Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Synthesis of the Pentasaccharide Repeating Unit of the *O*-antigen from *Enterobacter cloacae* C4115 containing the rare α-D-FucNAc

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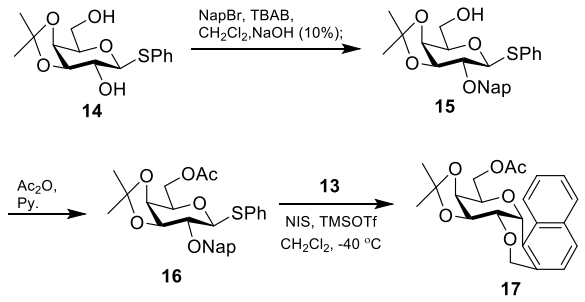
Undesired outcome from the glycosylation of donor 16 with acceptor 13:



Scheme S1: Preparation of D-galactosyl donor **23** and attempted disaccharide synthesis

Phenyl 6-*O*-acetyl-3,4-*O*-isopropylidene-2-*O*-(2′-methyl)naphthyl-1-thio-β-D-galactopyranoside [16]

Compound **14** (2.2 g, 7.05 mmol) was dissolved in CH_2Cl_2 (40 mL) along with NapBr (2.18 g, 9.87 mmol) and TBAB (2.5 g, 7.75 mmol). After stirring the reaction mixture for 10 minutes NaOH (10% aq., 10 mL) was added and the reaction mixture was allowed to stir overnight. After the completion of the reaction it was diluted with CH_2Cl_2 (20 mL) and washed with water (100 mL). The organic layer was collected and dried over anhydrous Na_2SO_4(s). The solvent was removed under reduced pressure to give the crude product which was purified by column chromatography (1:1 *n*-Hexane/EtOAc) to give the mono-alkylated product **15** (R_f = 0.5 1:1 *n*-Hexane/EtOAc).

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.87-7.26 (m, 12H, Ar*H*), 4.86 (d, 1H, *J*=11.5Hz, NapCH_2), 4.69 (d, 1H, *J*=11.5 Hz, NapCH_2), 4.33 (d, 1H, *J*=9.5 Hz, H-1), 4.33 (t, 3H, *J*= 6.0 Hz, H-3), 4.19 (d, 1H, *J*= 4.0 Hz, H-4), 3.98-3.94 (m, 1H, H-6a), 3.82-3.76 (m, 2H, H-6b, H-5), 3.62-3.59 (m, 1H, H-2), 1.40 (s, 3H, CH_3), 1.39 (s, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 125 MHz) δ: 135.2, 133.4, 133.2, 133.1, 129.0, 128.9, 128.0, 127.9, 127.6, 127.5, 127.0, 126.3, 126.0, 125.9, 110.4 (-*C*Me$_2$), 85.9 (C-1), 79.8 (C-3), 78.1 (C-2), 76.7 (C-5), 73.9 (C-4), 73.4 (Ar*C*H$_2$), 62.5 (C-6), 27.7, 26.3 (2×*C*H$_3$).

HRMS calculated for $C_{26}H_{28}O_5SNa$ $(M+Na)^+$: 475.1555, found: 475.1551.

This product **15** was dissolved in pyridine (15 mL) and acetic anhydride (2 mL) was added. The reaction mixture was stirred overnight. After the completion of the reaction the solvent was concentrated under reduced pressure and the crude residue was dissolved in CH_2Cl_2 (30 mL) and washed with ice-cold HCl (5% aq., 100 mL). The organic layer was collected and dried over anhydrous Na_2SO_4(s). The solvent was removed under reduced pressure to give the crude product which was purified by column chromatography (3.5:1 *n*-Hexane/EtOAc) to give the product **16** (R_f = 0.4 3:1 *n*-Hexane/EtOAc) (2.61 g, 75% over 2 steps).

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.85-7.26 (m, 12H, Ar*H*), 4.99 (d, 1H, *J*=11.5Hz, NapCH_2), 4.86 (d, 1H, *J*=11.5 Hz, NapCH_2), 4.66 (d, 1H, *J*=9.0 Hz, H-1), 4.35-4.30 (m, 3H, H-6a, H-6b, H-3), 4.19 (d, 1H, *J*=5.0 Hz, H-4), 3.95 (m, 1H, H-5), 3.60 (m, 1H, H-2), 2.06 (s, 3H, CH_3), 1.39 (s, 3H, CH_3), 1.35 (s, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 125 MHz) δ: 170.7 (*C*O), 135.1, 133.7, 133.2, 133.1, 132.0, 128.9, 128.7, 128.1, 127.9, 127.6, 127.4, 127.1, 126.3, 126.0, 125.9, 110.4 (O$_2$*C*Me$_2$), 86.1 (C-1), 79.5 (C-3), 78.0 (C-2), 74.1 (C-5), 73.5 (Ar*C*H$_2$), 73.4 (C-4), 63.7 (C-6), 27.6, 26.3 (2×*C*H$_3$), 20.8 (*C*H$_3$).

HRMS calculated for $C_{28}H_{30}O_6SNa$ $(M+Na)^+$: 517.1661, found: 517.1654.

((3aR,3bS,11bR,13R,13aS)-2,2-dimethyl-3a,3b,5,11b,13,13a-hexahydro-[1,3]dioxolo[4′,5′:4,5]pyrano[3,2 c]benzo[g]isochromen-13-yl)methyl acetate [17]

Donor **16** (176 mg, 0.36 mmol) and acceptor **13** (100 mg, 0.3 mmol) were dissolved in CH_2Cl_2 (10 mL) and stirred with 4Å MS (1g) and NIS (105 mg, 0.45 mmol) for 15 minutes under N_2 atmosphere. Thereafter the temperature was lowered to -40 °C and TMSOTf (0.012 mL, 0.06 mmol) was added and the reaction was allowed to continue for 1 hour. TLC (3:1 *n*-Hexane/EtOAc) at this point showed the glycosyl donor **21** to be completely consumed with the concomitant generation of a new spot located higher in the TLC (R_f = 0.5 3:1 *n*-Hexane/EtOAc) than the donor itself. The MS was filtered out and the filtrate was washed successively with $NaHCO_3$ aq. (50 mL), $Na_2S_2O_3$ (50 mL) and brine (50 mL). The organic layer was separated and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to give the crude residue which was purified by column chromatography (3:1 *n*-Hexane/EtOAc) to give the undesired product **17** (100 mg) in 73% yield.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 8.33 (d, 2H, *J*= 8.3 Hz, Ar*H*), 7.82 (d, 1H, *J*= 8.0 Hz, Ar*H*), 7.78 (d, 1H, *J*= 8.3 Hz, Ar*H*), 7.58 (t, 1H, *J*= 8.0 Hz, Ar*H*), 7.50 (t, 1H, *J*= 8.0 Hz, Ar*H*), 7.10 (d, 1H, *J*= 8.3 Hz, Ar*H*), 5.39 (d, 1H, *J*= 3.0 Hz, H-1), 4.95 (d, 1H, *J*= 15.0 Hz, ArCH_2), 4.82 (d, 1H, *J*=15.0 Hz, ArCH_2), 4.70 (dd, 1H, *J*= 2.7 Hz, 7.5 Hz, H-3), 4.39 (d, 1H, *J*= 7.7 Hz, H-4), 4.28-4.22 (m, 2H, H-5 H-6a), 4.18-4.17 (m, 1H, H-2), 4.09 (dd, 1H, *J*= 5.2 Hz, 10.3 Hz, H-6b), 1.71 (s, 3H, CH_3), 1.68 (s, 3H, CH_3), 1.47 (s, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 125 MHz) δ: 170.6 (*C*O), 132.9, 132.7, 132.3, 128.8, 128.2, 127.5, 126.6, 125.6, 124.9, 121.8 (Ar*C*), 110.4 (-*C*Me_2), 73.2 (C-3), 72.7 (C-4), 72.2 (C-2), 68.1 (Nap*C*H_2), 67.7 (C-5), 63.2 (C-1), 63.1 (C-6), 26.5, 25.1 (2×*C*H_3), 20.5 (CO*C*H_3).

HRMS calculated for $C_{22}H_{24}O_6Na$ $(M+Na)^+$: 407.1471, found: 407.1472.

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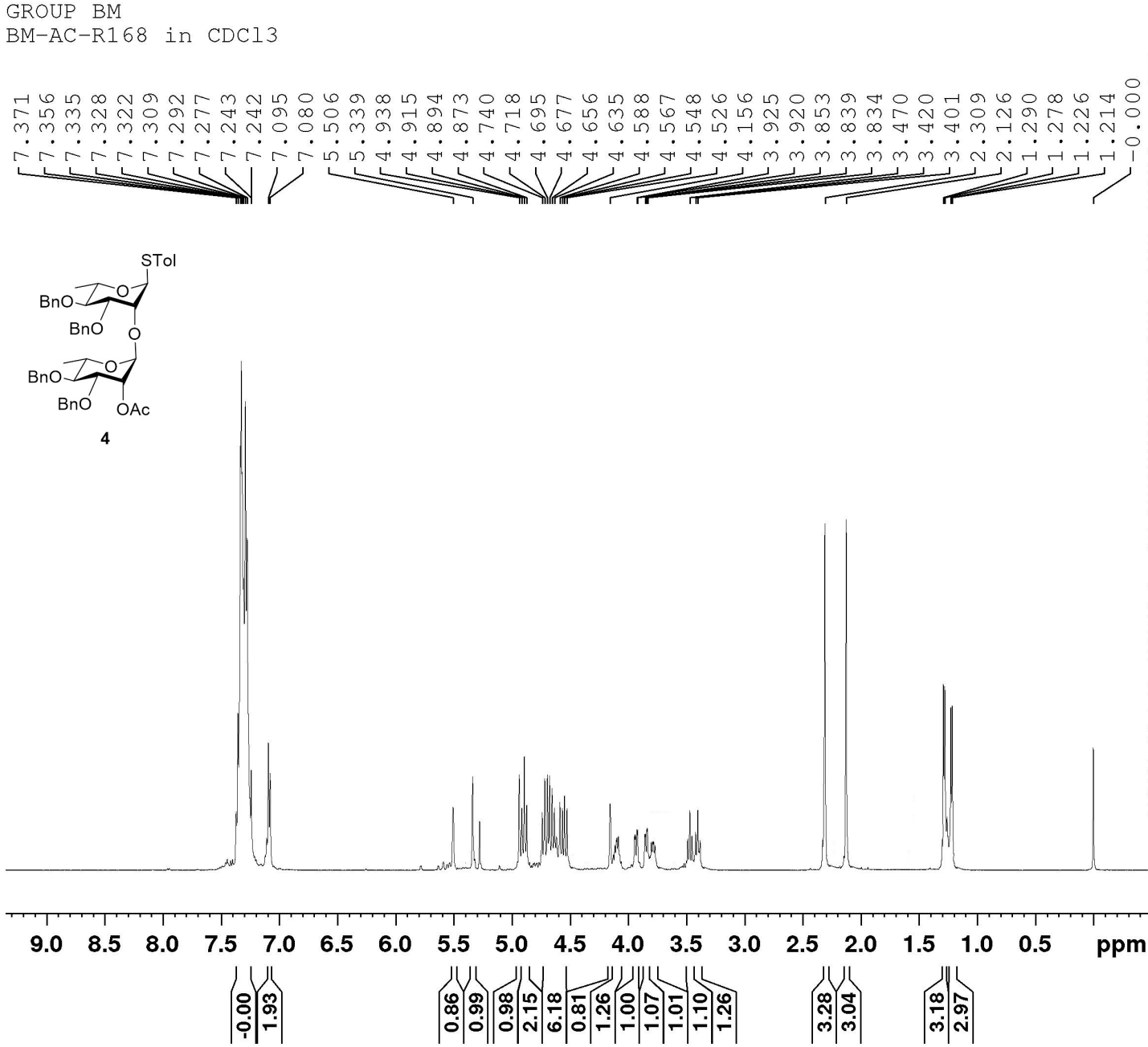

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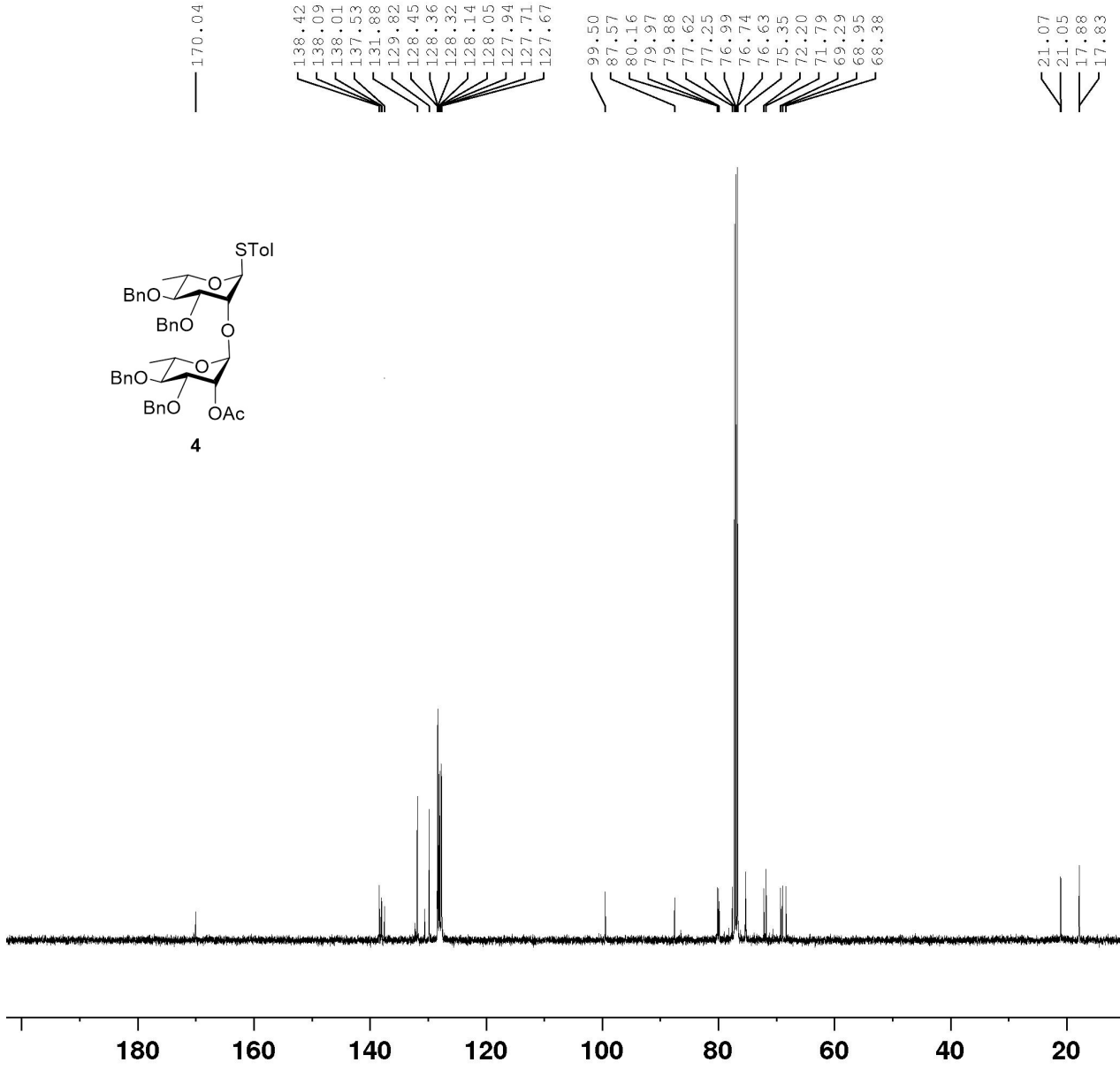

S-4

BRUKER

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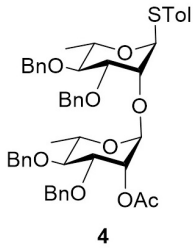

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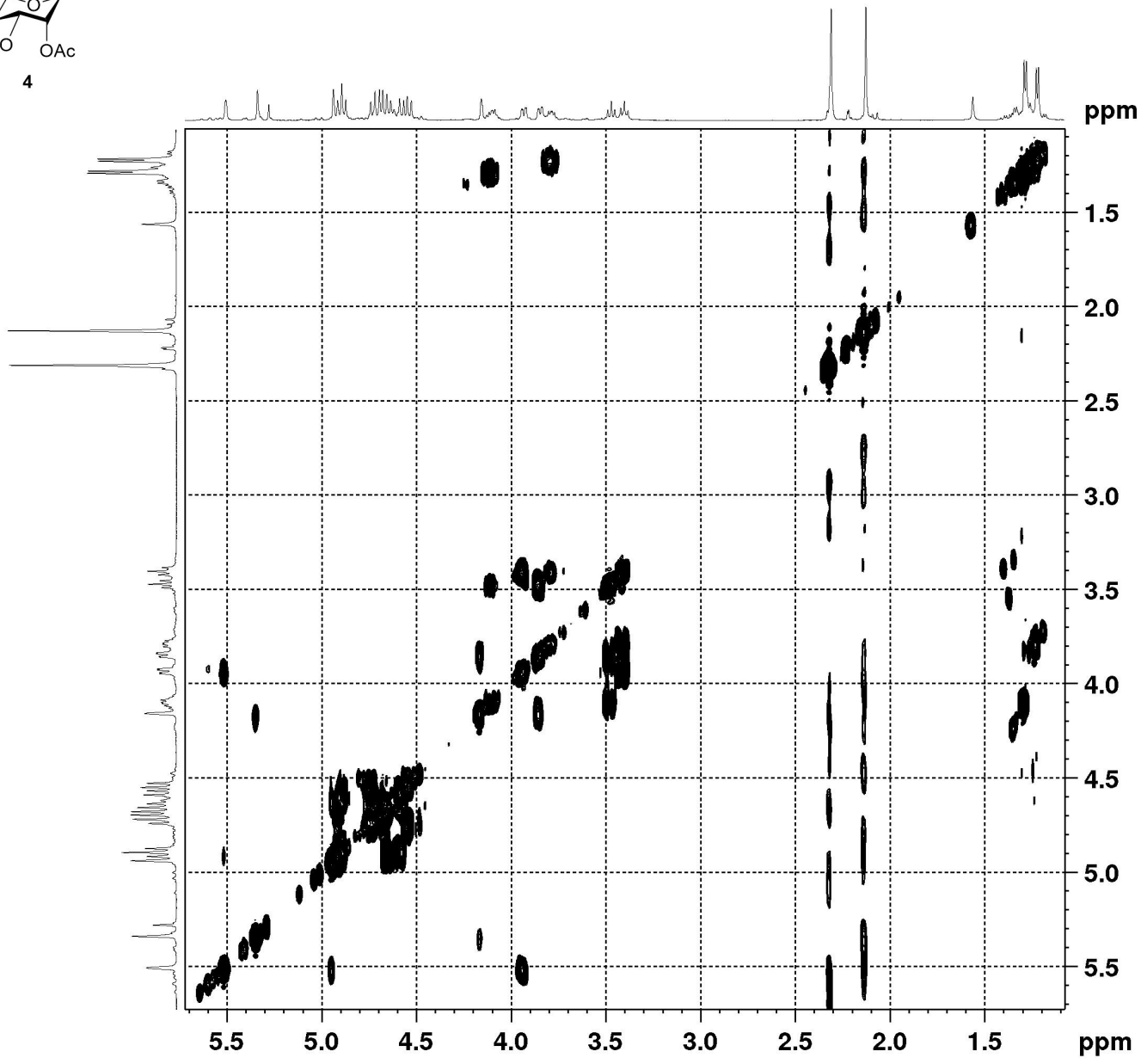


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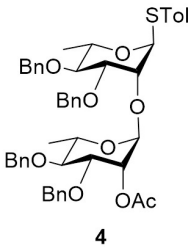

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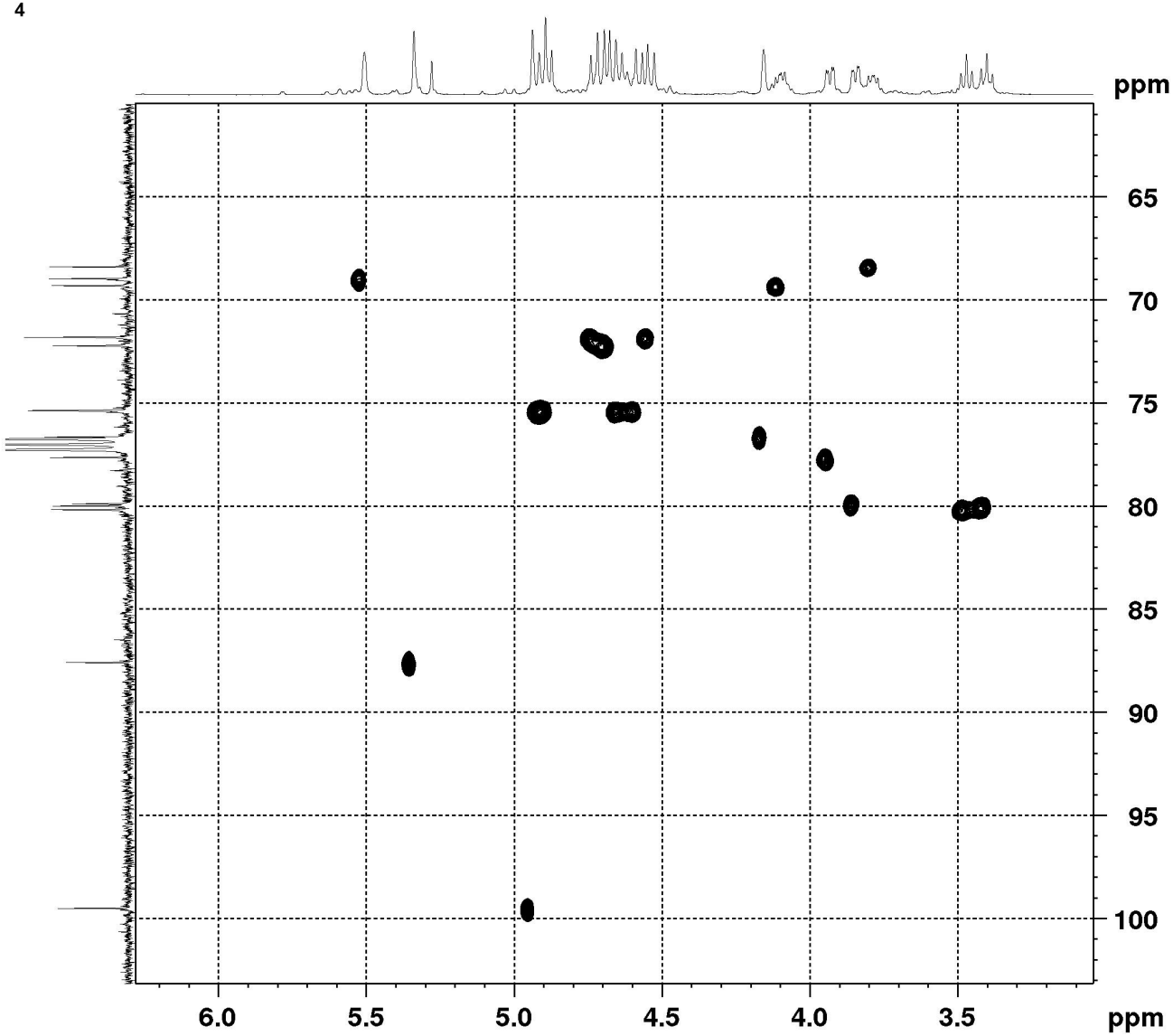


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ZGOPTNS

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CPDPRG[2             garp
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PCPD2             70.00 usec
PLW2        66.00000000 W
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GPZ3               11.00 %
GPZ4               -5.00 %
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P19              600.00 usec

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FnMODE     Echo-Antiecho

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F1 - Processing parameters
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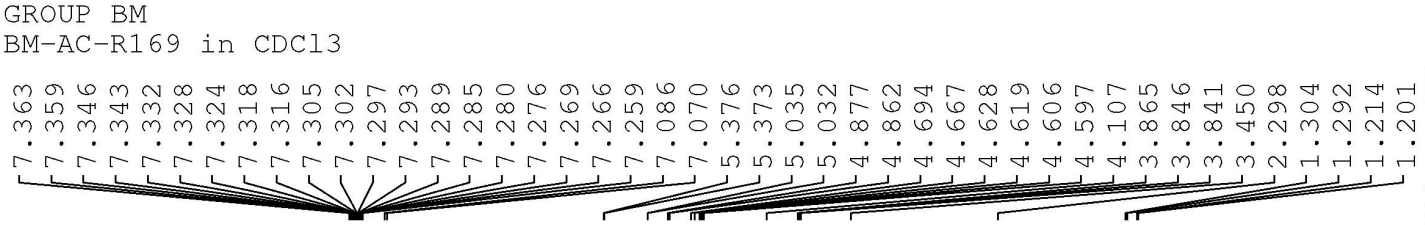

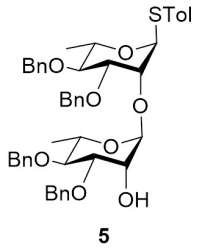

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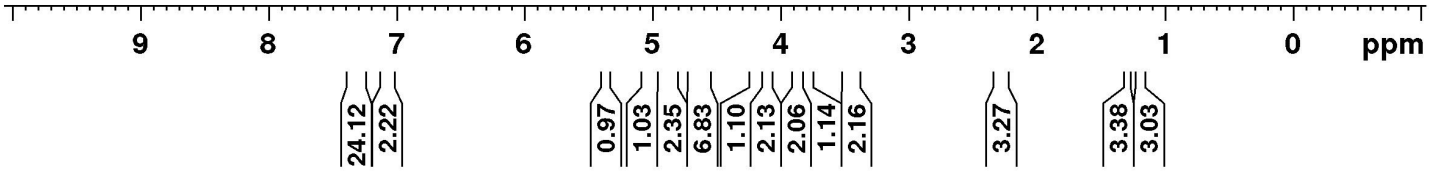

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NUC1 1H
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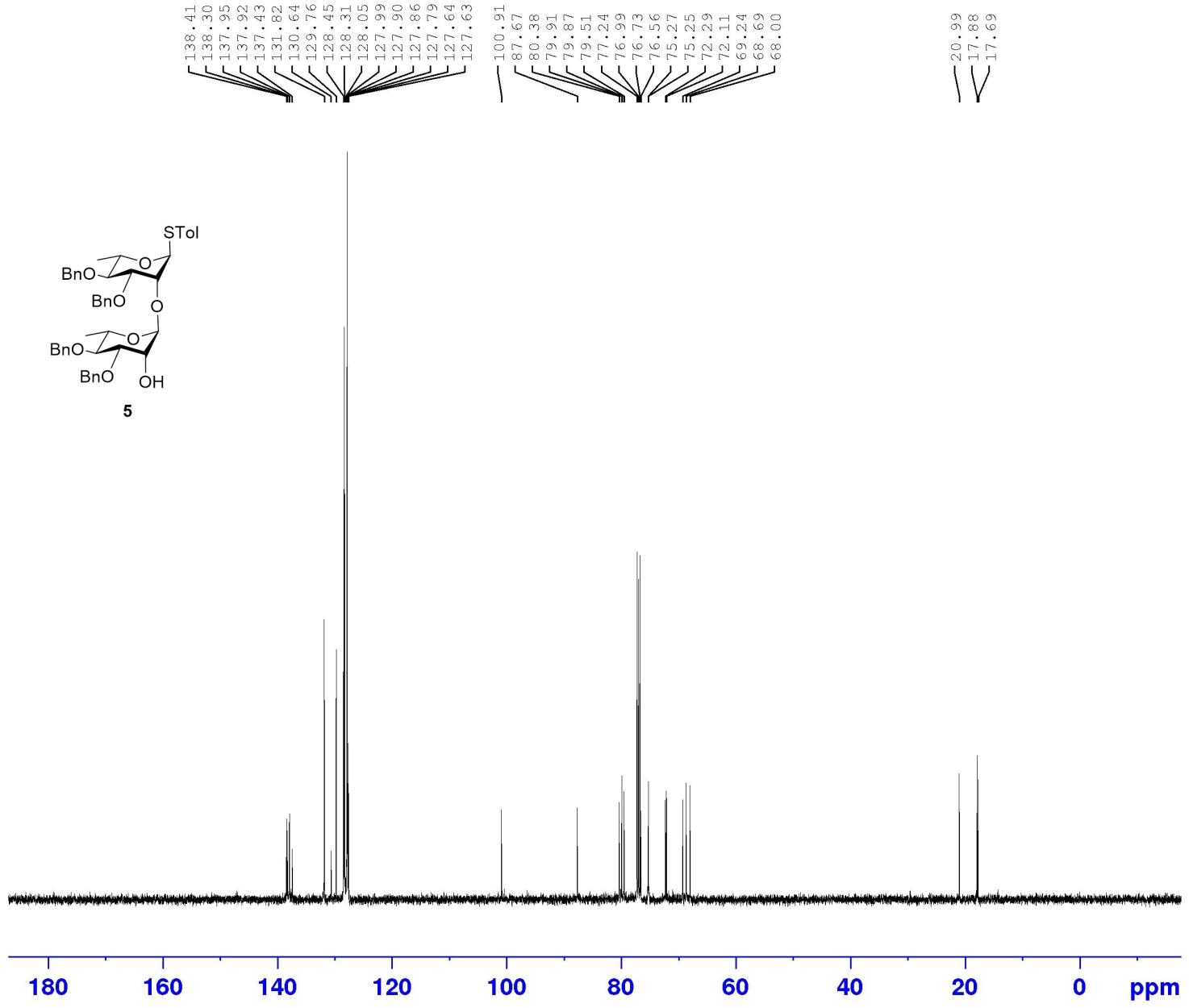


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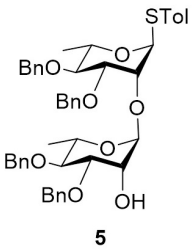

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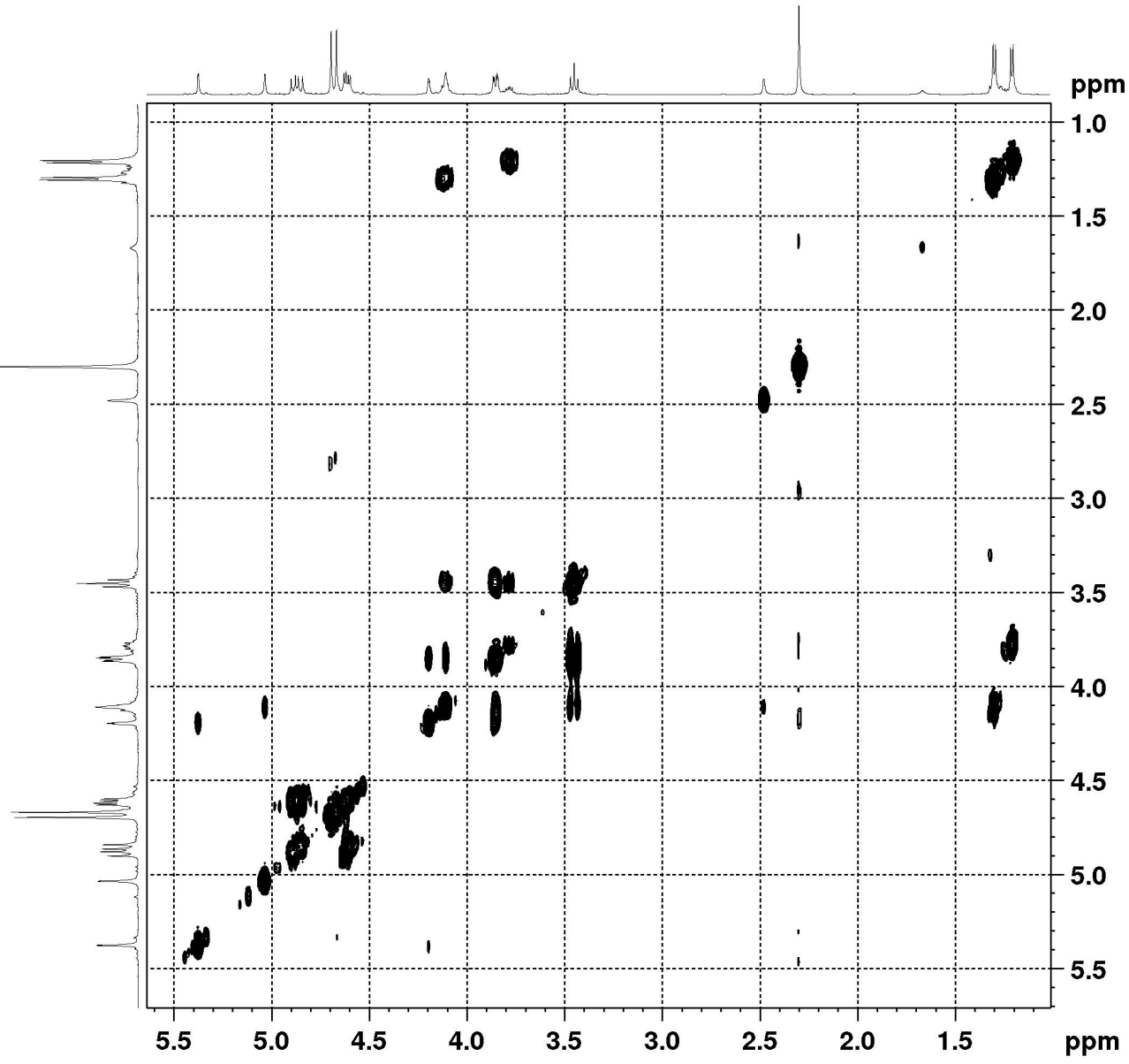


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FnMODE                QF

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LB        0 Hz
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PC                  1.00

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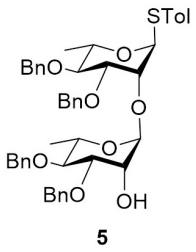

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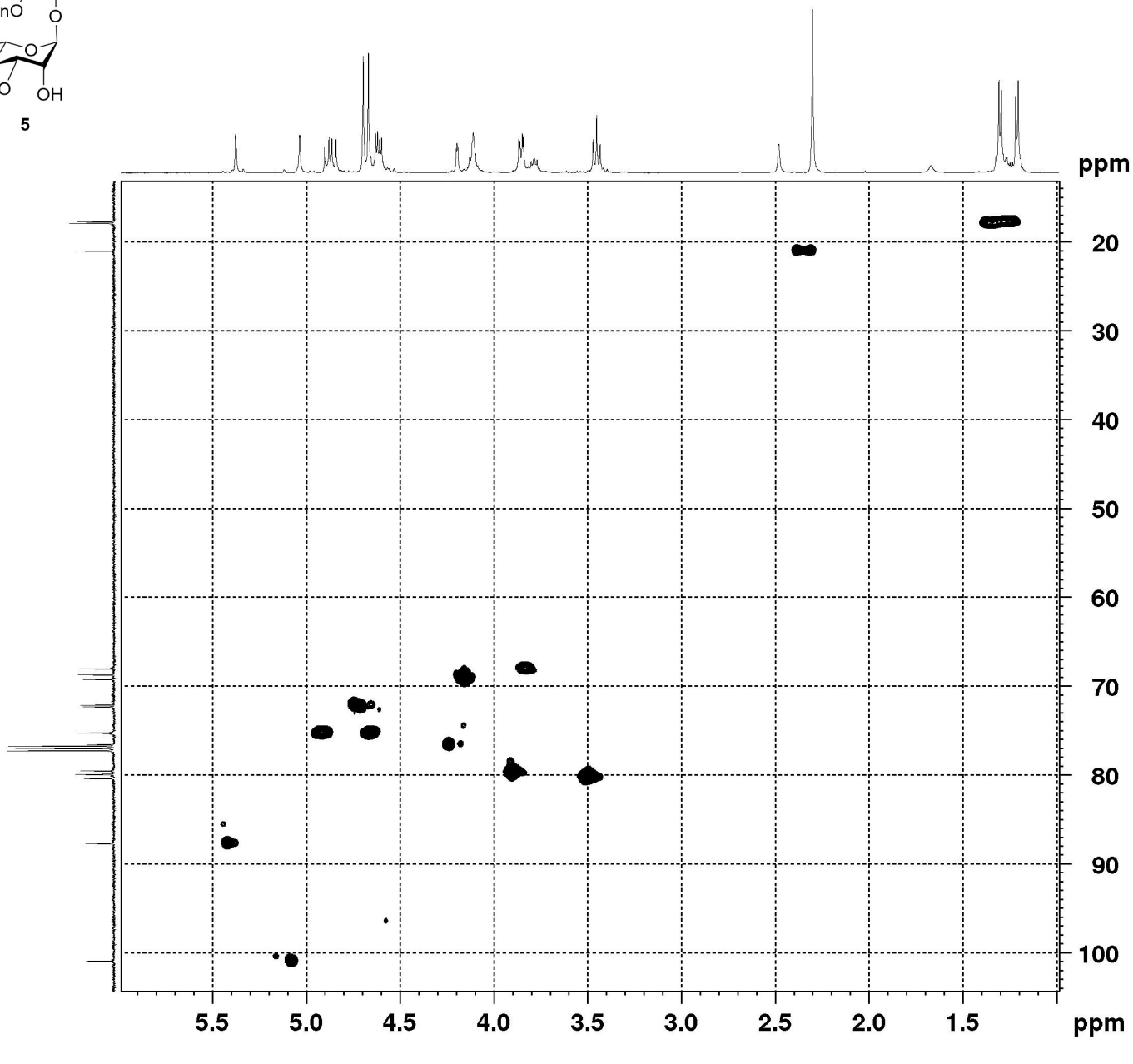


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D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

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P2                  35.00 usec
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PLW1        10.00000000 W

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CPDPRG[2             garp
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P4                  23.00 usec
PCPD2               70.00 usec
PLW2        66.00000000 W
PLW12        1.78129995 W

====== GRADIENT CHANNEL =====
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GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

F1 - Acquisition parameters
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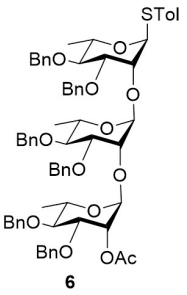
FIDRES        196.293976 Hz
SW                199.682 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF           500.3600191 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                    1.00

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF             125.8156381 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
```

GROUP BM
BM-AC-R80 in CDCl3

7.397 7.381 7.355 7.345 7.323 7.308 7.296 7.281 7.264 7.260 7.130 7.114 5.364 5.077 5.047 4.932 4.926 4.914 4.904 4.892 4.767 4.737 4.726 4.719 4.695 4.660 4.639 4.617 4.587 4.565 4.128 3.870 3.865 3.852 3.471 3.454 2.343 2.171 1.325 1.313 1.293 1.281 1.231 1.219



6

Current Data Parameters
NAME BM-AC-R80
EXPNO 60
PROCNO 1

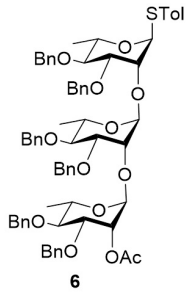
F2 - Acquisition Parameters
Date_ 20190426
Time 11.22
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 9469.697 Hz
FIDRES 0.142273 Hz
AQ 3.5143681 sec
RG 50.8
DW 52.800 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3445031 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3400116 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R80 in CDCl3

170.00
138.47
138.34
138.04
137.88
137.46
131.87
130.63
129.79
128.49
128.31
128.29
128.13
128.07
127.94
127.76
127.63
127.54
127.49
100.60
99.03
87.71
80.36
80.03
79.57
79.04
77.74
77.25
76.99
76.74
76.42
75.38
75.30
75.20
74.50
72.16
72.12
71.77
69.26
68.90
68.57
68.26
21.09
21.03
17.93
17.86



6

Current Data Parameters
NAME BM-AC-R80
EXPNO 61
PROCNO 1

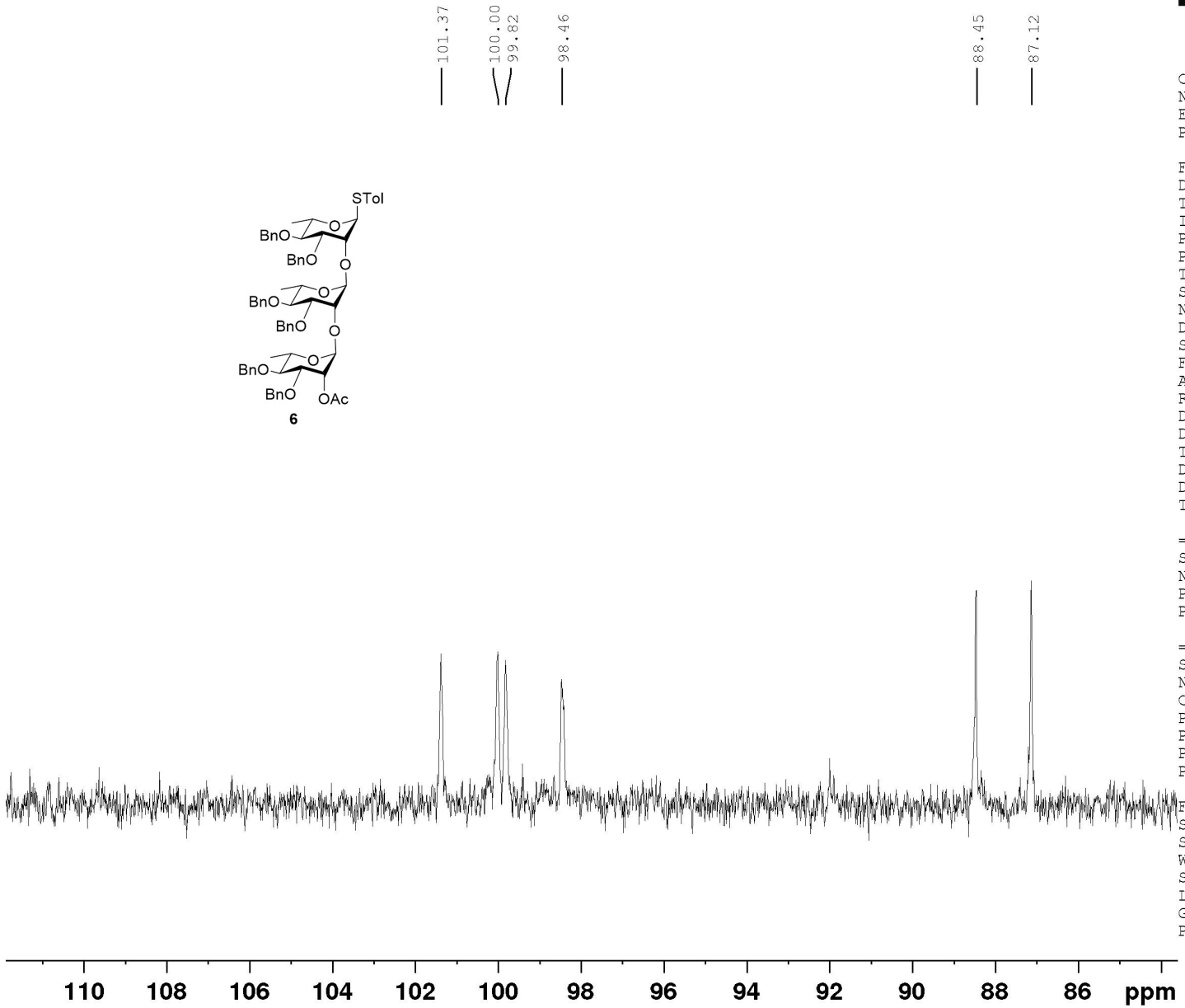
F2 - Acquisition Parameters
Date_ 20190426
Time 11.27
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8294646 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8106045 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

GROUP BM
BM-AC-R80 in CDCl3



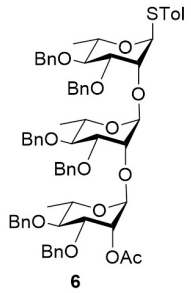

```
Current Data Parameters
NAME                 BM-AC-R80
EXPNO                      170
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20191217
Time                     20.29
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                      16065
DS                          4
SWH                37878.789 Hz
FIDRES              0.577984 Hz
AQ                  0.8650752 sec
RG                        203
DW                     13.200 usec
DE                      6.50 usec
TE                      276.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

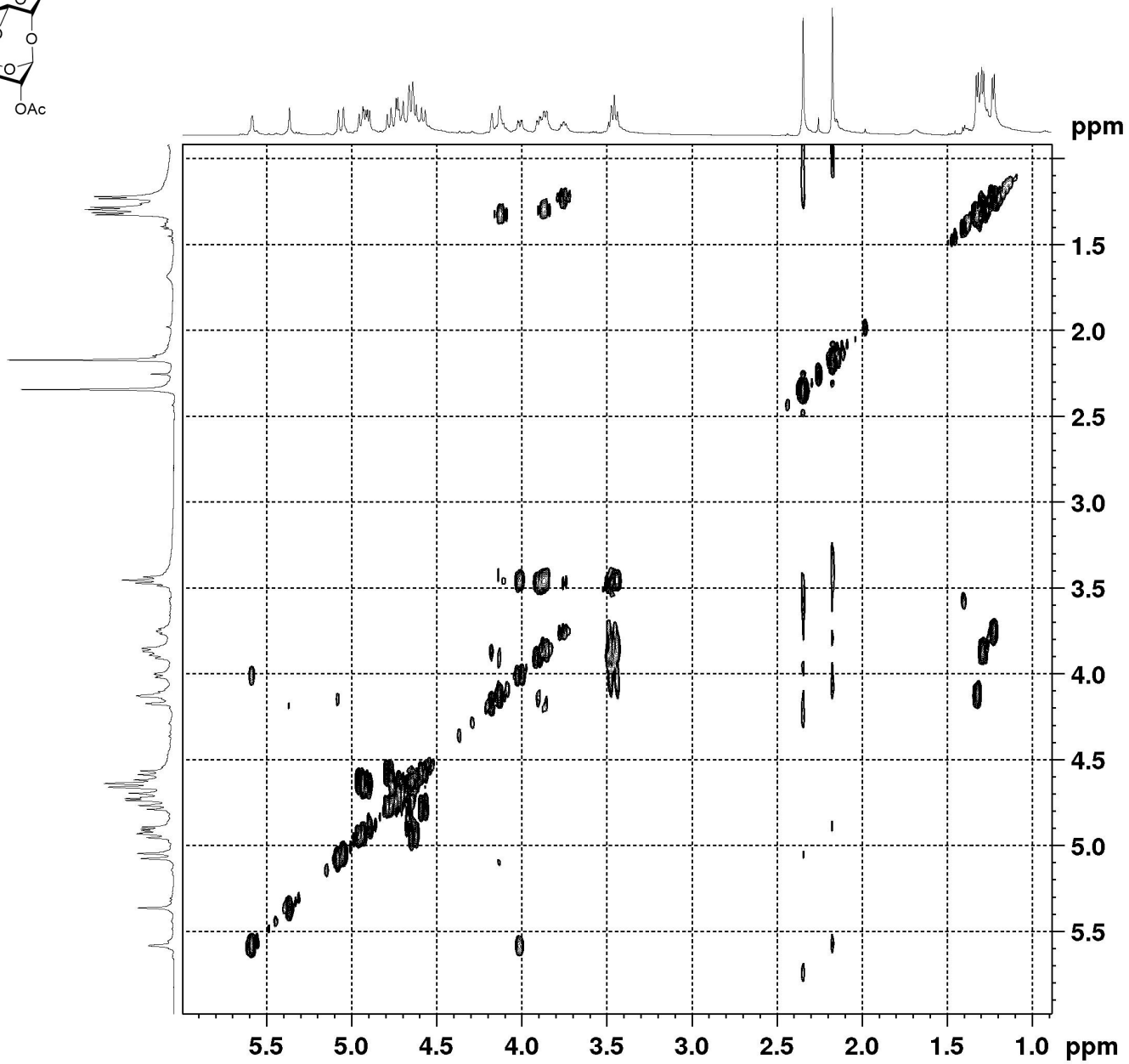
======== CHANNEL f1 ========
SFO1              125.8282036 MHz
NUC1                      13C
P1                     11.50 usec
PLW1              66.00000000 W

======== CHANNEL f2 ========
SFO2              500.3620014 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2          0 W
PLW12         0 W
PLW13         0 W

F2 - Processing parameters
SI                        32768
SF                125.8156220 MHz
WDW                          EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.35
```



6




```
Current Data Parameters
NAME                  BM-AC-R80
EXPNO                        62
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20190426
Time                     11.35
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                        2048
SOLVENT                 CDCl3
NS                            1
DS                            8
SWH                5000.000 Hz
FIDRES             2.441406 Hz
AQ                 0.2048000 sec
RG                        50.8
DW                  100.000 usec
DE                    6.50 usec
TE                   300.6 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00019980 sec

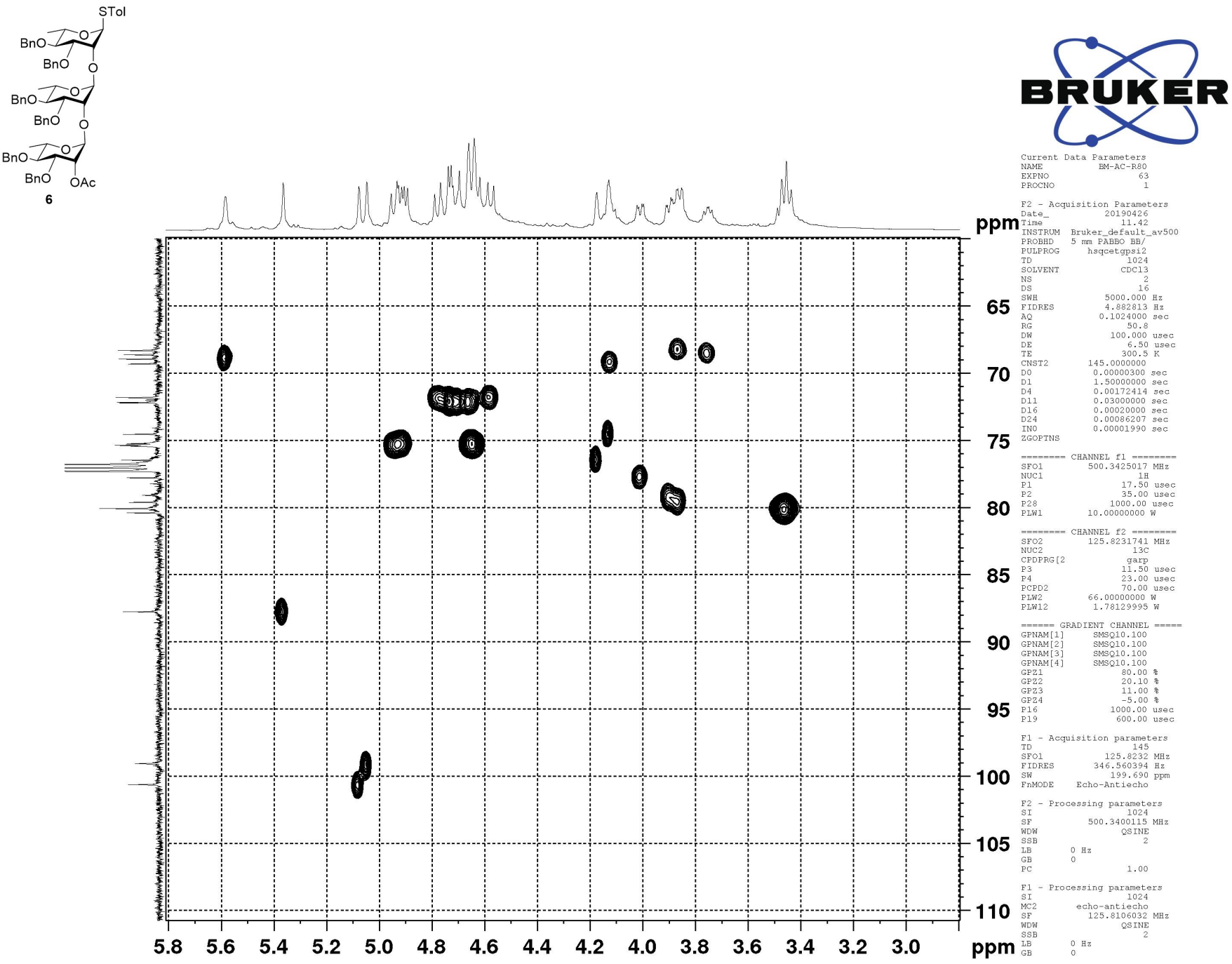
======== CHANNEL f1 ========
SFO1              500.3425017 MHz
NUC1                      1H
P0                     17.50 usec
P1                     17.50 usec
P17                  2500.00 usec
PLW1              10.00000000 W
PLW10              3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                  10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       128
SFO1                500.3425 MHz
FIDRES             78.203201 Hz
SW                    10.003 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       1024
SF                500.3400123 MHz
WDW                     QSINE
SSB          0
LB           0 Hz
GB           0
PC                        1.00

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                500.3400113 MHz
WDW                     QSINE
SSB          0
LB           0 Hz
GB           0
```



BRUKER

```
Current Data Parameters
NAME            BM-AC-R80
EXPNO                  63
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190426
Time                11.42
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                   1024
SOLVENT             CDCl3
NS                      2
DS                     16
SWH             5000.000 Hz
FIDRES          4.882813 Hz
AQ              0.1024000 sec
RG                   50.8
DW                100.000 usec
DE                  6.50 usec
TE                 300.5 K
CNST2          145.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D4              0.00172414 sec
D11             0.03000000 sec
D16             0.00020000 sec
D24             0.00086207 sec
IN0             0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          500.3425017 MHz
NUC1                    1H
P1                   17.50 usec
P2                   35.00 usec
P28                1000.00 usec
PLW1          10.00000000 W

======== CHANNEL f2 ========
SFO2          125.8231741 MHz
NUC2                   13C
CPDPRG[2               garp
P3                   11.50 usec
P4                   23.00 usec
PCPD2                70.00 usec
PLW2          66.00000000 W
PLW12          1.78129995 W

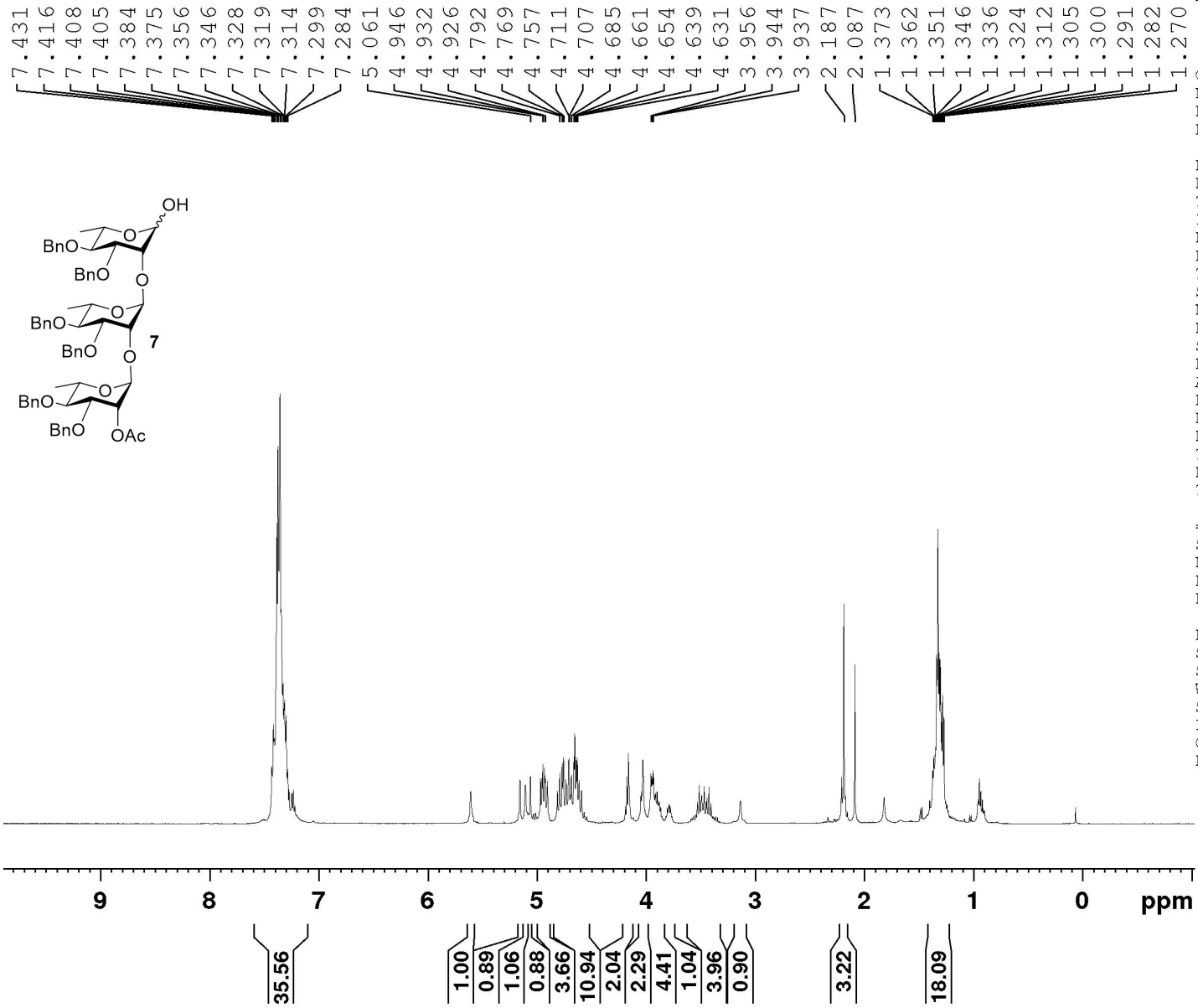
====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPNAM[3]       SMSQ10.100
GPNAM[4]       SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

F1 - Acquisition parameters
TD                     145
SFO1            125.8232 MHz
FIDRES         346.560394 Hz
SW                199.690 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF            500.3400115 MHz
WDW                   QSINE
SSB                       2
LB         0 Hz
GB         0
PC                     1.00

F1 - Processing parameters
SI                    1024
MC2         echo-antiecho
SF              125.8106032 MHz
WDW                   QSINE
SSB                       2
LB         0 Hz
GB         0
```

GROUP BM
BM-AC-R176 in CDCl3



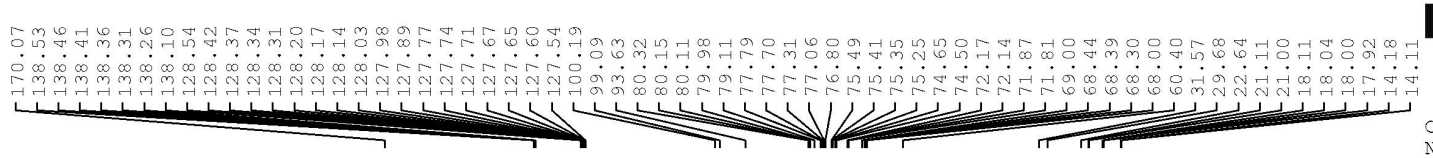
Current Data Parameters
NAME BM-AC-R176
EXPNO 290
PROCNO 1

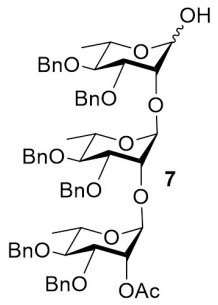
F2 - Acquisition Parameters
Date_ 20191226
Time 18.15
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 4
DS 2
SWH 12500.000 Hz
FIDRES 0.187800 Hz
AQ 2.6624000 sec
RG 32
DW 40.000 usec
DE 6.50 usec
TE -2434.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3625018 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3600047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R176 in CDCl3





Current Data Parameters
NAME BM-AC-R176
EXPNO 291
PROCNO 1

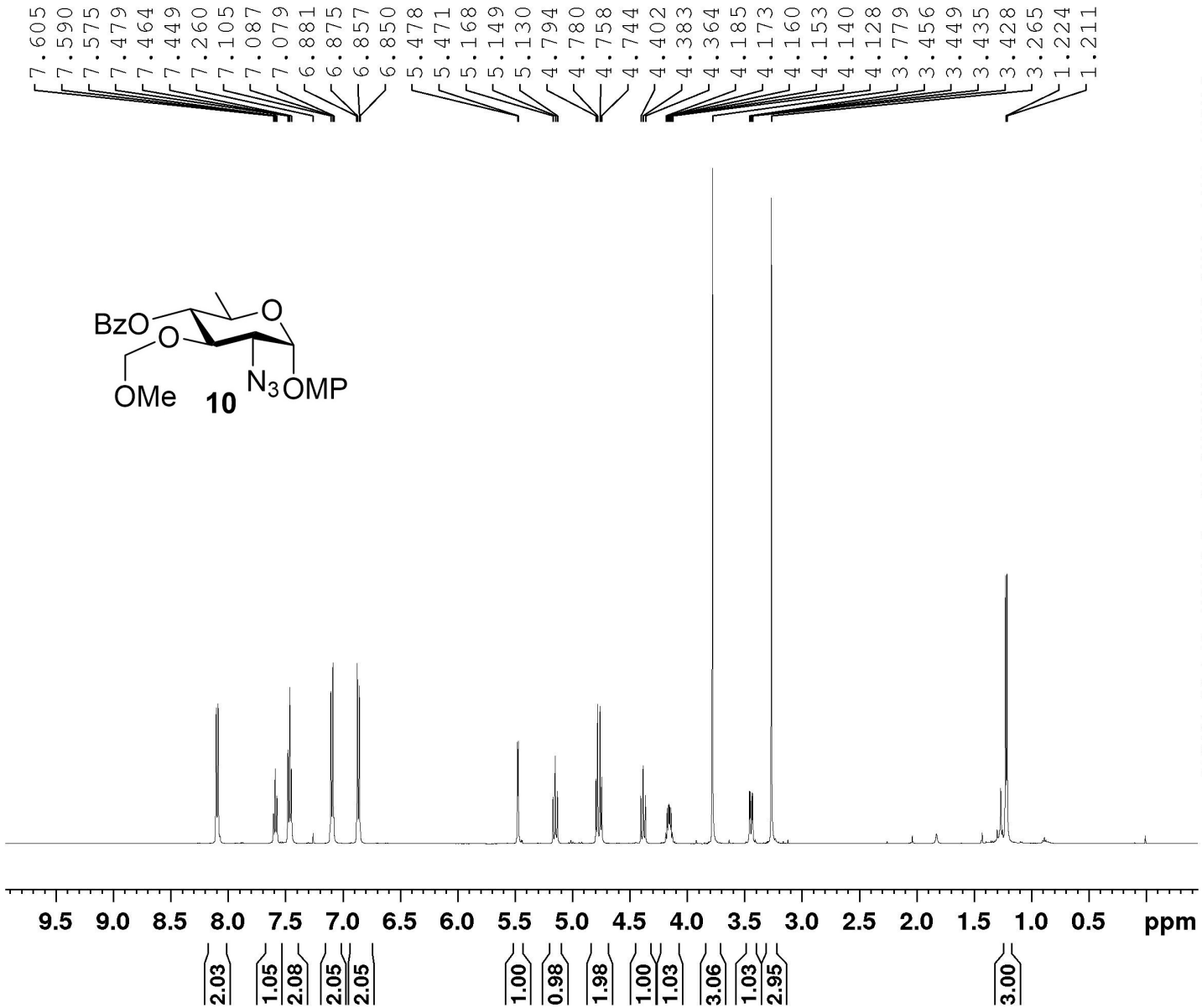
F2 - Acquisition Parameters
Date_ 20191226
Time 18.20
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 707
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 203
DW 13.200 usec
DE 6.50 usec
TE -2814.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8282036 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8156286 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.35

GROUP BM
BM-AC-R61 in CDCl3



Current Data Parameters
NAME BM-AC-R61
EXPNO 70
PROCNO 1

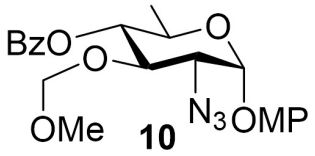
F2 - Acquisition Parameters
Date_ 20180607
Time 15.15
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.150240 Hz
AQ 3.3280001 sec
RG 40.3
DW 50.000 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3430898 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

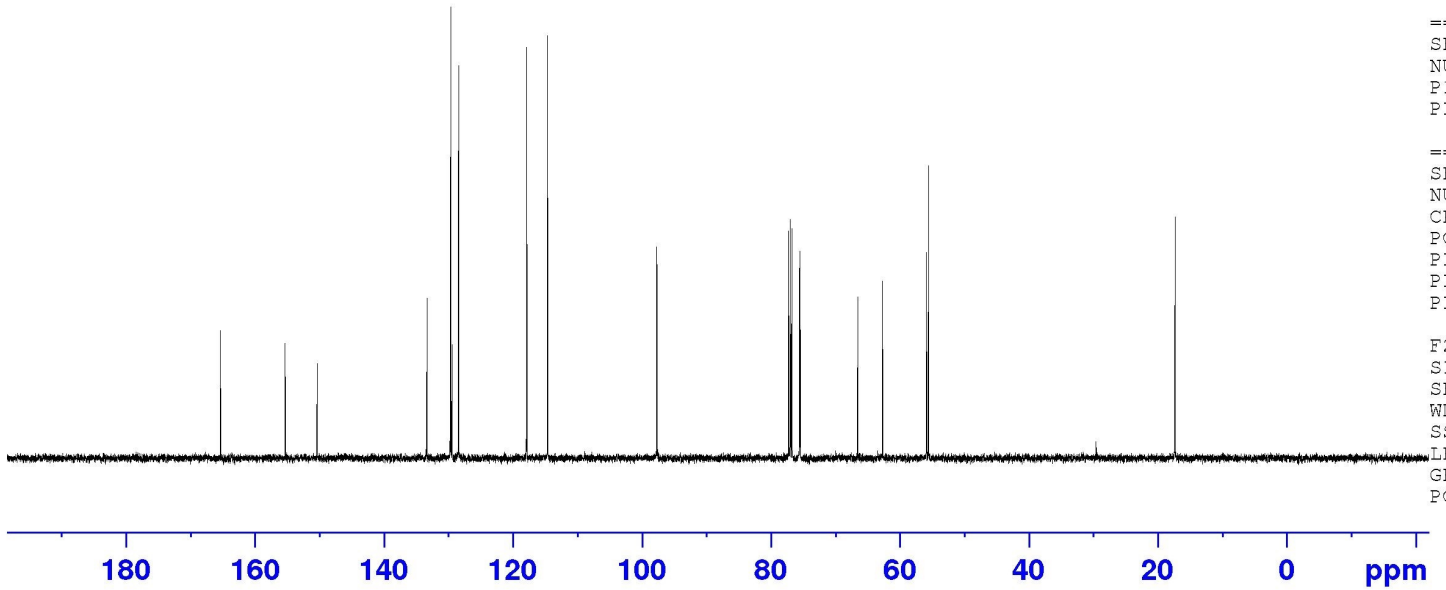
F2 - Processing parameters
SI 131072
SF 500.3400115 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R61 in CDCl3

165.37
155.33
150.38
133.33
129.67
129.43
128.44
117.87
114.63
97.68
97.65
77.25
76.99
76.74
75.55
75.44
66.52
62.67
55.86
55.51
17.31



10



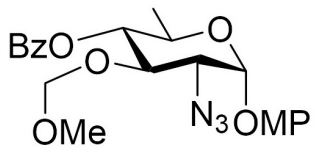
Current Data Parameters
NAME BM-AC-R61
EXPNO 71
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180607
Time 15.19
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

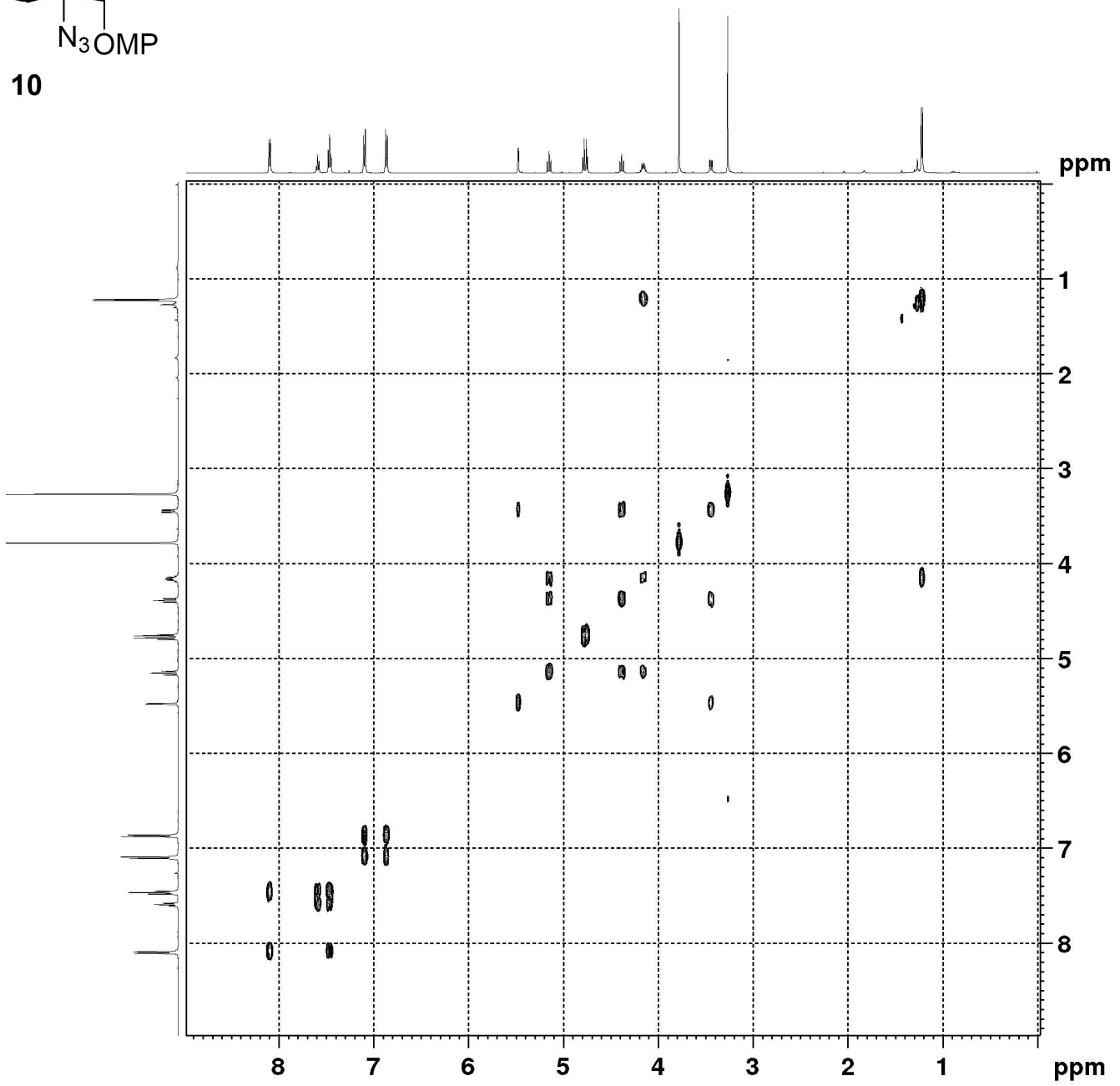
======== CHANNEL f1 ========
SFO1 125.8294646 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8106099 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10




```
Current Data Parameters
NAME                  BM-AC-R61
EXPNO                        72
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20180607
Time                     15.21
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                         2048
SOLVENT                  CDCl3
NS                            1
DS                            8
SWH                  4504.504 Hz
FIDRES               2.199465 Hz
AQ                   0.2273280 sec
RG                        40.3
DW                     111.000 usec
DE                       6.50 usec
TE                      299.6 K
D0                   0.00000300 sec
D1                   2.00000000 sec
D11                  0.03000000 sec
D12                  0.00002000 sec
D13                  0.00000400 sec
D16                  0.00020000 sec
IN0                  0.00022200 sec

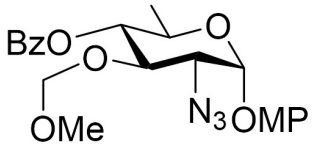
======== CHANNEL f1 ========
SFO1               500.3422515 MHz
NUC1                       1H
P0                      17.50 usec
P1                      17.50 usec
P17                   2500.00 usec
PLW1                10.00000000 W
PLW10                3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                    10.00 %
P16                   1000.00 usec

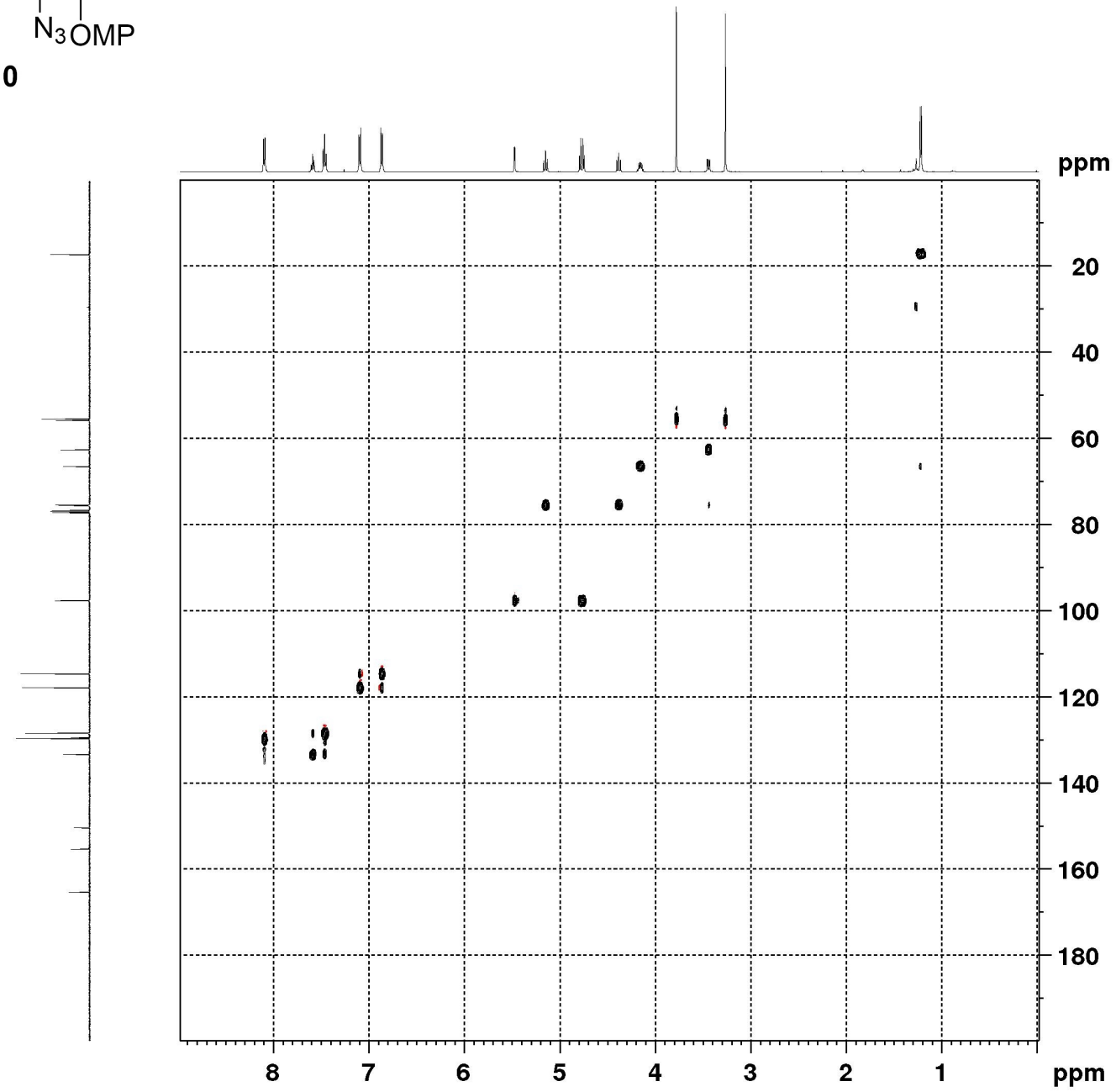
F1 - Acquisition parameters
TD                           87
SFO1                  500.3423 MHz
FIDRES               103.551826 Hz
SW                        9.003 ppm
FnMODE                       QF

F2 - Processing parameters
SI                         1024
SF                 500.3400120 MHz
WDW                      QSINE
SSB               0
LB                0 Hz
GB                0
PC                        1.00

F1 - Processing parameters
SI                         1024
MC2                          QF
SF                 500.3400144 MHz
WDW                      QSINE
SSB               0
LB                0 Hz
GB                0
```



10




```
Current Data Parameters
NAME                  BM-AC-R61
EXPNO                        73
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20180607
Time                      15.25
INSTRUM  Bruker_default_av500
PROBHD    5 mm PABBO BB/
PULPROG       hsqcetgpsi2
TD                        1024
SOLVENT                 CDCl3
NS                           2
DS                          16
SWH                 4504.504 Hz
FIDRES              4.398930 Hz
AQ                  0.1136640 sec
RG                         40.3
DW                    111.000 usec
DE                      6.50 usec
TE                     299.5 K
CNST2               145.0000000
D0                   0.00000300 sec
D1                   1.50000000 sec
D4                   0.00172414 sec
D11                  0.03000000 sec
D16                  0.00020000 sec
D24                  0.00086207 sec
IN0                  0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               500.3422515 MHz
NUC1                        1H
P1                       17.50 usec
P2                       35.00 usec
P28                    1000.00 usec
PLW1               10.00000000 W

======== CHANNEL f2 ========
SFO2               125.8231741 MHz
NUC2                       13C
CPDPRG[2                 garp
P3                       11.50 usec
P4                       23.00 usec
PCPD2                    70.00 usec
PLW2               66.00000000 W
PLW12               1.78129995 W

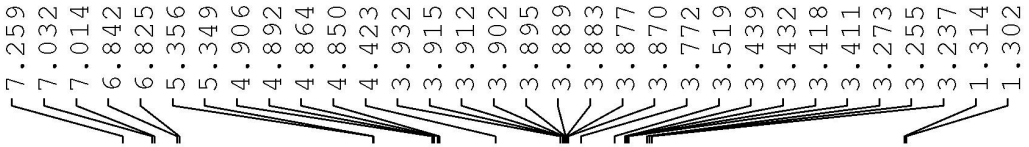
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                    80.00 %
GPZ2                    20.10 %
GPZ3                    11.00 %
GPZ4                    -5.00 %
P16                   1000.00 usec
P19                    600.00 usec

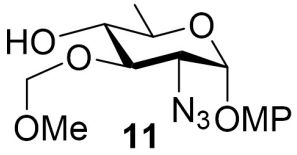
F1 - Acquisition parameters
TD                         137
SFO1                125.8232 MHz
FIDRES              366.797485 Hz
SW                     199.690 ppm
FnMODE     Echo-Antiecho

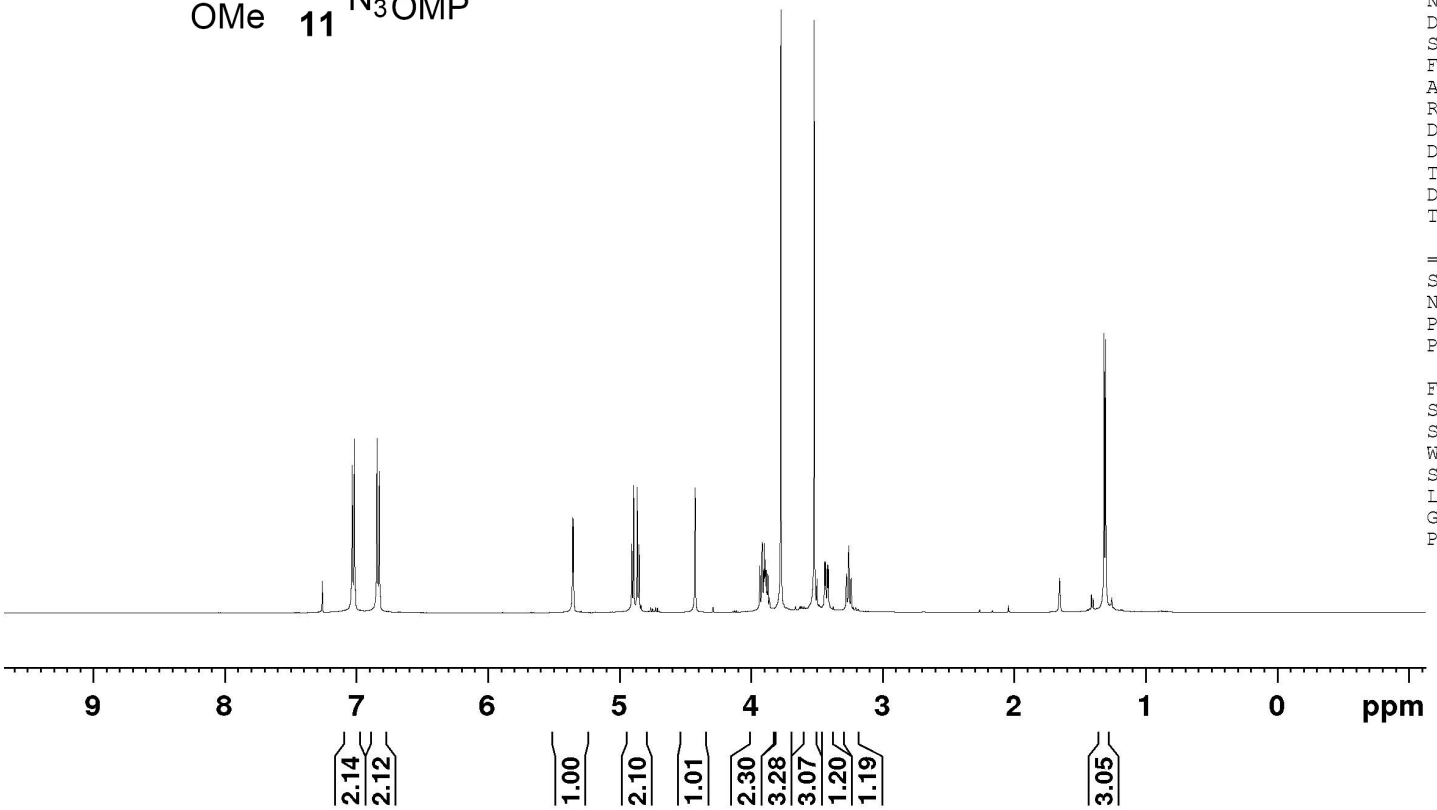
F2 - Processing parameters
SI                        1024
SF                 500.3400109 MHz
WDW                      QSINE
SSB                         2
LB          0 Hz
GB          0
PC                        1.00

F1 - Processing parameters
SI                        1024
MC2            echo-antiecho
SF                 125.8105931 MHz
WDW                      QSINE
SSB                         2
LB          0 Hz
GB          0
```

GROUP BM
BM-AC-R70 in CDCl3







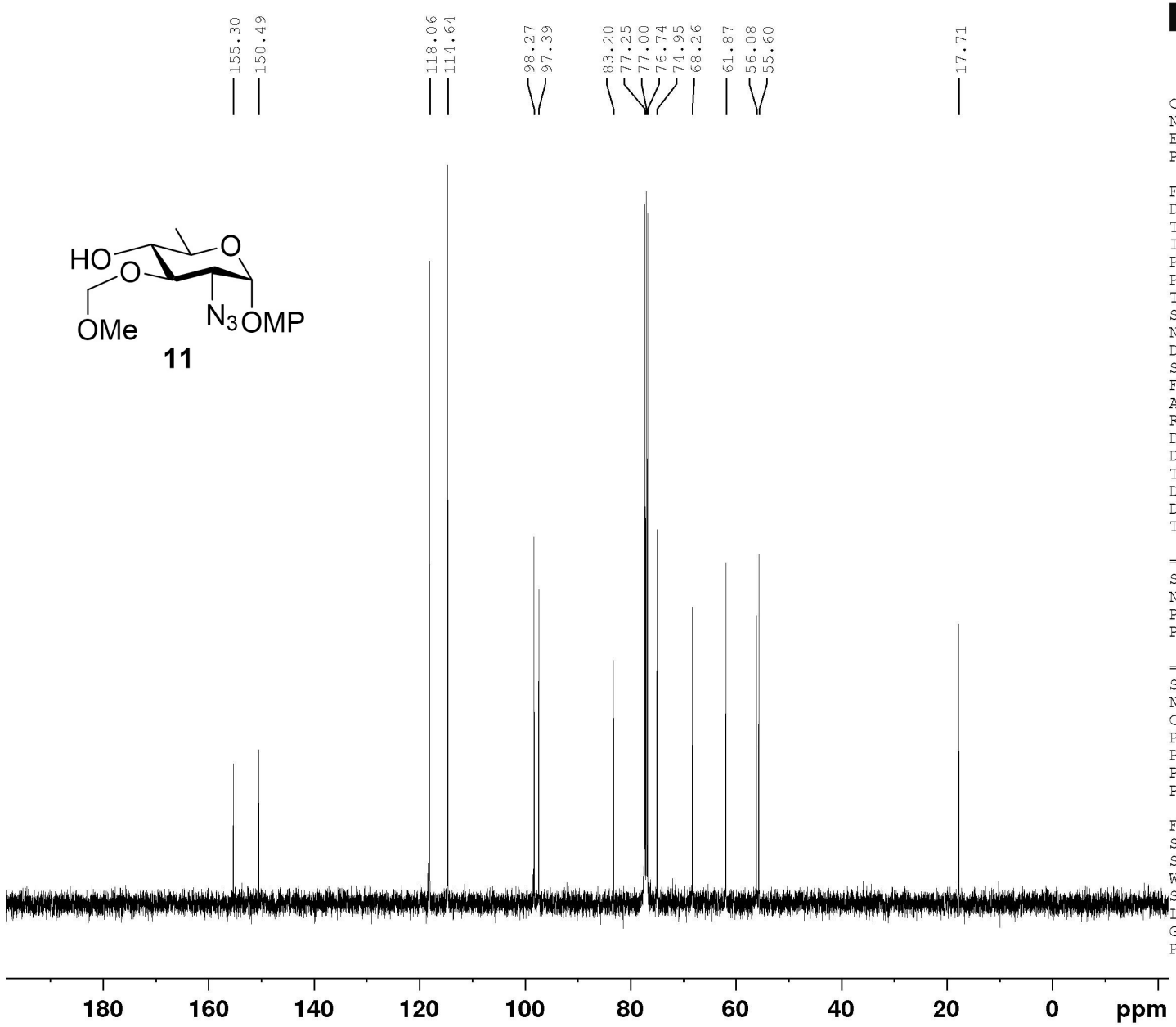
Current Data Parameters
NAME BM-AC-R70
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180720
Time 11.42
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.150240 Hz
AQ 3.3280001 sec
RG 90.5
DW 50.000 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3430898 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3400122 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R70 in CDCl3



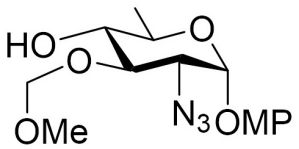
Current Data Parameters
NAME BM-AC-R70
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180720
Time 11.57
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 77
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

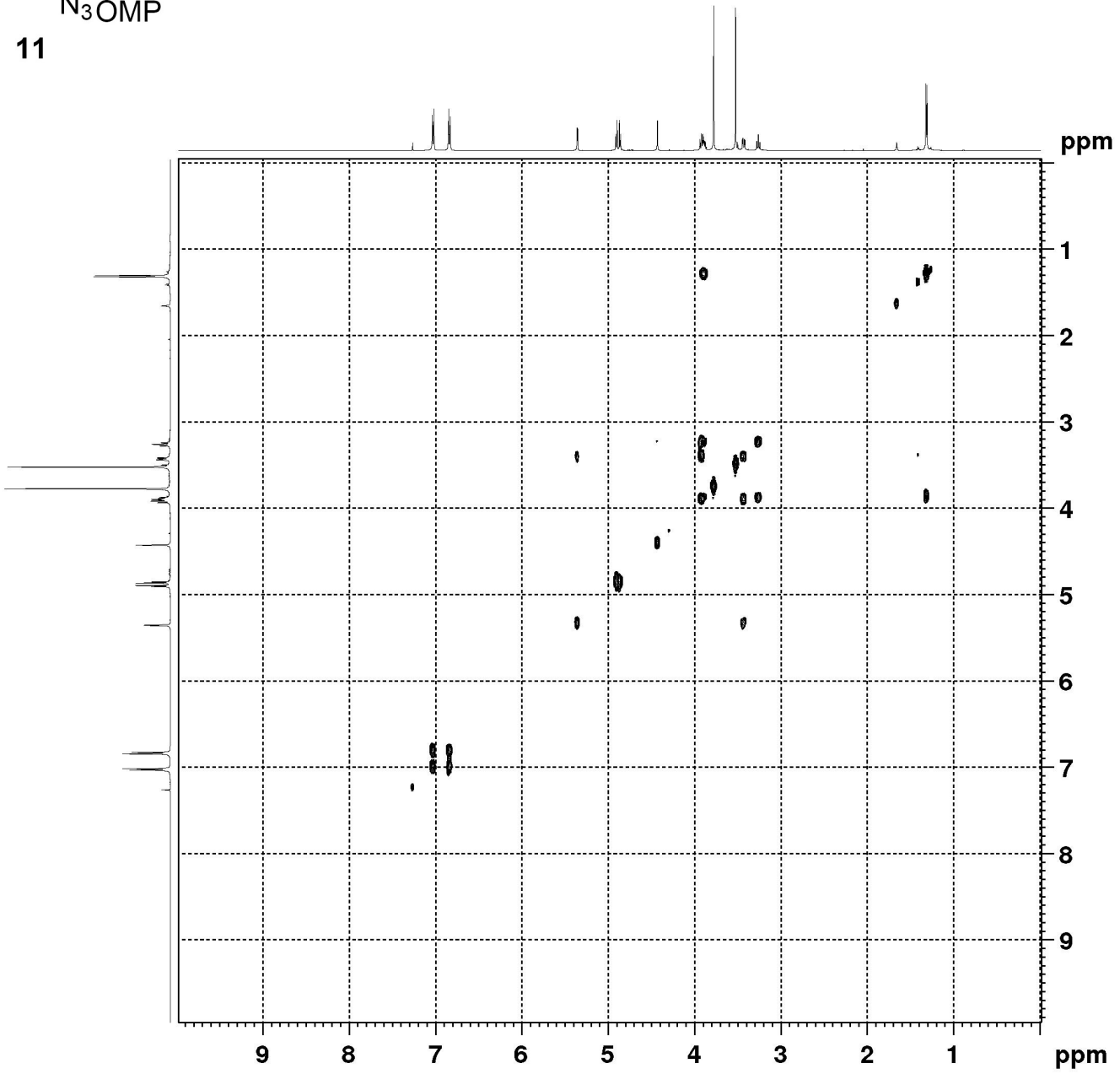
======== CHANNEL f1 ========
SFO1 125.8294646 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8105990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



11




```
Current Data Parameters
NAME            BM-AC-R70
EXPNO                  22
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180720
Time               11.45
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     1
DS                     8
SWH             5000.000 Hz
FIDRES          2.441406 Hz
AQ              0.2048000 sec
RG                  90.5
DW               100.000 usec
DE                  6.50 usec
TE                 299.1 K
D0              0.00000300 sec
D1              2.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00019980 sec

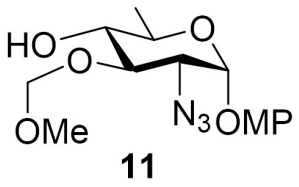
======== CHANNEL f1 ========
SFO1          500.3425017 MHz
NUC1                   1H
P0                  17.50 usec
P1                  17.50 usec
P17               2500.00 usec
PLW1          10.00000000 W
PLW10          3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1            500.3425 MHz
FIDRES          78.203201 Hz
SW                10.003 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF            500.3400107 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.00

F1 - Processing parameters
SI                   1024
MC2                    QF
SF            500.3400211 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```



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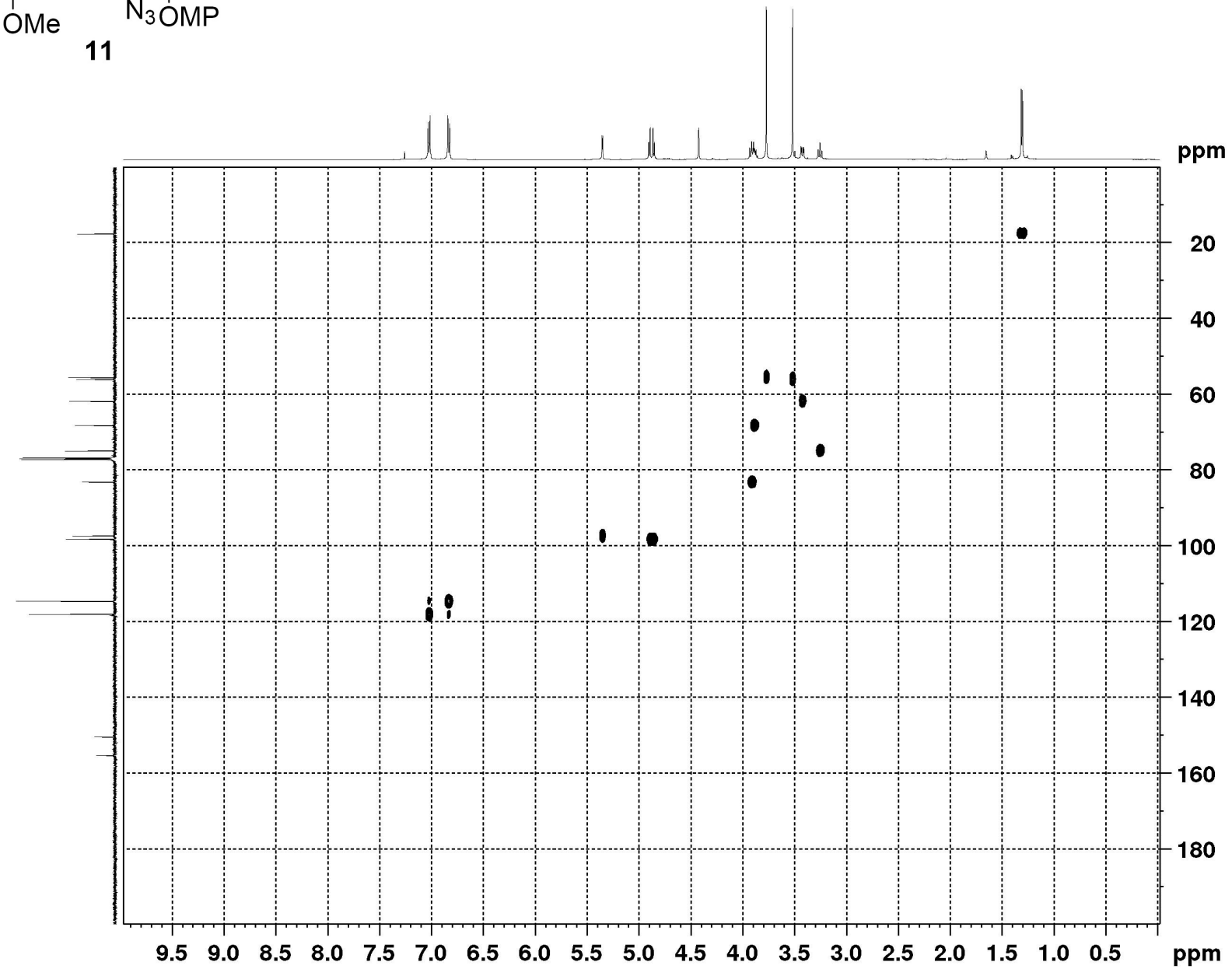



```
Current Data Parameters
NAME                  BM-AC-R70
EXPNO                        23
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20180720
Time                      11.59
INSTRUM   Bruker_default_av500
PROBHD    5 mm PABBO BB/
PULPROG       hsqcetgpsi2
TD                        1024
SOLVENT                 CDCl3
NS                            2
DS                           16
SWH                  5000.000 Hz
FIDRES               4.882813 Hz
AQ                   0.1024000 sec
RG                        45.2
DW                    100.000 usec
DE                      6.50 usec
TE                     299.5 K
CNST2              145.0000000
D0                   0.00000300 sec
D1                   1.50000000 sec
D4                   0.00172414 sec
D11                  0.03000000 sec
D16                  0.00020000 sec
D24                  0.00086207 sec
IN0                  0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               500.3425017 MHz
NUC1                         1H
P1                        17.50 usec
P2                        35.00 usec
P28                     1000.00 usec
PLW1              10.00000000 W

======== CHANNEL f2 ========
SFO2               125.8231741 MHz
NUC2                        13C
CPDPRG[2                  garp
P3                        11.50 usec
P4                        23.00 usec
PCPD2                     70.00 usec
PLW2              66.00000000 W
PLW12              1.78129995 W

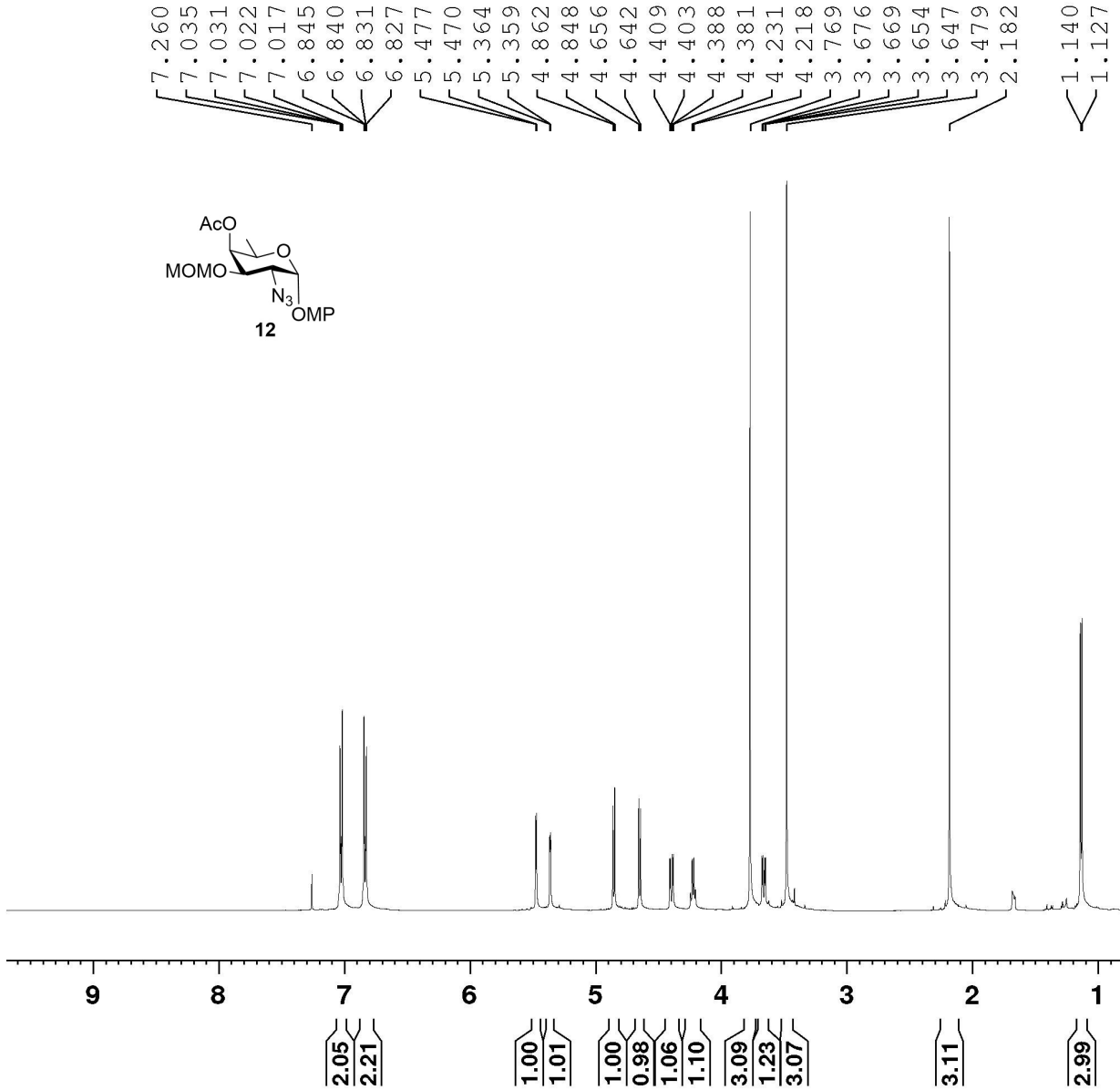
====== GRADIENT CHANNEL =====
GPNAM[1]           SMSQ10.100
GPNAM[2]           SMSQ10.100
GPNAM[3]           SMSQ10.100
GPNAM[4]           SMSQ10.100
GPZ1                    80.00 %
GPZ2                    20.10 %
GPZ3                    11.00 %
GPZ4                    -5.00 %
P16                   1000.00 usec
P19                    600.00 usec

F1 - Acquisition parameters
TD                           102
SFO1                 125.8232 MHz
FIDRES            492.659363 Hz
SW                   199.690 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                          1024
SF                 500.3400127 MHz
WDW                       QSINE
SSB                           2
LB          0 Hz
GB          0
PC                         1.00

F1 - Processing parameters
SI                          1024
MC2              echo-antiecho
SF                 125.8105931 MHz
WDW                       QSINE
SSB                           2
LB          0 Hz
GB          0
```

GROUP BM
BM-AC-R71 in CDCl3



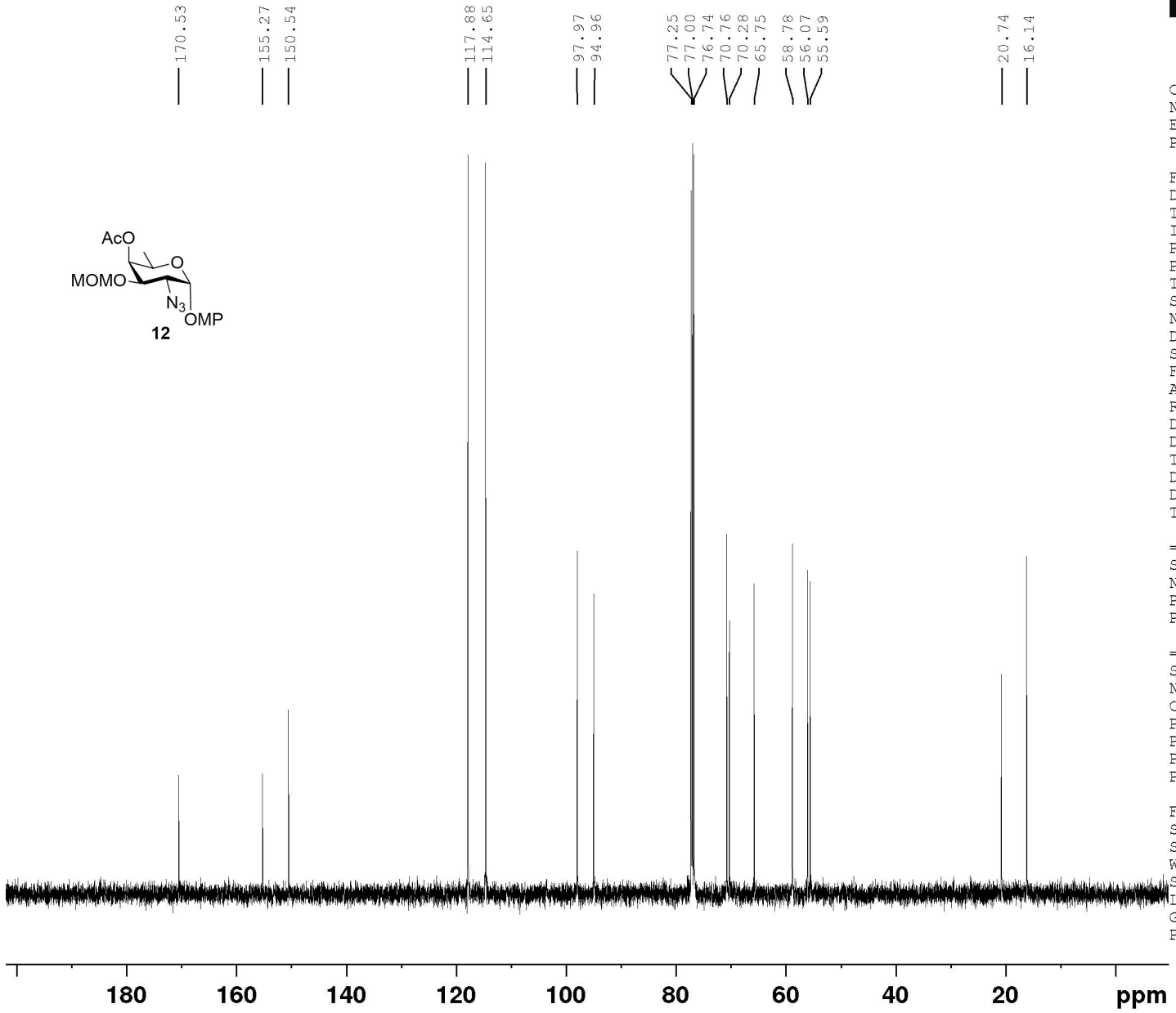
Current Data Parameters
NAME BM-AC-R71
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180725
Time 12.55
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.150240 Hz
AQ 3.3280001 sec
RG 71.8
DW 50.000 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3430898 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3400119 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R71 in CDCl3



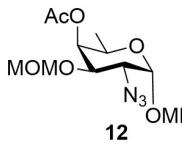
Current Data Parameters
NAME BM-AC-R71
EXPNO 91
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180725
Time 12.59
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 89
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8294646 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8106006 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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```
Current Data Parameters
NAME                  BM-AC-R71
EXPNO                        92
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20180725
Time                     13.04
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                        2048
SOLVENT                  CDCl3
NS                            1
DS                            8
SWH                5000.000 Hz
FIDRES             2.441406 Hz
AQ                 0.2048000 sec
RG                        71.8
DW                  100.000 usec
DE                    6.50 usec
TE                    298.1 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00019980 sec

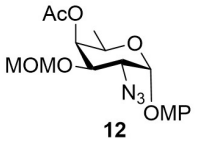
======== CHANNEL f1 ========
SFO1              500.3425017 MHz
NUC1                       1H
P0                      17.50 usec
P1                      17.50 usec
P17                   2500.00 usec
PLW1               10.00000000 W
PLW10               3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPZ1                   10.00 %
P16                  1000.00 usec

F1 - Acquisition parameters
TD                         128
SFO1                500.3425 MHz
FIDRES             78.203201 Hz
SW                    10.003 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        1024
SF                500.3400119 MHz
WDW                     QSINE
SSB          0
LB           0 Hz
GB           0
PC                        1.00

F1 - Processing parameters
SI                        1024
MC2                         QF
SF                500.3400155 MHz
WDW                     QSINE
SSB          0
LB           0 Hz
GB           0
```



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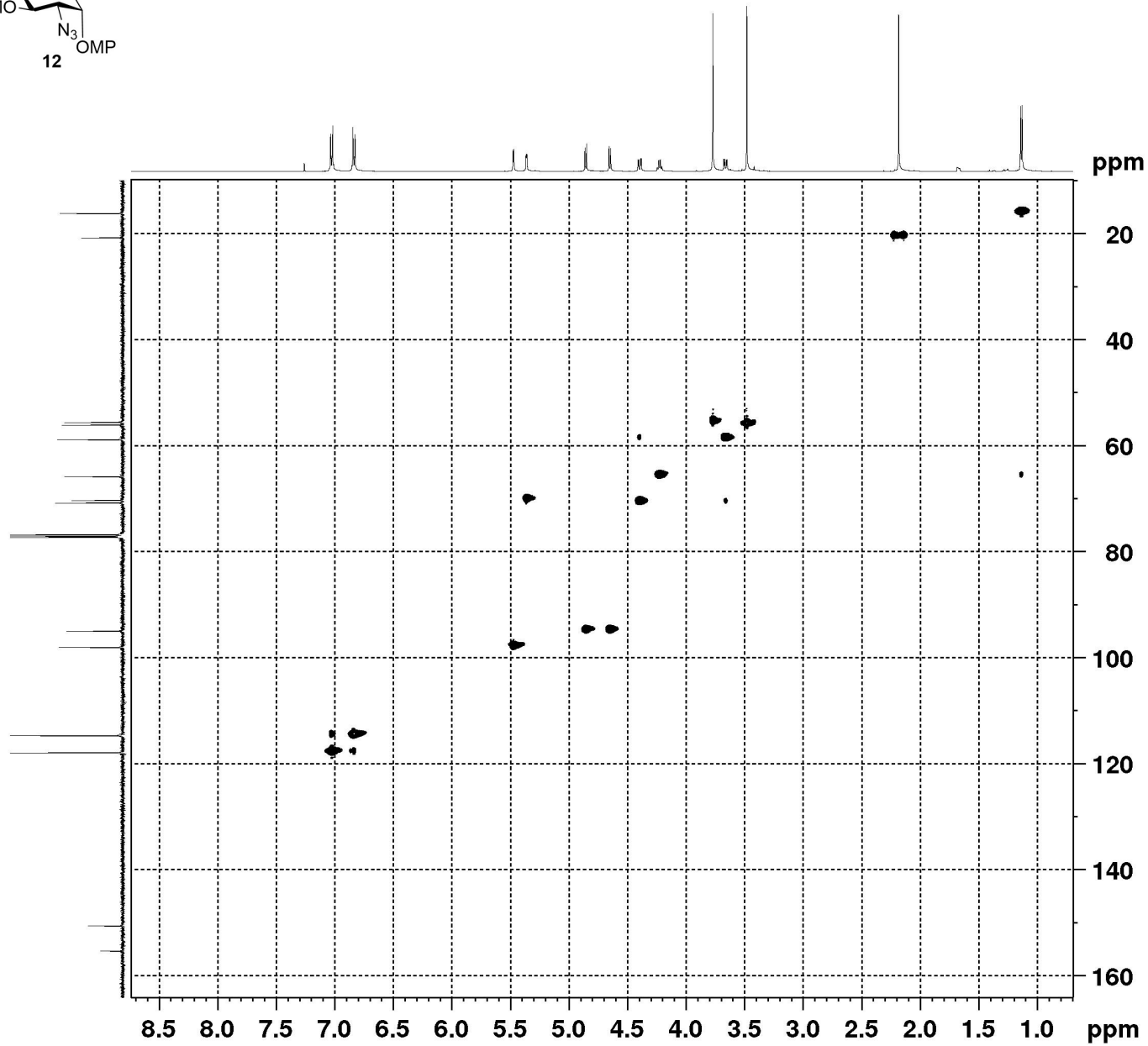


BRUKER

```
Current Data Parameters
NAME                  BM-AC-R71
EXPNO                        93
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20180725
Time                      13.13
INSTRUM  Bruker_default_av500
PROBHD    5 mm PABBO BB/
PULPROG          hsqcetgpsi2
TD                        1024
SOLVENT                 CDCl3
NS                           2
DS                          16
SWH                5000.000 Hz
FIDRES              4.882813 Hz
AQ                 0.1024000 sec
RG                        71.8
DW                   100.000 usec
DE                     6.50 usec
TE                     298.0 K
CNST2              145.0000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D4                  0.00172414 sec
D11                 0.03000000 sec
D16                 0.00020000 sec
D24                 0.00086207 sec
IN0                 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               500.3425017 MHz
NUC1                       1H
P1                      17.50 usec
P2                      35.00 usec
P28                   1000.00 usec
PLW1              10.00000000 W

======== CHANNEL f2 ========
SFO2               125.8231741 MHz
NUC2                       13C
CPDPRG[2                 garp
P3                      11.50 usec
P4                      23.00 usec
PCPD2                   70.00 usec
PLW2              66.00000000 W
PLW12              1.78129995 W

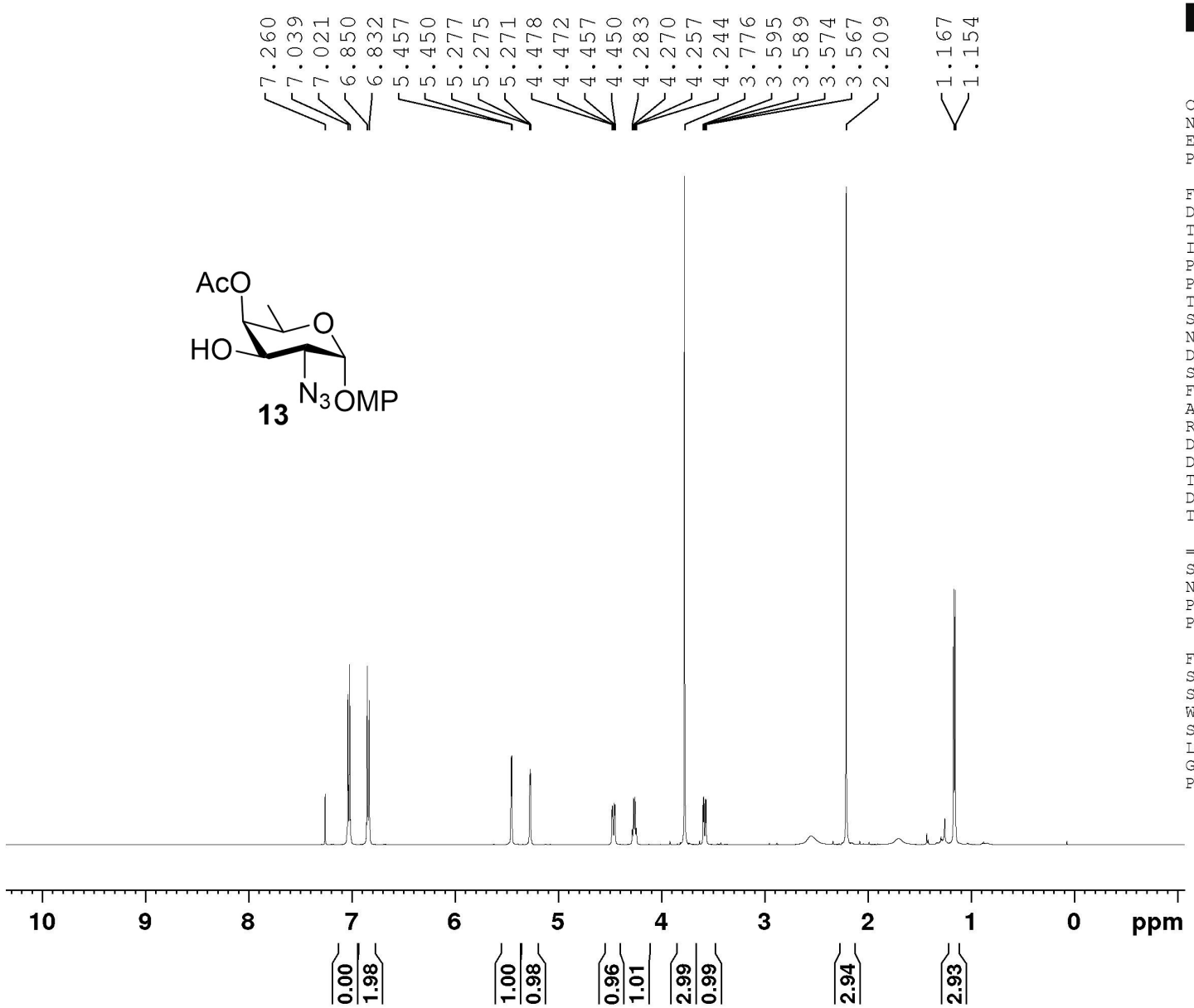
====== GRADIENT CHANNEL =====
GPNAM[1]          SMSQ10.100
GPNAM[2]          SMSQ10.100
GPNAM[3]          SMSQ10.100
GPNAM[4]          SMSQ10.100
GPZ1                    80.00 %
GPZ2                    20.10 %
GPZ3                    11.00 %
GPZ4                    -5.00 %
P16                   1000.00 usec
P19                    600.00 usec

F1 - Acquisition parameters
TD                         256
SFO1                125.8232 MHz
FIDRES             196.293976 Hz
SW                     199.690 ppm
FnMODE         Echo-Antiecho

F2 - Processing parameters
SI                        1024
SF                 500.3400111 MHz
WDW                       QSINE
SSB                          2
LB              0 Hz
GB              0
PC                        1.00

F1 - Processing parameters
SI                        1024
MC2             echo-antiecho
SF                 125.8106252 MHz
WDW                       QSINE
SSB                          2
LB              0 Hz
GB              0
```

GROUP BM
BM-AC-R78 in CDCl3



Current Data Parameters
NAME BM-AC-R78
EXPNO 10
PROCNO 1

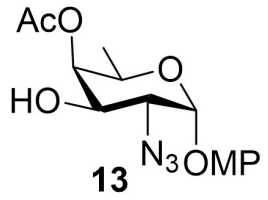
F2 - Acquisition Parameters
Date_ 20181002
Time 11.22
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.150240 Hz
AQ 3.3280001 sec
RG 144
DW 50.000 usec
DE 6.50 usec
TE 2135.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3430898 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3400122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R78 in CDCl3

171.54
155.36
150.67
117.98
114.71
98.04
77.25
76.99
76.74
73.09
67.30
65.68
60.02
55.64
20.76
16.13



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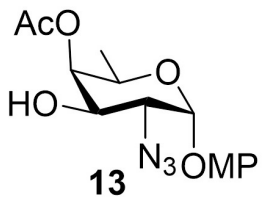
Current Data Parameters
NAME BM-AC-R78
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181002
Time 11.25
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 70
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 2131.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8294646 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8105979 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.10



13


```
Current Data Parameters
NAME            BM-AC-R78
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20181002
Time                11.28
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      1
DS                      8
SWH              5000.000 Hz
FIDRES           2.441406 Hz
AQ              0.2048000 sec
RG                    144
DW                100.000 usec
DE                  6.50 usec
TE                2145.8 K
D0              0.00000300 sec
D1              2.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00019980 sec

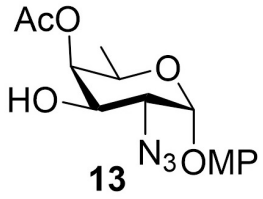
======== CHANNEL f1 ========
SFO1          500.3425017 MHz
NUC1                   1H
P0                  17.50 usec
P1                  17.50 usec
P17               2500.00 usec
PLW1         10.00000000 W
PLW10         3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     91
SFO1             500.3425 MHz
FIDRES         110.000107 Hz
SW                 10.003 ppm
FnMODE                 QF

F2 - Processing parameters
SI                   1024
SF            500.3400139 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                   1.00

F1 - Processing parameters
SI                   1024
MC2                    QF
SF            500.3400134 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```



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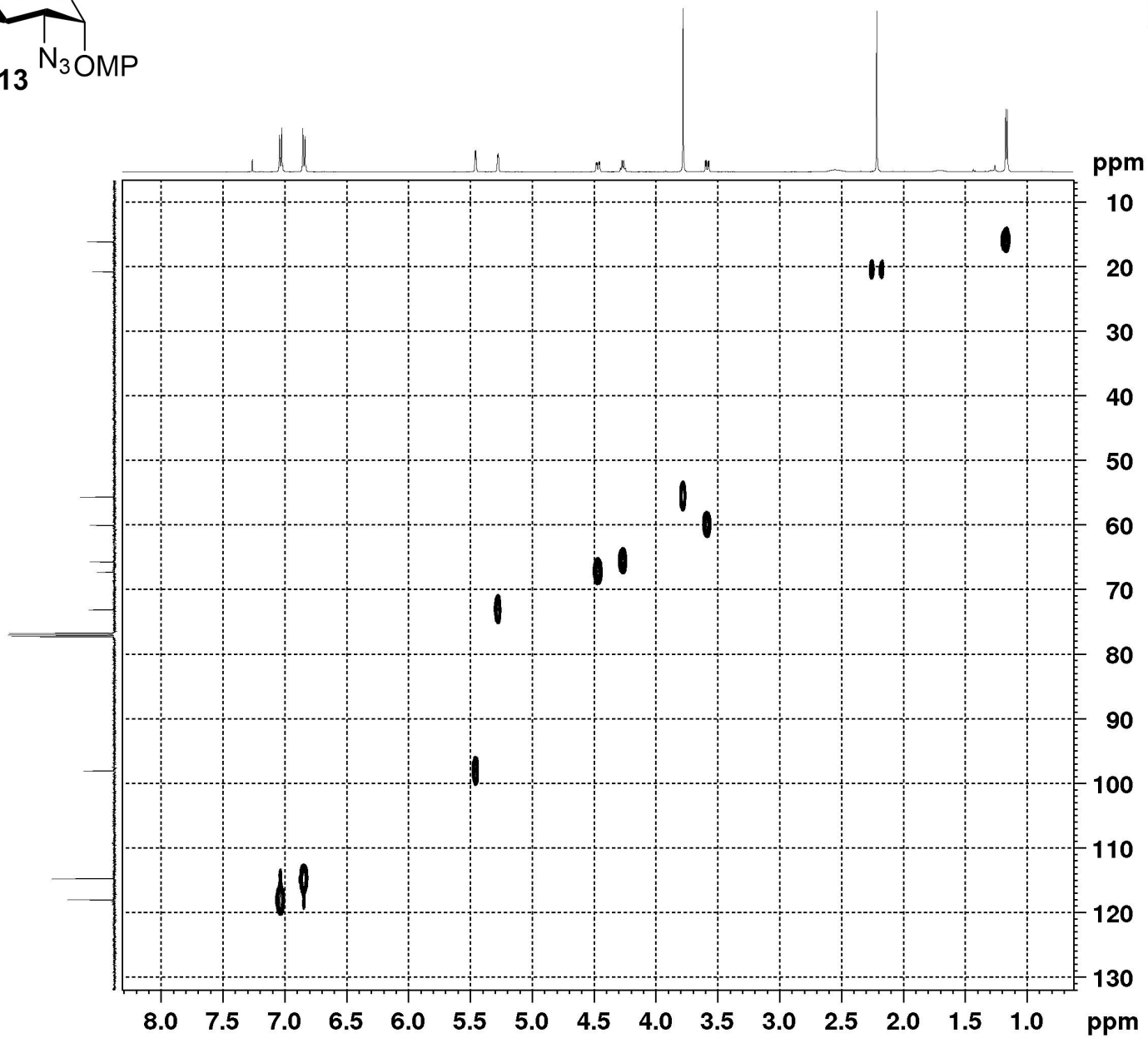



```
Current Data Parameters
NAME                  BM-AC-R78
EXPNO                        13
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20181002
Time                      11.33
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG          hsqcetgpsi2
TD                        1024
SOLVENT                 CDCl3
NS                            2
DS                           16
SWH                5000.000 Hz
FIDRES             4.882813 Hz
AQ                 0.1024000 sec
RG                          144
DW                   100.000 usec
DE                     6.50 usec
TE                    2134.8 K
CNST2              145.0000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D4                  0.00172414 sec
D11                 0.03000000 sec
D16                 0.00020000 sec
D24                 0.00086207 sec
IN0                 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               500.3425017 MHz
NUC1                       1H
P1                       17.50 usec
P2                       35.00 usec
P28                    1000.00 usec
PLW1               10.00000000 W

======== CHANNEL f2 ========
SFO2               125.8231741 MHz
NUC2                       13C
CPDPRG[2                  garp
P3                       11.50 usec
P4                       23.00 usec
PCPD2                    70.00 usec
PLW2               66.00000000 W
PLW12               1.78129995 W

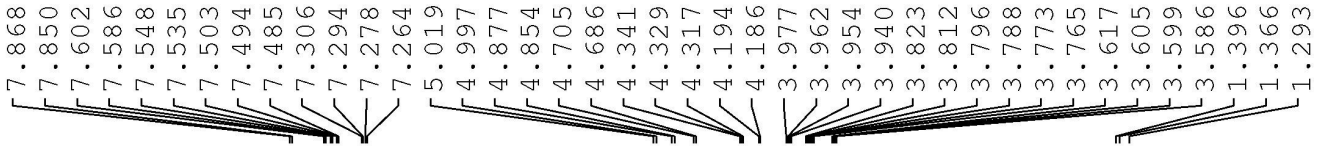
====== GRADIENT CHANNEL =====
GPNAM[1]           SMSQ10.100
GPNAM[2]           SMSQ10.100
GPNAM[3]           SMSQ10.100
GPNAM[4]           SMSQ10.100
GPZ1                    80.00 %
GPZ2                    20.10 %
GPZ3                    11.00 %
GPZ4                    -5.00 %
P16                   1000.00 usec
P19                    600.00 usec

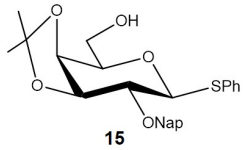
F1 - Acquisition parameters
TD                           76
SFO1                125.8232 MHz
FIDRES             661.200745 Hz
SW                     199.690 ppm
FnMODE          Echo-Antiecho

F2 - Processing parameters
SI                         1024
SF                 500.3400123 MHz
WDW                       QSINE
SSB                           2
LB              0 Hz
GB              0
PC                         1.00

F1 - Processing parameters
SI                         1024
MC2             echo-antiecho
SF                 125.8105942 MHz
WDW                       QSINE
SSB                           2
LB              0 Hz
GB              0
```

GROUP BM
BM-AC-R57SI in CDCl3





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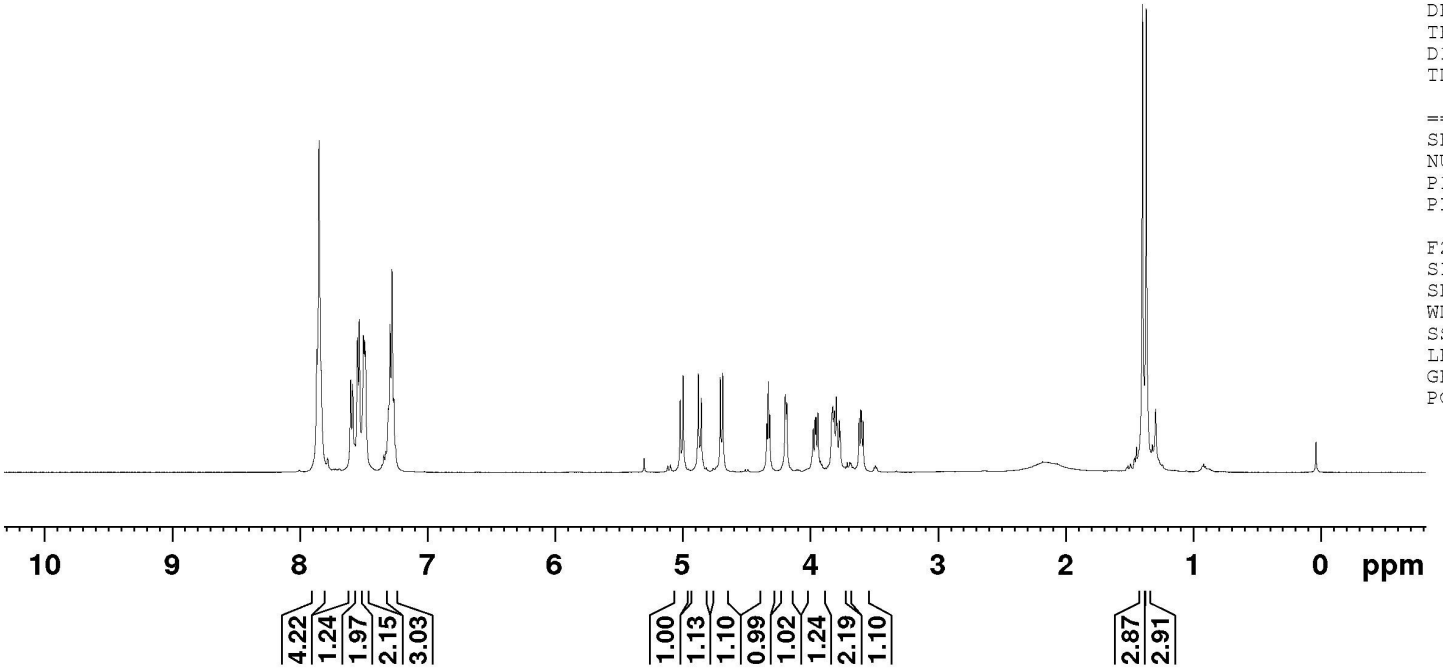


Current Data Parameters
NAME BM-AC-R57SI
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191218
Time 13.11
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 4
DS 2
SWH 12500.000 Hz
FIDRES 0.187800 Hz
AQ 2.6624000 sec
RG 64
DW 40.000 usec
DE 6.50 usec
TE 277.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3625018 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

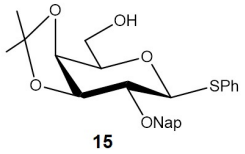
F2 - Processing parameters
SI 131072
SF 500.3600047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R57SI in CDCl3

135.19
133.38
133.20
133.07
131.94
131.42
129.04
128.87
128.05
127.90
127.65
127.50
127.07
126.27
125.99
125.86
110.32

85.91
79.76
78.13
77.28
77.03
76.77
73.88
73.42
62.55

27.68
26.30



15

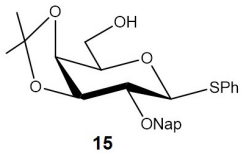
Current Data Parameters
NAME BM-AC-R57SI
EXPNO 71
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191218
Time 13.15
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 53
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 203
DW 13.200 usec
DE 6.50 usec
TE 277.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

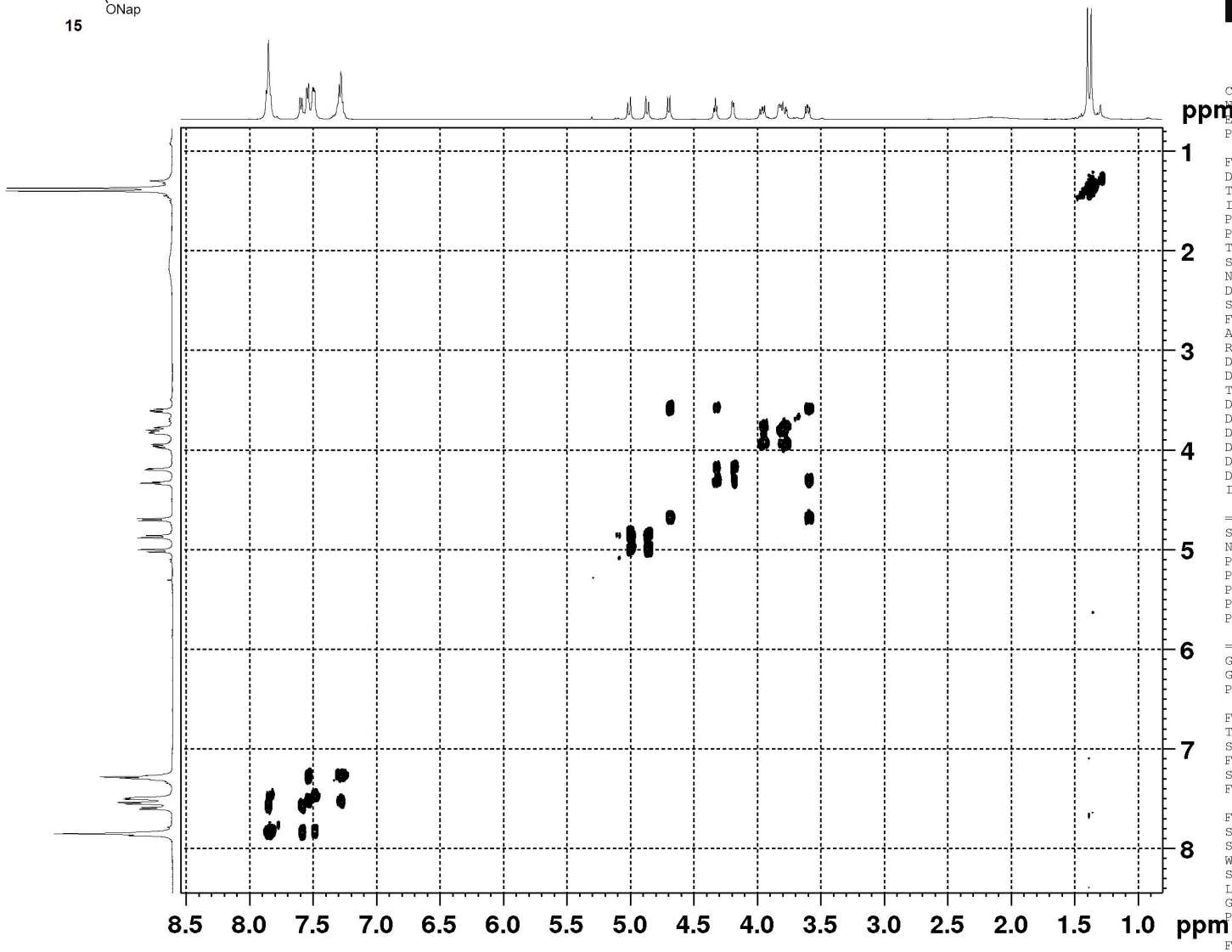
======== CHANNEL f1 ========
SFO1 125.8282036 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8156286 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.35



15




```
Current Data Parameters
NAME          BM-AC-R57SI
EXPNO                  72
PROCNO                  1

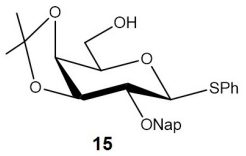
F2 - Acquisition Parameters
Date_            20191218
Time                13.18
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      1
DS                      8
SWH              5000.000 Hz
FIDRES           2.441406 Hz
AQ               0.2048000 sec
RG                   80.6
DW                100.000 usec
DE                  6.50 usec
TE                 277.5 K
D0               0.00000300 sec
D1               2.00000000 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00019980 sec

======== CHANNEL f1 ========
SFO1          500.3625017 MHz
NUC1                  1H
P0                 17.50 usec
P1                 17.50 usec
P17              2500.00 usec
PLW1          10.00000000 W
PLW10          3.40280008 W

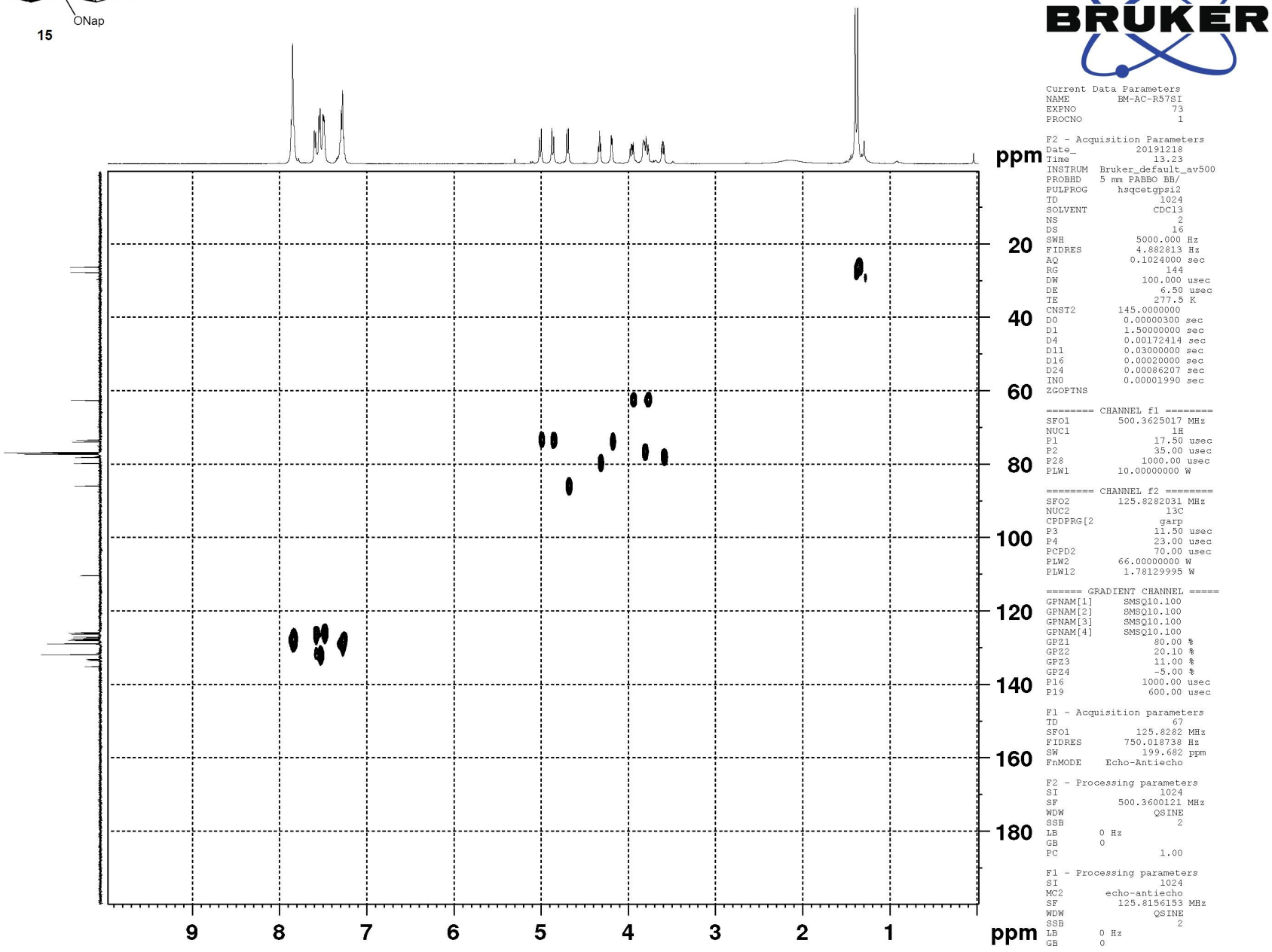
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1            500.3625 MHz
FIDRES          78.203201 Hz
SW                10.003 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF            500.3600123 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.00
F1 - Processing parameters
SI                   1024
MC2                    QF
SF            500.3600123 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```



15




```
Current Data Parameters
NAME         BM-AC-R57SI
EXPNO                 73
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191218
Time              13.23
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                  1024
SOLVENT             CDCl3
NS                     2
DS                    16
SWH            5000.000 Hz
FIDRES         4.882813 Hz
AQ           0.1024000 sec
RG                   144
DW             100.000 usec
DE               6.50 usec
TE              277.5 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1         500.3625017 MHz
NUC1                   1H
P1                 17.50 usec
P2                 35.00 usec
P28              1000.00 usec
PLW1        10.00000000 W

======== CHANNEL f2 ========
SFO2         125.8282031 MHz
NUC2                  13C
CPDPRG[2              garp
P3                 11.50 usec
P4                 23.00 usec
PCPD2              70.00 usec
PLW2        66.00000000 W
PLW12        1.78129995 W

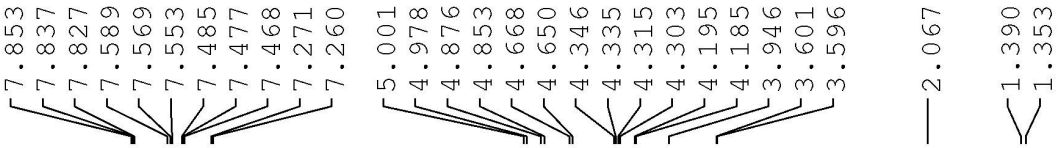
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

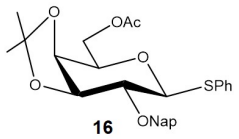
F1 - Acquisition parameters
TD                    67
SFO1           125.8282 MHz
FIDRES         750.018738 Hz
SW                199.682 ppm
FnMODE     Echo-Antiecho

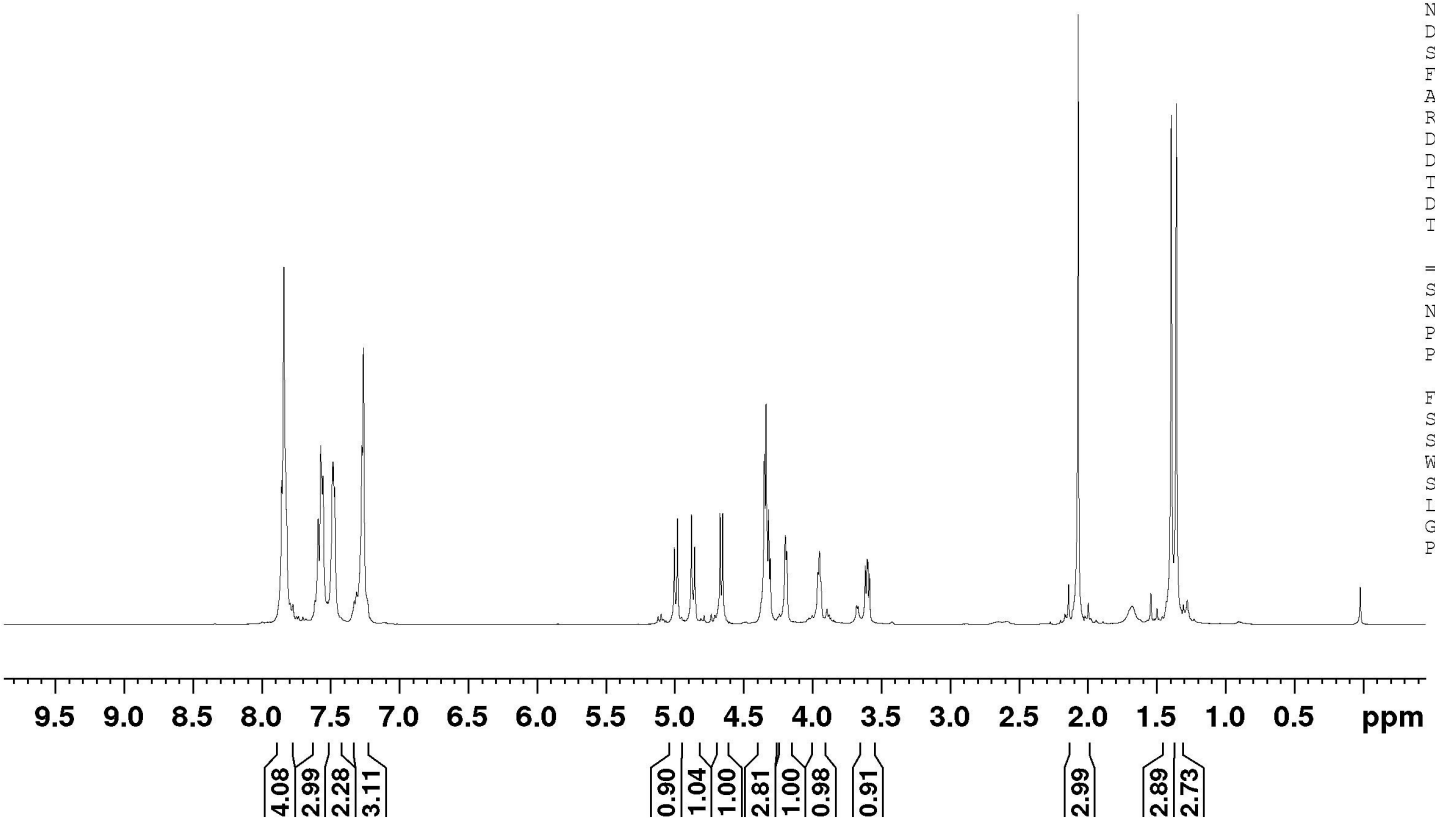
F2 - Processing parameters
SI                  1024
SF           500.3600121 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.00

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           125.8156153 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

GROUP BM
BM-AC-R57 S-II in CDCl3








```
Current Data Parameters
NAME       BM-AC-R57 SII
EXPNO               250
PROCNO                1

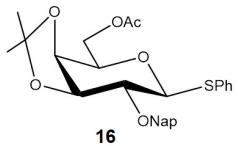
F2 - Acquisition Parameters
Date_          20190926
Time              18.24
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                66560
SOLVENT           CDCl3
NS                    4
DS                    2
SWH           10000.000 Hz
FIDRES            0.150240 Hz
AQ            3.3280001 sec
RG                 90.5
DW                50.000 usec
DE                 6.50 usec
TE                458.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.3625018 MHz
NUC1                1H
P1                17.50 usec
PLW1        10.00000000 W

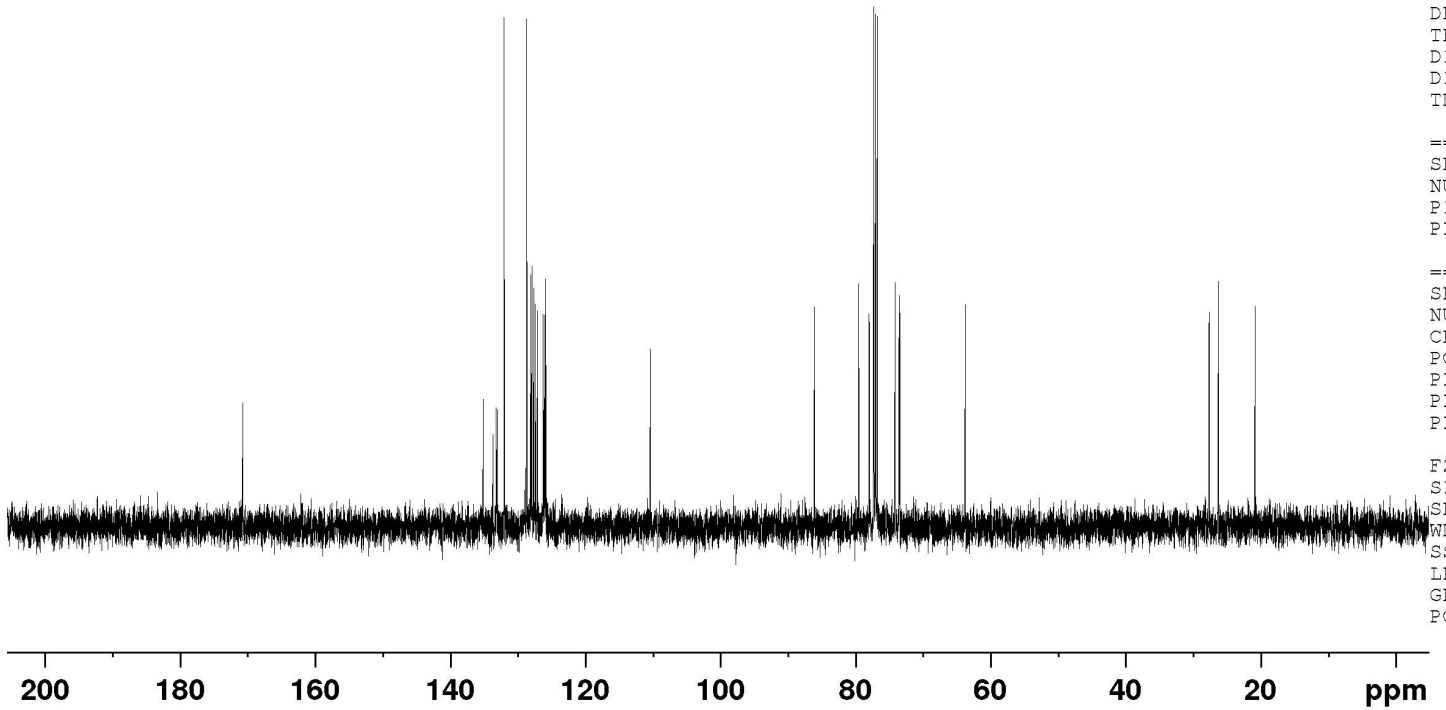
F2 - Processing parameters
SI                131072
SF           500.3600121 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

GROUP BM
BM-AC-R57 S-II in CDCl3

170.75
135.14
133.68
133.20
133.08
132.05
128.92
128.70
128.07
127.91
127.65
127.43
127.11
126.27
126.00
125.87
110.39
86.08
79.50
77.97
77.28
77.03
76.77
74.12
73.53
73.44
63.74
27.62
26.26
20.81



16



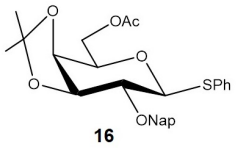
Current Data Parameters
NAME BM-AC-R57 SII
EXPNO 253
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190926
Time 18.40
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 28
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 90.5
DW 13.200 usec
DE 6.50 usec
TE -1163.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

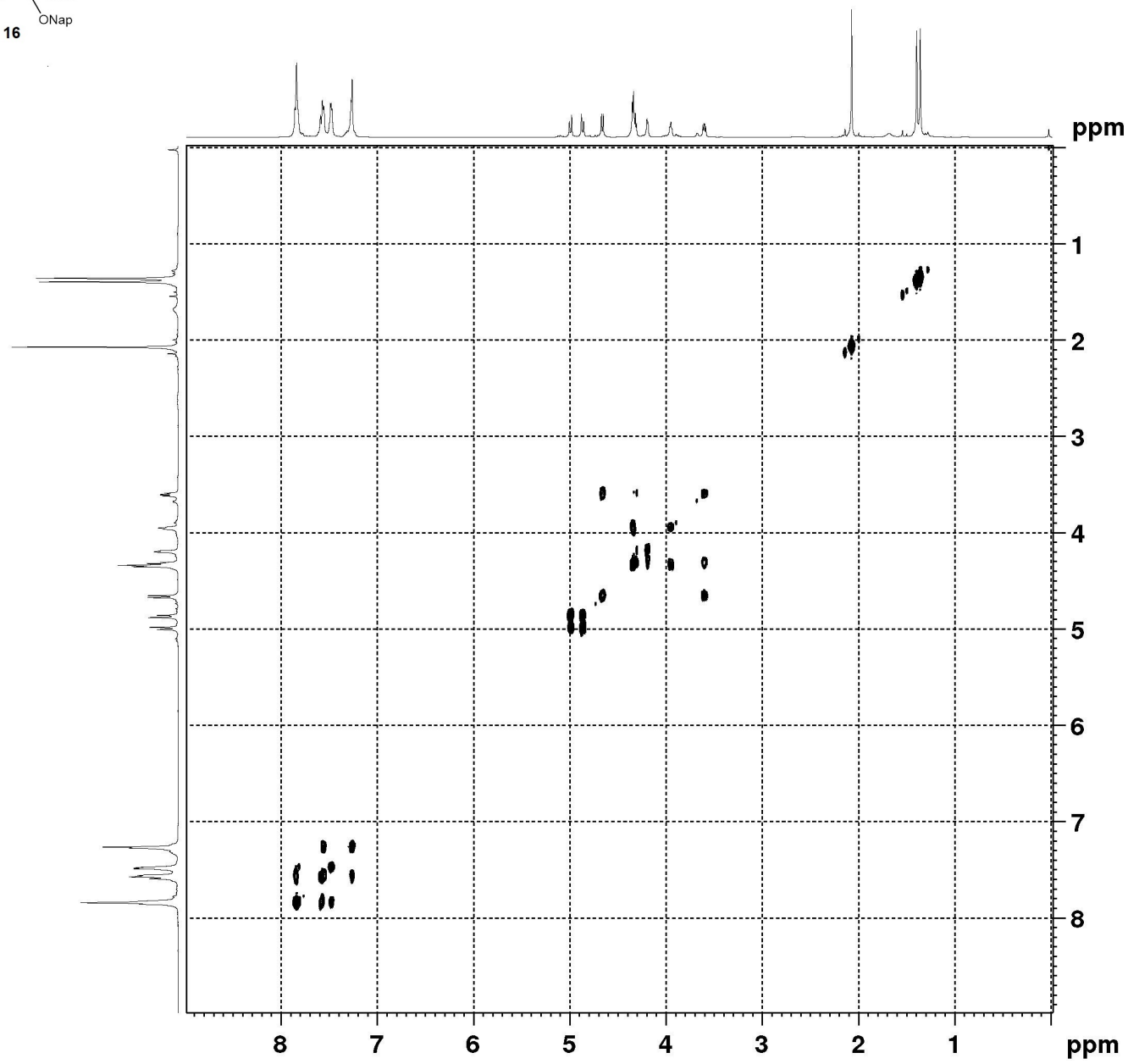
======== CHANNEL f1 ========
SFO1 125.8282036 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8156282 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



16




```
Current Data Parameters
NAME       BM-AC-R57 SII
EXPNO              251
PROCNO               1

F2 - Acquisition Parameters
Date_         20190926
Time             18.26
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT           CDCl3
NS                   1
DS                   8
SWH          5000.000 Hz
FIDRES       2.441406 Hz
AQ           0.2048000 sec
RG                90.5
DW           100.000 usec
DE              6.50 usec
TE             660.7 K
D0           0.00000300 sec
D1           2.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00019980 sec

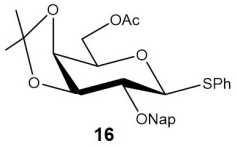
======== CHANNEL f1 ========
SFO1       500.3625017 MHz
NUC1               1H
P0              17.50 usec
P1              17.50 usec
P17           2500.00 usec
PLW1       10.00000000 W
PLW10       3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1            10.00 %
P16           1000.00 usec

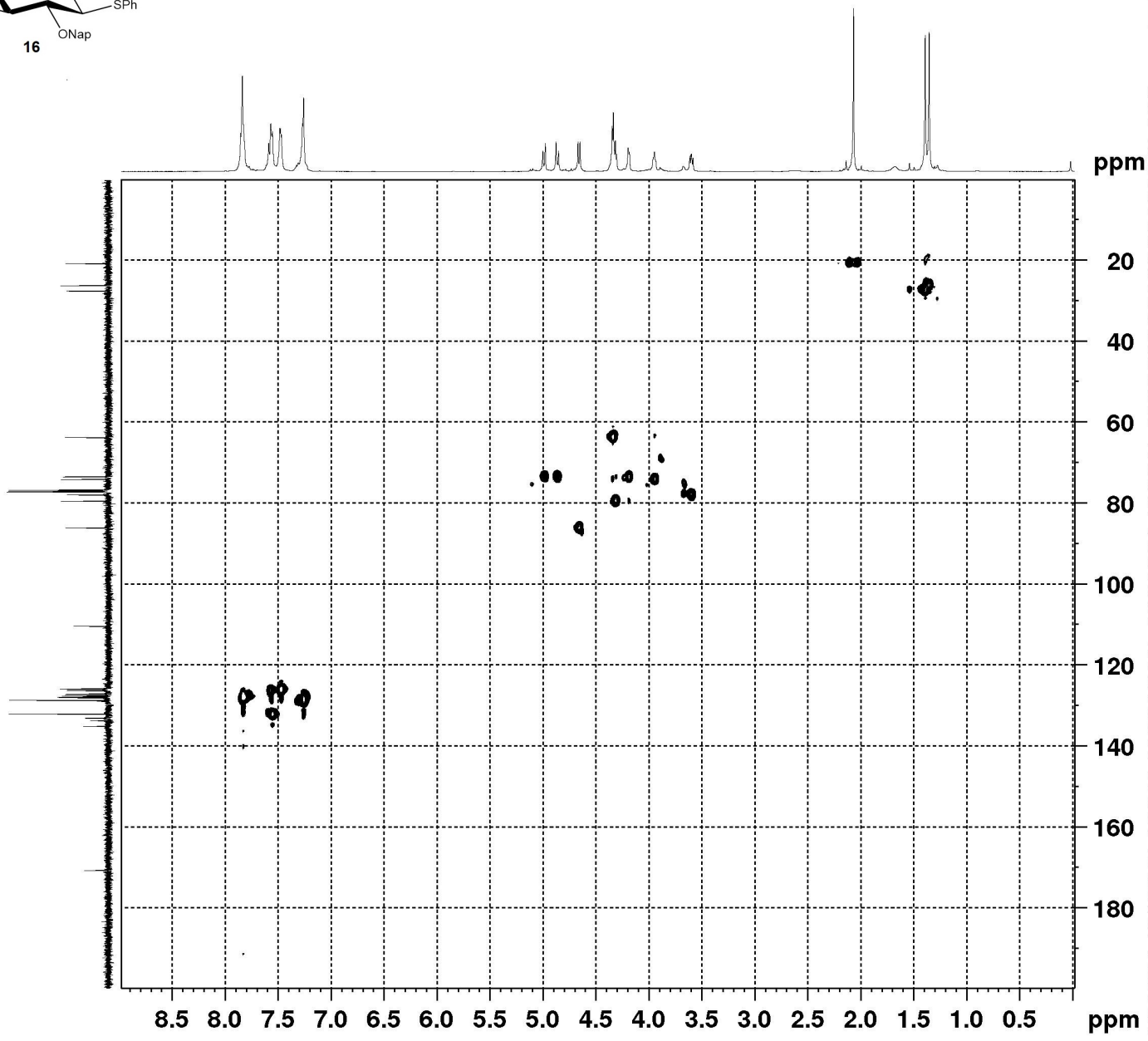
F1 - Acquisition parameters
TD                 128
SFO1          500.3625 MHz
FIDRES       78.203201 Hz
SW             10.003 ppm
FnMODE              QF

F2 - Processing parameters
SI                1024
SF          500.3600123 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
PC                1.00

F1 - Processing parameters
SI                1024
MC2                 QF
SF          500.3600123 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
```



16




```
Current Data Parameters
NAME       BM-AC-R57 SII
EXPNO               252
PROCNO                1

F2 - Acquisition Parameters
Date_          20190926
Time              18.32
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                 1024
SOLVENT            CDCl3
NS                    2
DS                   16
SWH           5000.000 Hz
FIDRES        4.882813 Hz
AQ            0.1024000 sec
RG                 71.8
DW             100.000 usec
DE               6.50 usec
TE              584.1 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1         500.3625017 MHz
NUC1                   1H
P1                 17.50 usec
P2                 35.00 usec
P28              1000.00 usec
PLW1        10.00000000 W

======== CHANNEL f2 ========
SFO2         125.8282031 MHz
NUC2                  13C
CPDPRG[2             garp
P3                 11.50 usec
P4                 23.00 usec
PCPD2              70.00 usec
PLW2        66.00000000 W
PLW12        1.78129995 W

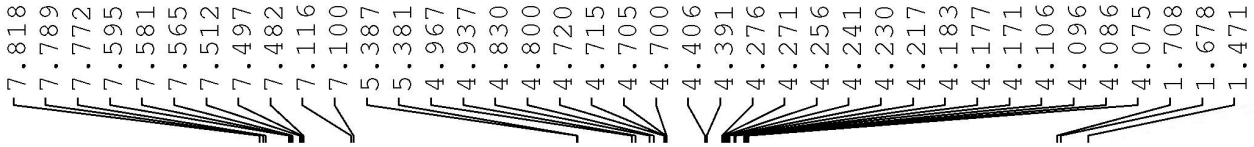
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

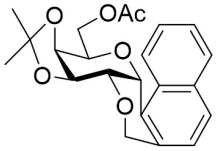
F1 - Acquisition parameters
TD                  131
SFO1          125.8282 MHz
FIDRES        383.597382 Hz
SW               199.682 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          500.3600121 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                  1.00

F1 - Processing parameters
SI                 1024
MC2        echo-antiecho
SF            125.8156153 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
```

GROUP BM
BM-AC-R81 in CDCl3





17

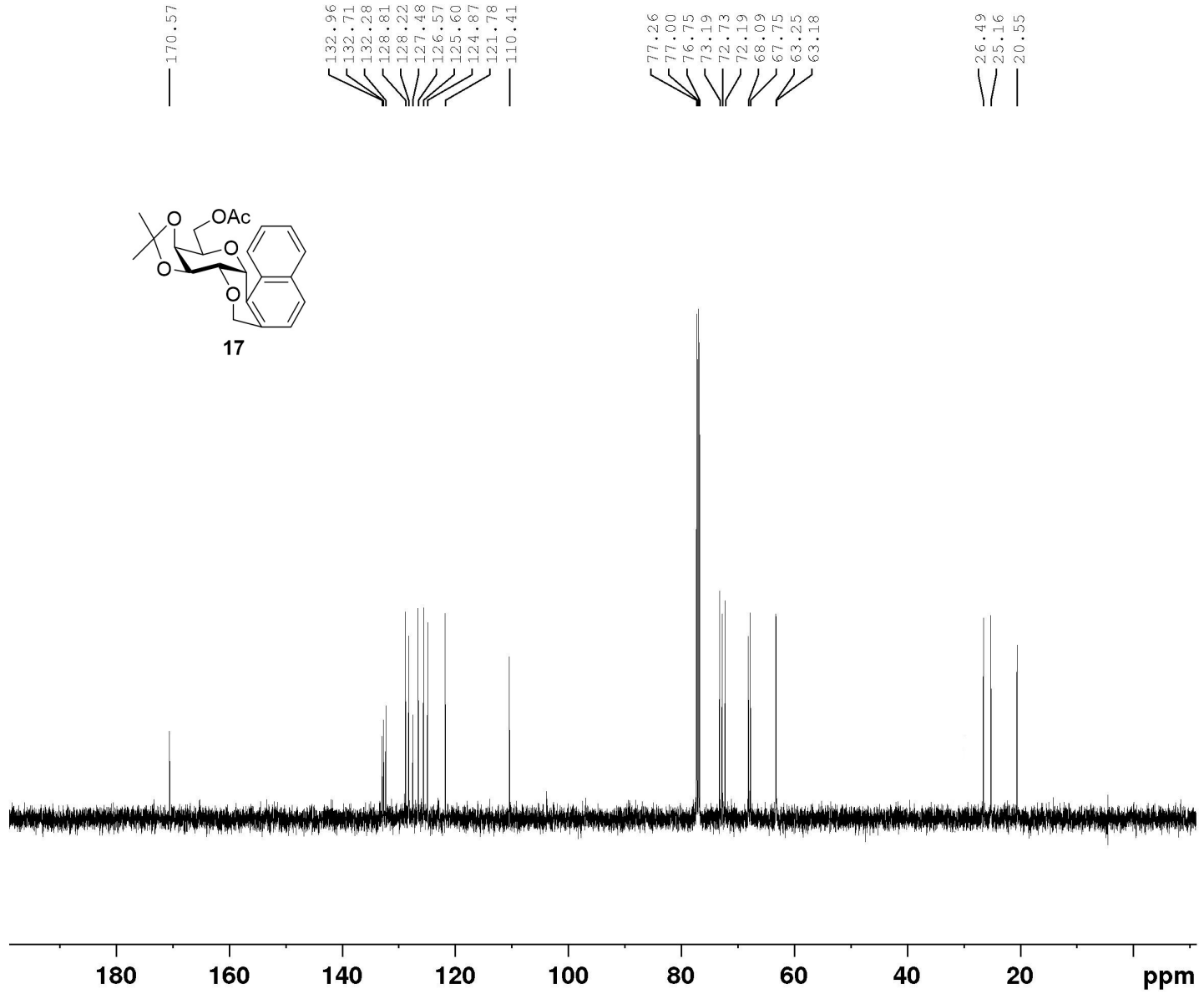
Current Data Parameters
NAME BM-AC-R81
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 17.59
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 4
DS 2
SWH 12500.000 Hz
FIDRES 0.187800 Hz
AQ 2.6624000 sec
RG 64
DW 40.000 usec
DE 6.50 usec
TE -1425.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3625018 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3600047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R81 in CDCl3



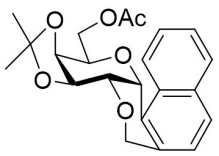

```
Current Data Parameters
NAME            BM-AC-R81
EXPNO                 331
PROCNO                  1

F2 - Acquisition Parameters
Date_            20191219
Time                18.03
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     28
DS                      4
SWH             37878.789 Hz
FIDRES           0.577984 Hz
AQ               0.8650752 sec
RG                    203
DW                 13.200 usec
DE                  6.50 usec
TE                -1486.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          125.8282036 MHz
NUC1                  13C
P1                 11.50 usec
PLW1          66.00000000 W

======== CHANNEL f2 ========
SFO2          500.3620014 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          10.00000000 W
PLW12          0.47852001 W
PLW13          0.24068999 W

F2 - Processing parameters
SI                  32768
SF            125.8156286 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.35
```



17


```
Current Data Parameters
NAME                  BM-AC-R81
EXPNO                       332
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20191219
Time                      18.06
INSTRUM  Bruker_default_av500
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                         2048
SOLVENT                  CDCl3
NS                            1
DS                            8
SWH                5000.000 Hz
FIDRES                2.441406 Hz
AQ                 0.2048000 sec
RG                         80.6
DW                  100.000 usec
DE                    6.50 usec
TE                   -1585.9 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00019980 sec

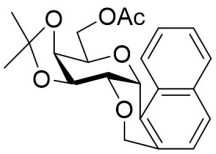
======== CHANNEL f1 ========
SFO1               500.3625017 MHz
NUC1                        1H
P0                       17.50 usec
P1                       17.50 usec
P17                    2500.00 usec
PLW1               10.00000000 W
PLW10               3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]           SMSQ10.100
GPZ1                      10.00 %
P16                    1000.00 usec

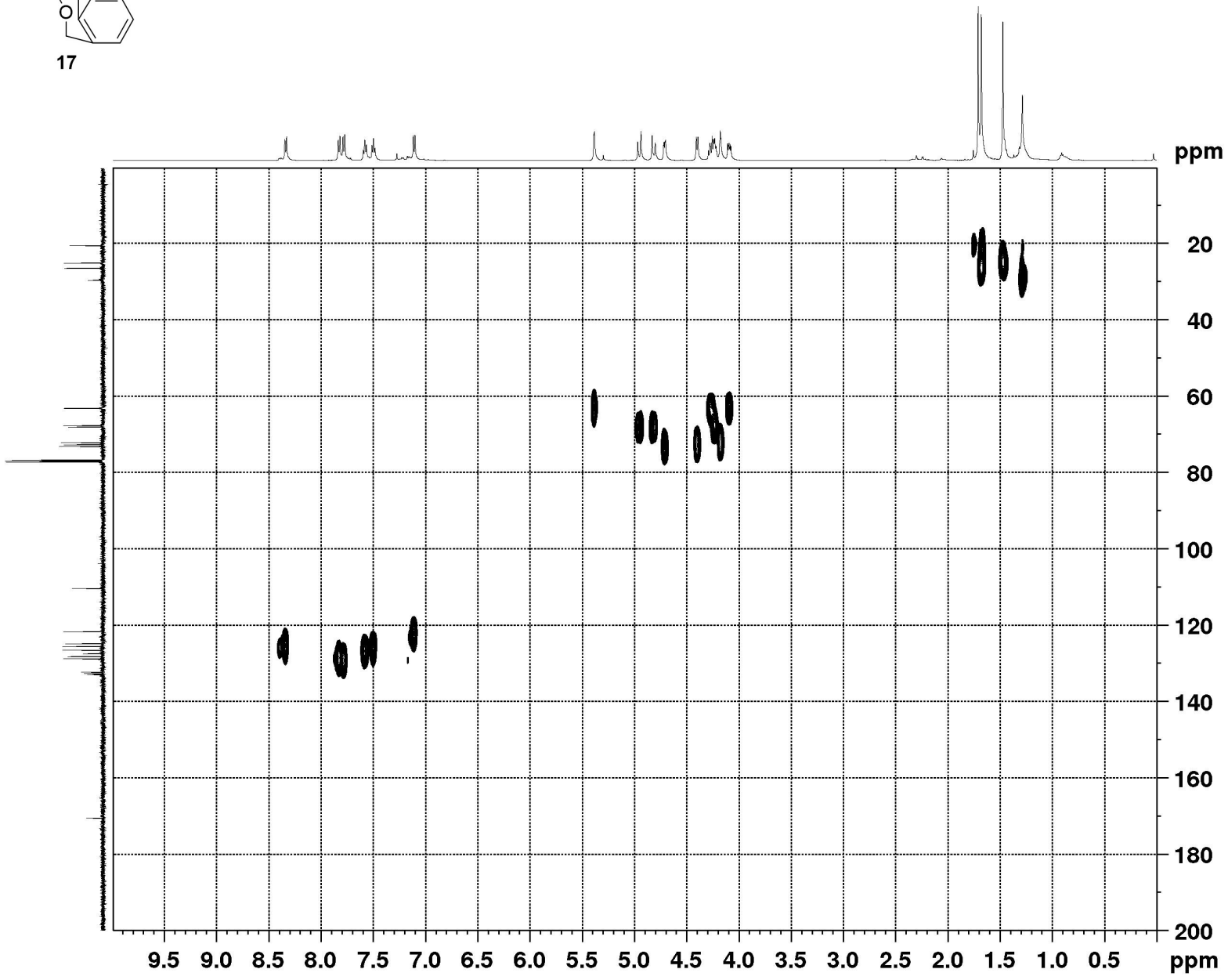
F1 - Acquisition parameters
TD                          128
SFO1                 500.3625 MHz
FIDRES                78.203201 Hz
SW                       10.003 ppm
FnMODE                       QF

F2 - Processing parameters
SI                         1024
SF                 500.3600028 MHz
WDW                      QSINE
SSB             0
LB              0 Hz
GB              0
PC                         1.00

F1 - Processing parameters
SI                         1024
MC2                          QF
SF                 500.3600034 MHz
WDW                      QSINE
SSB             0
LB              0 Hz
GB              0
```



17




```
Current Data Parameters
NAME                  BM-AC-R81
EXPNO                       333
PROCNO                        1

F2 - Acquisition Parameters
Date_              20191219
Time                    18.13
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                      1024
SOLVENT              CDCl3
NS                         2
DS                        16
SWH                5000.000 Hz
FIDRES                4.882813 Hz
AQ                 0.1024000 sec
RG                       144
DW                   100.000 usec
DE                     6.50 usec
TE                  -1707.6 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D16                0.00020000 sec
D24                0.00086207 sec
IN0                0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               500.3625017 MHz
NUC1                       1H
P1                       17.50 usec
P2                       35.00 usec
P28                    1000.00 usec
PLW1              10.00000000 W

======== CHANNEL f2 ========
SFO2               125.8282031 MHz
NUC2                       13C
CPDPRG[2                 garp
P3                       11.50 usec
P4                       23.00 usec
PCPD2                    70.00 usec
PLW2              66.00000000 W
PLW12              1.78129995 W

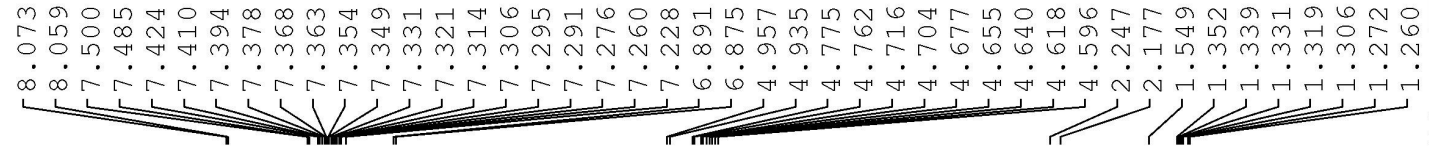
====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPNAM[3]       SMSQ10.100
GPNAM[4]       SMSQ10.100
GPZ1                    80.00 %
GPZ2                    20.10 %
GPZ3                    11.00 %
GPZ4                    -5.00 %
P16                   1000.00 usec
P19                    600.00 usec

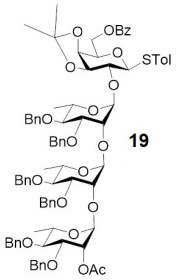
F1 - Acquisition parameters
TD                         37
SFO1                125.8282 MHz
FIDRES           1358.142090 Hz
SW                   199.682 ppm
FnMODE     Echo-Antiecho

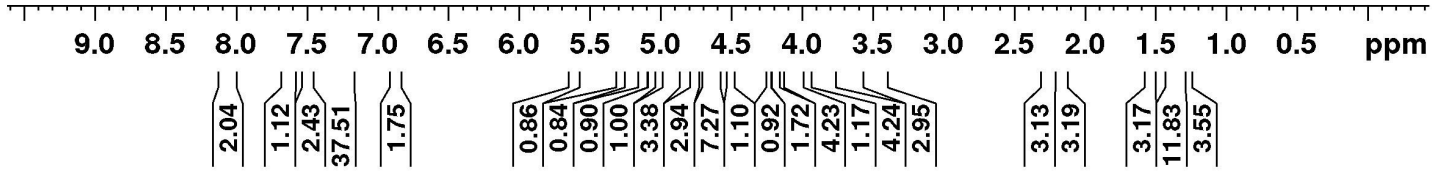
F2 - Processing parameters
SI                      1024
SF                500.3600028 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
PC                      1.00

F1 - Processing parameters
SI                      1024
MC2          echo-antiecho
SF                125.8156016 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
```

GROUP BM
BM-AC-124 in CDCl3







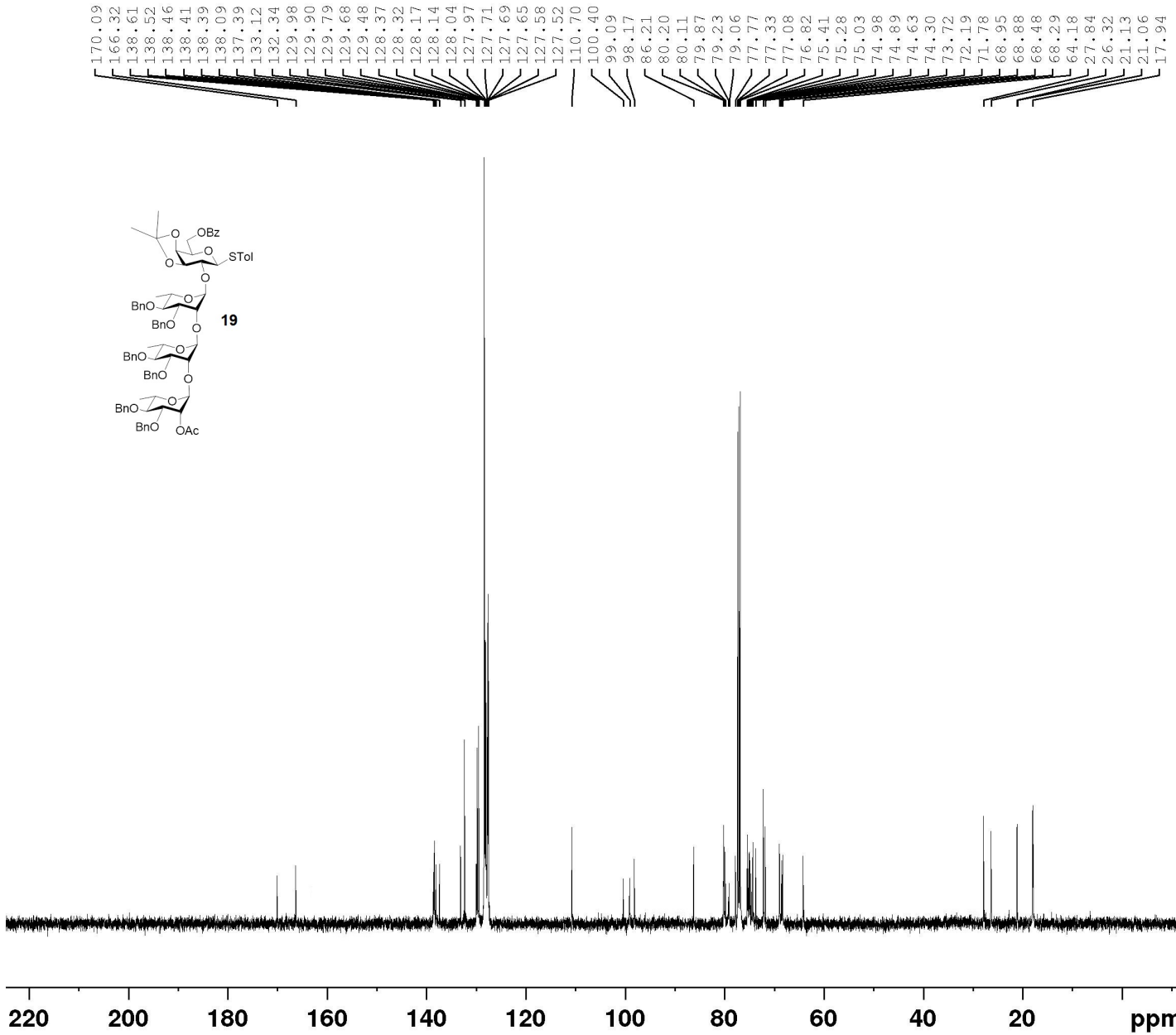
Current Data Parameters
NAME BM-AC-R124
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190516
Time 17.45
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 9469.697 Hz
FIDRES 0.142273 Hz
AQ 3.5143681 sec
RG 32
DW 52.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3445031 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3400113 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-124 in CDCl3



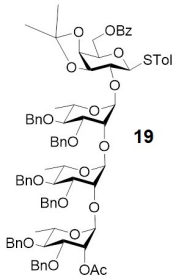
Current Data Parameters
NAME BM-AC-R124
EXPNO 293
PROCNO 1

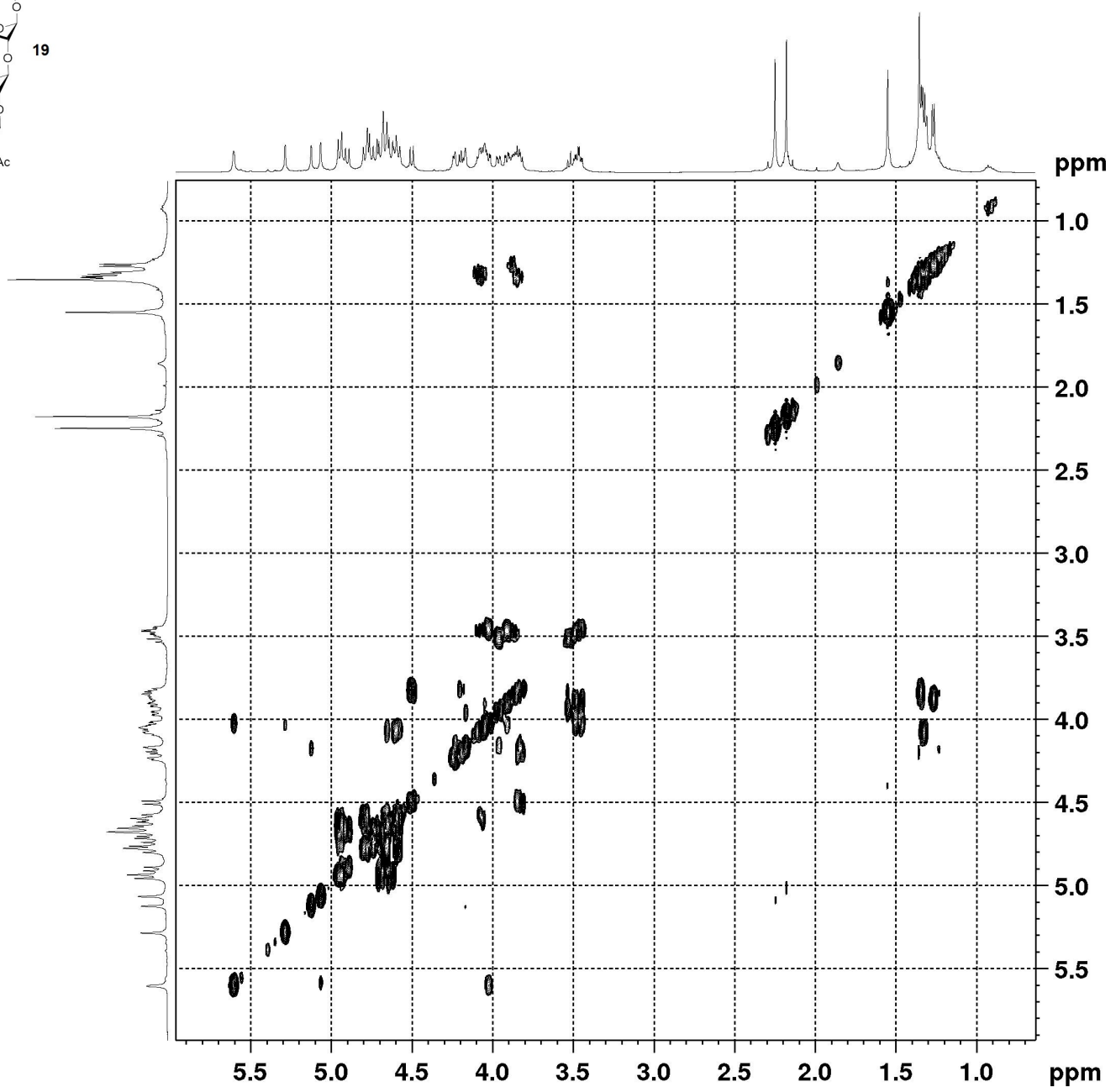
F2 - Acquisition Parameters
Date_ 20190516
Time 18.02
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 90.5
DW 11.400 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8294646 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8106005 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





BRUKER

```
Current Data Parameters
NAME          BM-AC-R124
EXPNO                291
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190516
Time               17.47
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     1
DS                     8
SWH             5000.000 Hz
FIDRES          2.441406 Hz
AQ             0.2048000 sec
RG                    32
DW              100.000 usec
DE                6.50 usec
TE                299.7 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00019980 sec

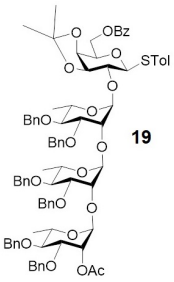
======== CHANNEL f1 ========
SFO1          500.3425017 MHz
NUC1                   1H
P0                 17.50 usec
P1                 17.50 usec
P17              2500.00 usec
PLW1          10.00000000 W
PLW10          3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1            500.3425 MHz
FIDRES          78.203201 Hz
SW                10.003 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF            500.3400094 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.00

F1 - Processing parameters
SI                   1024
MC2                    QF
SF            500.3400109 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
```



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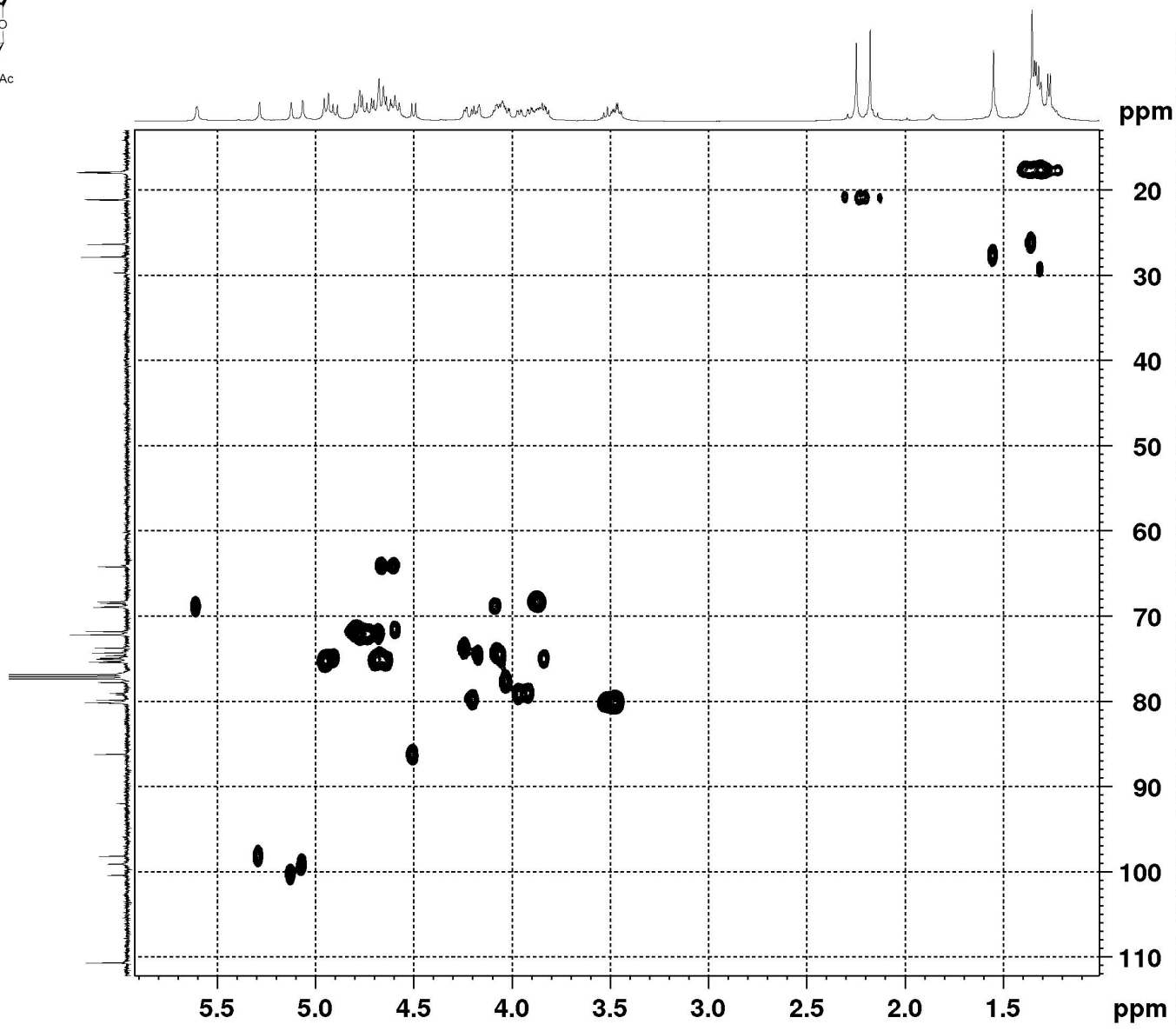



```
Current Data Parameters
NAME          BM-AC-R124
EXPNO                292
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190516
Time              17.52
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                  1024
SOLVENT             CDCl3
NS                     2
DS                    16
SWH            5000.000 Hz
FIDRES          4.882813 Hz
AQ             0.1024000 sec
RG                    32
DW              100.000 usec
DE                6.50 usec
TE                299.8 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          500.3425017 MHz
NUC1                    1H
P1                  17.50 usec
P2                  35.00 usec
P28               1000.00 usec
PLW1         10.00000000 W

======== CHANNEL f2 ========
SFO2          125.8231741 MHz
NUC2                   13C
CPDPRG[2             garp
P3                  11.50 usec
P4                  23.00 usec
PCPD2               70.00 usec
PLW2         66.00000000 W
PLW12         1.78129995 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

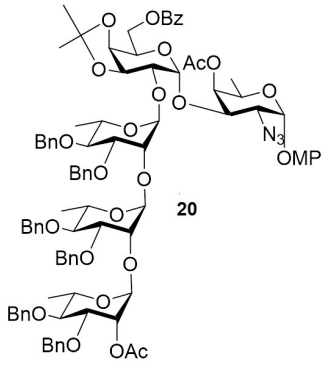
F1 - Acquisition parameters
TD                   114
SFO1           125.8232 MHz
FIDRES        440.800507 Hz
SW                199.690 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF            500.3400094 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.00

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF            125.8106032 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
```

GROUP BM
BM-AC-R125 in CDCl3

8.090 8.074 7.346 7.337 7.327 7.311 7.300 7.280 7.275 7.262 7.250 7.236 6.915 6.897 6.788 6.770 4.901 4.731 4.716 4.648 4.633 4.625 4.617 4.610 4.604 4.583 4.105 4.100 3.825 3.786 3.780 2.146 2.037 1.523 1.326 1.314 1.301 1.294 1.281 1.272 1.232 1.219 1.052 1.039



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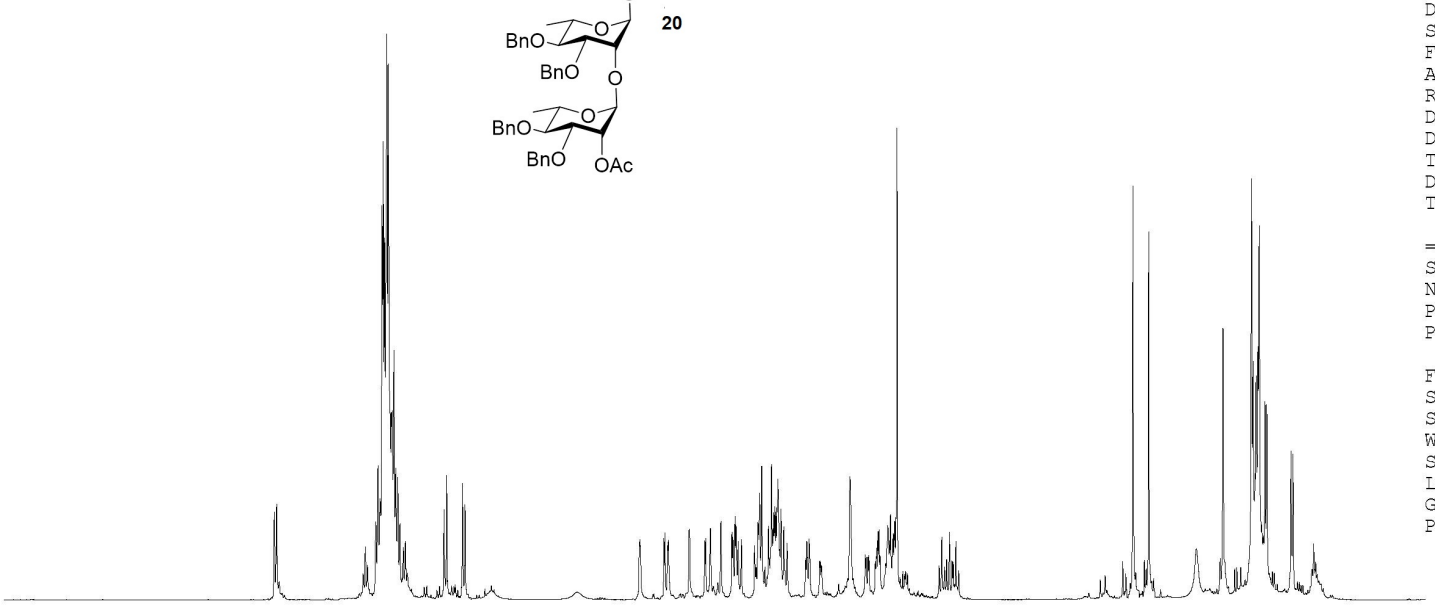
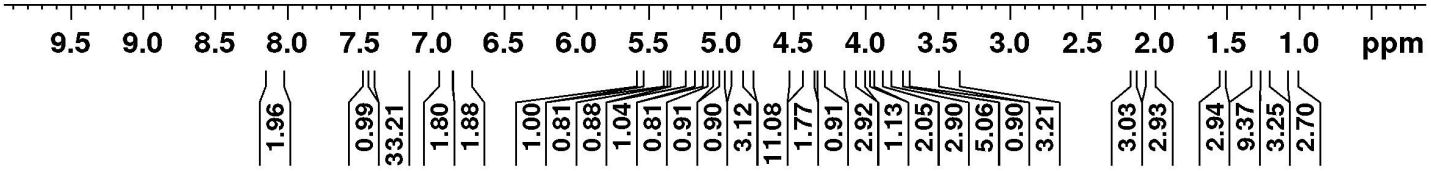




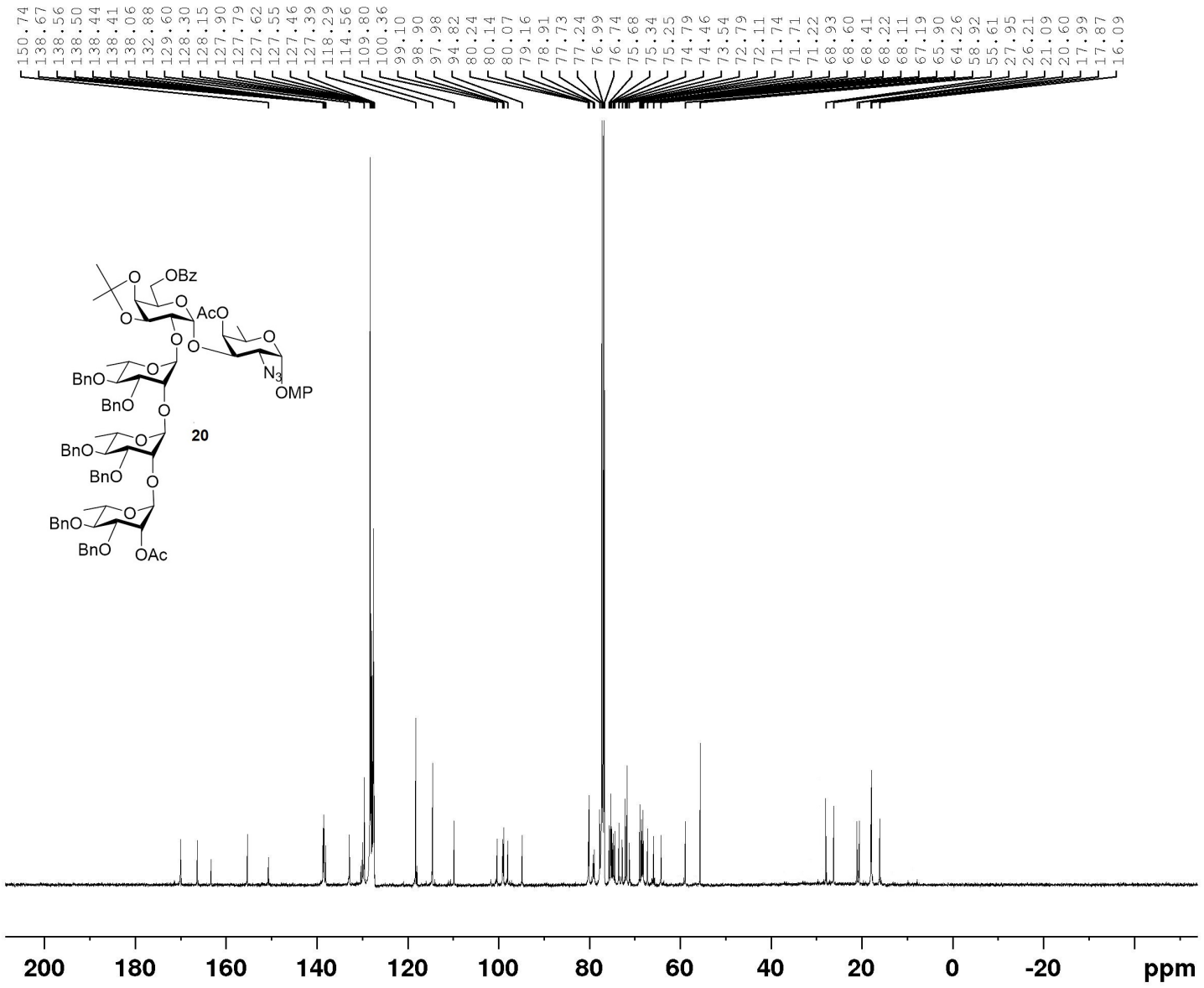
Current Data Parameters
NAME BM-AC-R125US
EXPNO 470
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190527
Time 17.57
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 12500.000 Hz
FIDRES 0.187800 Hz
AQ 2.6624000 sec
RG 80.6
DW 40.000 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3637527 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3600115 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-R125 in CDCl3



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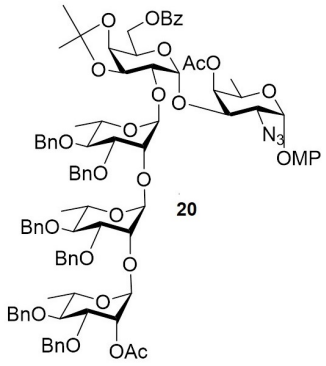
Current Data Parameters
NAME BM-AC-R125US
EXPNO 590
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190603
Time 20.19
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 18000
DS 4
SWH 75757.578 Hz
FIDRES 1.155969 Hz
AQ 0.4325376 sec
RG 203
DW 6.600 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

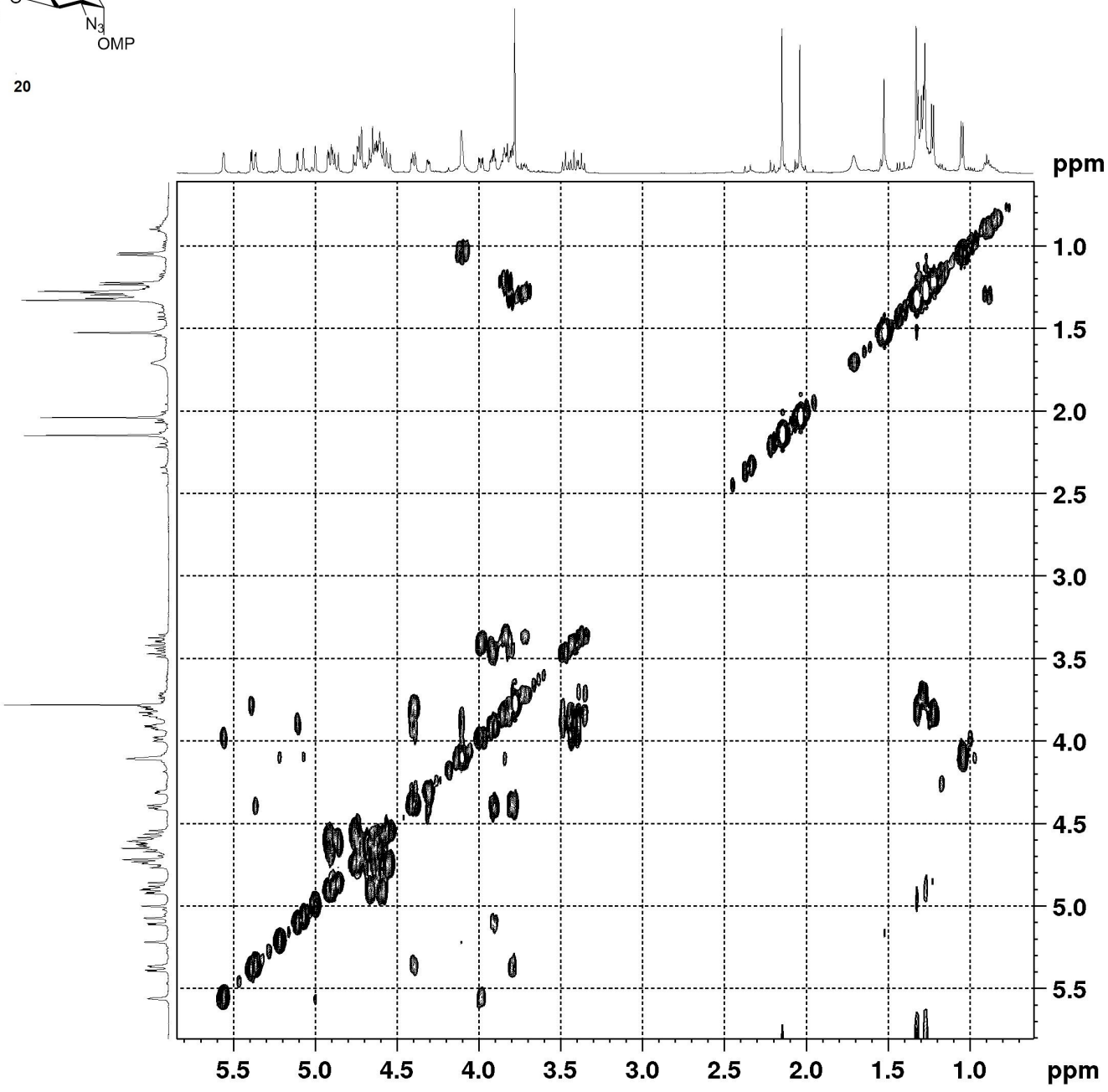
======== CHANNEL f1 ========
SFO1 125.8407841 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8156307 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



20




```
Current Data Parameters
NAME        BM-AC-R125US
EXPNO                390
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190528
Time               14.19
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     2
DS                     8
SWH             5000.000 Hz
FIDRES          2.441406 Hz
AQ             0.2048000 sec
RG                  90.5
DW               100.000 usec
DE                  6.50 usec
TE                299.2 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00019980 sec

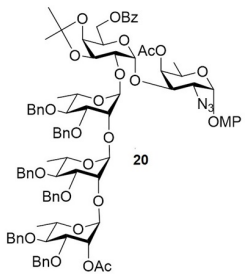
======== CHANNEL f1 ========
SFO1         500.3625017 MHz
NUC1                1H
P0                17.50 usec
P1                17.50 usec
P17             2500.00 usec
PLW1         10.00000000 W
PLW10         3.40280008 W

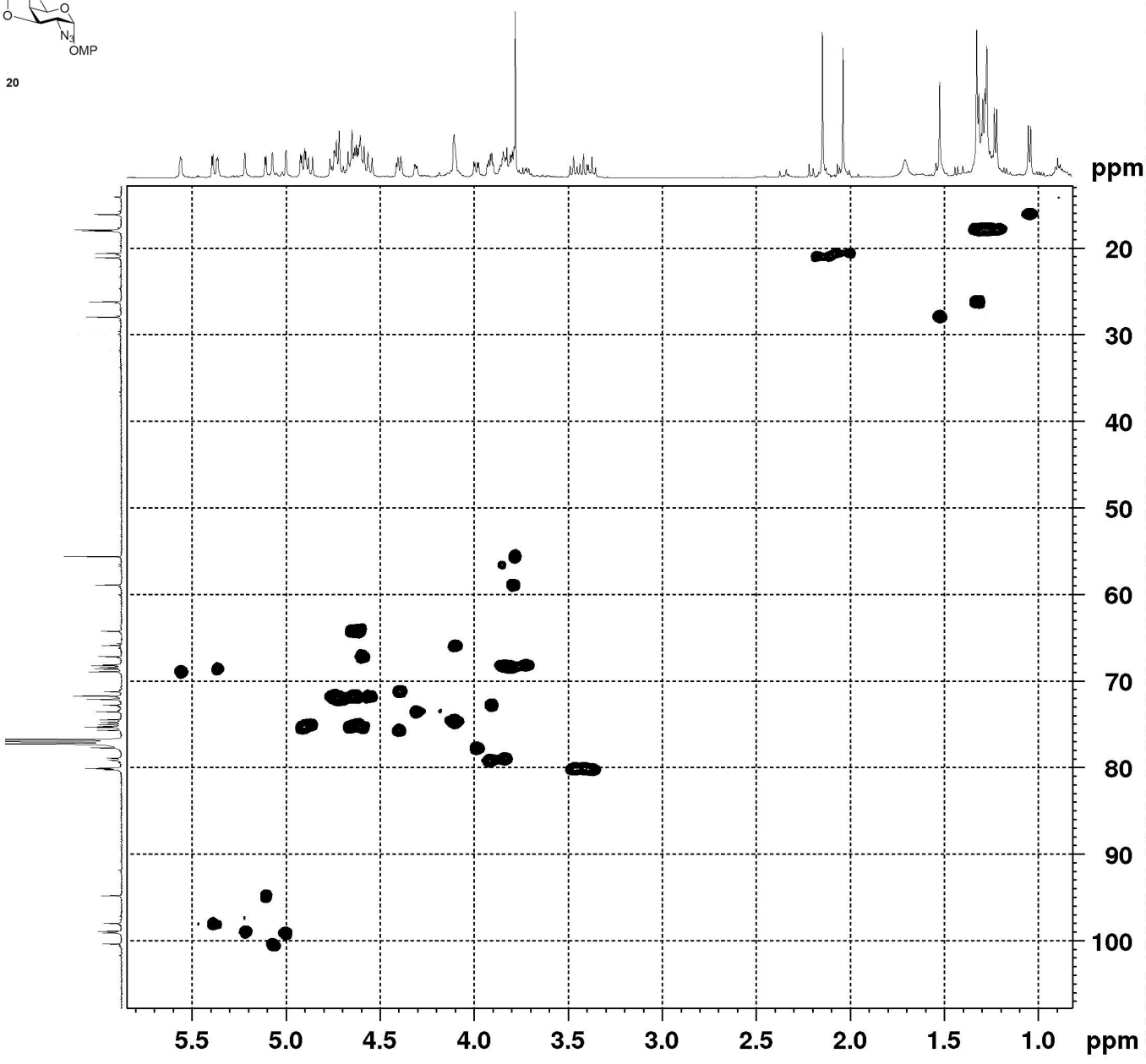
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1            500.3625 MHz
FIDRES          78.203201 Hz
SW                10.003 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           500.3600115 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.00

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           500.3600115 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```






```
Current Data Parameters
NAME        BM-AC-R125US
EXPNO                391
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190528
Time               14.33
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                  1024
SOLVENT             CDCl3
NS                     2
DS                    16
SWH            5000.000 Hz
FIDRES         4.882813 Hz
AQ             0.1024000 sec
RG                   161
DW              100.000 usec
DE                6.50 usec
TE                299.2 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          500.3625017 MHz
NUC1                    1H
P1                  17.50 usec
P2                  35.00 usec
P28               1000.00 usec
PLW1         10.00000000 W

======== CHANNEL f2 ========
SFO2          125.8282031 MHz
NUC2                   13C
CPDPRG[2              garp
P3                  11.50 usec
P4                  23.00 usec
PCPD2               70.00 usec
PLW2         66.00000000 W
PLW12         1.78129995 W

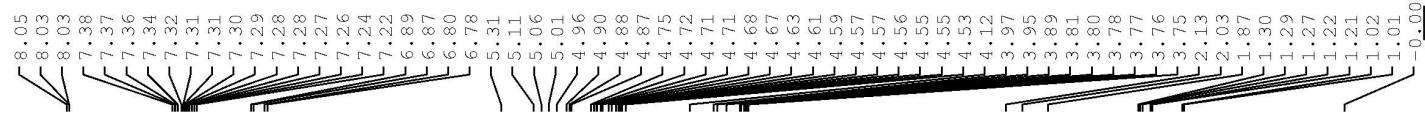
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

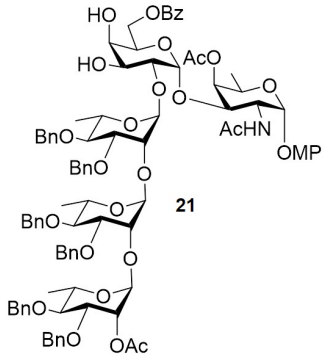
F1 - Acquisition parameters
TD                   244
SFO1           125.8282 MHz
FIDRES         205.947769 Hz
SW                199.682 ppm
FnMODE     Echo-Antiecho

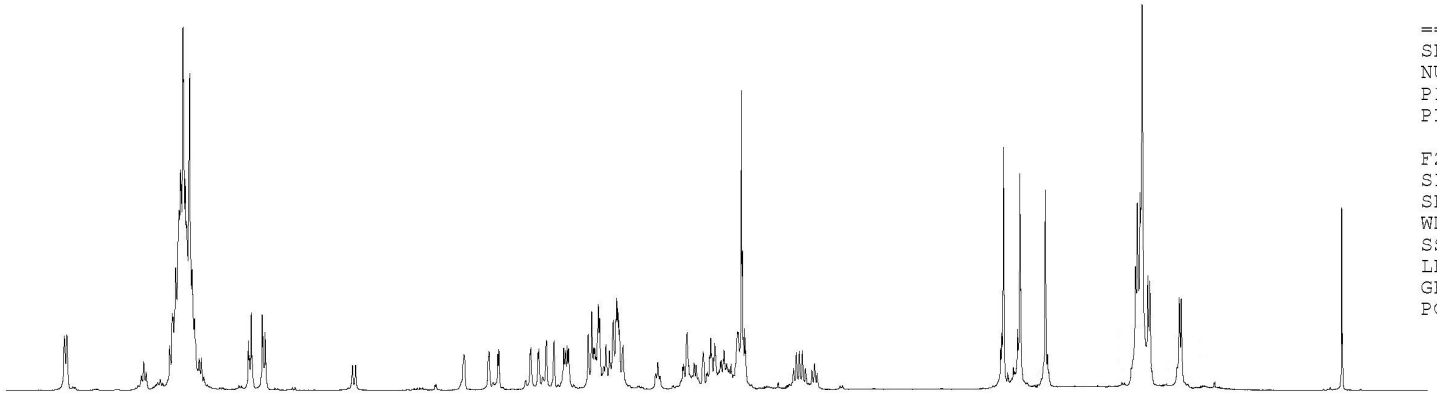
F2 - Processing parameters
SI                  1024
SF           500.3600115 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.00

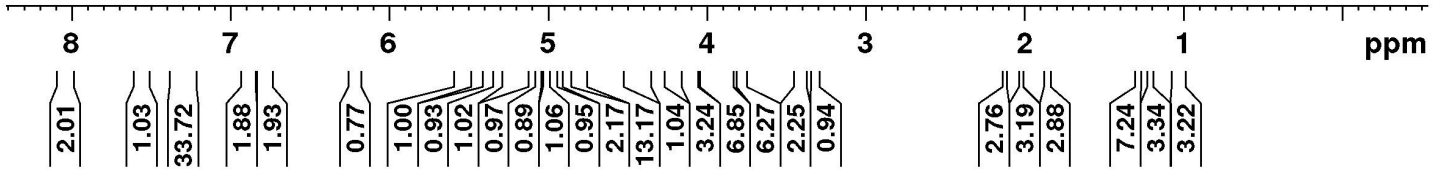
F1 - Processing parameters
SI                  1024
MC2         echo-antiecho
SF           125.8156220 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
```

GROUP BM
BM-AC-R132 in CDCl3









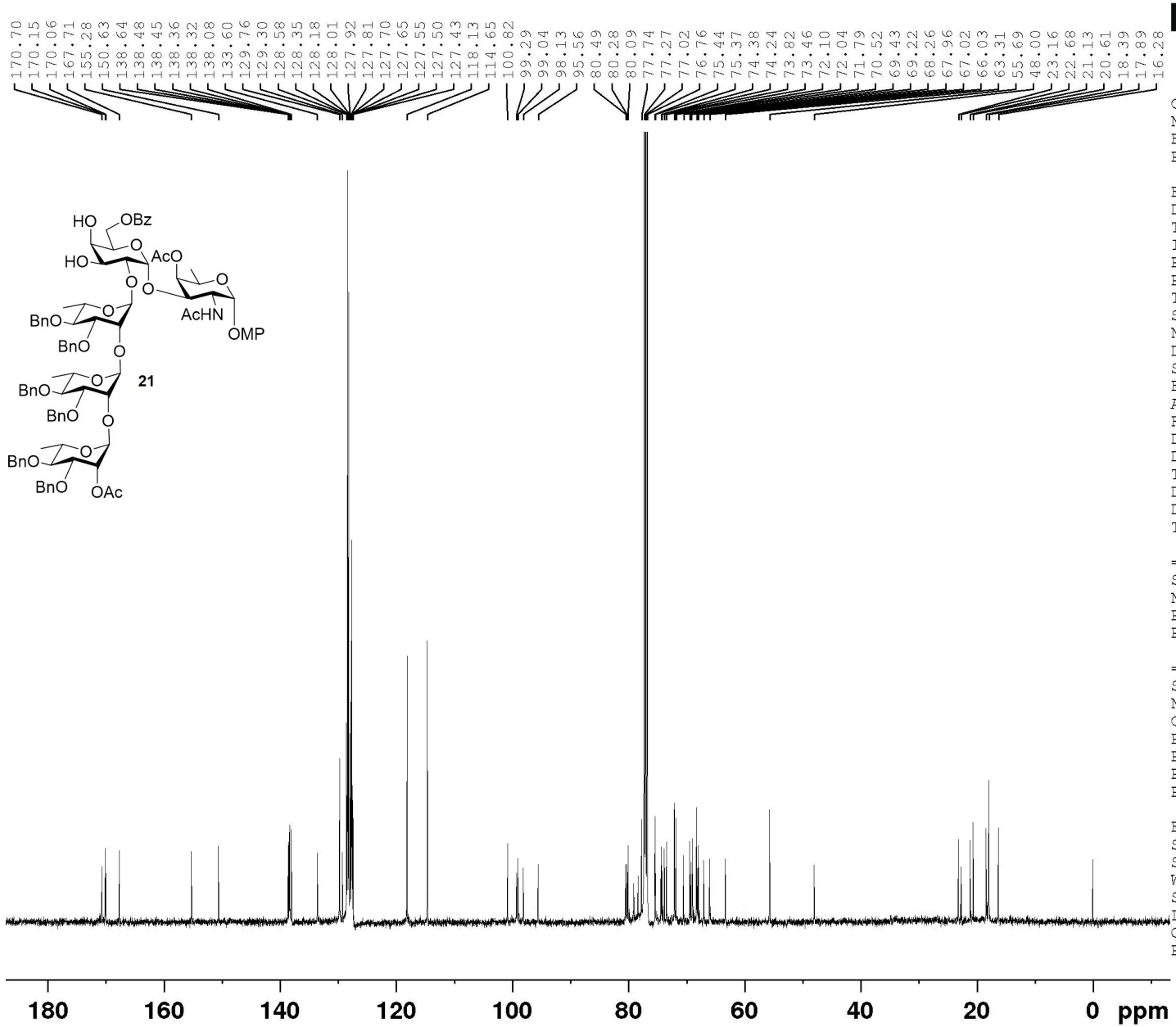

```
Current Data Parameters
NAME          BM-AC-R132
EXPNO                480
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190617
Time               20.23
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 66560
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           12500.000 Hz
FIDRES            0.187800 Hz
AQ             2.6624000 sec
RG                   128
DW                40.000 usec
DE                 6.50 usec
TE                298.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.3637527 MHz
NUC1                   1H
P1                 17.50 usec
PLW1         10.00000000 W

F2 - Processing parameters
SI                131072
SF           500.3600142 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

GROUP BM
BM-AC-R132 in CDCl3



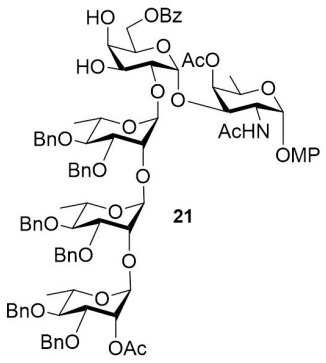

```
Current Data Parameters
NAME          BM-AC-R132
EXPNO                483
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190617
Time               20.52
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                17410
DS                    4
SWH           75757.578 Hz
FIDRES         1.155969 Hz
AQ            0.4325376 sec
RG                  203
DW                6.600 usec
DE                6.50 usec
TE                299.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.8407841 MHz
NUC1                13C
P1                11.50 usec
PLW1        66.00000000 W

======== CHANNEL f2 ========
SFO2        500.3620014 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        10.00000000 W
PLW12        0.47852001 W
PLW13        0.24068999 W

F2 - Processing parameters
SI                32768
SF          125.8156233 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



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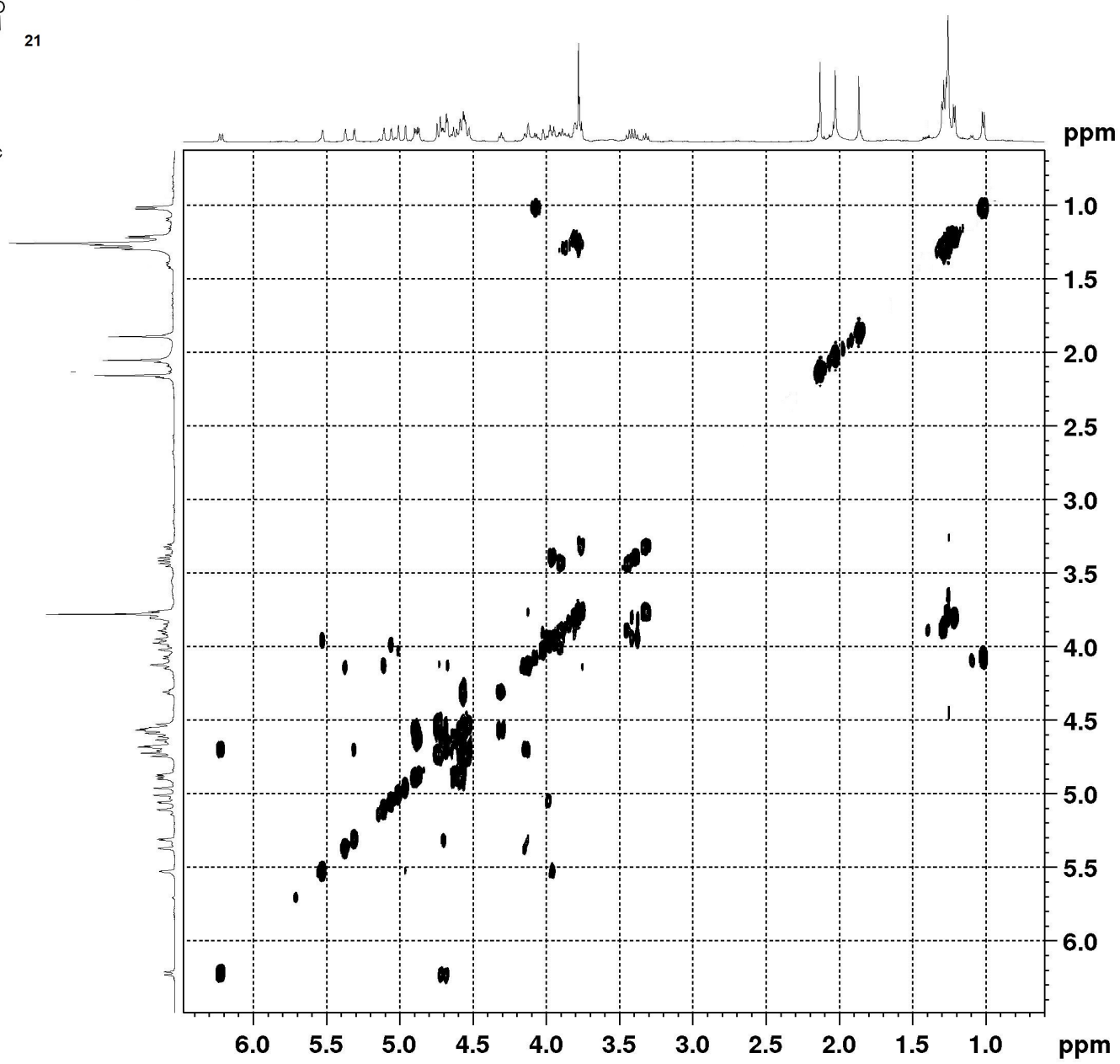



```
Current Data Parameters
NAME          BM-AC-R132
EXPNO                481
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190617
Time               20.25
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     2
DS                     8
SWH           5000.000 Hz
FIDRES        2.441406 Hz
AQ           0.2048000 sec
RG                   128
DW             100.000 usec
DE               6.50 usec
TE              298.9 K
D0           0.00000300 sec
D1           2.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00019980 sec

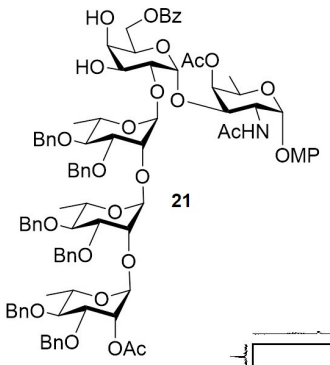
======== CHANNEL f1 ========
SFO1        500.3625017 MHz
NUC1                1H
P0                17.50 usec
P1                17.50 usec
P17             2500.00 usec
PLW1         10.00000000 W
PLW10         3.40280008 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1          500.3625 MHz
FIDRES       78.203201 Hz
SW             10.003 ppm
FnMODE              QF

F2 - Processing parameters
SI                  1024
SF          500.3600126 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.00

F1 - Processing parameters
SI                  1024
MC2                 QF
SF          500.3600126 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```



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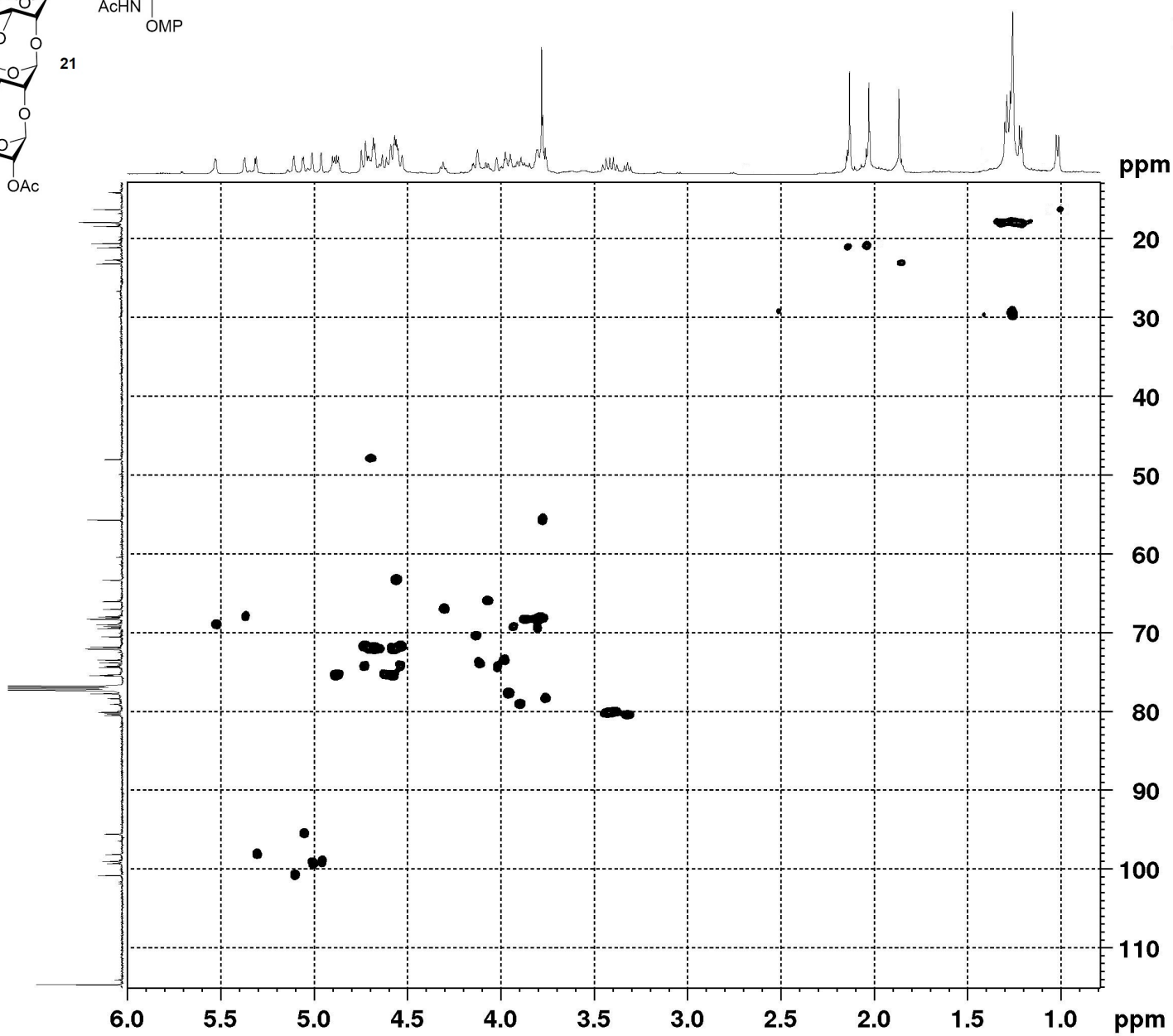


BRUKER

```
Current Data Parameters
NAME          BM-AC-R132
EXPNO                482
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190617
Time                20.36
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                  1024
SOLVENT             CDCl3
NS                     2
DS                    16
SWH             5000.000 Hz
FIDRES          4.882813 Hz
AQ              0.1024000 sec
RG                   128
DW               100.000 usec
DE                 6.50 usec
TE                298.9 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          500.3625017 MHz
NUC1                  1H
P1                 17.50 usec
P2                 35.00 usec
P28              1000.00 usec
PLW1          10.00000000 W

======== CHANNEL f2 ========
SFO2          125.8282031 MHz
NUC2                 13C
CPDPRG[2             garp
P3                 11.50 usec
P4                 23.00 usec
PCPD2              70.00 usec
PLW2          66.00000000 W
PLW12          1.78129995 W

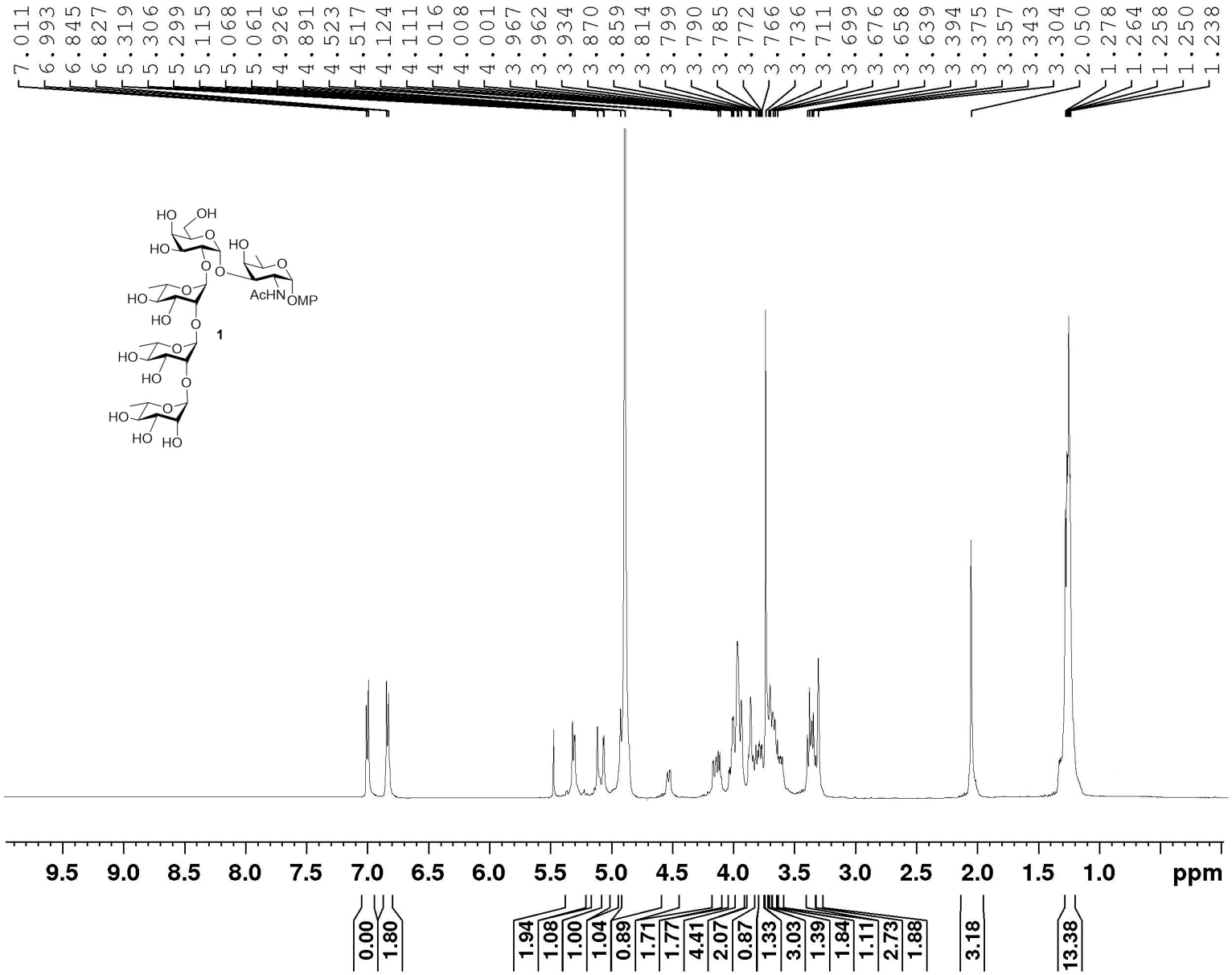
====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPNAM[3]       SMSQ10.100
GPNAM[4]       SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            125.8282 MHz
FIDRES        196.293976 Hz
SW               199.682 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF            500.3600152 MHz
WDW                 QSINE
SSB                    2
LB        0 Hz
GB        0
PC                  1.00

F1 - Processing parameters
SI                  1024
MC2         echo-antiecho
SF           125.8156233 MHz
WDW                 QSINE
SSB                    2
LB        0 Hz
GB        0
```

GROUP BM
BM-AC-160C 8 in CD3OD



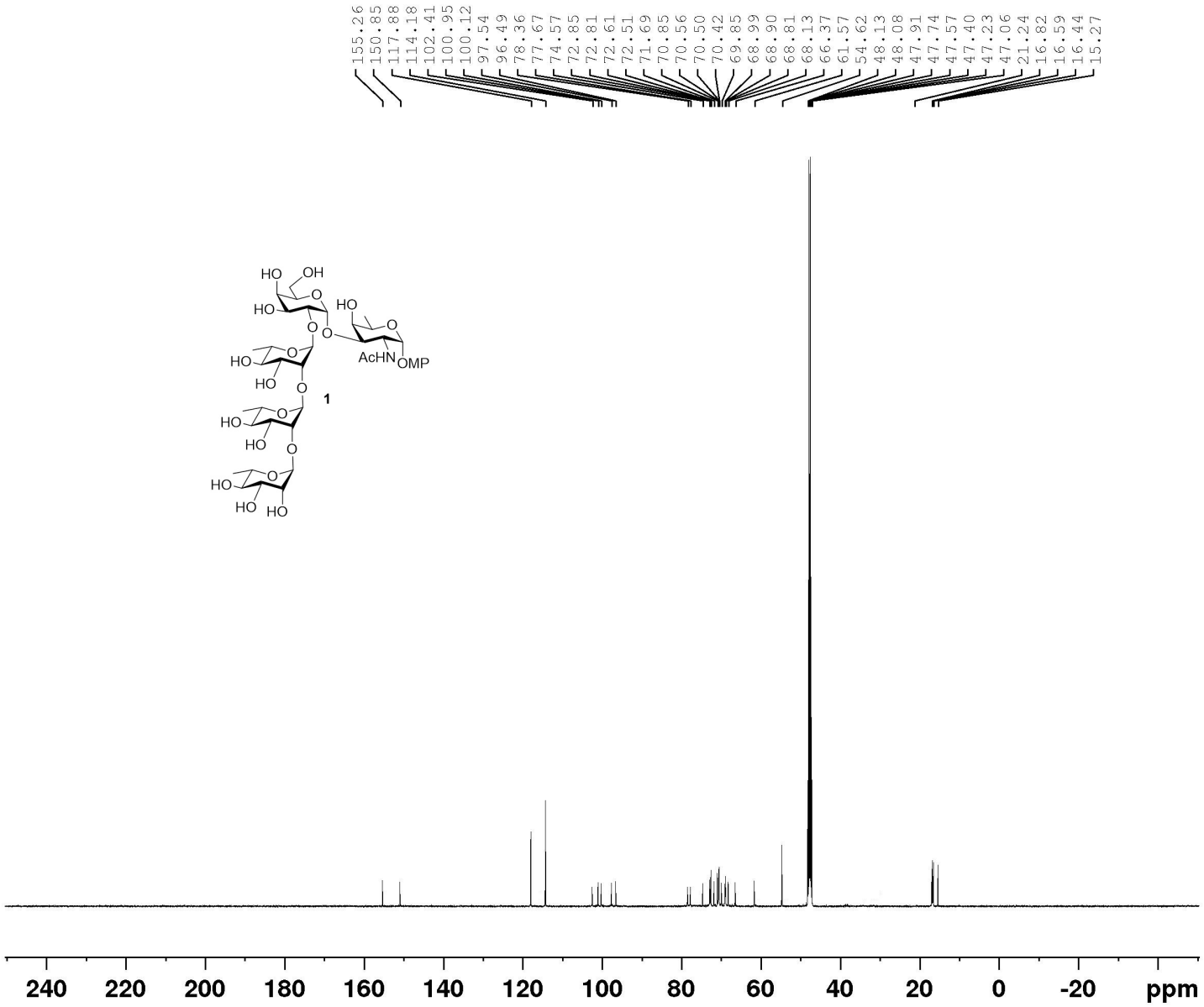
Current Data Parameters
NAME BM-AC-R160C
EXPNO 481
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190919
Time 22.55
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 66560
SOLVENT MeOD
NS 8
DS 2
SWH 10000.000 Hz
FIDRES 0.150240 Hz
AQ 3.3280001 sec
RG 80.6
DW 50.000 usec
DE 6.50 usec
TE -0.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3625018 MHz
NUC1 1H
P1 17.50 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 131072
SF 500.3600118 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

GROUP BM
BM-AC-160C 8000 in CD3OD



Current Data Parameters
NAME BM-AC-R160C
EXPNO 483
PROCNO 1

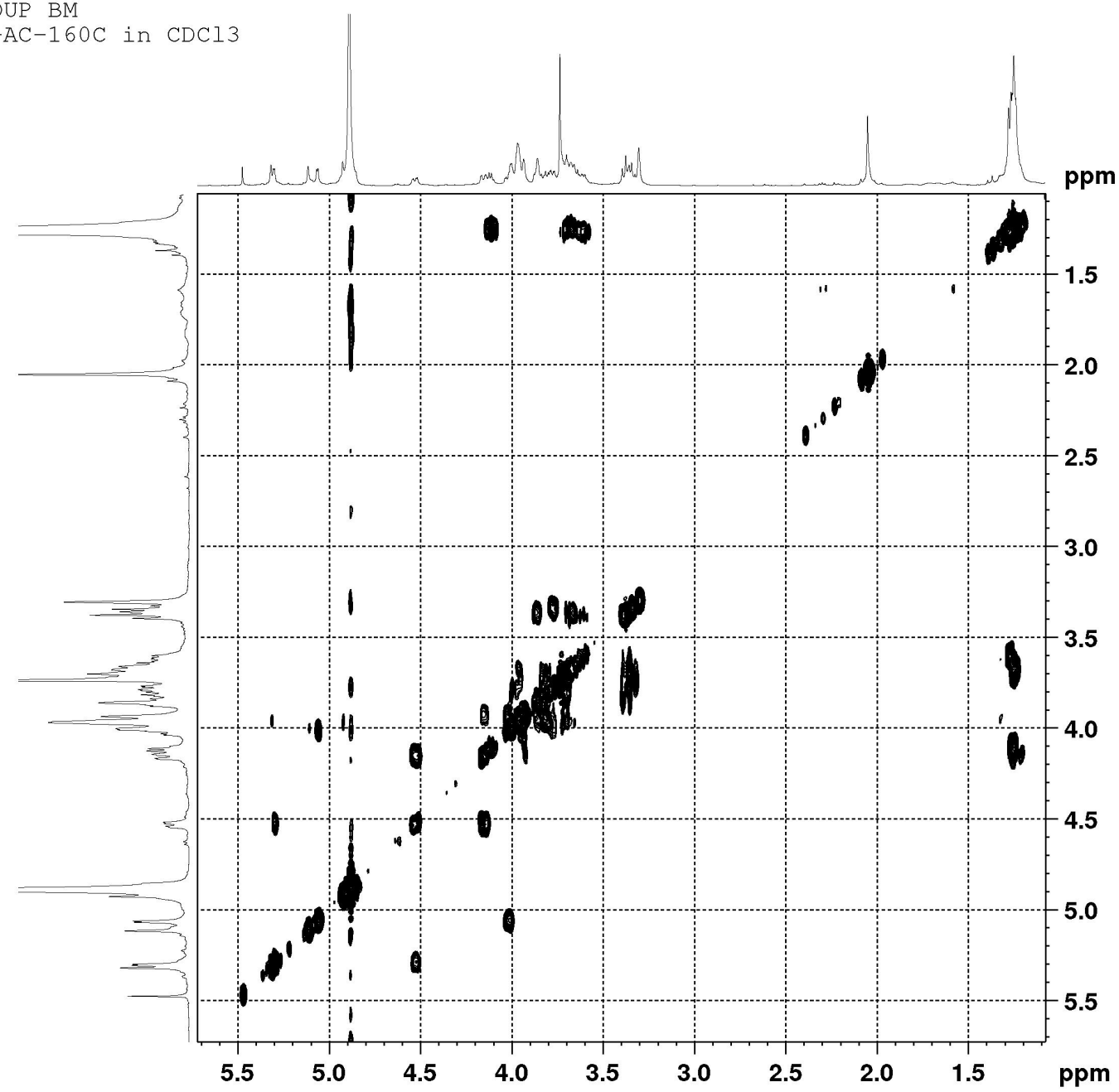
F2 - Acquisition Parameters
Date_ 20190920
Time 0.48
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 7568
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 90.5
DW 13.200 usec
DE 6.50 usec
TE 730.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8282036 MHz
NUC1 13C
P1 11.50 usec
PLW1 66.00000000 W

======== CHANNEL f2 ========
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

F2 - Processing parameters
SI 32768
SF 125.8156323 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

GROUP BM
BM-AC-160C in CDCl3



Current Data Parameters
NAME BM-AC-R160C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190920
Time 6.31
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT MeOD
NS 2
DS 8
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048000 sec
RG 80.6
DW 100.000 usec
DE 6.50 usec
TE 3451.2 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019980 sec

======== CHANNEL f1 ========
SFO1 500.3625017 MHz
NUC1 1H
P0 17.50 usec
P1 17.50 usec
P17 2500.00 usec
PLW1 10.00000000 W
PLW10 3.40280008 W

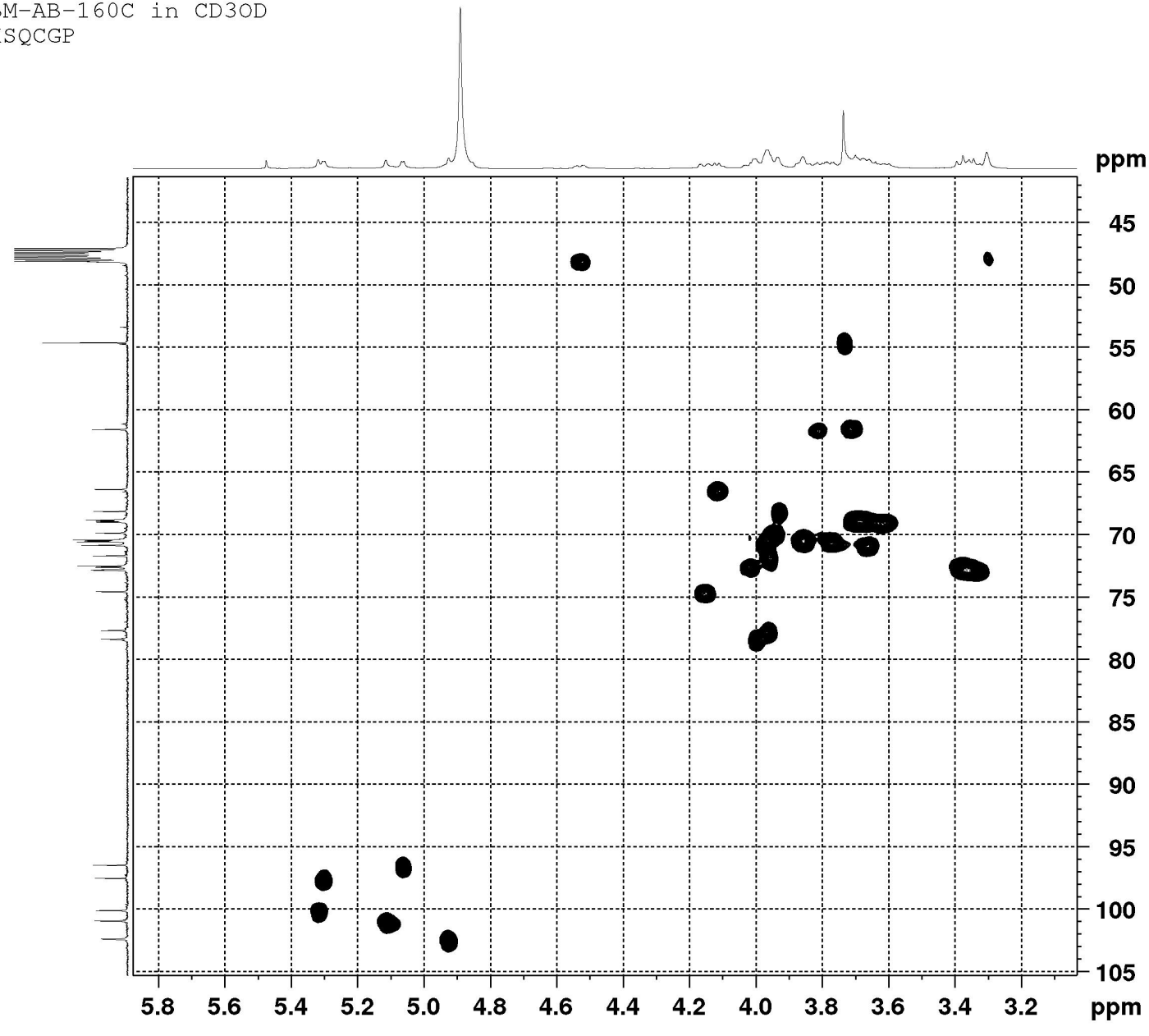
====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.3625 MHz
FIDRES 78.203201 Hz
SW 10.003 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 500.3600123 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.3600123 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

GROUP BM
BM-AB-160C in CD3OD
HSQCGP




```
Current Data Parameters
NAME         BM-AC-R160C
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190920
Time                6.44
INSTRUM  Bruker_default_av500
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                  1024
SOLVENT              MeOD
NS                     4
DS                    16
SWH            5000.000 Hz
FIDRES          4.882813 Hz
AQ             0.1024000 sec
RG                  80.6
DW              100.000 usec
DE                6.50 usec
TE                528.1 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          500.3625017 MHz
NUC1                    1H
P1                  17.50 usec
P2                  35.00 usec
P28               1000.00 usec
PLW1         10.00000000 W

======== CHANNEL f2 ========
SFO2          125.8282031 MHz
NUC2                   13C
CPDPRG[2               garp
P3                  11.50 usec
P4                  23.00 usec
PCPD2               70.00 usec
PLW2         66.00000000 W
PLW12         1.78129995 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

F1 - Acquisition parameters
TD                    195
SFO1           125.8282 MHz
FIDRES        257.698761 Hz
SW                199.682 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF            500.3600121 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                    1.00

F1 - Processing parameters
SI                   1024
MC2         echo-antiecho
SF            125.8156153 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
```

Pentasaccharide Deprotected.
Exp: 934.3532 Fr: $C_{39}H_{61}NNaO_{23}$
Obs: 934.3532

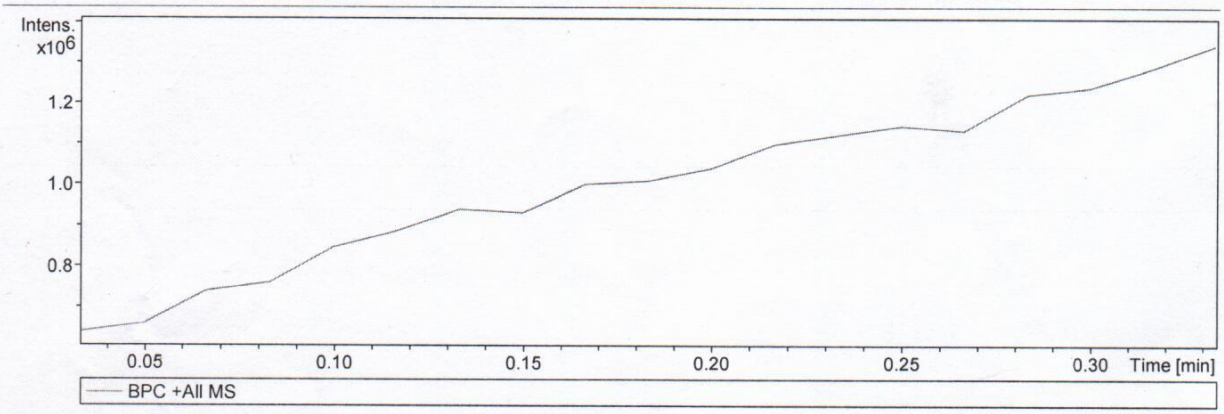
Display Report

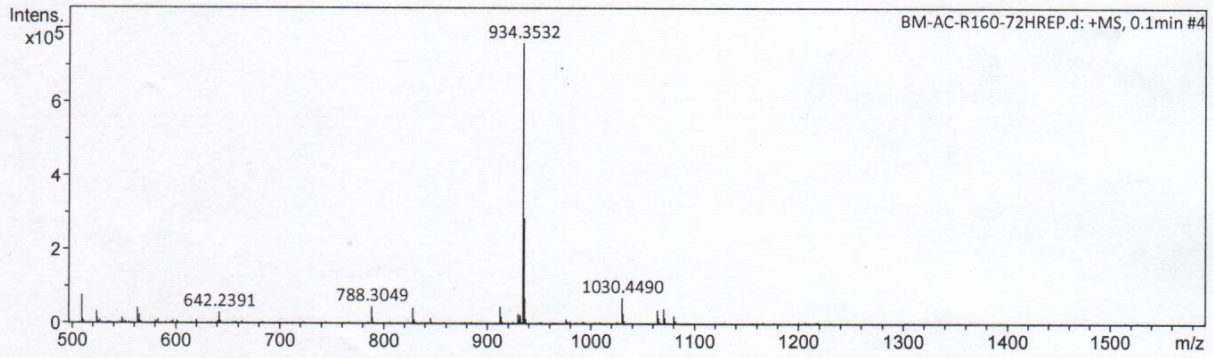
Analysis Info

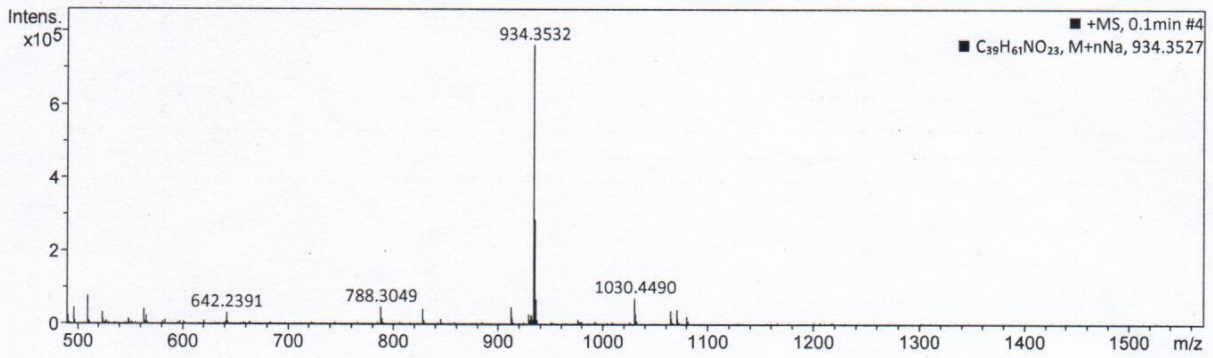
Analysis Name	D:\Data\User data\2019\SEP\BM-AC-R160-72HREP.d	Acquisition Date	9/24/2019 3:37:12 PM
Method	Tune_pos_Mid.m	Operator	IISER Kalyani
Sample Name	BM-AC-R160-72HREP	Instrument	maXis impact 8282001.00127
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C







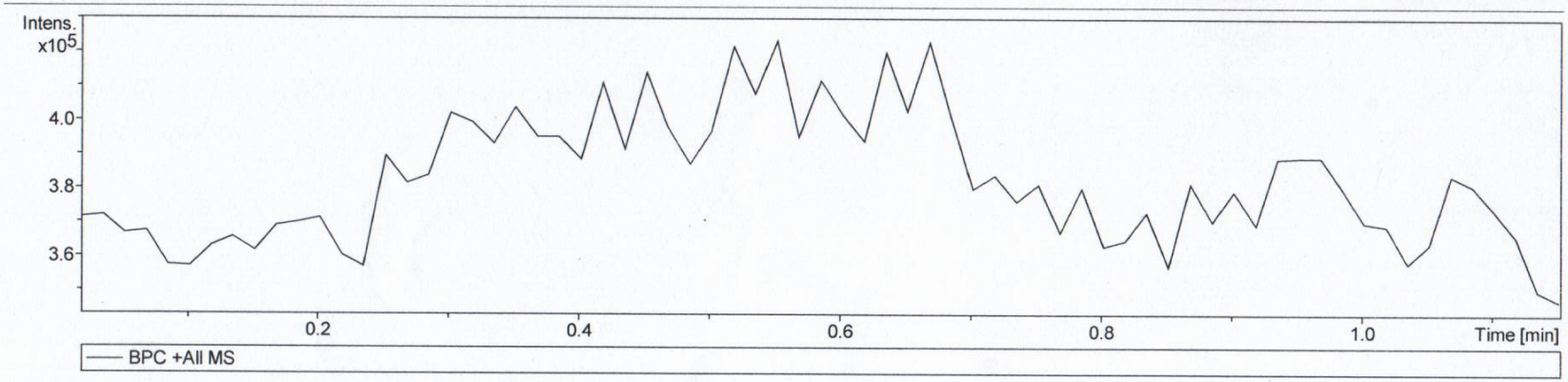
Display Report

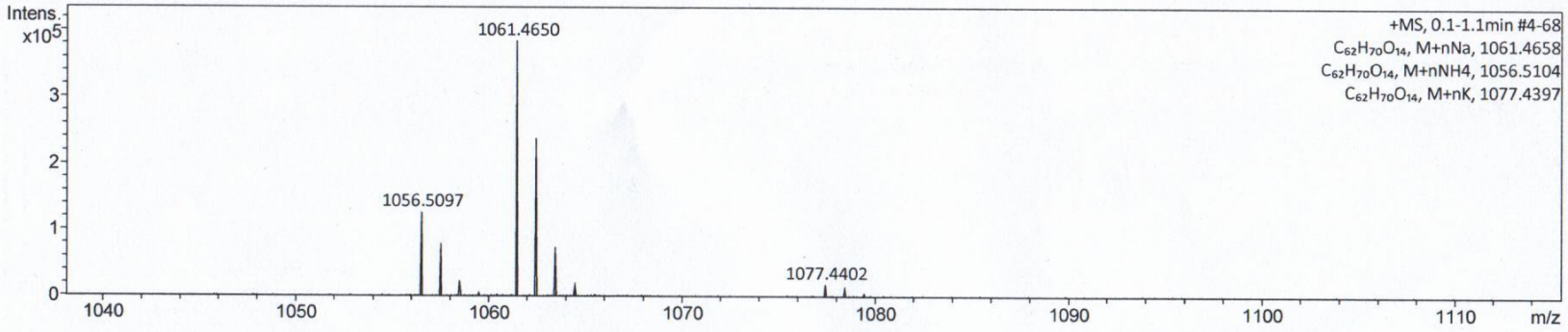
Analysis Info

Analysis Name	D:\Data\User data\2019\DEC\BM-AC-TRIOH.d	Acquisition Date	12/24/2019 12:54:04 PM
Method	Tune_pos_Mid.m	Operator	IISER Kalyani
Sample Name	BM-AC-TRIOH	Instrument	maXis impact 8282001.00127
Comment	pyrrrole -COOH and -COOET		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





BM-AC-TRIOH.d