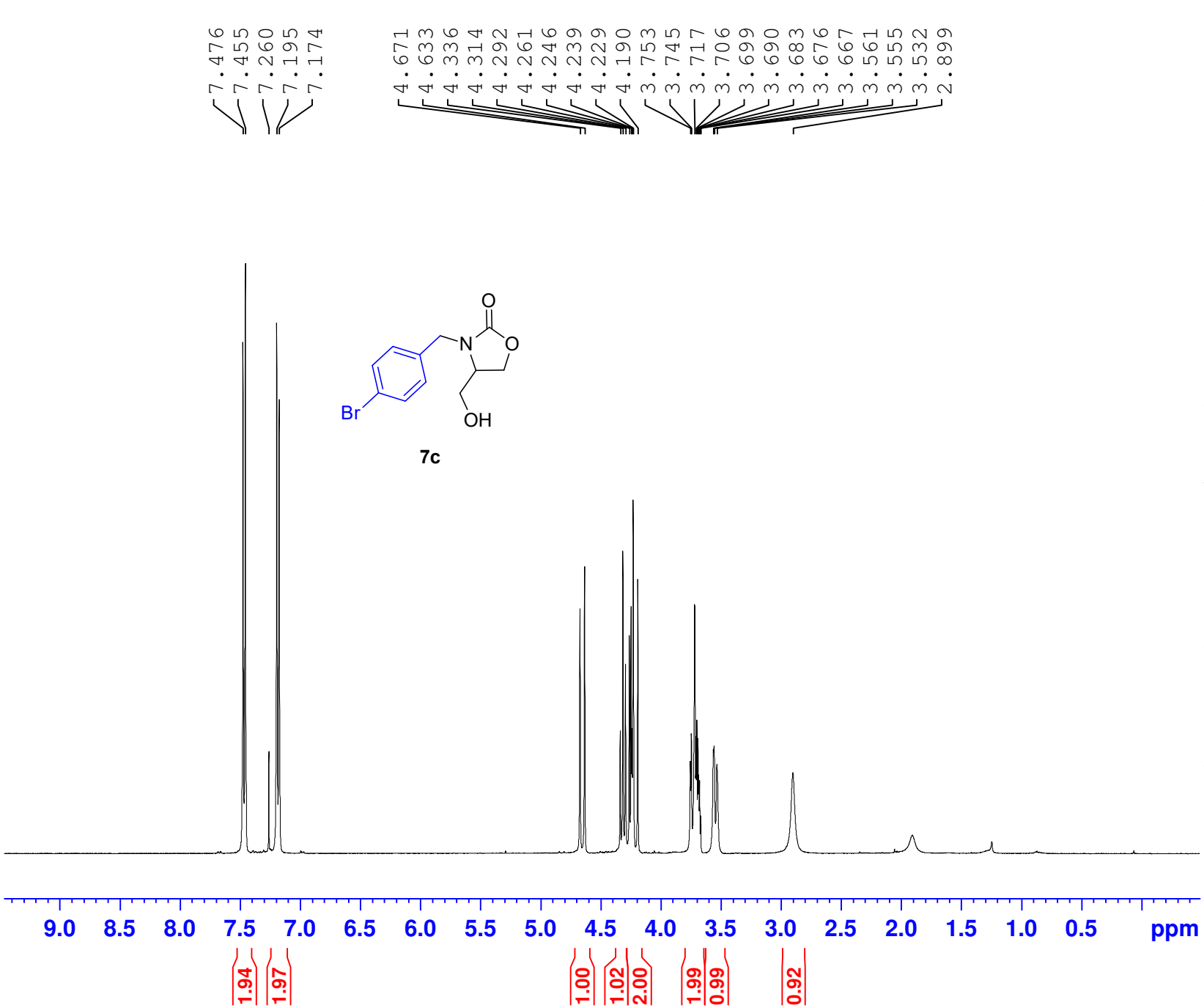
Current Data Parameters
NAME zrw-1518
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180913
Time 19.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.84
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


159.30
159.07
129.40
127.93
114.22
77.32
77.00
76.68
64.46
60.32
55.69
55.23
45.67
PMBN
O
O
HO
7b
Current Data Parameters
NAME zrw-1518
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180913
Time 19.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 72
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W
F2 - Processing parameters
SI 32768
SF 100.6127773 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

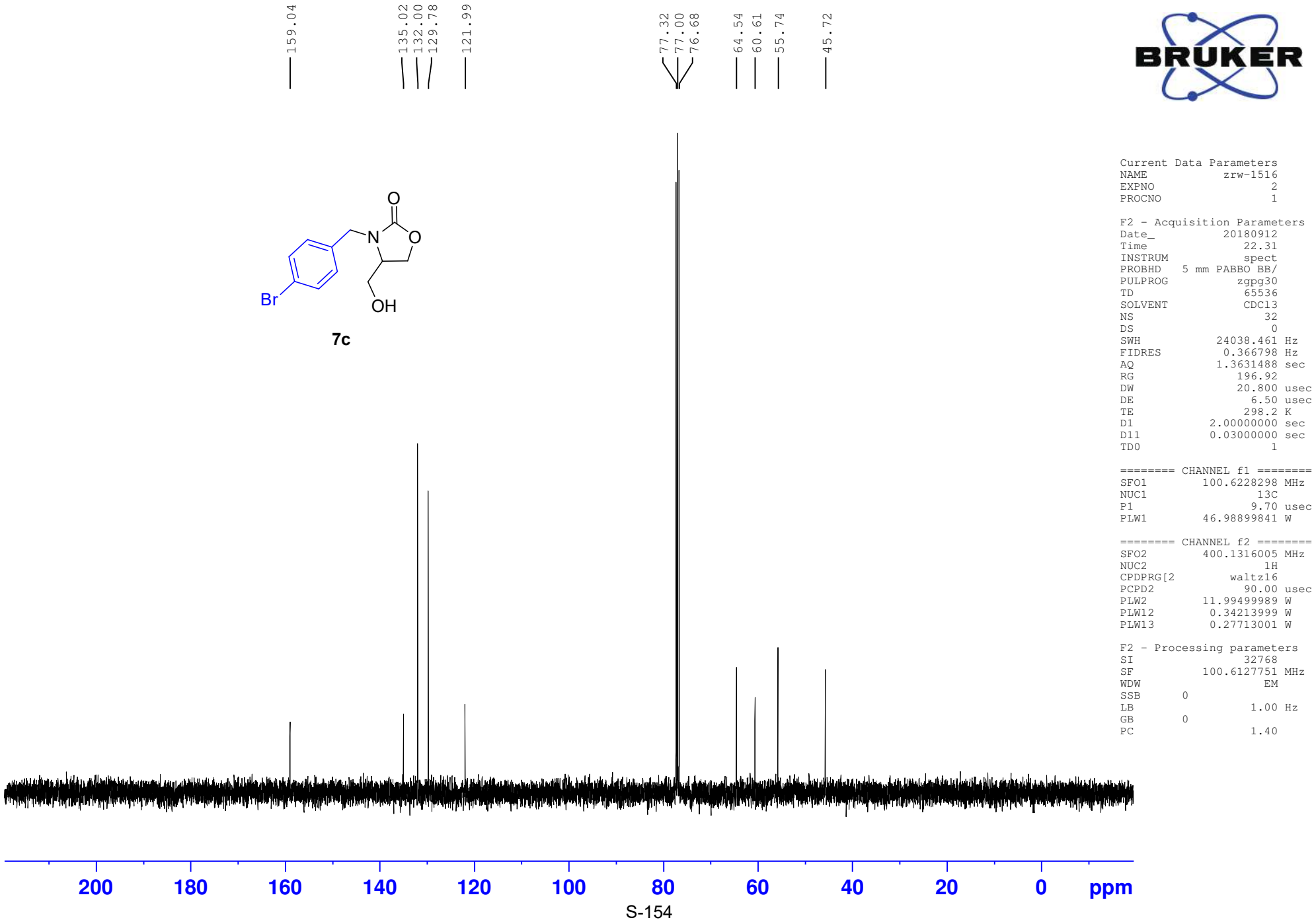


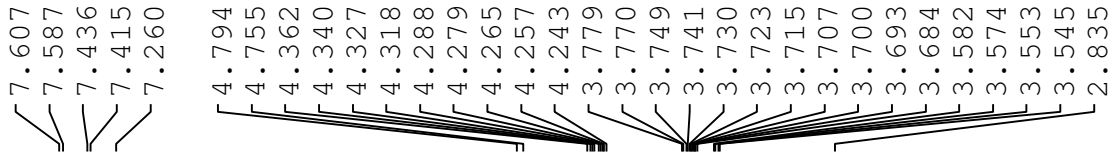

```
Current Data Parameters
NAME                 zrw-1516
EXPNO                       1
PROCNO                      1

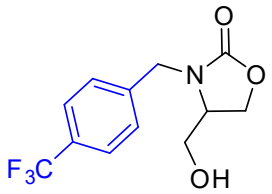
F2 - Acquisition Parameters
Date_               20180912
Time                   22.29
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         4
DS                         0
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                    126.97
DW                    62.400 usec
DE                     6.50 usec
TE                    297.5 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                       1H
P1                    14.50 usec
PLW1            11.99499989 W

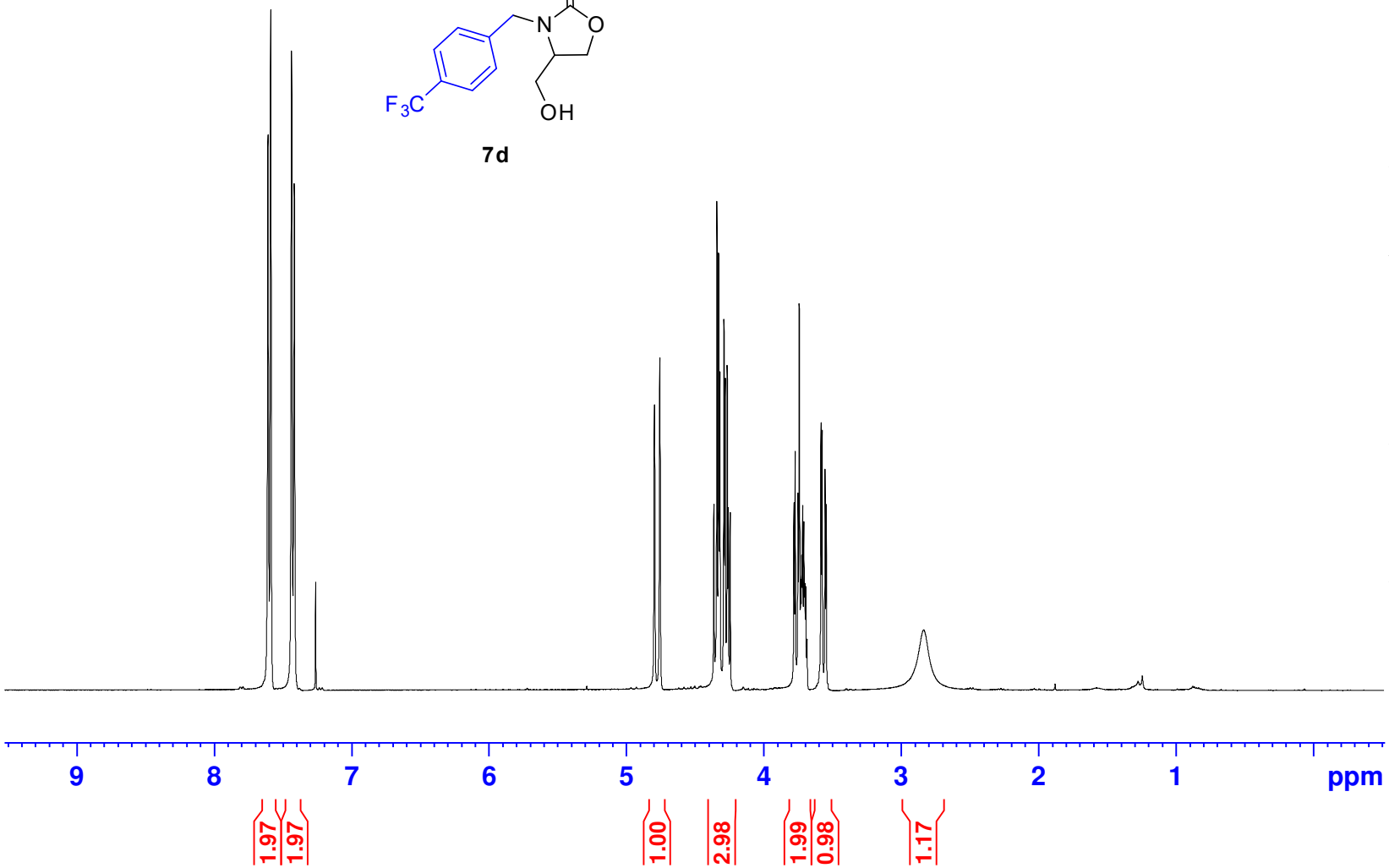
F2 - Processing parameters
SI                         65536
SF              400.1300104 MHz
WDW                        EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```


159.04
135.02
132.00
129.78
121.99
77.32
77.00
76.68
64.54
60.61
55.74
45.72
O
N
O
Br
OH
7c
Current Data Parameters
NAME zrw-1516
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180912
Time 22.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W
F2 - Processing parameters
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm





7d

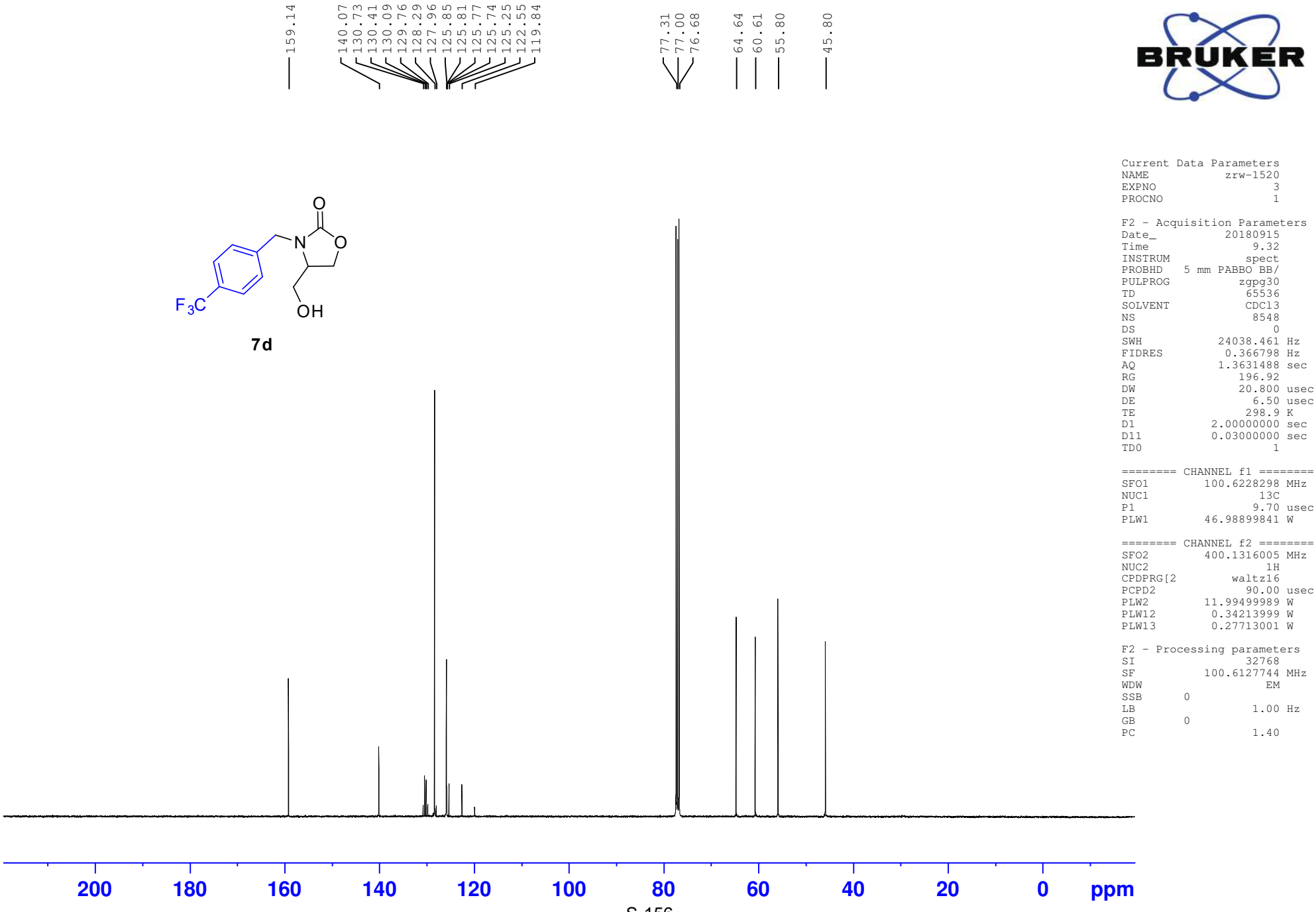



```
Current Data Parameters
NAME                  zrw-1520
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180913
Time                     21.57
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           4
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                      103.52
DW                      62.400 usec
DE                       6.50 usec
TE                      297.2 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                       65536
SF               400.1300103 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                       1.00
```



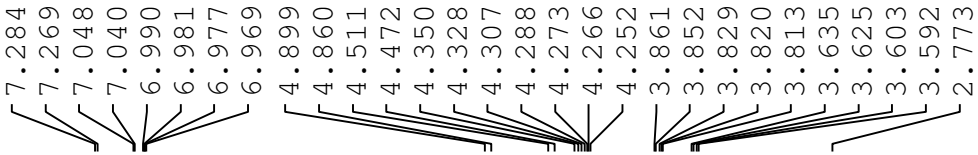

```
Current Data Parameters
NAME            zrw-1520
EXPNO                  3
PROCNO                 1

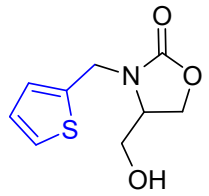
F2 - Acquisition Parameters
Date_           20180915
Time                9.32
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  8548
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               298.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

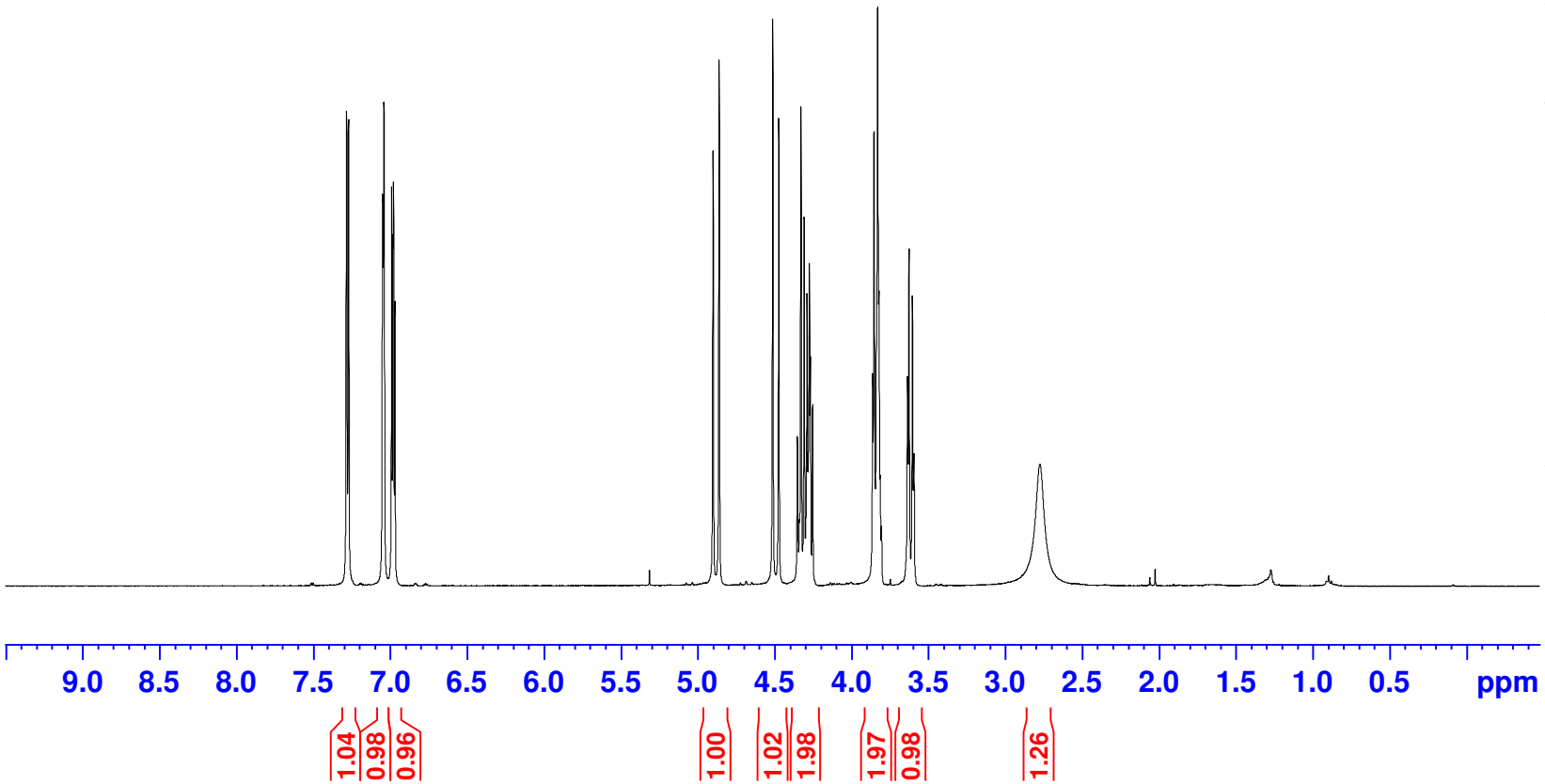
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127744 MHz
WDW                 EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





7e

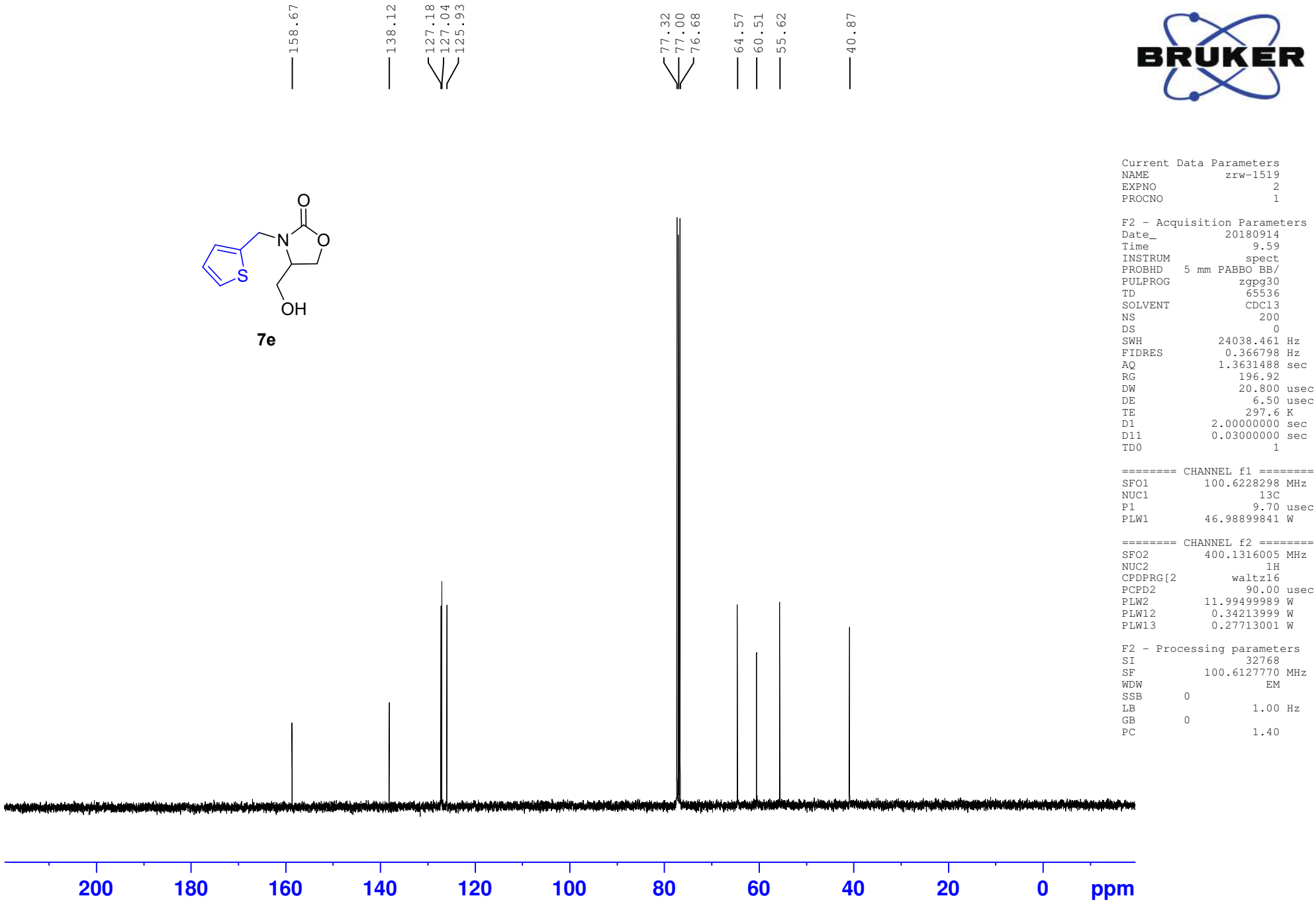



```
Current Data Parameters
NAME                 zrw-1519
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180914
Time                    9.47
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                          4
DS                          0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                      88.84
DW                     62.400 usec
DE                      6.50 usec
TE                     296.7 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                         65536
SF               400.1300000 MHz
WDW                          EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



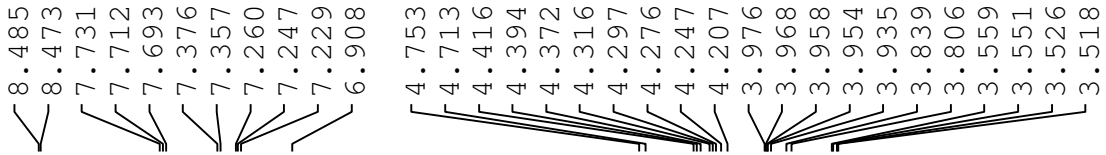

```
Current Data Parameters
NAME            zrw-1519
EXPNO                  2
PROCNO                 1

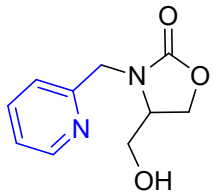
F2 - Acquisition Parameters
Date_           20180914
Time                9.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                9.70 usec
PLW1        46.98899841 W

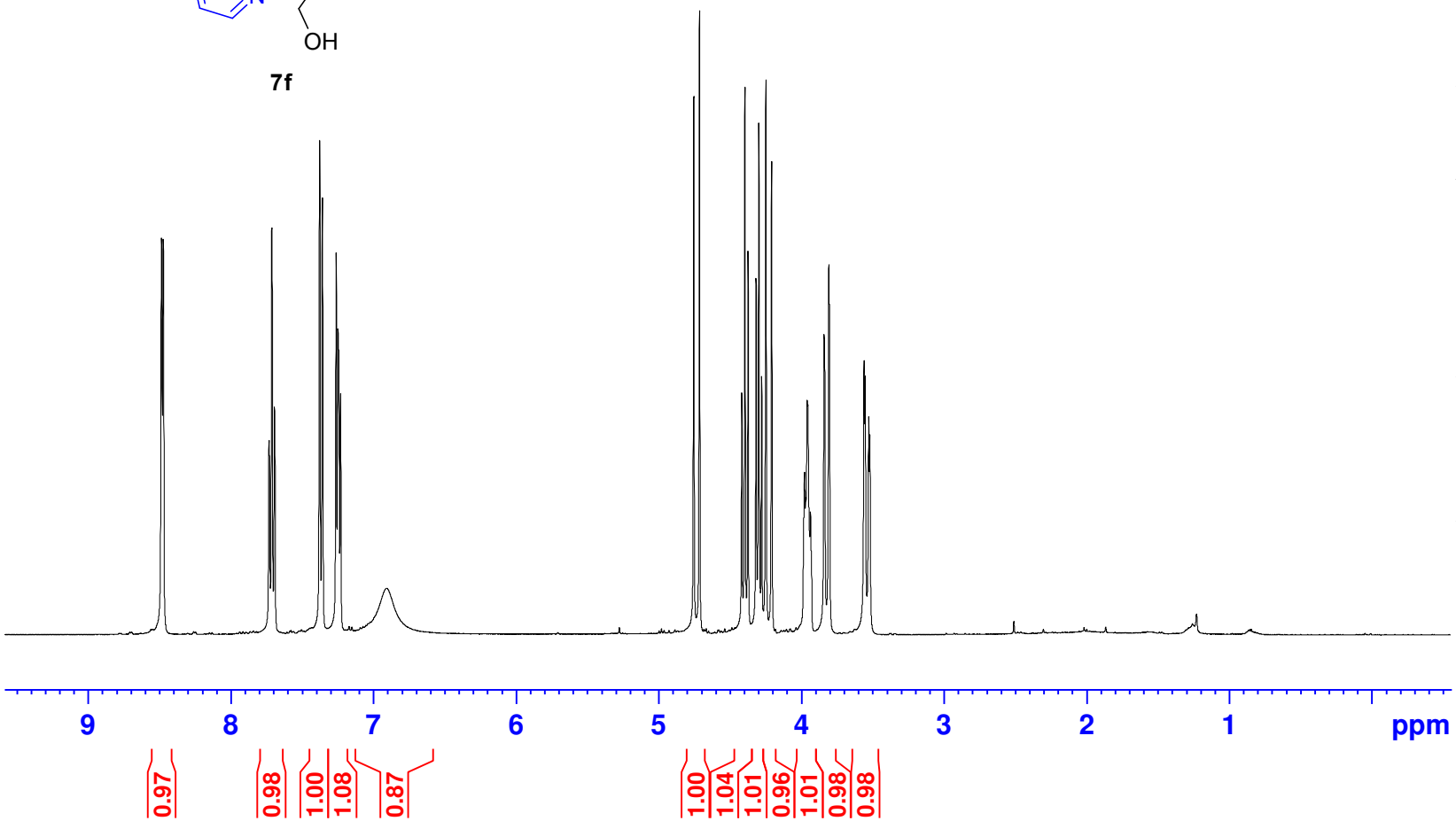
======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127770 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```





7f

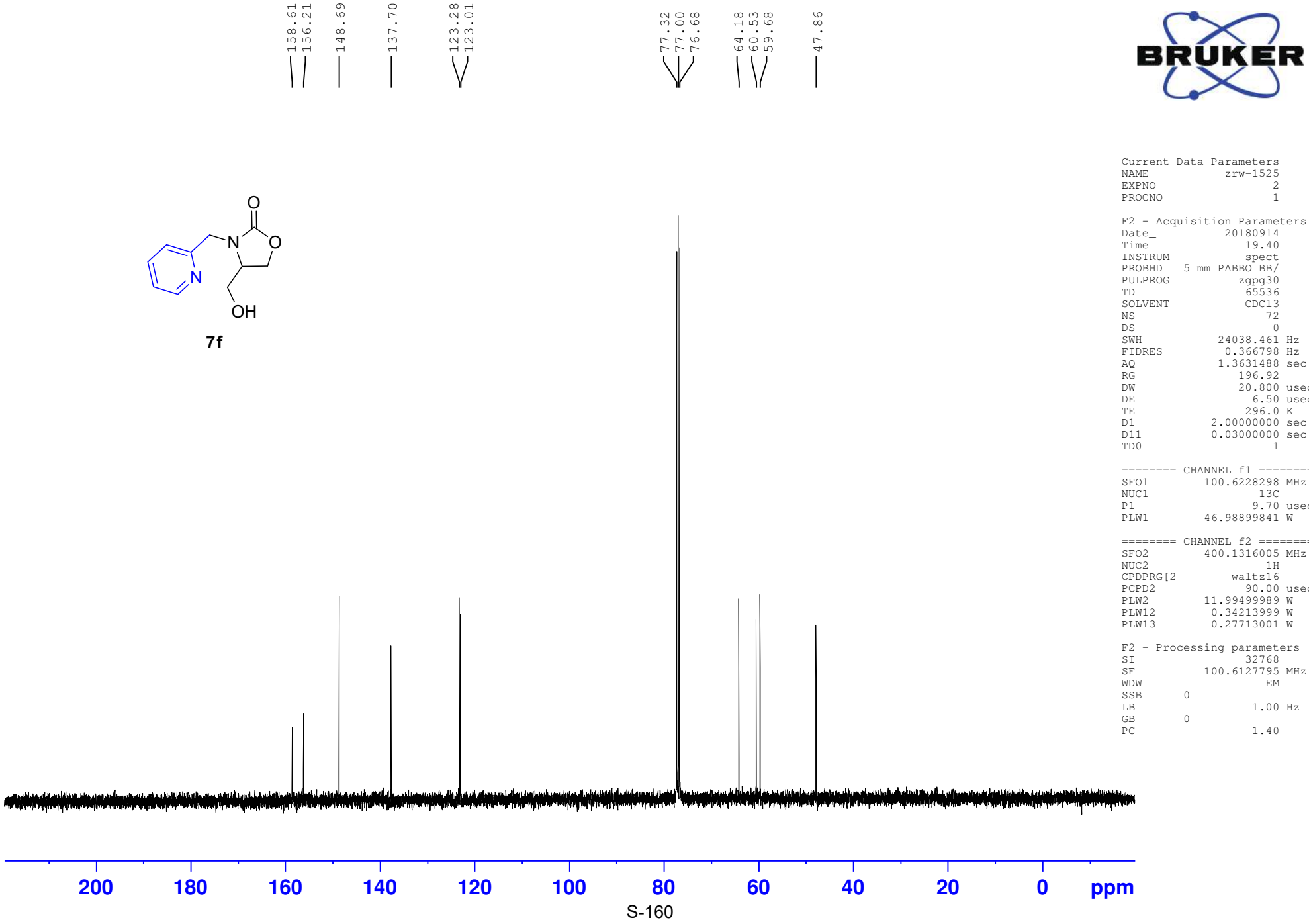


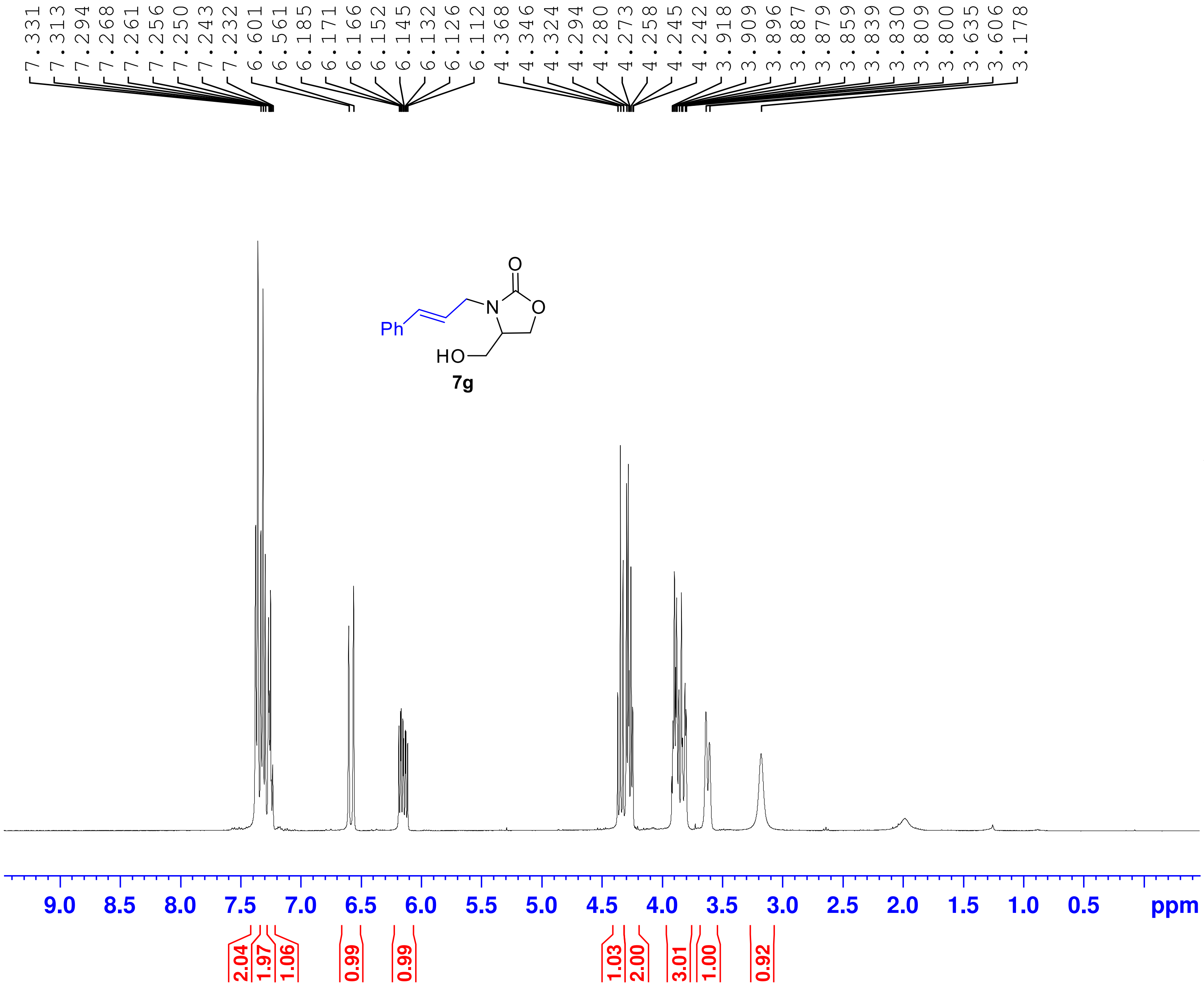

```
Current Data Parameters
NAME                  zrw-1525
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180914
Time                     19.36
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       88.84
DW                     62.400 usec
DE                      6.50 usec
TE                      295.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                           65536
SF                 400.1300106 MHz
WDW                             EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```


158.61
156.21
148.69
137.70
123.28
123.01
77.32
77.00
76.68
64.18
60.53
59.68
47.86
O
N
O
N
OH
7f
Current Data Parameters
NAME zrw-1525
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180914
Time 19.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 72
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W
F2 - Processing parameters
SI 32768
SF 100.6127795 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

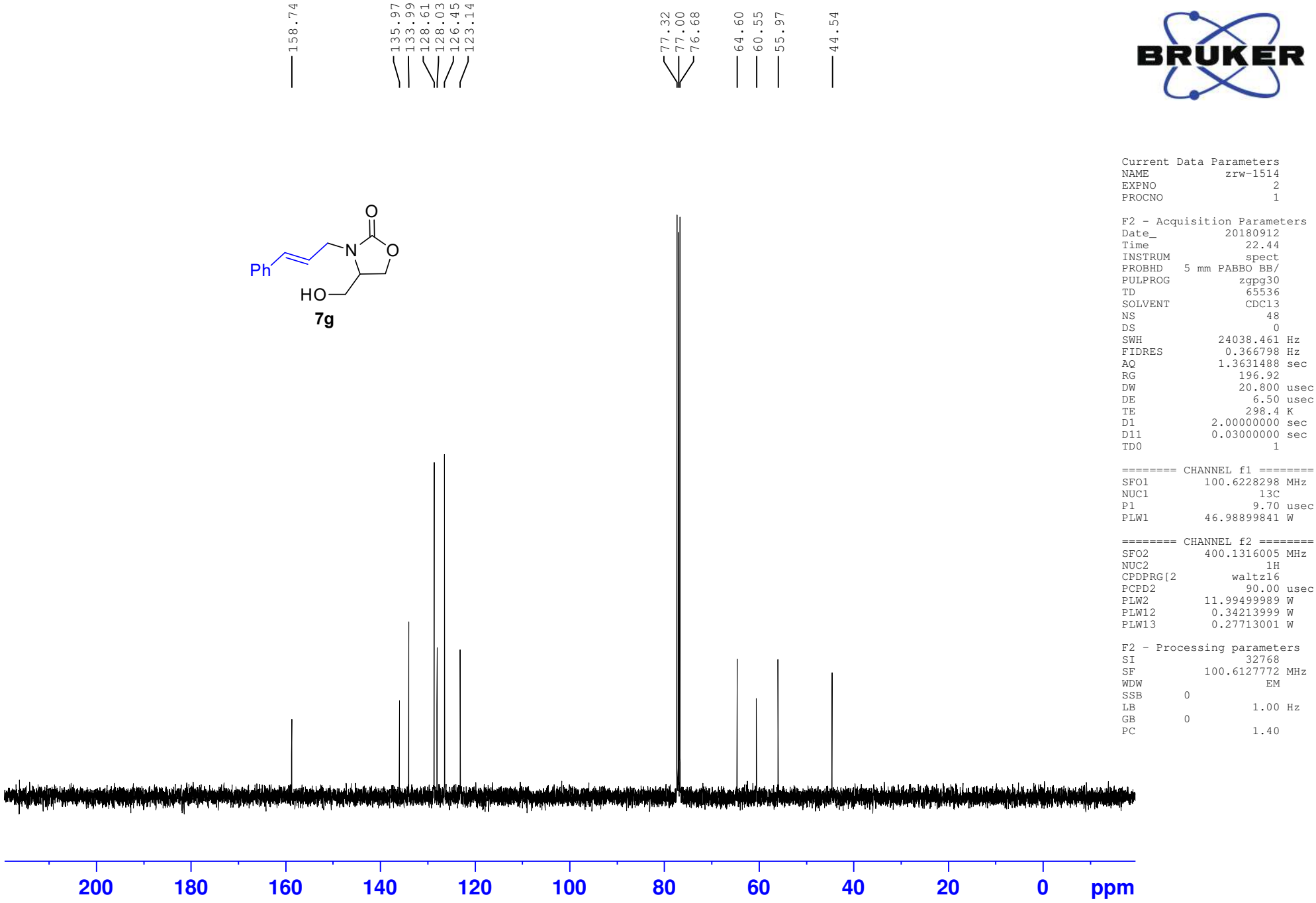



```
Current Data Parameters
NAME               zrw-1514
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180912
Time                  22.41
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                    70.97
DW               62.400 usec
DE                 6.50 usec
TE                  297.7 K
D1           1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                     1H
P1                14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                    65536
SF          400.1300102 MHz
WDW                      EM
SSB        0
LB                  0.30 Hz
GB         0
PC                     1.00
```



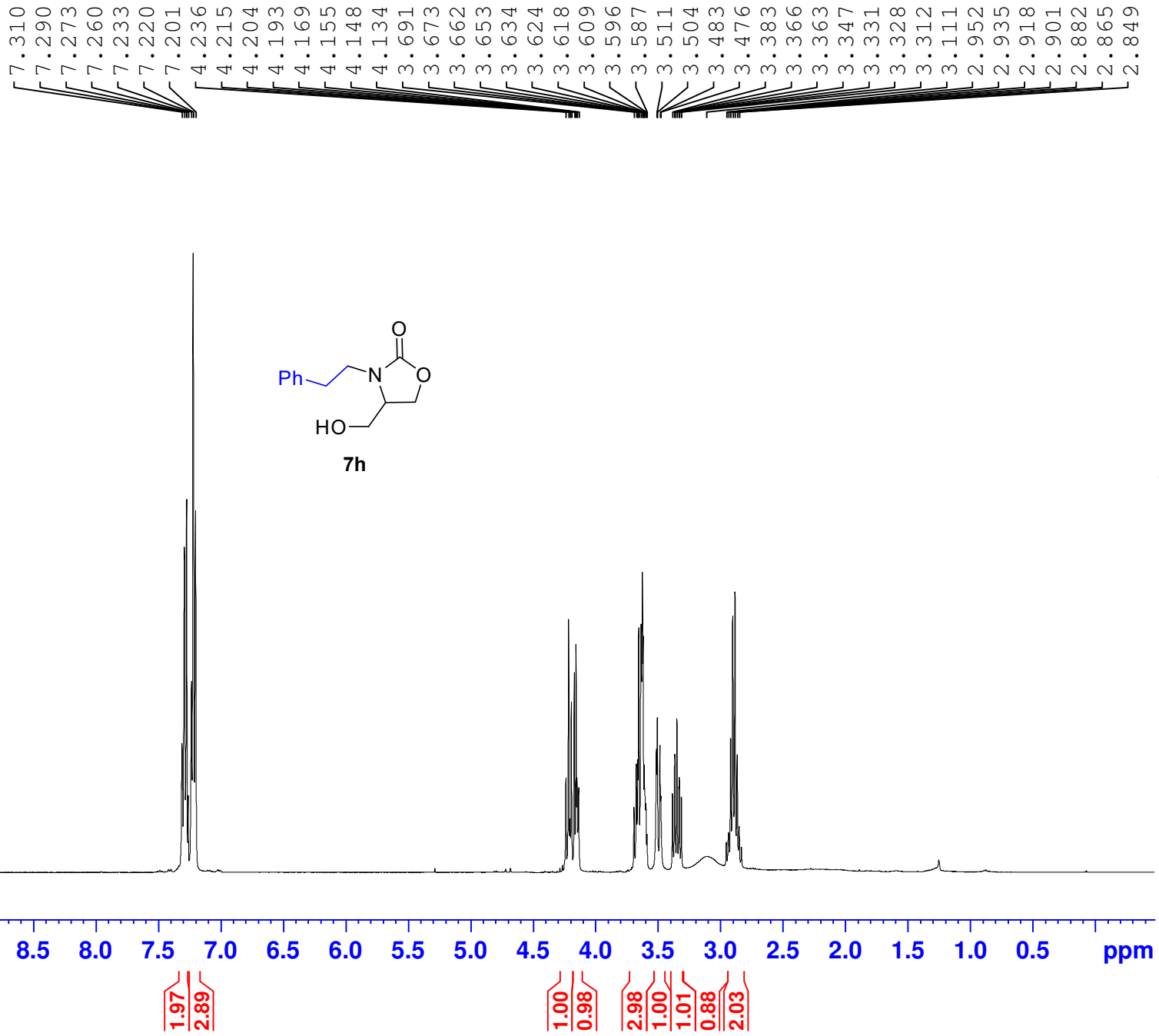

```
Current Data Parameters
NAME                 zrw-1514
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180912
Time                   22.44
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         48
DS                          0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     298.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                      9.70 usec
PLW1              46.98899841 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              11.99499989 W
PLW12              0.34213999 W
PLW13              0.27713001 W

F2 - Processing parameters
SI                      32768
SF               100.6127772 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

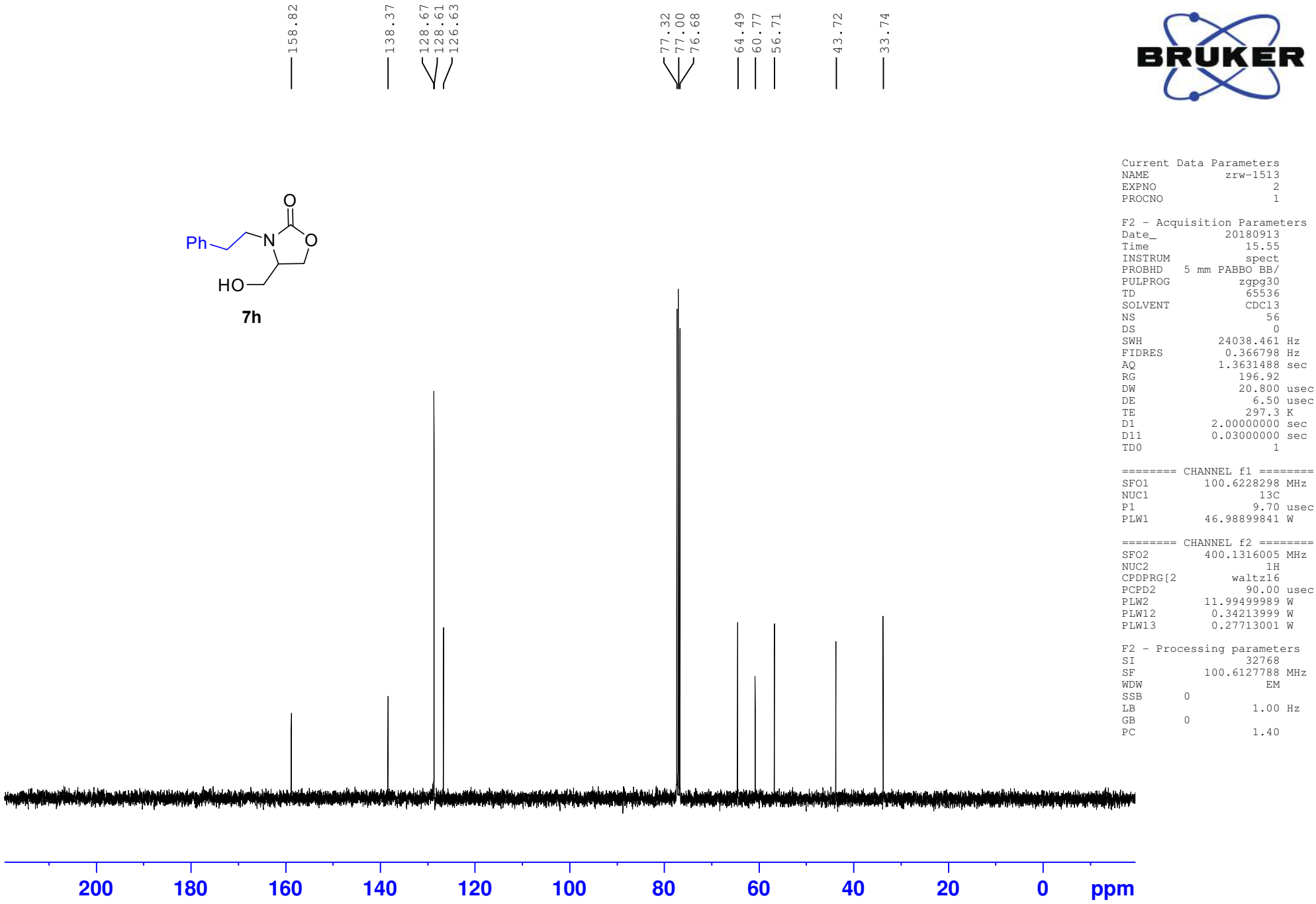



```
Current Data Parameters
NAME                  zrw-1513
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180913
Time                     15.52
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           4
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       70.97
DW                     62.400 usec
DE                      6.50 usec
TE                      296.5 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1               11.99499989 W

F2 - Processing parameters
SI                       65536
SF                 400.1300102 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                       1.00
```



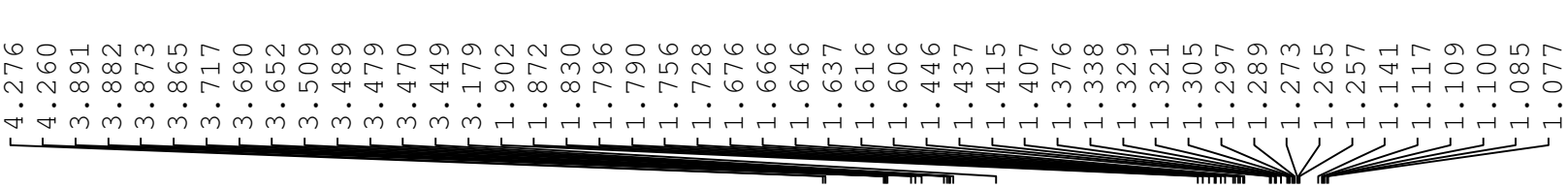

```
Current Data Parameters
NAME            zrw-1513
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180913
Time               15.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   56
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

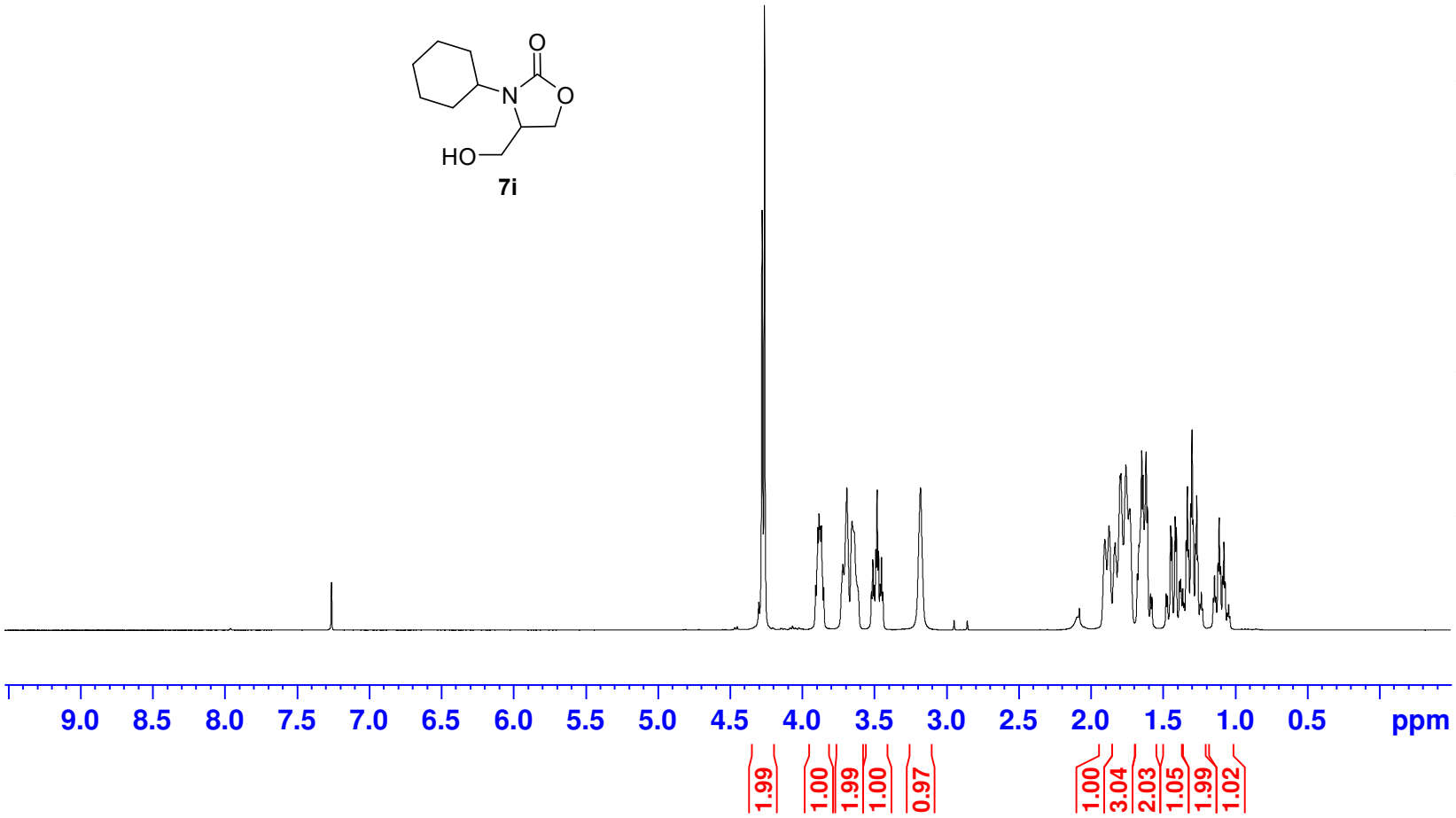
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                  32768
SF           100.6127788 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



7i

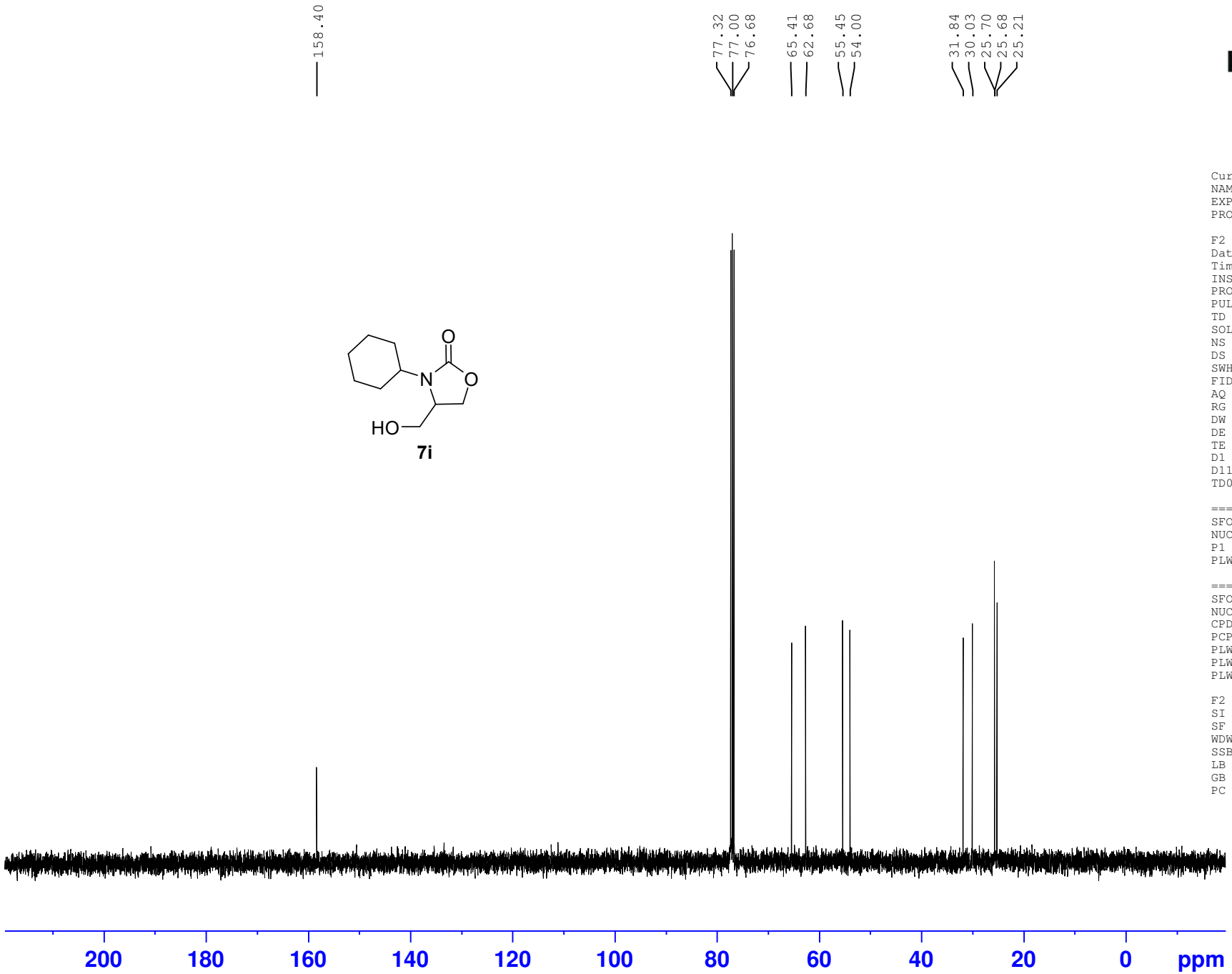



```
Current Data Parameters
NAME                 zrw-1523
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180914
Time                   19.23
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                     62.93
DW                    62.400 usec
DE                     6.50 usec
TE                    295.1 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                         65536
SF               400.1300103 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



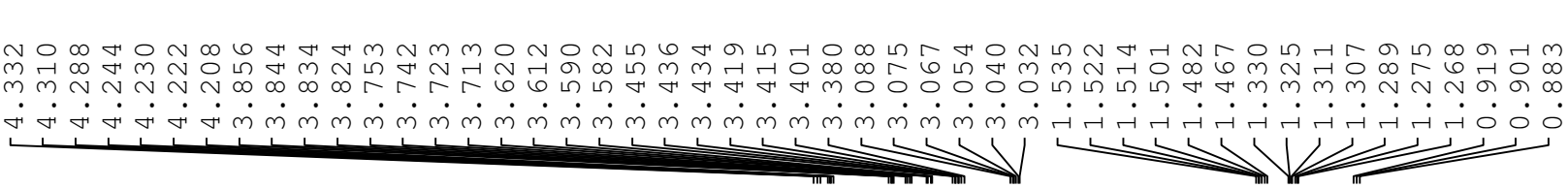

```
Current Data Parameters
NAME                 zrw-1523
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180914
Time                   19.26
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         40
DS                          0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     295.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

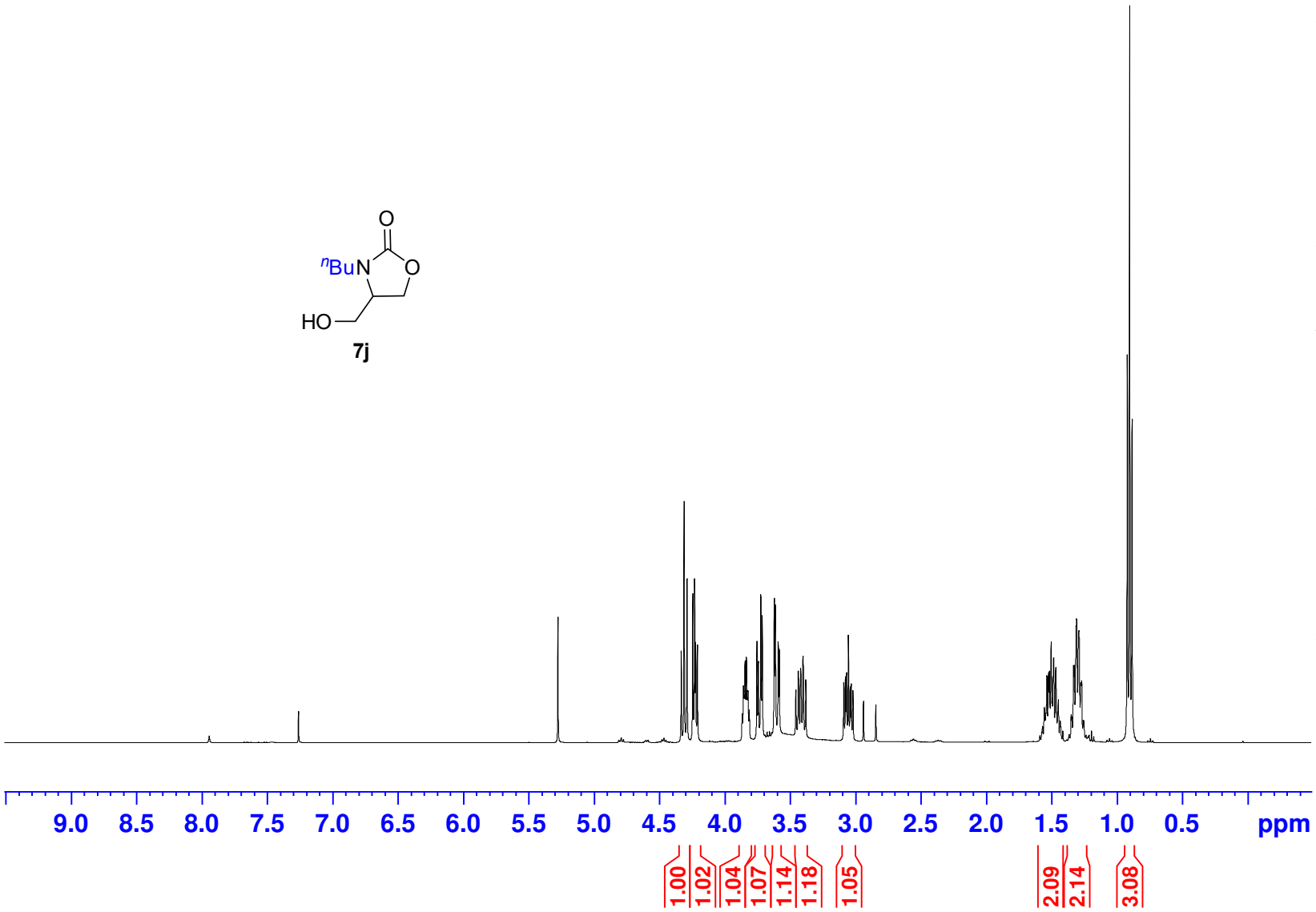
======== CHANNEL f1 ========
SFO1              100.6228298 MHz
NUC1                      13C
P1                      9.70 usec
PLW1              46.98899841 W

======== CHANNEL f2 ========
SFO2              400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              11.99499989 W
PLW12              0.34213999 W
PLW13              0.27713001 W

F2 - Processing parameters
SI                      32768
SF                100.6127780 MHz
WDW                        EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



7j

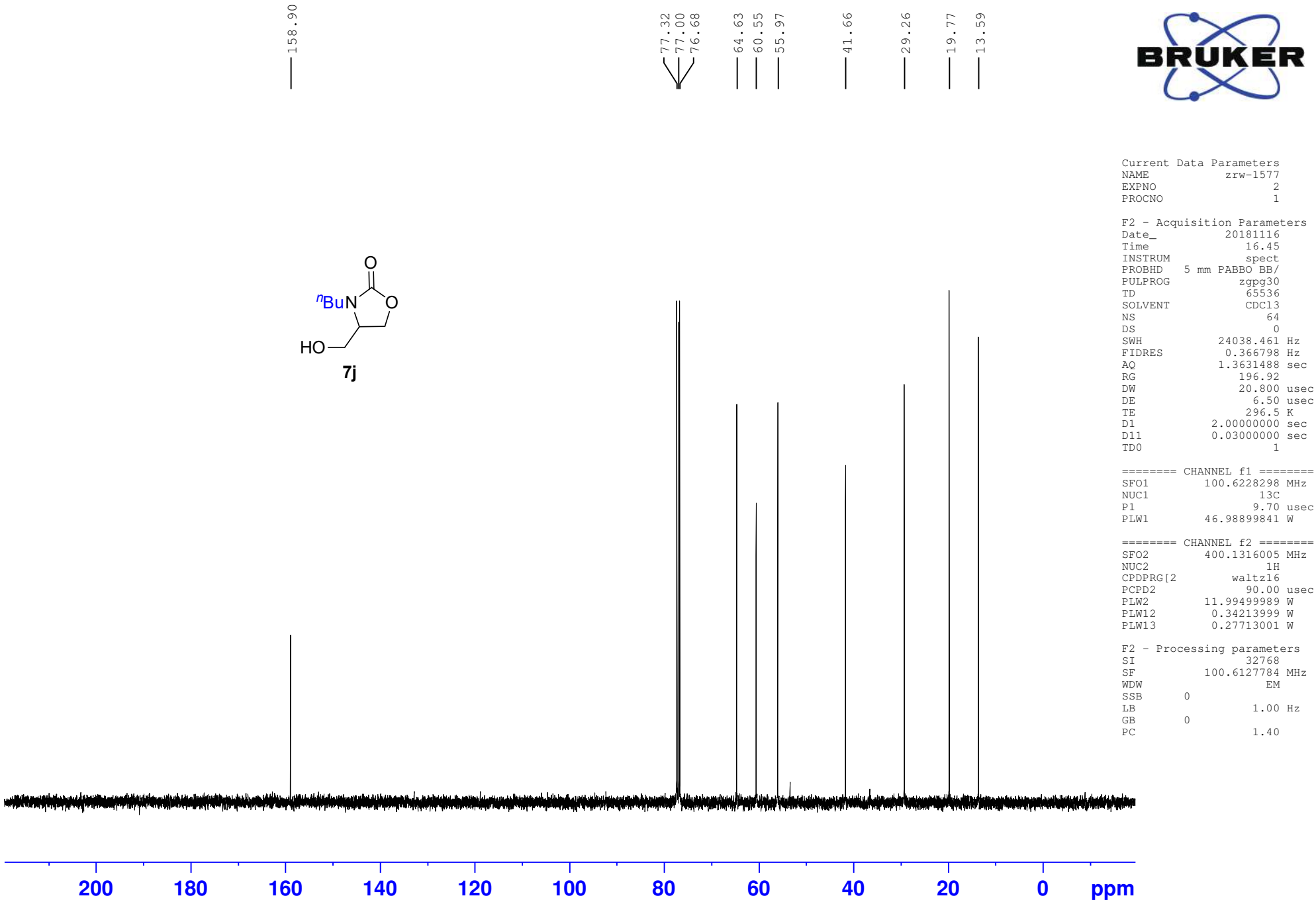



```
Current Data Parameters
NAME                  zrw-1577
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20181116
Time                     16.41
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       31.55
DW                     62.400 usec
DE                      6.50 usec
TE                      295.7 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                       65536
SF               400.1300101 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                       1.00
```



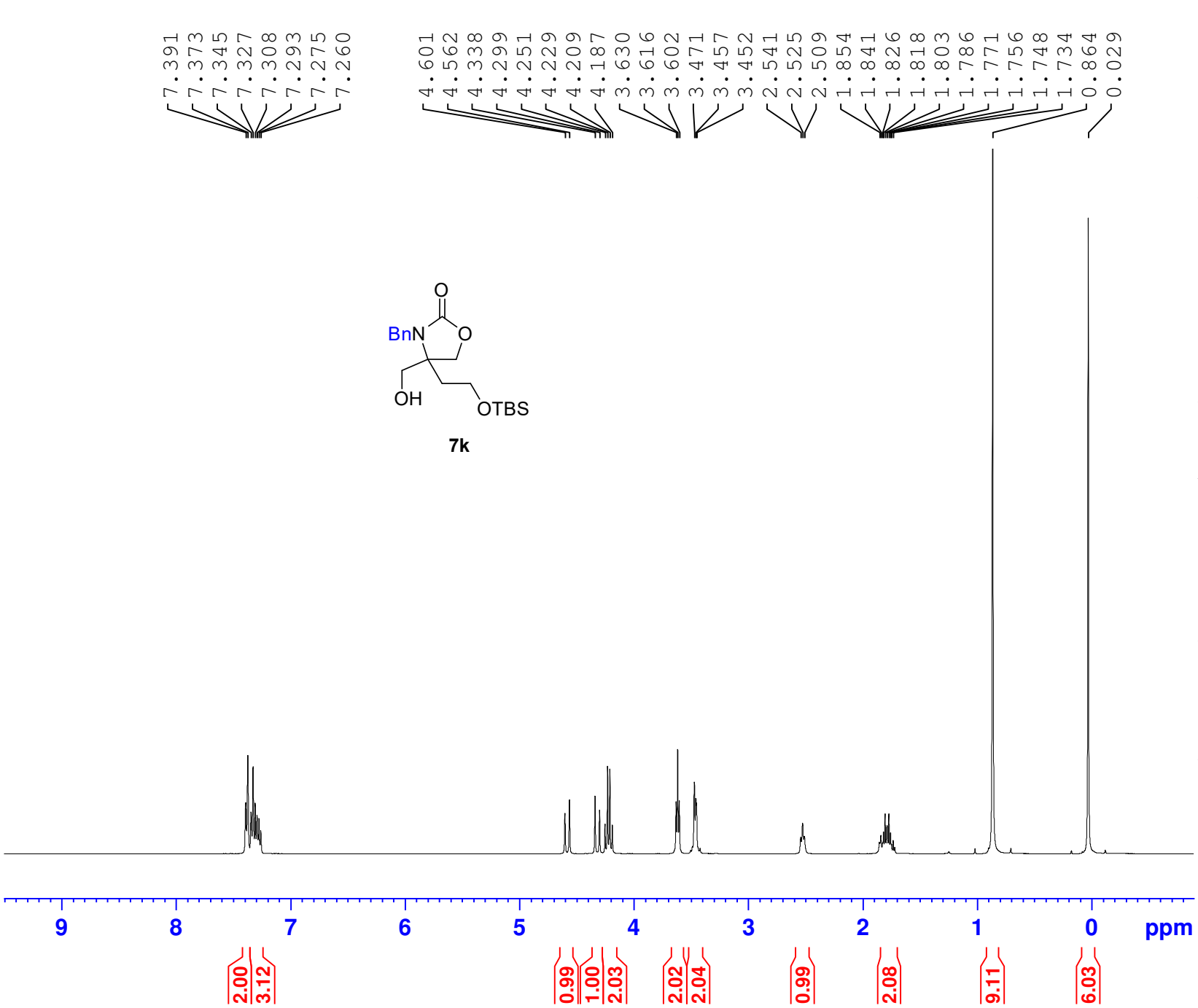

```
Current Data Parameters
NAME            zrw-1577
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181116
Time               16.45
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   64
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127784 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

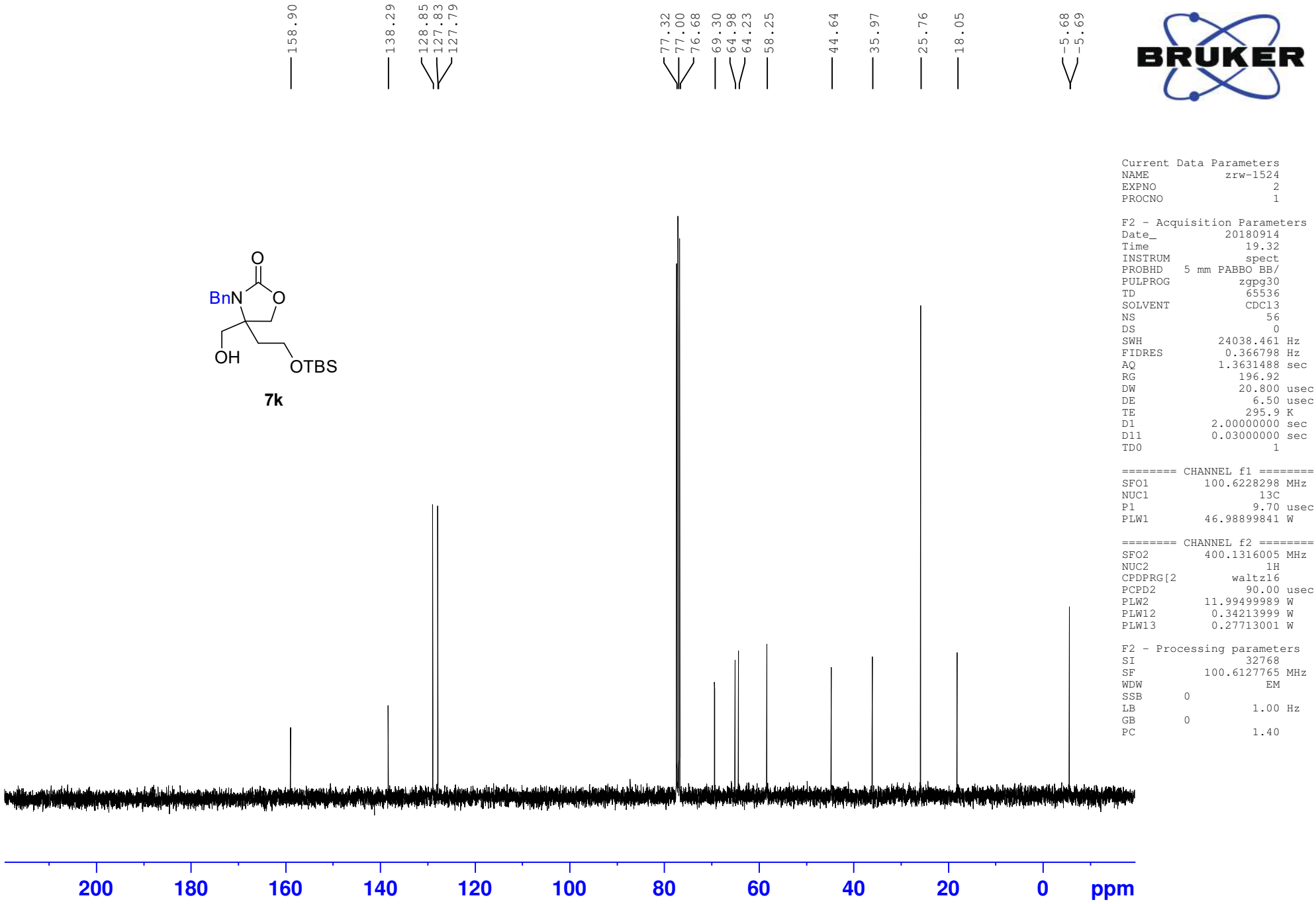


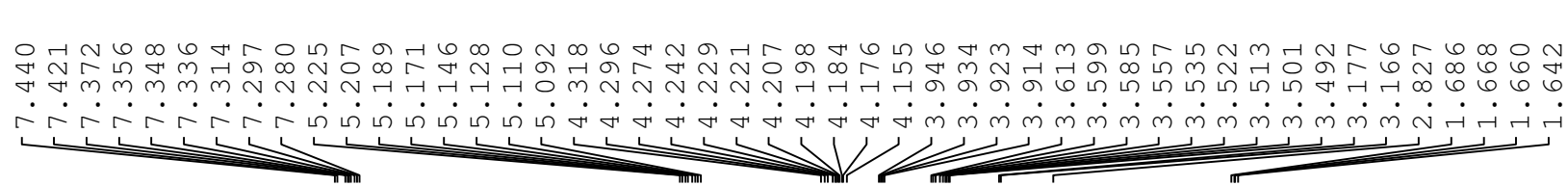
Current Data Parameters
NAME zrw-1524
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180914
Time 19.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 54.81
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

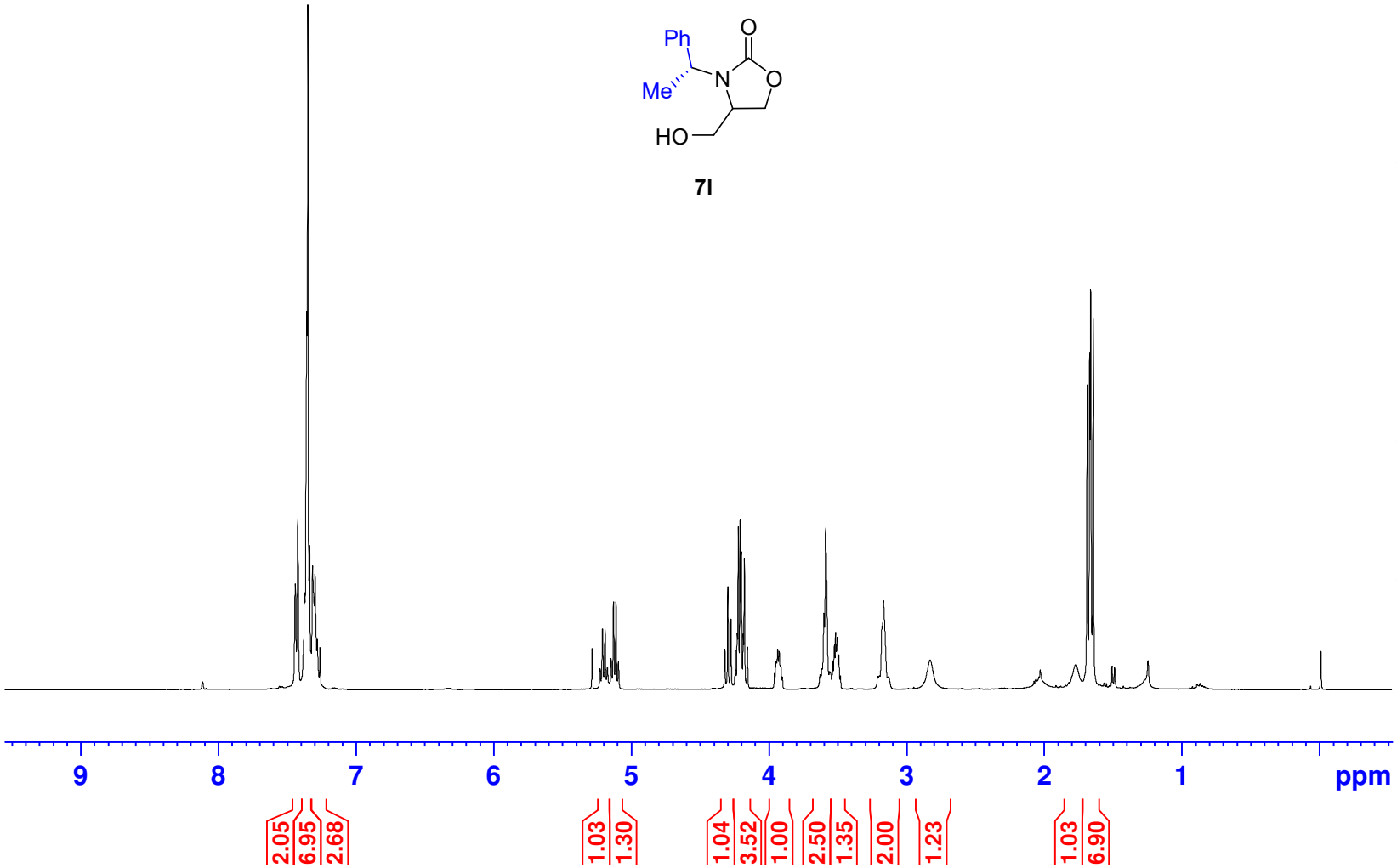
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


158.90
138.29
128.85
127.83
127.79
77.32
77.00
76.68
69.30
64.98
64.23
58.25
44.64
35.97
25.76
18.05
-5.68
-5.69
BnN
O
O
OH
OTBS
7k
Current Data Parameters
NAME zrw-1524
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180914
Time 19.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 56
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W
F2 - Processing parameters
SI 32768
SF 100.6127765 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



7l

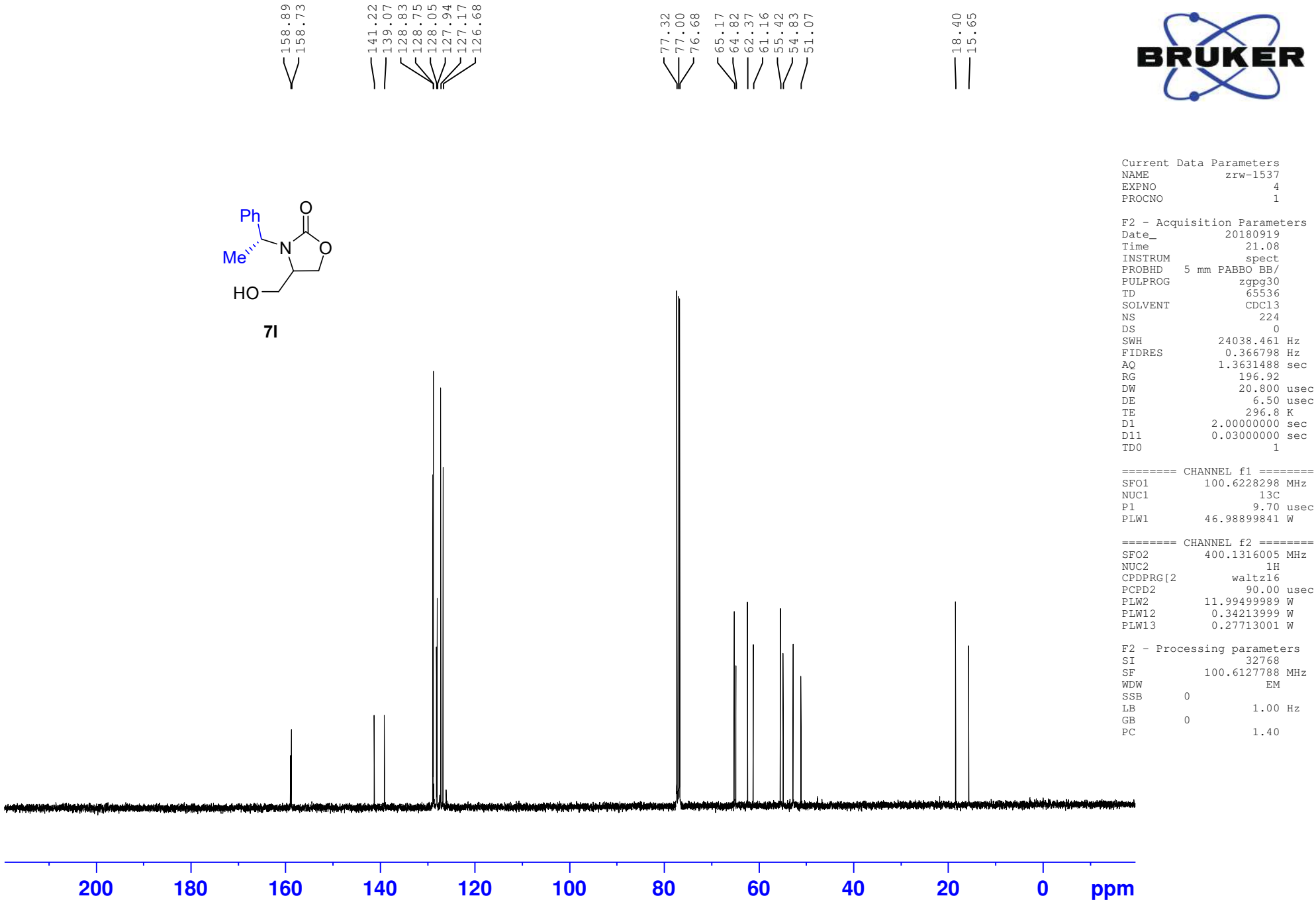



```
Current Data Parameters
NAME                  zrw-1537
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180919
Time                     20.55
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       34.77
DW                     62.400 usec
DE                      6.50 usec
TE                      295.4 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                       65536
SF               400.1300103 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                       1.00
```



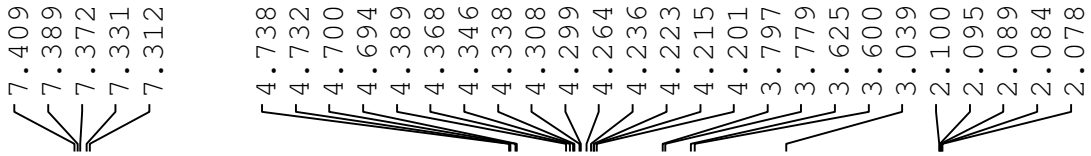

```
Current Data Parameters
NAME            zrw-1537
EXPNO                  4
PROCNO                 1

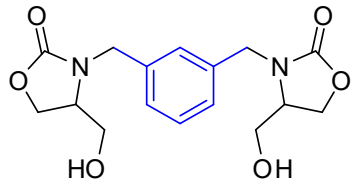
F2 - Acquisition Parameters
Date_           20180919
Time               21.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  224
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

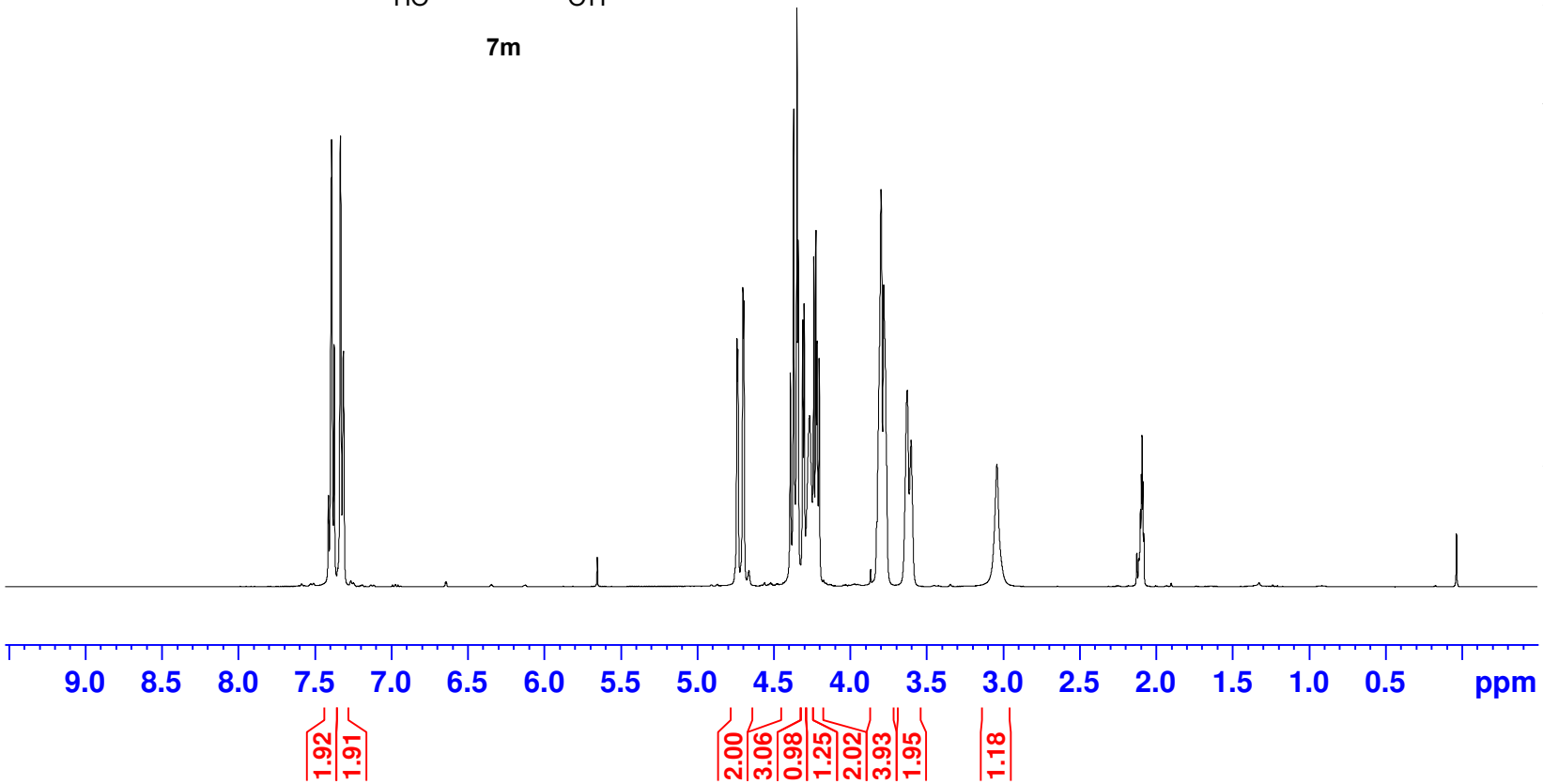
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                  32768
SF           100.6127788 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





7m

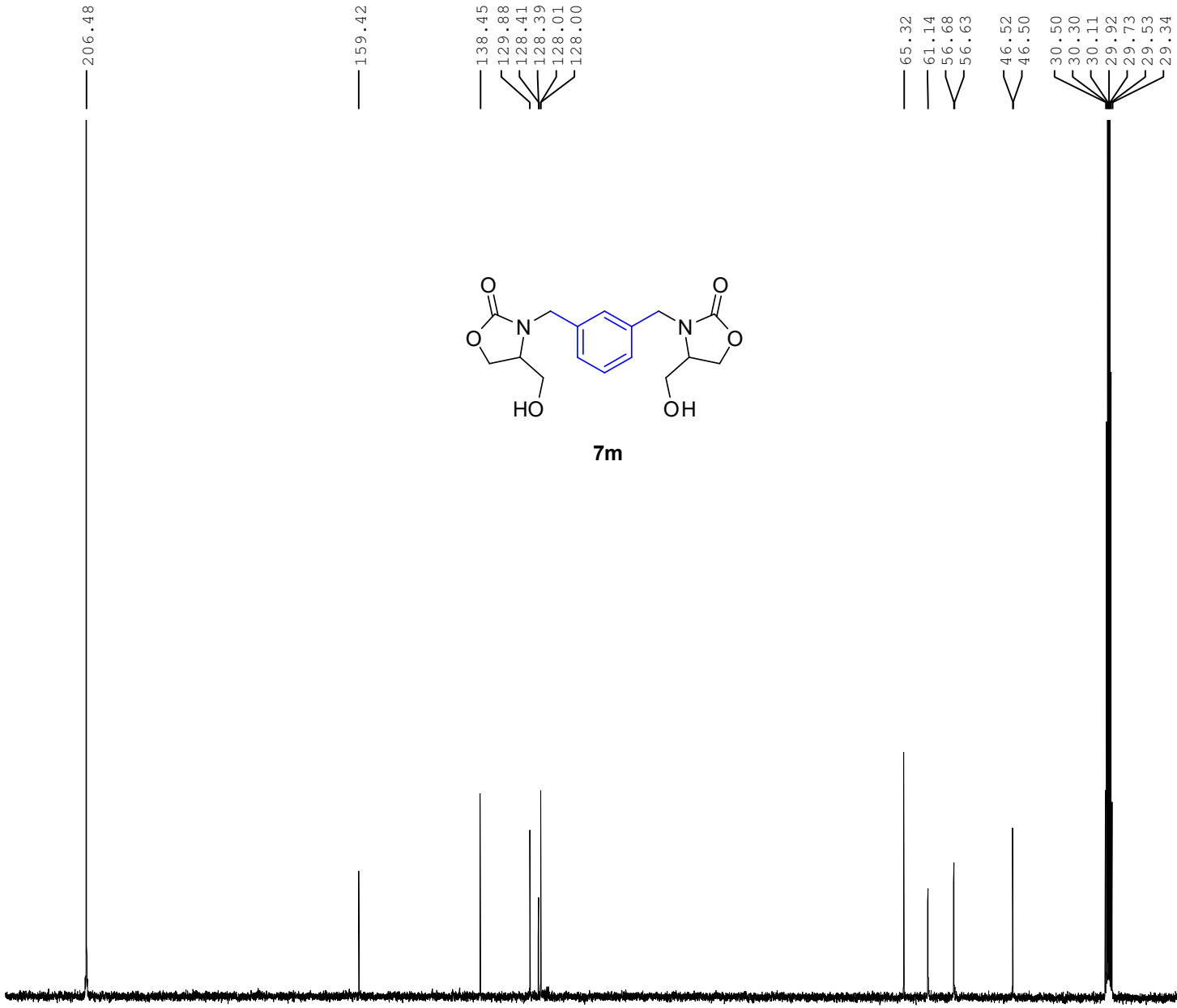



```
Current Data Parameters
NAME                 zrw-1530
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180915
Time                   21.34
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT              Acetone
NS                          8
DS                          0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                     70.97
DW                    62.400 usec
DE                     6.50 usec
TE                     297.9 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                         65536
SF               400.1299916 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



BRUKER

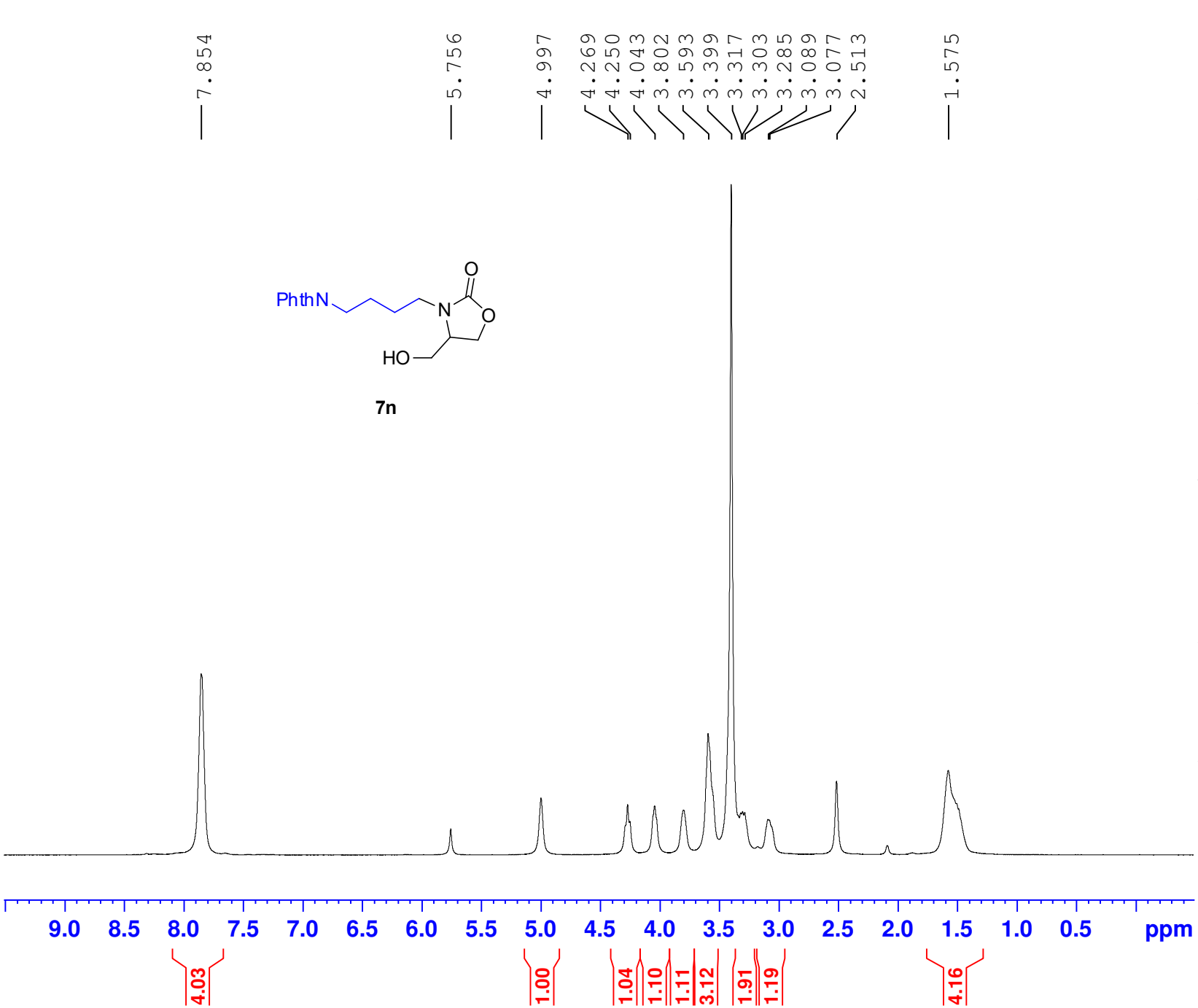
```
Current Data Parameters
NAME                 zrw-1530
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180915
Time                   21.46
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT               Acetone
NS                          400
DS                            0
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631488 sec
RG                      196.92
DW                      20.800 usec
DE                       6.50 usec
TE                      298.9 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                        9.70 usec
PLW1               46.98899841 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2               11.99499989 W
PLW12               0.34213999 W
PLW13               0.27713001 W

F2 - Processing parameters
SI                        32768
SF                 100.6126761 MHz
WDW                          EM
SSB             0
LB                        1.00 Hz
GB              0
PC                        1.40
```



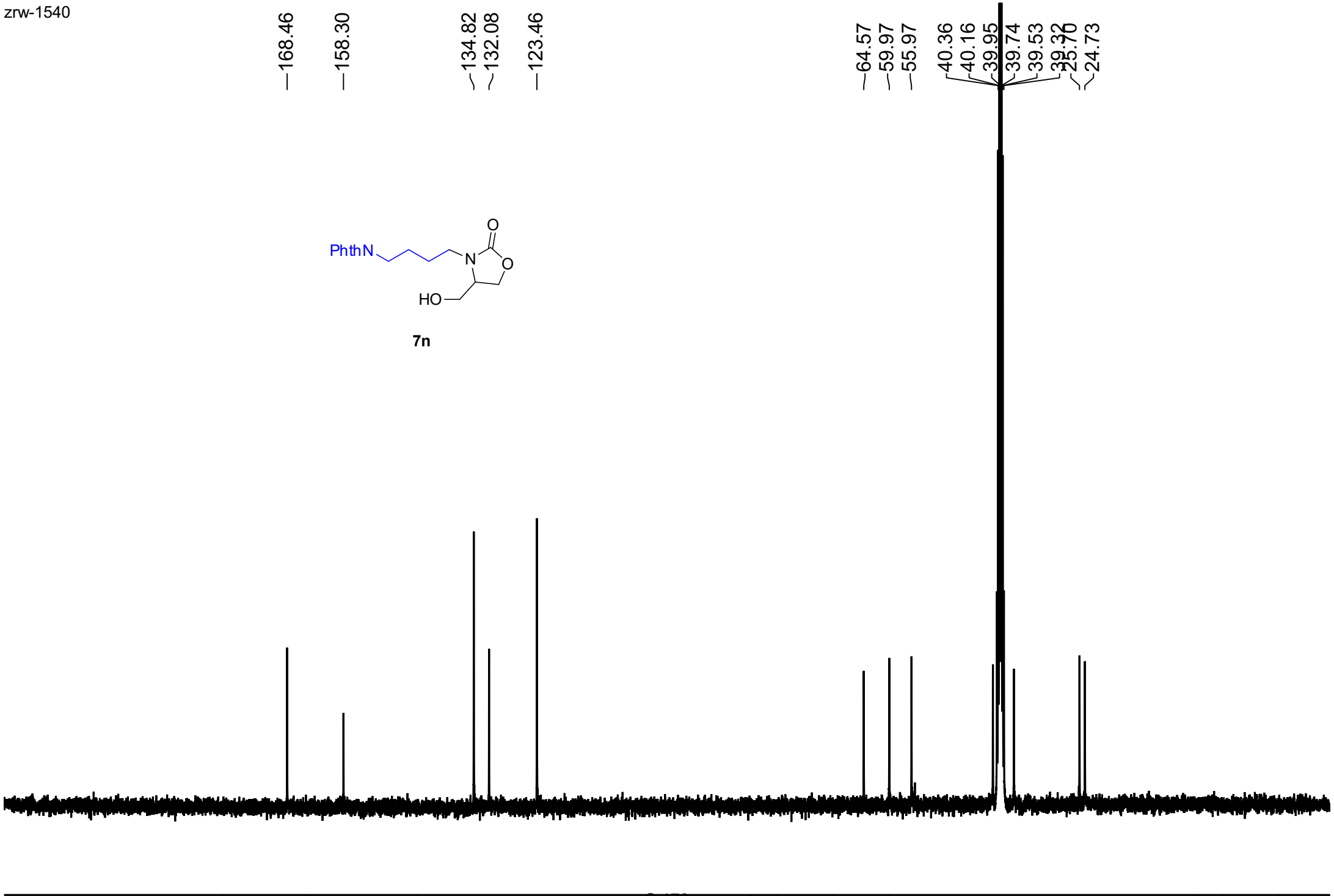

```
Current Data Parameters
NAME                  zrw-1540
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180920
Time                     11.53
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
NS                          4
DS                          0
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       70.97
DW                      62.400 usec
DE                       6.50 usec
TE                      295.5 K
D1                   1.00000000 sec
TD0                         1

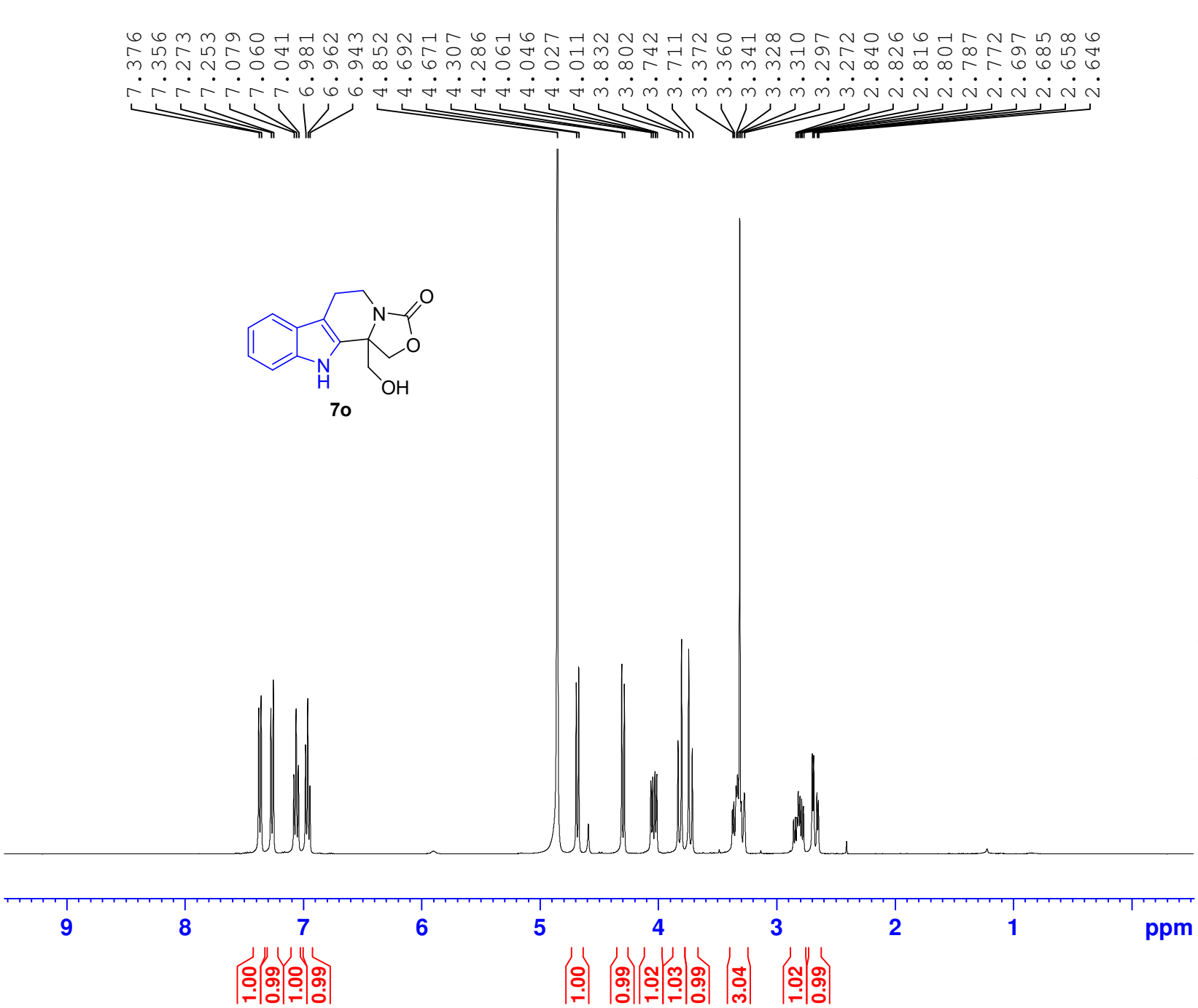
======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1               11.99499989 W

F2 - Processing parameters
SI                      65536
SF                 400.1300000 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

zrw-1540


168.46
158.30
134.82
132.08
123.46
64.57
59.97
55.97
40.36
40.16
39.95
39.74
39.53
39.32
25.70
24.73
PhthN
N
O
O
HO
O

7n

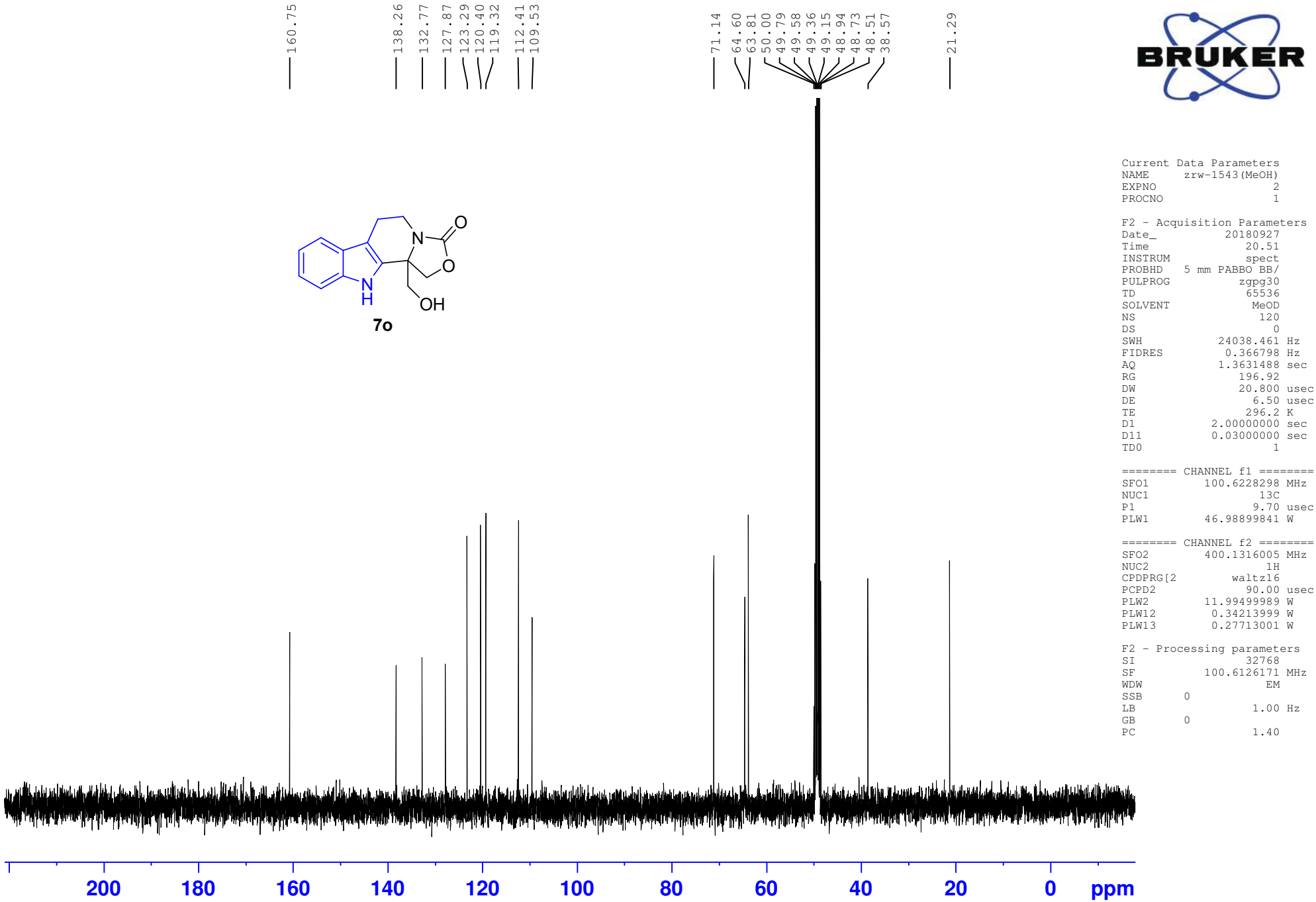



```
Current Data Parameters
NAME      zrw-1543(MeOH)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180927
Time               20.44
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 70.97
DW                62.400 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300237 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```


160.75
138.26
132.77
127.87
123.29
120.40
119.32
112.41
109.53
71.14
64.60
63.81
50.00
49.79
49.58
49.36
49.15
48.94
48.73
48.51
38.57
21.29
BRUKER
Current Data Parameters
NAME zrw-1543(MeOH)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180927
Time 20.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 120
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
PLW1 46.98899841 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.34213999 W
PLW13 0.27713001 W
F2 - Processing parameters
SI 32768
SF 100.6126171 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
O
O
N
H
OH
7o
200
180
160
140
120
100
80
60
40
20
0
ppm