Supplementary Data

Metal Trifluoromethanesulfonate-Catalyzed Regioselective Acylation of *myo*-Inositol 1,3,5-Orthoformate

Laxmansingh T. Padiyar, Yuh-Sheng Wen and Shang-Cheng Hung*

General Procedure for $M(OTf)_n$-Catalyzed Regioselective Benzoylation of *myo*-Inositol 1,3,5-orthoformate 1. A mixture of compound **1** (100 mg, 0.52 mmol), $M(OTf)_n$ (1 mol%), and Bz_2O (130 mg, 0.57 mmol) was dried under vacuum for 1 h. Anhydrous 1,4-dioxane (4 mL) was added to the mixture under nitrogen atmosphere, and the solution was kept stirring at 25 ^oC or 40 ^oC. After the starting material **1** was totally consumed, 1,4-dioxane was removed under reduced pressure. The crude residue was purified by flash column chromatography on silica gel (hexane/EtOAc, 2/1 to 1/1) to yield **5**, **(±)-6**, and **(±)-7**.

2-*O*-Benzoyl-*myo*-inositol 1,3,5-Orthoformate (5). ^1H NMR (400 MHz, CD_3OD) δ 8.12 (dd, *J* = 8.5, 1.1 Hz, 2H, Bz-H), 7.65-7.61 (m, 1H, Bz-H), 7.52-7.47 (m, 2H, Bz-H), 5.58-5.57 (m, 1H), 5.52 (d, *J* = 1.4 Hz, 1H, orthoformate-H), 4.52-4.49 (m, 2H), 4.35-4.33 (m, 2H), 4.25-4.23 (m, 1H); ^{13}C NMR (100 MHz, CD_3OD) δ 167.3 (C), 134.5 (CH), 131.2 (C), 130.8 (2 x CH), 129.6 (2 x CH), 103.9 (CH), 73.7 (2 x CH), 70.9 (CH), 69.0 (2 x CH), 65.3 (CH); HRMS (ESI, MNa^+) calcd for $C_{14}H_{14}O_7Na$ 317.0637, found 317.0642.

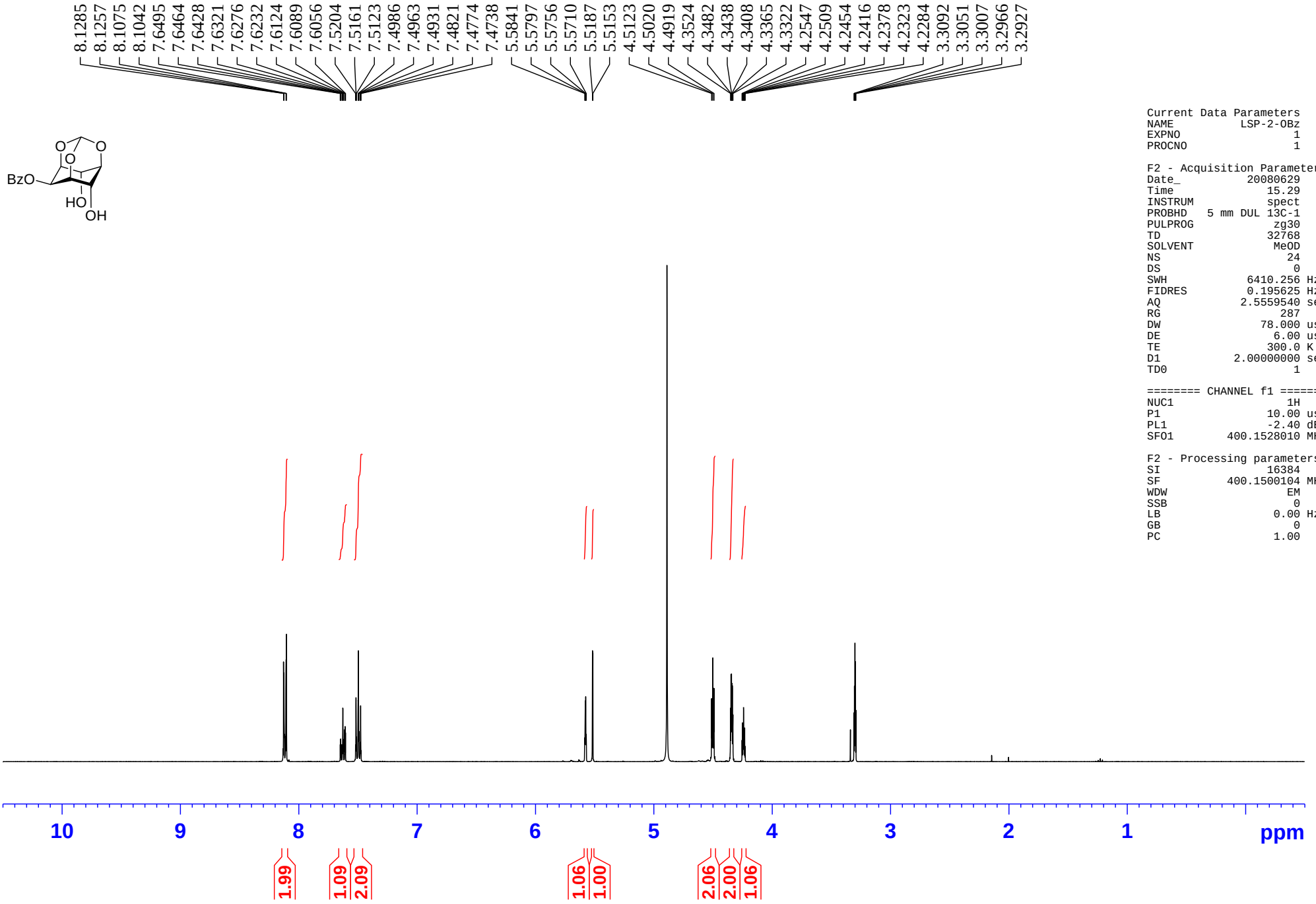
4(6)-*O*-Benzoyl-*myo*-inositol 1,3,5-Orthoformate (6). ^1H NMR (400 MHz, CD_3OD) δ 8.04 (dd, *J* = 8.3, 1.1 Hz, 2H, Bz-H), 7.62-7.58 (m, 1H, Bz-H), 7.49-7.44 (m, 2H, Bz-H), 5.63 (td, *J* = 3.7, 1.8 Hz, 1H, 4/6-H), 5.51 (d, *J* = 1.2 Hz, 1H, orthoformate-H), 4.51 (td, *J* = 3.9, 1.7 Hz, 1H), 4.43-4.41 (m, 1H), 4.26-4.24 (m, 2H), 4.13-4.10 (m, 1H); ^{13}C NMR (100 MHz, CD_3OD) δ 166.9 (C), 134.5 (CH), 130.9 (C), (2 x CH), 129.6 (2 x CH), 104.5 (CH), 75.8 (CH), 73.5 (CH), 70.3 (2 x CH), 68.1 (CH), 61.7 (CH); HRMS (ESI, MNa^+) calcd for HRMS (ESI, MNa^+) calcd for $C_{14}H_{14}O_7Na$ 317.0637, found 317.0643

2,4(6)-Di-*O*-benzoyl-*myo*-inositol 1,3,5-Orthoformate (7). ^1H NMR (600 MHz, $CDCl_3$) δ 8.14-8.13 (m, 2H, Ar-H), 8.03-8.02 (m, 2H, Ar-H), 7.59-7.56 (m, 2H, Ar-H), 7.46-7.43 (m, 4H, Ar-H), 5.83 (td, *J* = 3.9, 1.6 Hz, 1H, 4/6-H), 5.65-5.64 (m, 1H, 2-H), 5.64 (d, *J* = 1.2 Hz, 1H, orthoformate-H), 4.73-4.72 (m, 1H), 4.62-4.60 (m,1H), 4.60-4.58 (m, 1H), 4.49-4.48 (m, 1H), 2.48 (d, *J* = 5.9 Hz, 1H, OH); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.2 (C), 165.0 (C), 133.8 (CH),

133.5 (CH), 130.0 (2 x CH), 129.9 (2 x CH), 129.4 (C), 129.9 (C), 128.7 (2 x CH), 128.5 (2 x CH), 102.9 (CH), 71.8 (CH), 69.6 (CH), 68.51 (CH), 68.48 (CH), 67.4 (CH), 63.7 (CH); HRMS (ESI, MNa^+) calcd for $C_{21}H_{18}O_8Na$ 421.0899, found 421.0894.

(1*S*)-(-)-Camphanic Anhydride (8). (1*S*)-(-)-Camphanic acid (4.00 g, 20.2 mmol) was dissolved in THF (12 mL) at room temperature under nitrogen atmosphere. The flask was immersed in an ice bath, and a solution of dicyclohexylcarbodiimide (2.08 g, 10.1 mmol) in THF (4 mL) was added to the mixture. The ice bath was removed, and the solution was kept stirring at room temperature overnight. The mixture was filtered through celite, the solid was washed with THF, and the filtrate was concentrated *in vacuo*. The crude mass was recrystallized from ethyl acetate to give the corresponding anhydride **8** (2.84 g, 76%) as a colorless solid. $[\alpha]^{25}_D$ –16.5 (*c* 1.0, 1,4-dioxane); mp 157 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.49-2.44 (m, 2H), 2.16-2.12 (m, 2H), 1.97-1.93 (m, 2H), 1.74-1.69 (m, 2H), 1.12 (s, 6H), 1.10 (s, 6H), 1.04 (s, 6H); ^{13}C NMR (150 MHz $CDCl_3$) δ 177.1 (C), 163.4 (C), 90.5 (C), 55.3 (C), 55.1 (C), 30.9 (CH_2), 28.8 (CH_2), 16.65 (CH_3), 16.56 (CH_3), 9.6 (CH_3); HRMS (FAB, MH^+) calcd for $C_{20}H_{27}O_7$ 379.1757 found 379.1754.

6-*O*-[(1*S*)-camphanoyl]-D-*myo*-inositol 1,3,5-orthoformate (9). A mixture of compound **1** (190 mg, 1.00 mmol), $Yb(OTf)_3$ (1 mol%), and (1*S*)-(-)-camphanic anhydride **8** (130 mg, 0.57 mmol) was dried under vacuum for 1 h. Anhydrous 1,4-dioxane (8 mL) was added to the mixture under nitrogen atmosphere, and the solution was stirred at 40 °C for 3 d. The solvent was removed under reduced pressure, the crude residue was dissolved in dichloromethane (50 mL), and the mixture was sequentially washed by saturated aq. $NaHCO_{3(aq)}$ (2 x 30 mL) and water (2 x 20 mL). The organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated in *vacuo*. The residue was purified by flash column chromatography on silica gel (2% MeOH in $CHCl_3$) to yield a mixture of diols **9** and **10** (2.3/1, 288 mg, 78%). Recrystallization of this mixture from ethanol furnished the desired major diol **9** as colorless crystals. $[\alpha]^{25}_D$ –11.0 (*c* 1.0, 1,4-dioxane); mp 201 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.66 (td, *J* = 3.9, 1.7 Hz, 1H), 5.49 (d, *J* = 1.0 Hz, orthoformate-H), 4.59 (br, 1H), 4.45-4.44 (m, 1H), 4.23-4.24 (m, 1H), 4.22-4.20 (m, 1H), 4.04 (br, 1H), 2.42-2.37 (m, 1H), 2.04-2.00 (m, 1H), 1.94-1.89 (m, 1H), 1.70-1.65 (m, 1H), 1.09 (s, 3H), 1.05 (s, 3H), 0.94 (s, 3H); ^{13}C NMR (150 MHz $CDCl_3$) δ 177.4 (C), 165.9 (C), 102.9 (CH), 90.7 (C), 74.3 (CH), 71.4 (CH), 69.4 (CH), 67.6 (CH), 67.3 (CH), 60.6 (CH), 54.9 (C), 54.5 (C), 30.9 (CH_2), 28.7 (CH_2), 16.7 (CH_3), 16.48 (CH_3), 9.6 (CH_3); HRMS (ESI, MNa^+) calcd for $C_{17}H_{22}O_9Na$ 393.1162 found 393.1159.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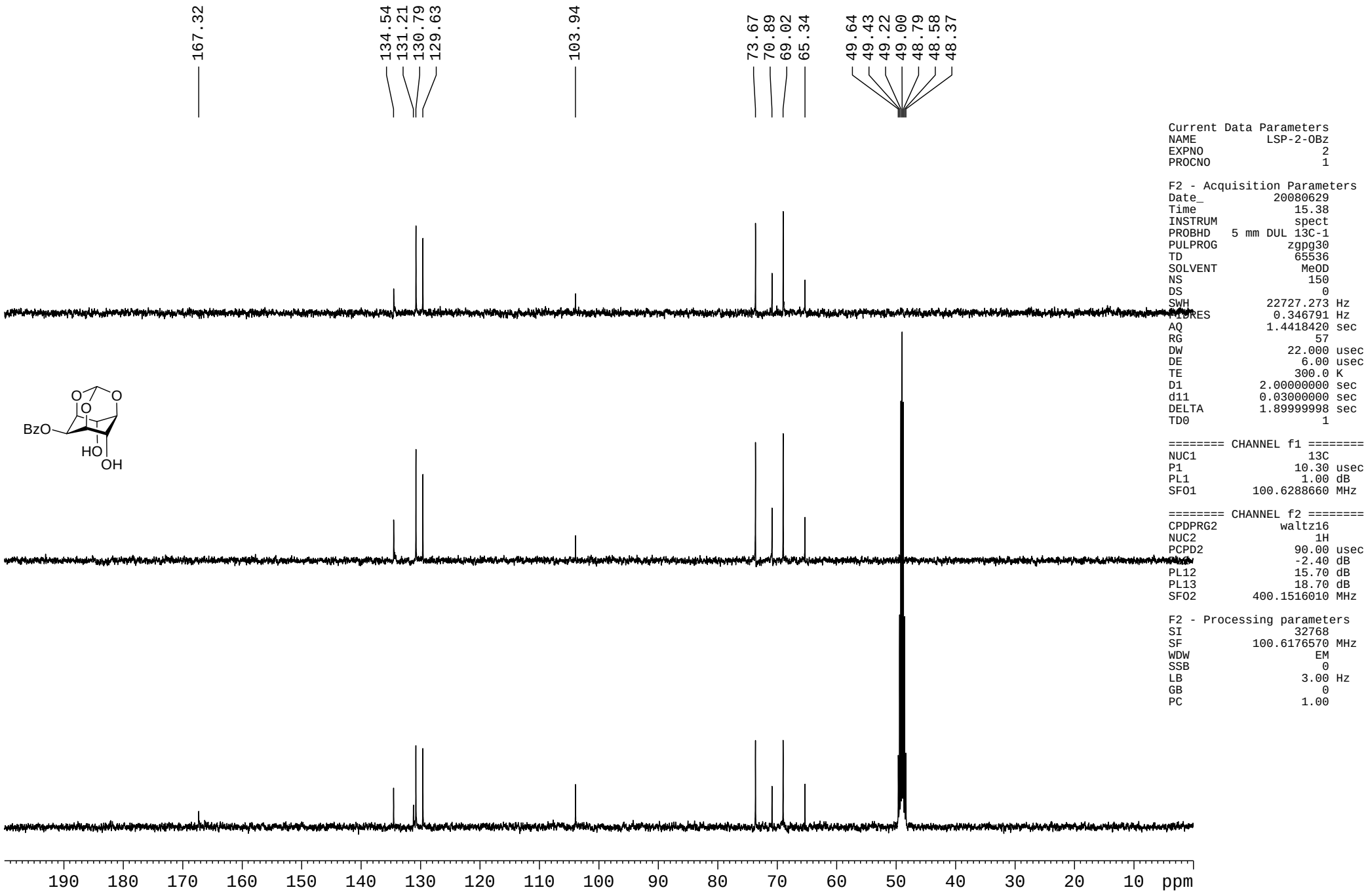
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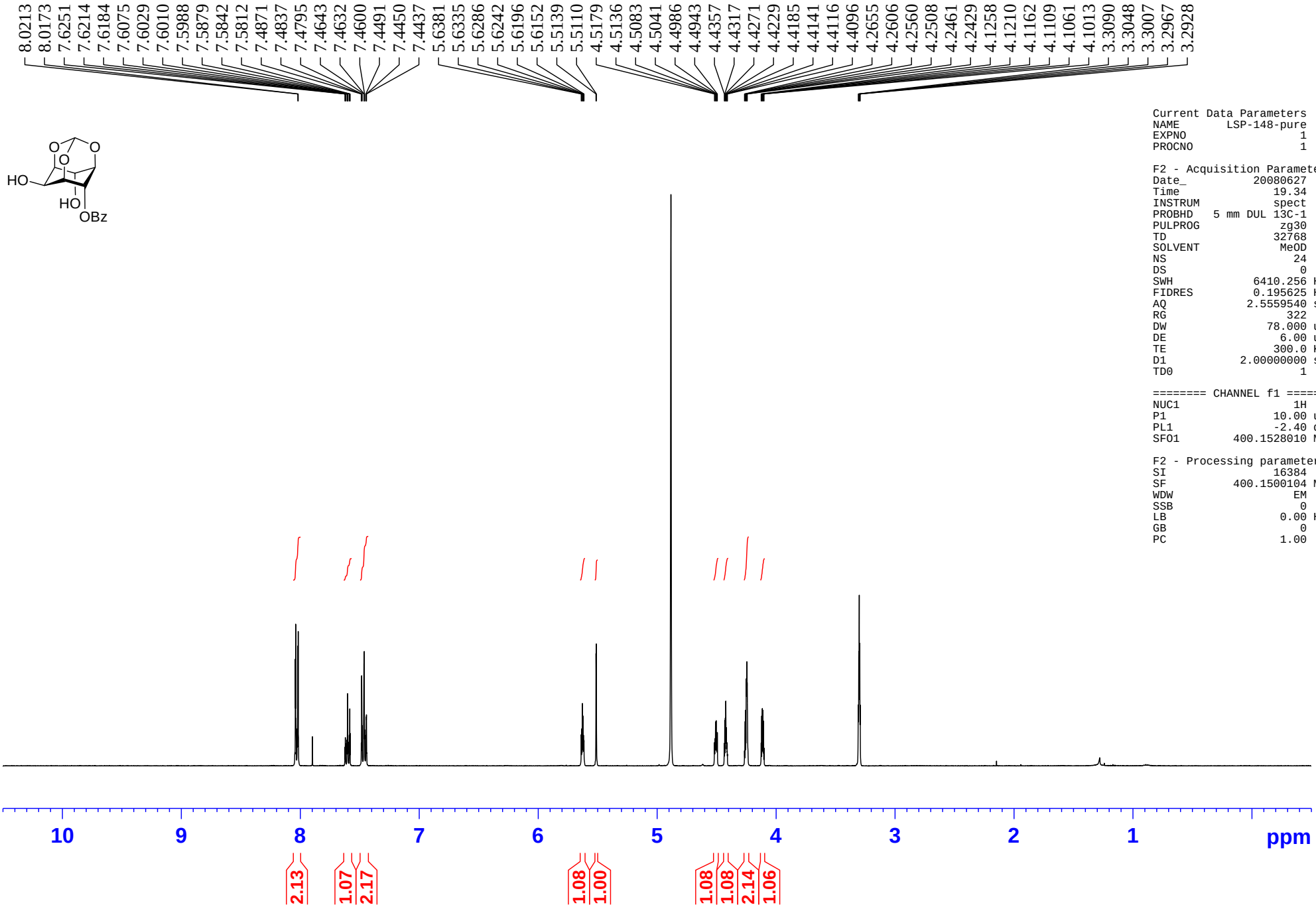
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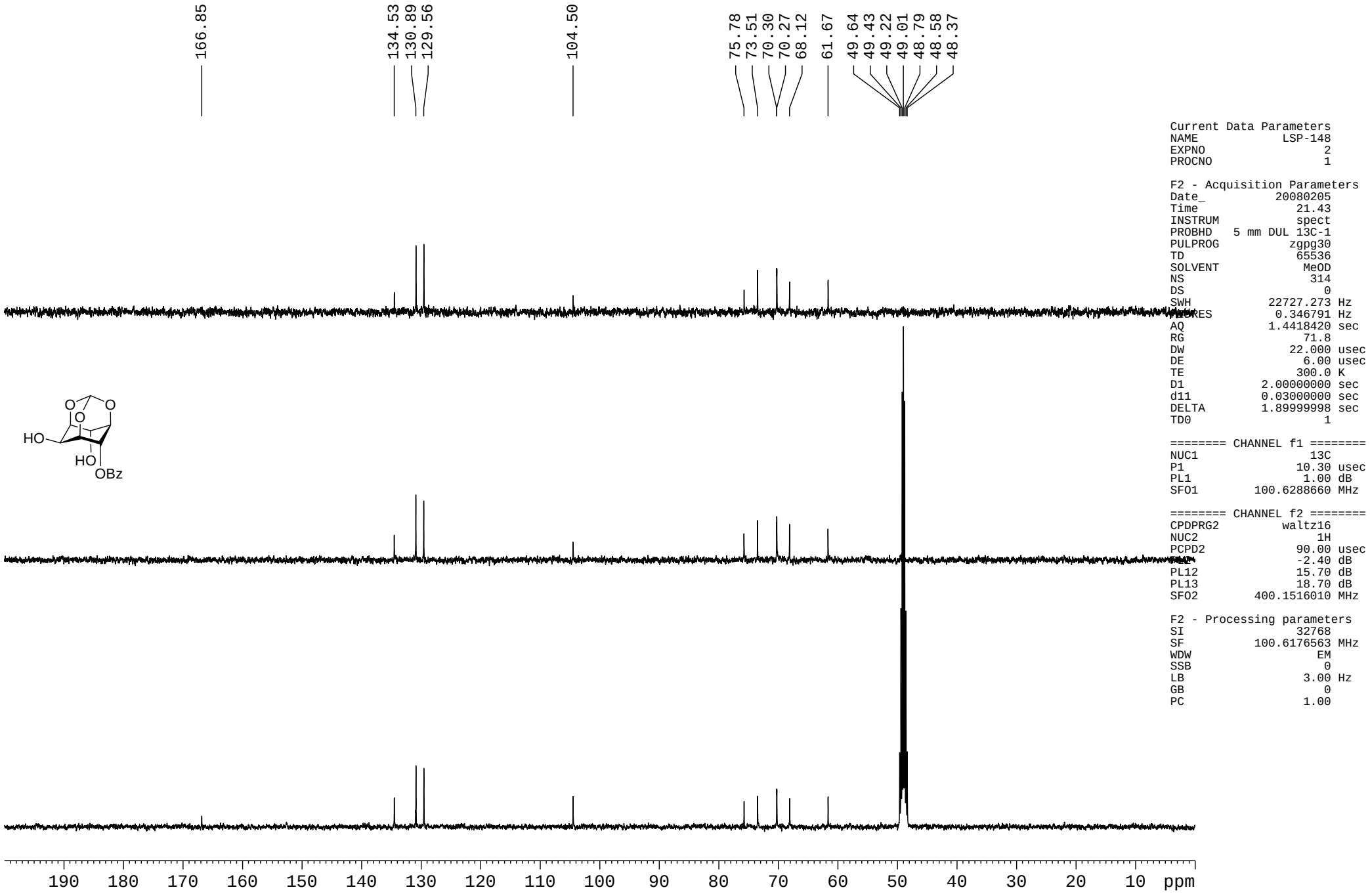


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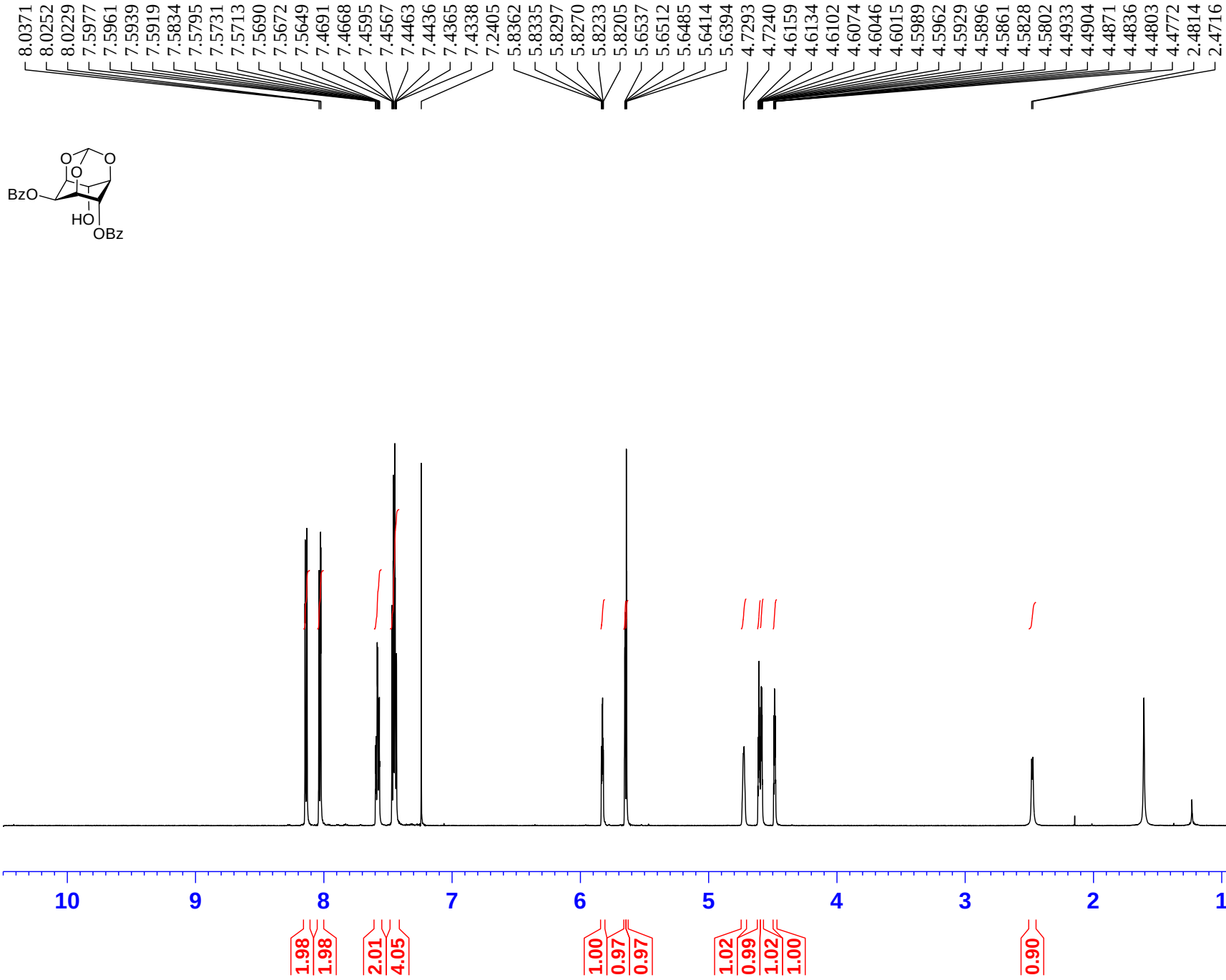
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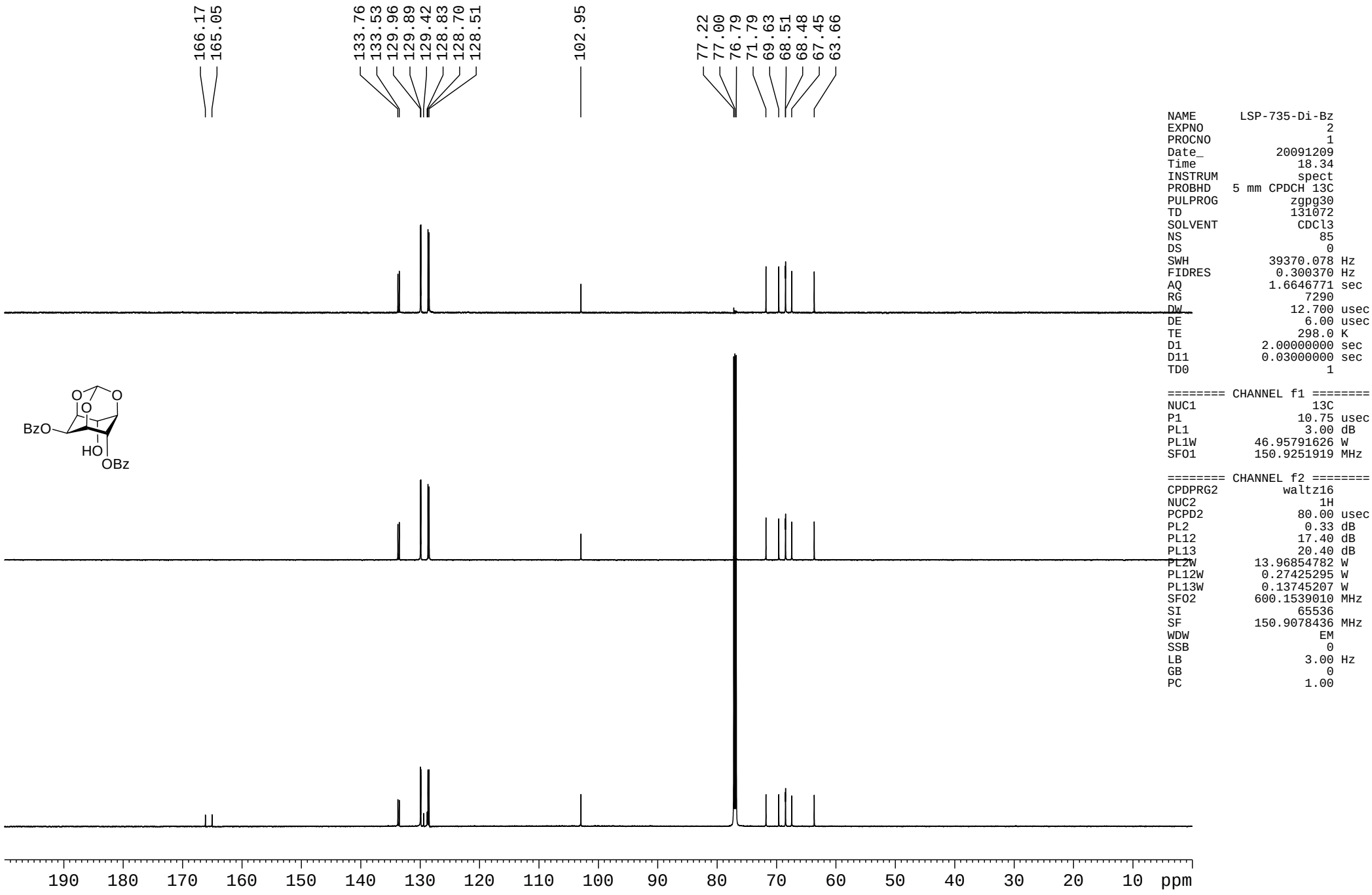

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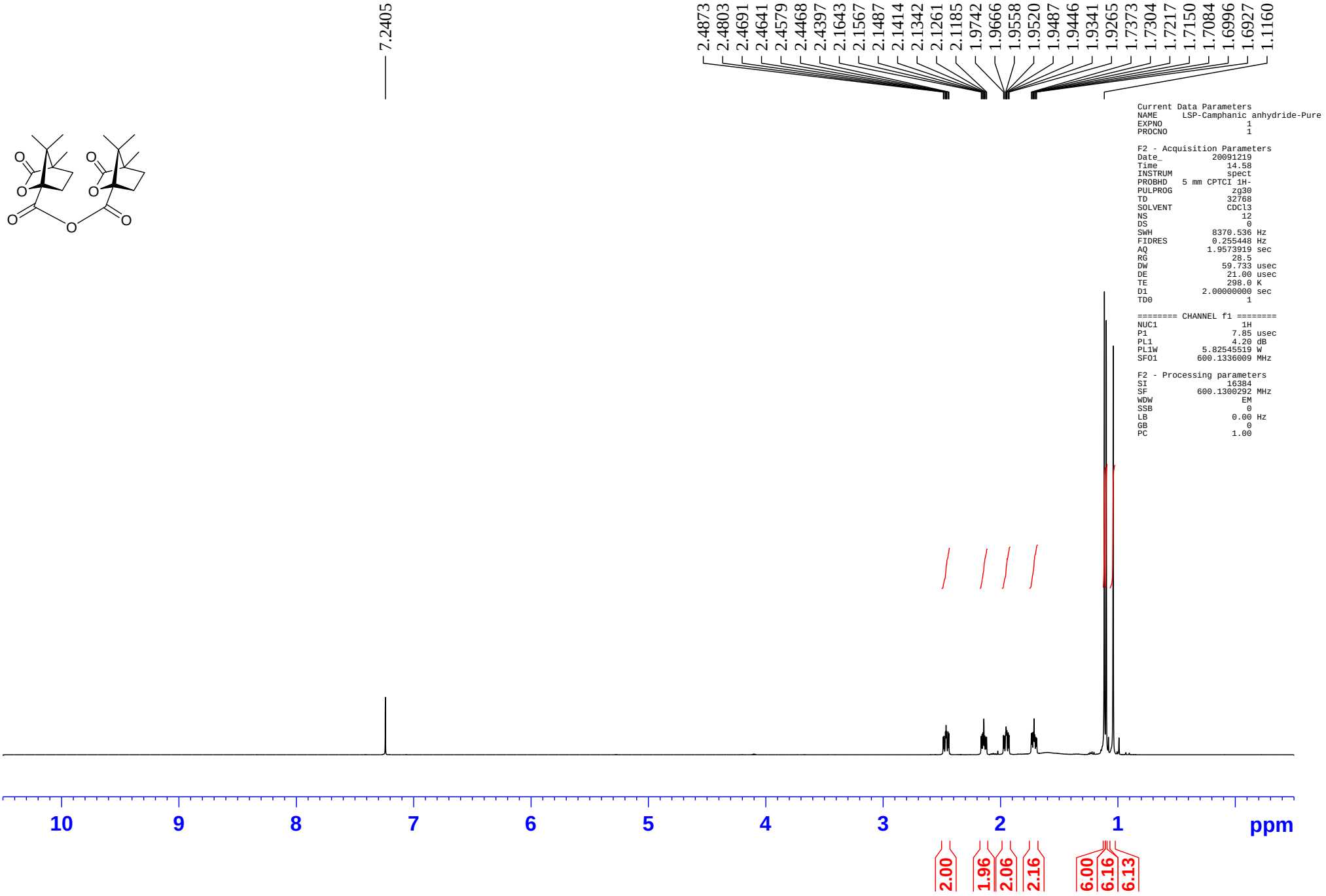
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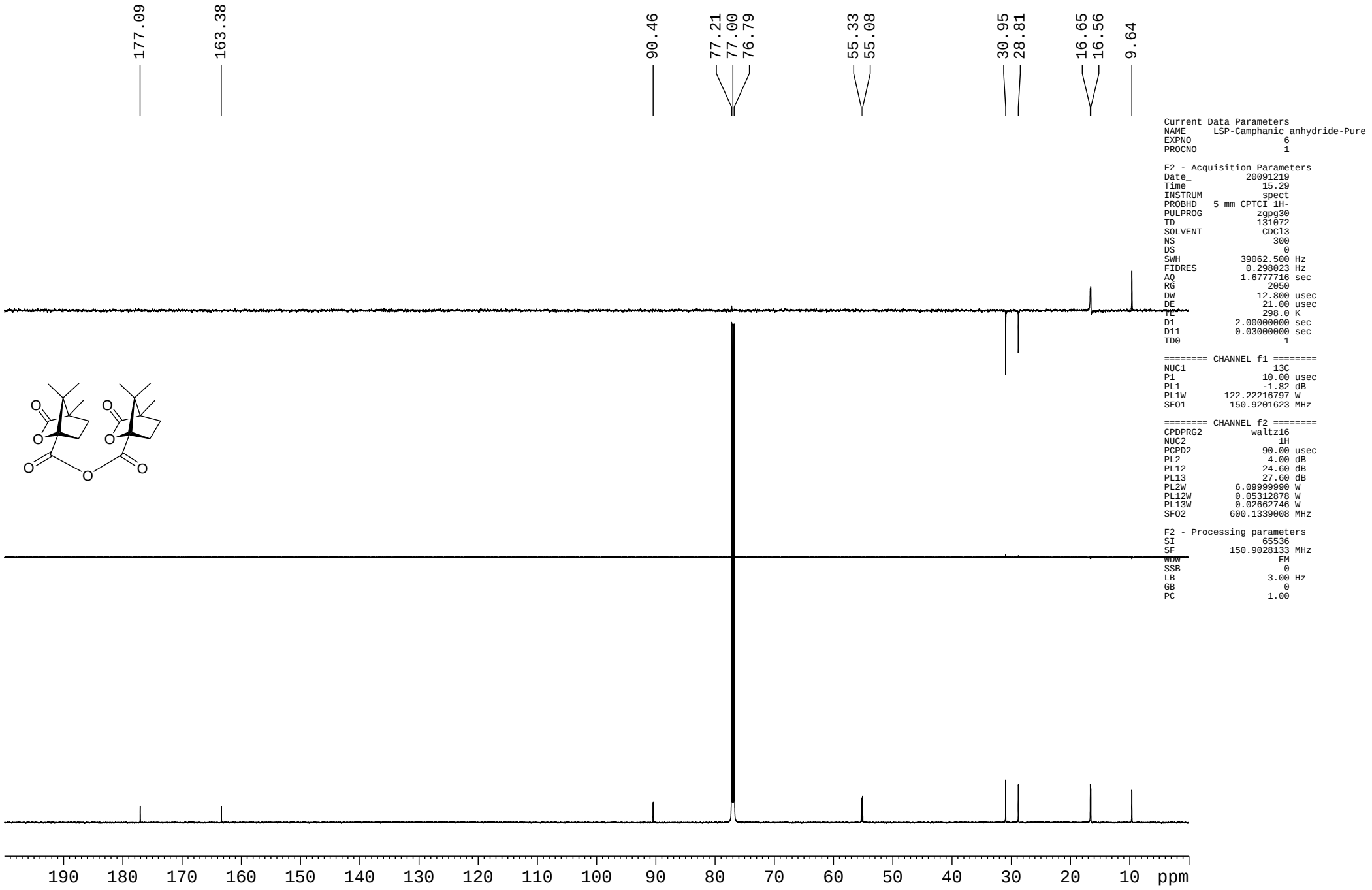
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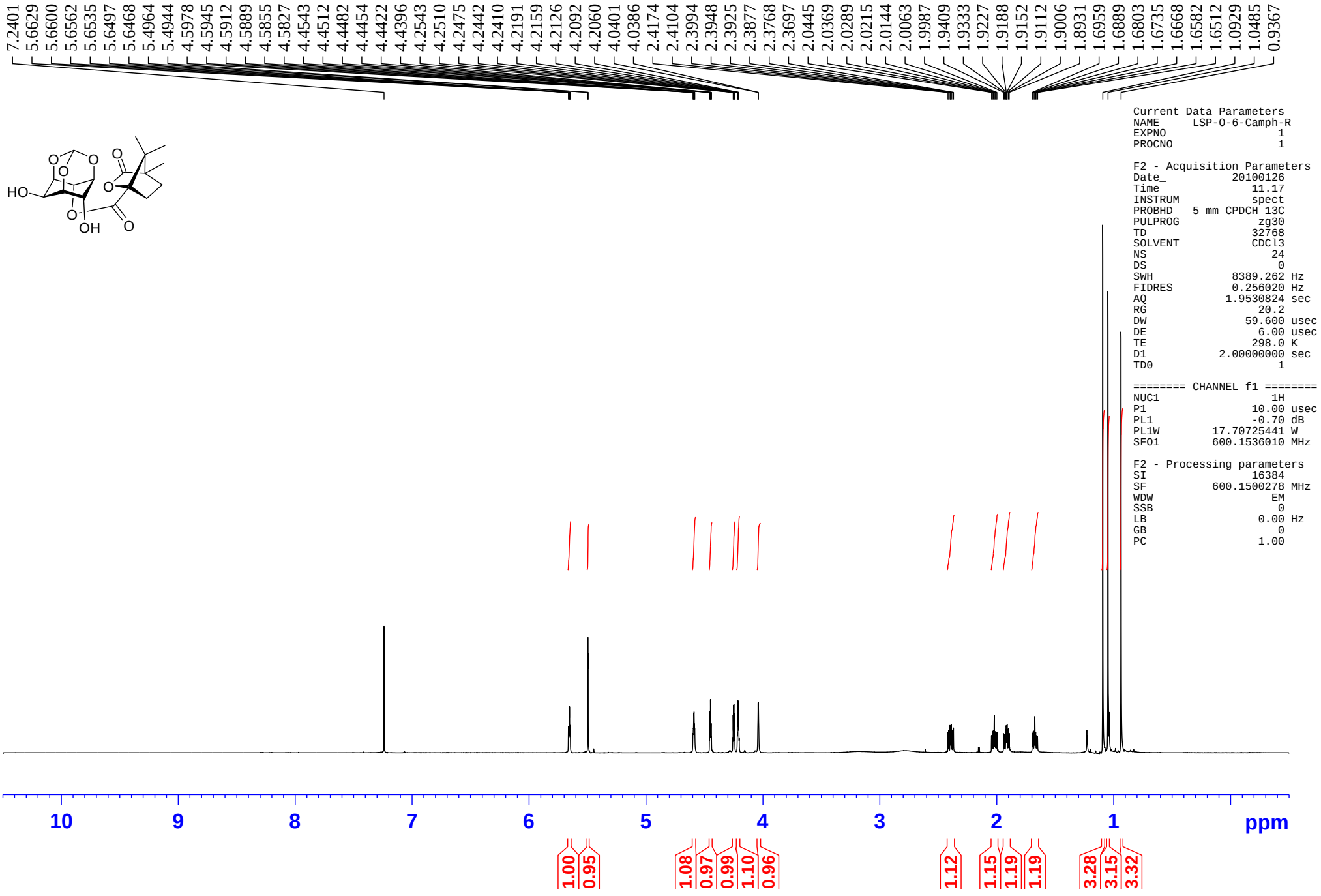
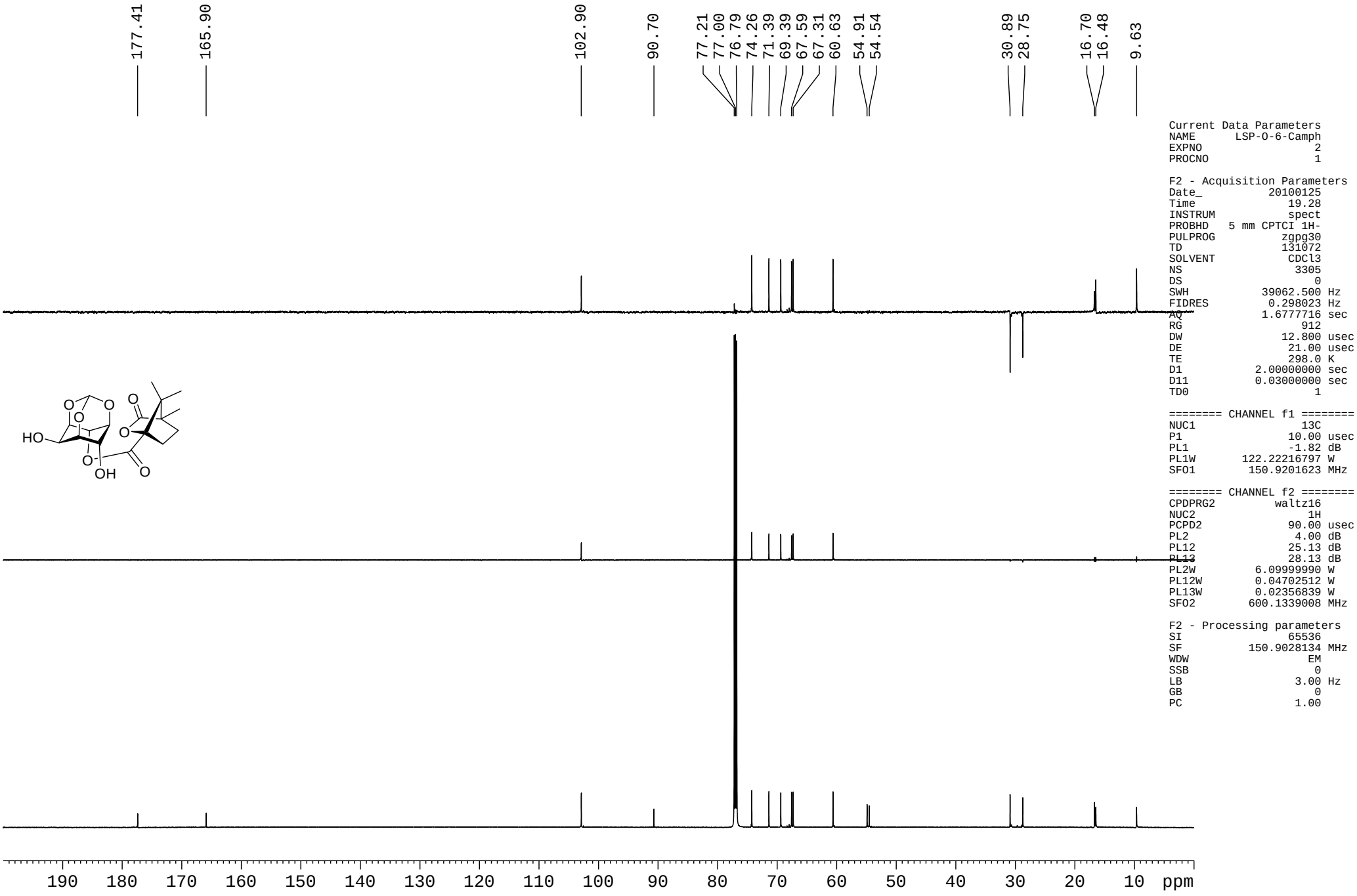
ppm


7.2401 5.6629 5.6600 5.6562 5.6535 5.6497 5.6468 5.4964 5.4944 4.5978 4.5945 4.5912 4.5889 4.5855 4.5827 4.4543 4.4512 4.4482 4.4454 4.4422 4.4396 4.2543 4.2510 4.2475 4.2442 4.2410 4.2191 4.2159 4.2126 4.2092 4.2060 4.0401 4.0386 2.4174 2.4104 2.3994 2.3948 2.3925 2.3877 2.3768 2.3697 2.0445 2.0369 2.0289 2.0215 2.0144 2.0063 1.9987 1.9409 1.9333 1.9227 1.9188 1.9152 1.9112 1.9006 1.8931 1.6959 1.6889 1.6803 1.6735 1.6668 1.6582 1.6512 1.0929 1.0485 0.9367
HO
O
OH
Current Data Parameters
NAME LSP-O-6-Camph-R
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100126
Time 11.17
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530824 sec
RG 20.2
DW 59.600 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -0.70 dB
PL1W 17.70725441 W
SFO1 600.1536010 MHz
F2 - Processing parameters
SI 16384
SF 600.1500278 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 0.95 1.08 0.97 0.99 1.10 0.96 1.12 1.15 1.19 1.19 3.28 3.15 3.32



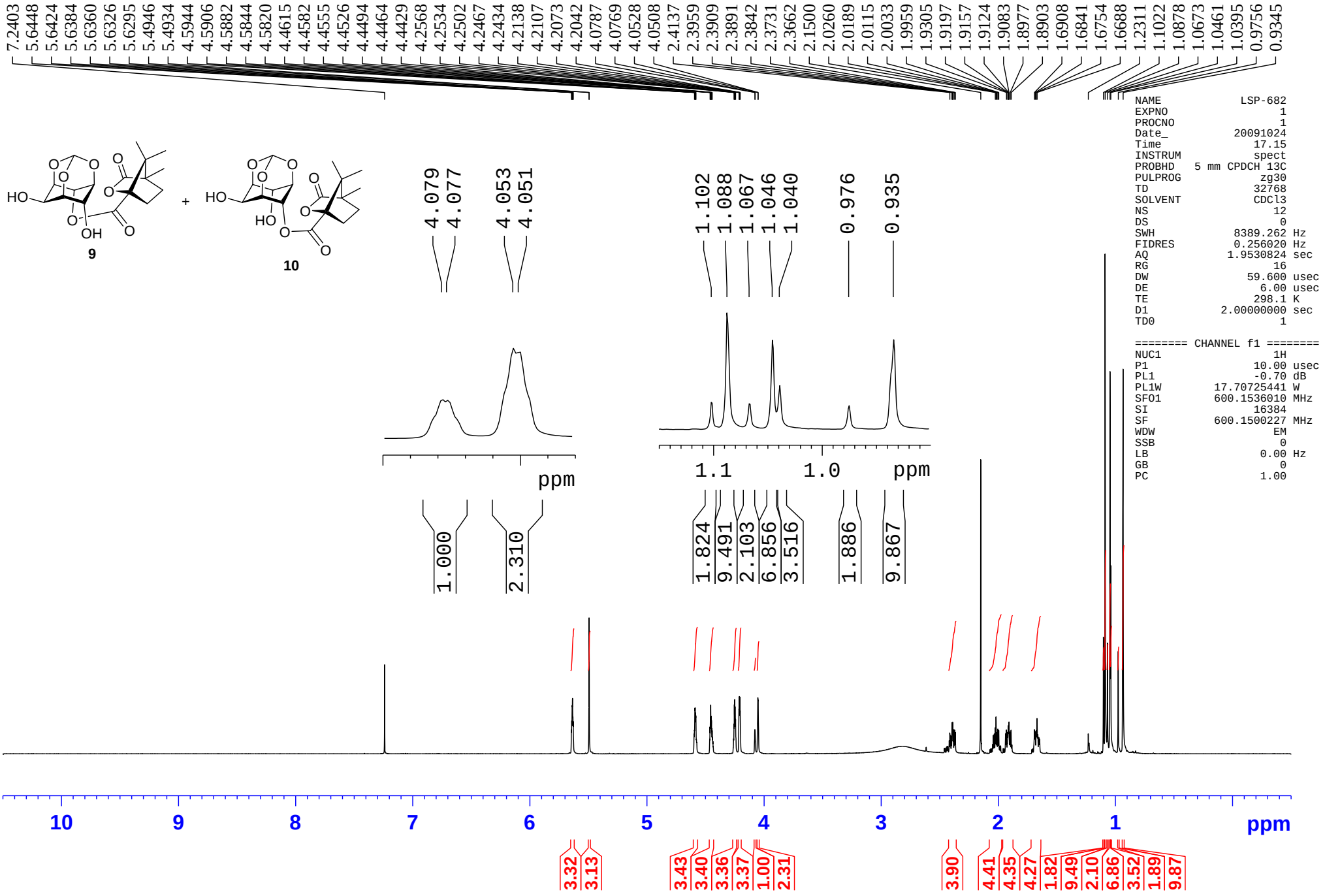

```
Current Data Parameters
NAME      LSP-O-6-Camph
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20100125
Time              19.28
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD               131072
SOLVENT            CDCl3
NS                  3305
DS                     0
SWH          39062.500 Hz
FIDRES        0.298023 Hz
AQ            1.6777716 sec
RG                   912
DW              12.800 usec
DE              21.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.82 dB
PL1W       122.22216797 W
SFO1        150.9201623 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                4.00 dB
PL12              25.13 dB
PL13              28.13 dB
PL2W         6.09999990 W
PL12W        0.04702512 W
PL13W        0.02356839 W
SFO2        600.1339008 MHz

F2 - Processing parameters
SI                65536
SF          150.9028134 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
```


7.2403 5.6448 5.6424 5.6384 5.6360 5.6326 5.6295 5.4946 5.4934 4.5944 4.5906 4.5882 4.5844 4.5820 4.4615 4.4582 4.4555 4.4526 4.4494 4.4464 4.4429 4.2568 4.2534 4.2502 4.2467 4.2434 4.2138 4.2107 4.2073 4.2042 4.0787 4.0769 4.0528 4.0508 2.4137 2.3959 2.3909 2.3891 2.3842 2.3731 2.3662 2.1500 2.0260 2.0189 2.0115 2.0033 1.9959 1.9305 1.9197 1.9157 1.9124 1.9083 1.8977 1.8903 1.6908 1.6841 1.6754 1.6688 1.2311 1.1022 1.0878 1.0673 1.0461 1.0395 0.9756 0.9345
HO
O
OH
9
10
4.079 4.077 4.053 4.051
1.102 1.088 1.067 1.046 1.040 0.976 0.935
ppm
1.1
1.0
1.000 2.310
1.824 9.491 2.103 6.856 3.516 1.886 9.867
NAME LSP-682
EXPNO 1
PROCNO 1
Date_ 20091024
Time 17.15
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530824 sec
RG 16
DW 59.600 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -0.70 dB
PL1W 17.70725441 W
SFO1 600.1536010 MHz
SI 16384
SF 600.1500227 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
3.32 3.13 3.43 3.40 3.36 3.37 1.00 2.31 3.90 4.41 4.35 4.27 1.82 9.49 2.10 6.86 3.52 1.89 9.87