

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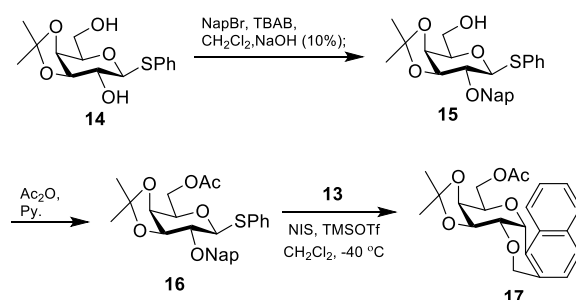
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Undesired outcome from the glycosylation of donor **16** with acceptor **13**:



Scheme S1: Preparation of α -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 $\text{Na}_2\text{SO}_4(\text{s})$. 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).

^1H NMR (CDCl_3 , 500 MHz) δ : 7.87-7.26 (m, 12H, ArH), 4.86 (d, 1H, $J=11.5\text{ Hz}$, NapCH₂), 4.69 (d, 1H, $J=11.5\text{ Hz}$, NapCH₂), 4.33 (d, 1H, $J=9.5\text{ Hz}$, H-1), 4.33 (t, 3H, $J=6.0\text{ Hz}$, H-3), 4.19 (d, 1H, $J=4.0\text{ Hz}$, 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, CH₃), 1.39 (s, 3H, CH₃).

^{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 (-CMe₂), 85.9 (C-1), 79.8 (C-3), 78.1 (C-2), 76.7 (C-5), 73.9 (C-4), 73.4 (ArCH₂), 62.5 (C-6), 27.7, 26.3 (2 $\times$ CH₃).

HRMS calculated for $\text{C}_{26}\text{H}_{28}\text{O}_5\text{SNa}$ ($\text{M}+\text{Na}^+$): 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 $\text{Na}_2\text{SO}_4(\text{s})$. 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).

^1H NMR (CDCl_3 , 500 MHz) δ : 7.85-7.26 (m, 12H, ArH), 4.99 (d, 1H, $J=11.5\text{ Hz}$, NapCH₂), 4.86 (d, 1H, $J=11.5\text{ Hz}$, NapCH₂), 4.66 (d, 1H, $J=9.0\text{ Hz}$, H-1), 4.35-4.30 (m, 3H, H-6a, H-6b, H-3), 4.19 (d, 1H, $J=5.0\text{ Hz}$, H-4), 3.95 (m, 1H, H-5), 3.60 (m, 1H, H-2), 2.06 (s, 3H, CH₃), 1.39 (s, 3H, CH₃), 1.35 (s, 3H, CH₃).

^{13}C NMR (CDCl_3 , 125 MHz) δ : 170.7 (CO), 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 (O₂CMe₂), 86.1 (C-1), 79.5 (C-3), 78.0 (C-2), 74.1 (C-5), 73.5 (ArCH₂), 73.4 (C-4), 63.7 (C-6), 27.6, 26.3 (2 $\times$ CH₃), 20.8 (CH₃).

HRMS calculated for $\text{C}_{28}\text{H}_{30}\text{O}_6\text{SNa}$ ($\text{M}+\text{Na}^+$): 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**]

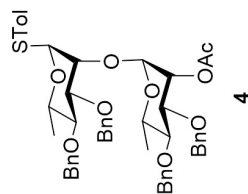
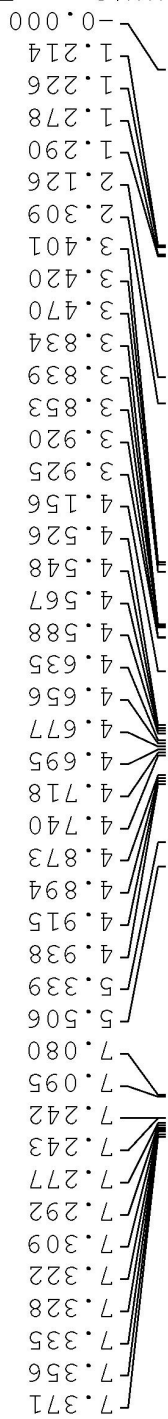
Donor **16** (176 mg, 0.36 mmol) and acceptor **13** (100 mg, 0.3 mmol) were dissolved in CH₂Cl₂ (10 mL) and stirred with 4Å MS (1g) and NIS (105 mg, 0.45 mmol) for 15 minutes under N₂ atmosphere. Thereafter the temperature was lowered to -40 °C and TMSOTf (0.012 mL, 0.06 mmol) was added and the reaction 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 NaHCO₃ aq. (50 mL), Na₂S₂O₃ (50 mL) and brine (50 mL). The organic layer was separated and dried over anhydrous Na₂SO₄. 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.

¹H NMR (CDCl₃, 500 MHz) δ: 8.33 (d, 2H, *J* = 8.3 Hz, ArH), 7.82 (d, 1H, *J* = 8.0 Hz, ArH), 7.78 (d, 1H, *J* = 8.3 Hz, ArH), 7.58 (t, 1H, *J* = 8.0 Hz, ArH), 7.50 (t, 1H, *J* = 8.0 Hz, ArH), 7.10 (d, 1H, *J* = 8.3 Hz, ArH), 5.39 (d, 1H, *J* = 3.0 Hz, H-1), 4.95 (d, 1H, *J* = 15.0 Hz, ArCH₂), 4.82 (d, 1H, *J* = 15.0 Hz, ArCH₂), 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, CH₃), 1.68 (s, 3H, CH₃), 1.47 (s, 3H, CH₃).

¹³C NMR (CDCl₃, 125 MHz) δ: 170.6 (CO), 132.9, 132.7, 132.3, 128.8, 128.2, 127.5, 126.6, 125.6, 124.9, 121.8 (ArC), 110.4 (-CMe₂), 73.2 (C-3), 72.7 (C-4), 72.2 (C-2), 68.1 (NapCH₂), 67.7 (C-5), 63.2 (C-1), 63.1 (C-6), 26.5, 25.1 (2×CH₃), 20.5 (COCH₃).

HRMS calculated for C₂₂H₂₄O₆Na (M+Na)⁺: 407.1471, found: 407.1472.

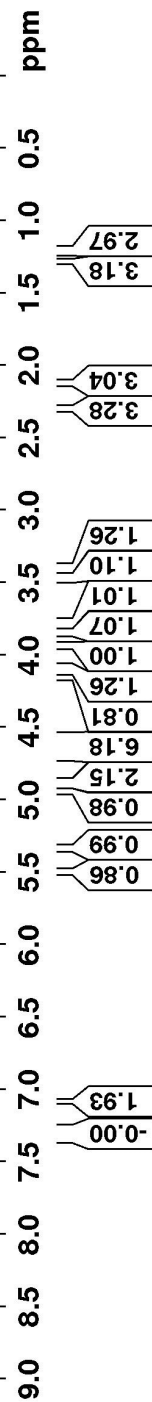
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BM-AC-R168 in CDCl3



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PROCNO 1

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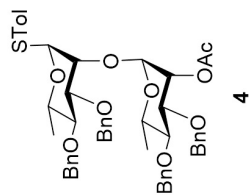
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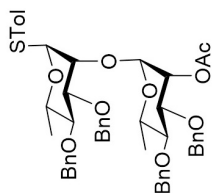
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71.79
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68.38

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138.09
138.01
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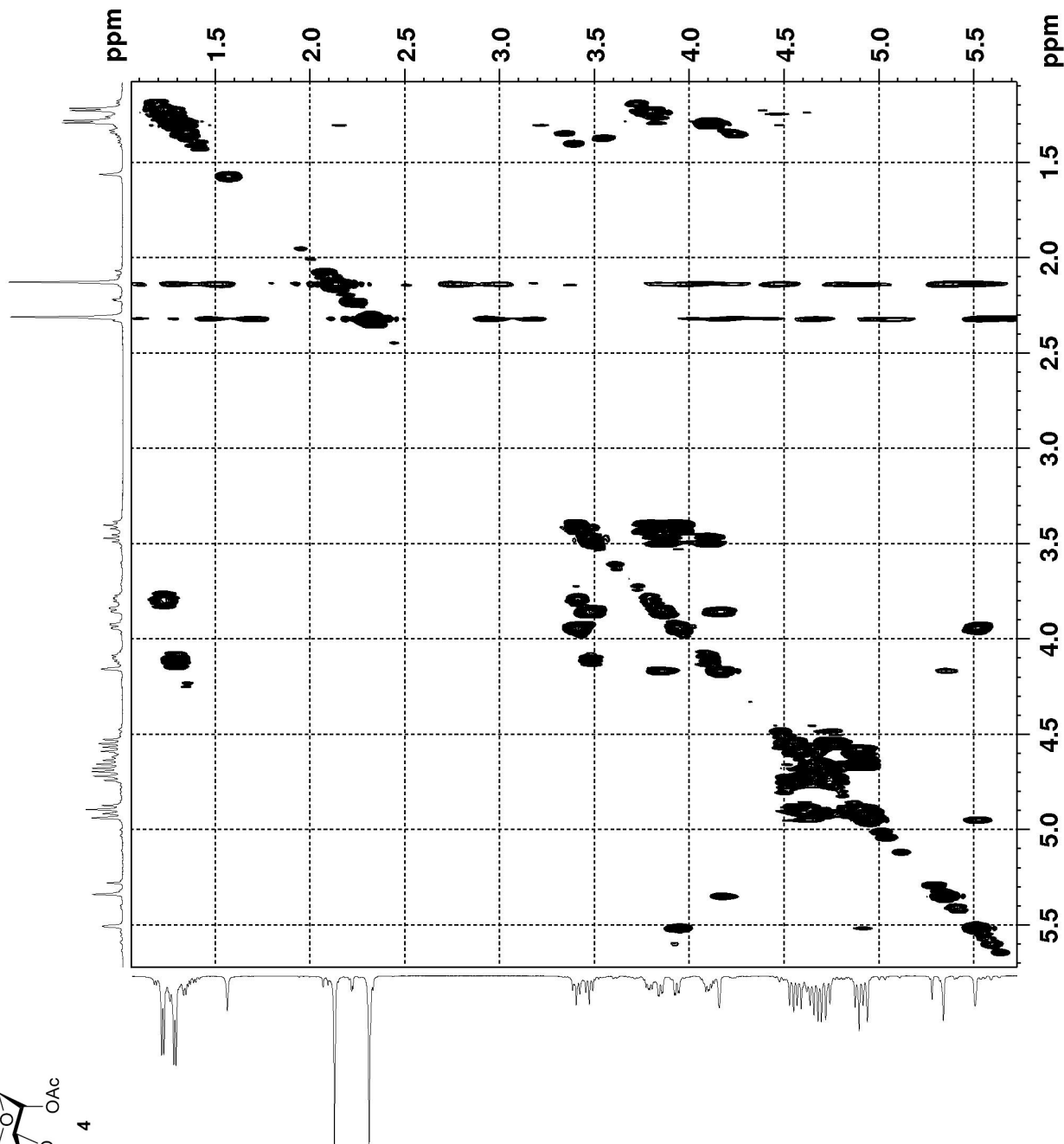
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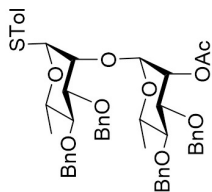
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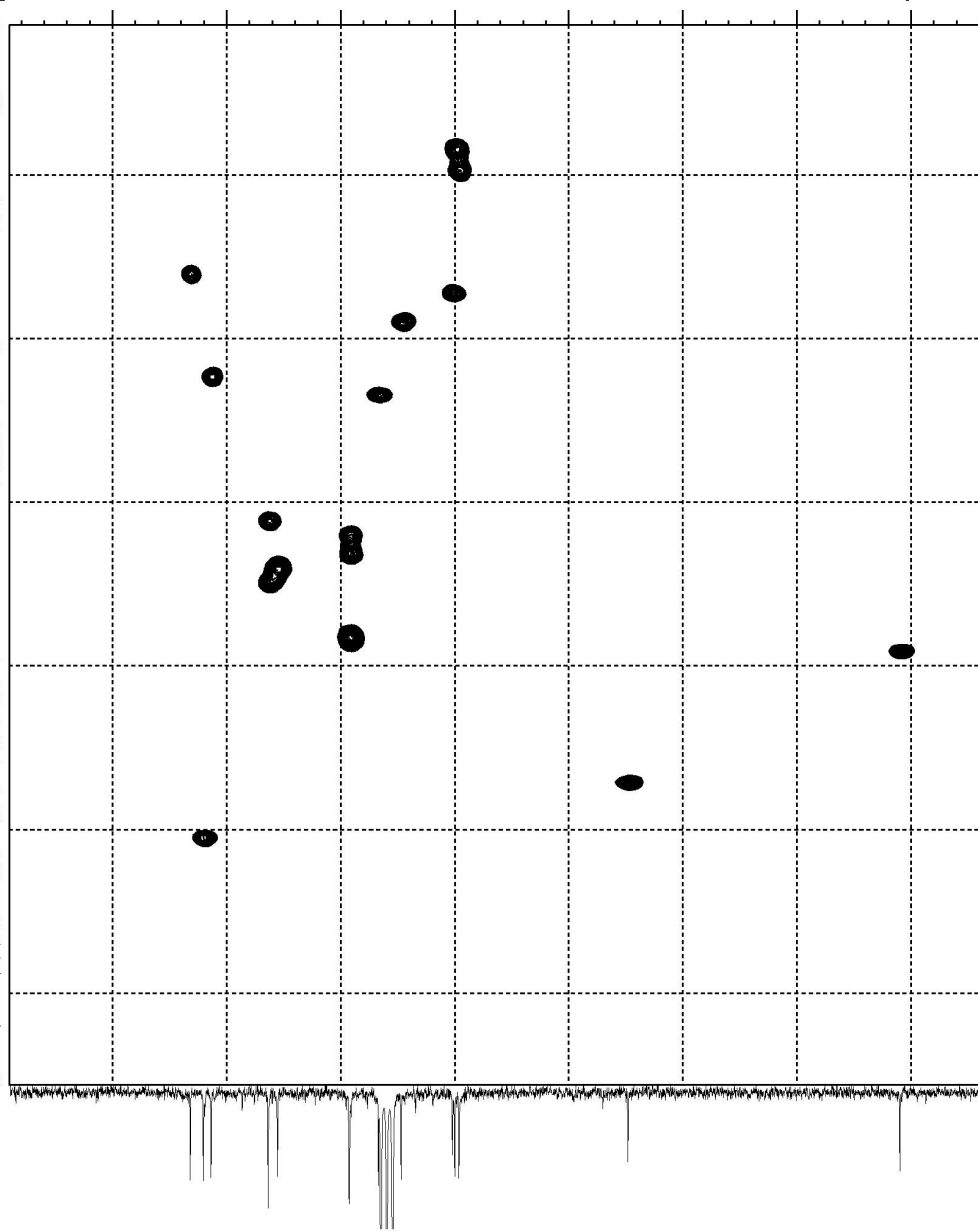




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ppm



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CHANNEL f2
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GPZ3 11.00 %
GPZ4 5.00 %
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PC 1.00

F1 - Processing parameters
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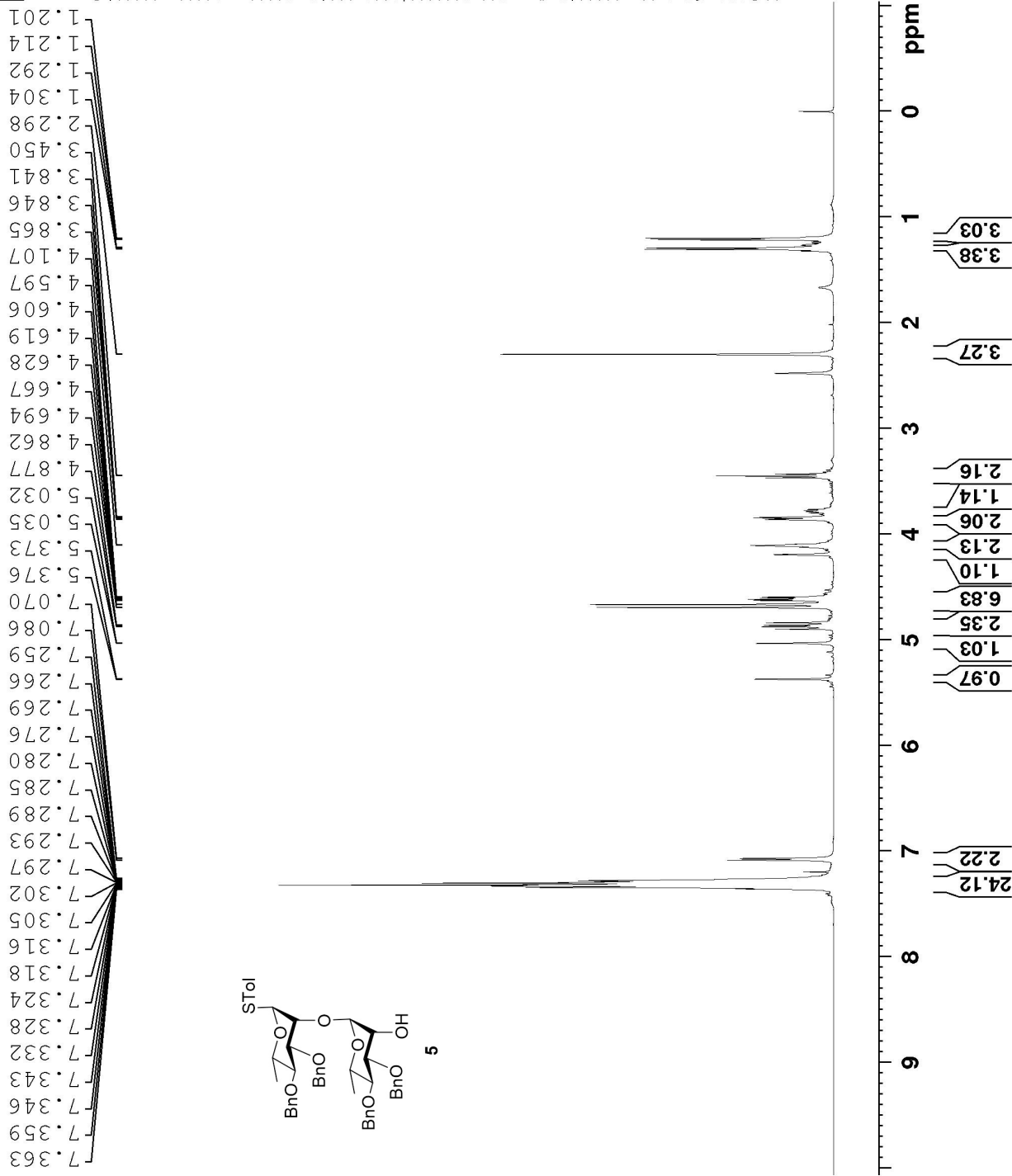
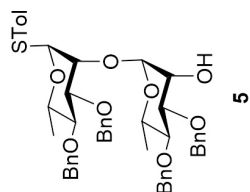


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GROUP BM
BM-AC-R169 in CDCl3



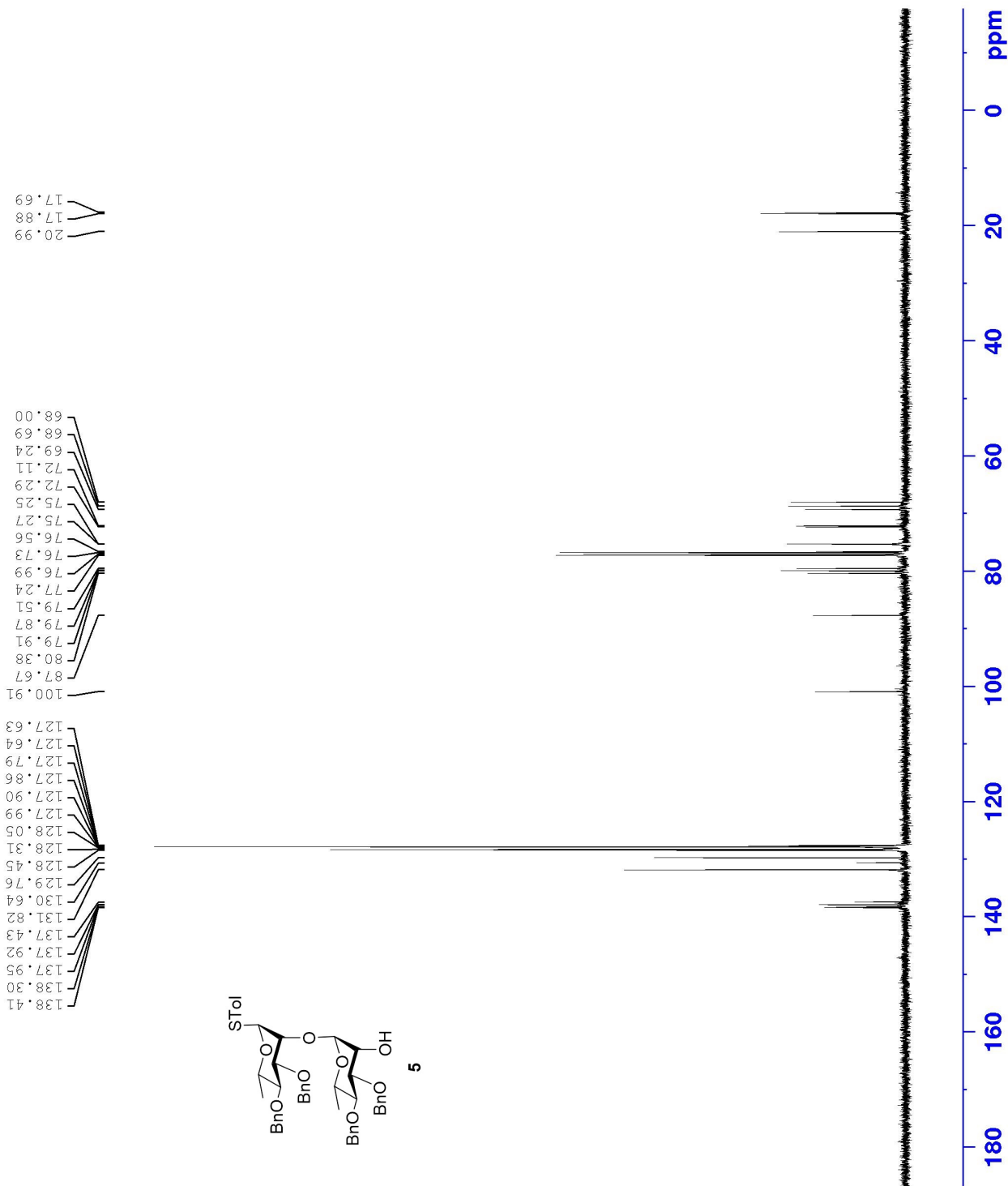
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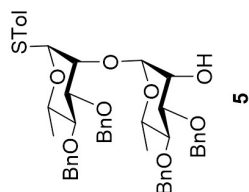
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TE 630.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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PLW1 66.00000000 W

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PLW13 0.24068999 W

F2 - Processing parameters
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LB 1.00 Hz
GB 0
PC 1.35





Current Data Parameters
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 PROCNO 1

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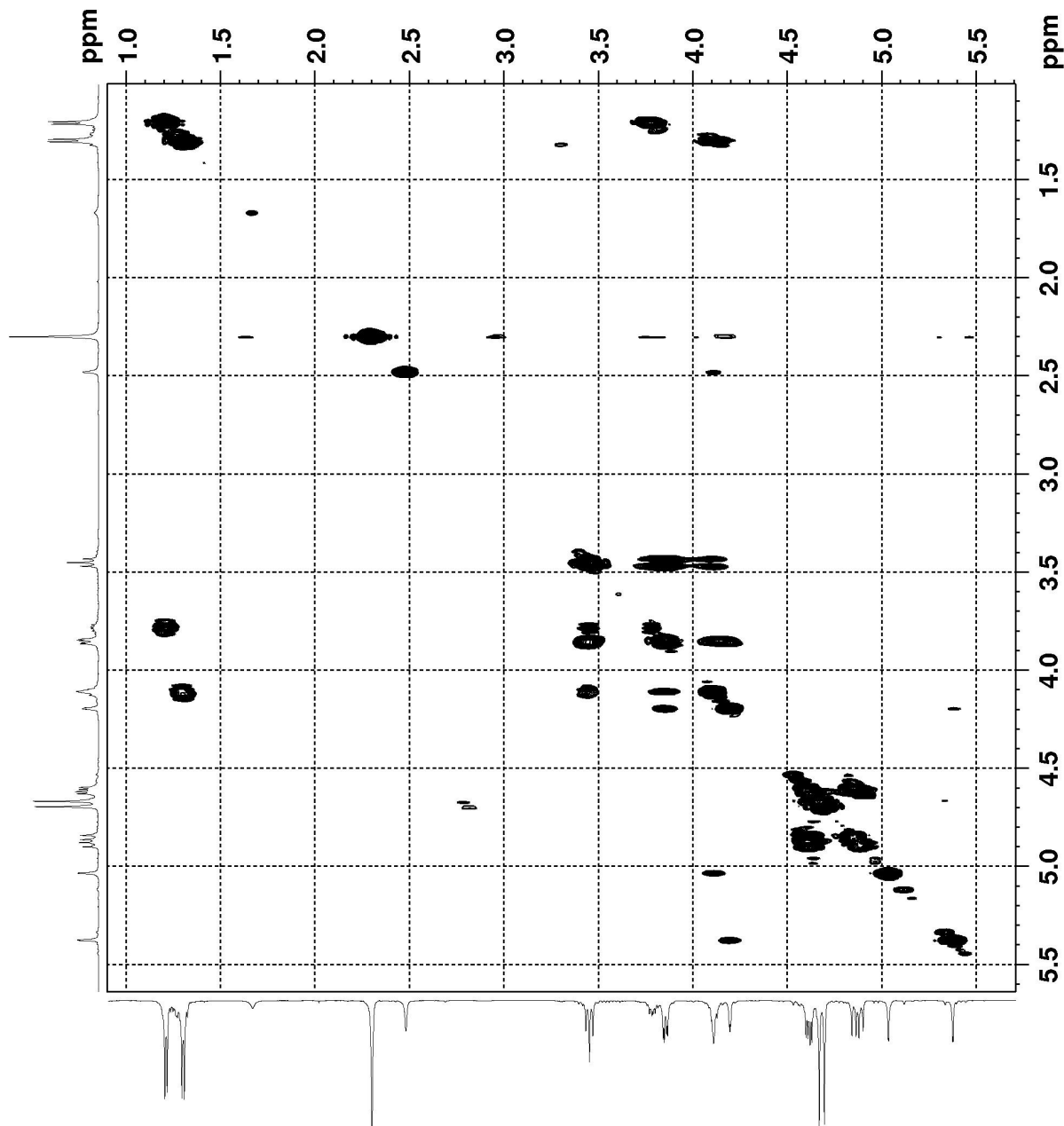
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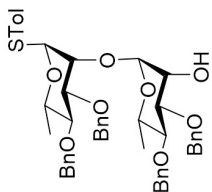
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 LB 0
 GB 0
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F1 - Processing parameters
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5



Current Data Parameters
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PROCNO 1

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DE 6.50 usec
TE 300.2 K
CNS12 145.000000 sec
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00000000 sec
D26 0.00082007 sec
D36 0.00000000 sec
INO 0.00001990 sec
ZGPG30

===== CHANNEL f1 =====
SFO1 500.362501 MHz
NUC1 13C
P1 17.50 usec
P2 35.00 usec
P28 1000.00 usec
PLW1 10.00000000 W

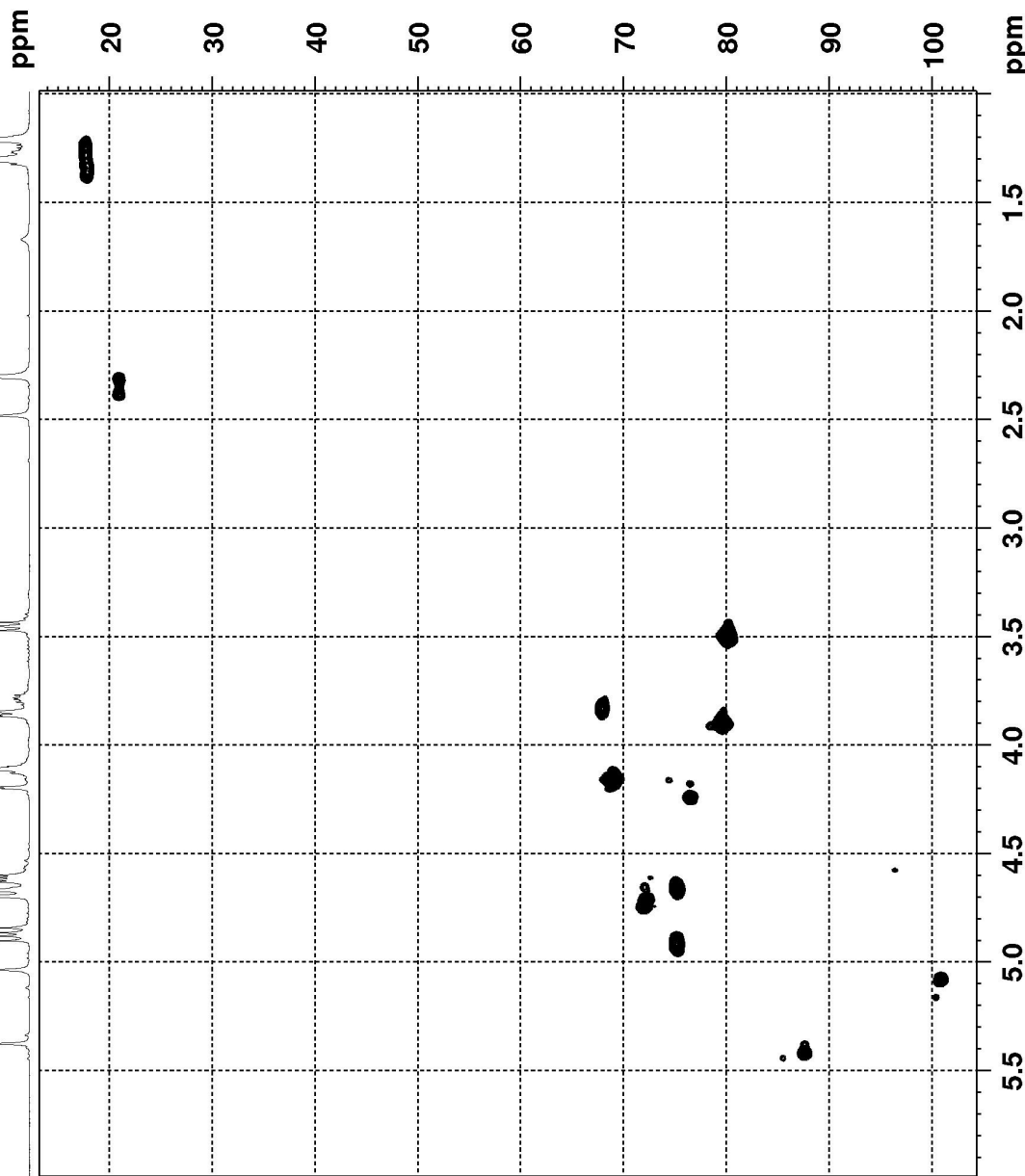
===== CHANNEL f2 =====
SFO2 125.828031 MHz
NUC2 13C
P1 11.50 usec
P2 23.00 usec
P28 1000.00 usec
PLW2 66.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GP21 80.00 %
GP22 20.10 %
GP23 11.00 %
GP24 11.00 %
P10 1000.00 usec
P19 600.00 usec

F1 - Acquisition Parameters
TD 256
SFO1 125.8282 MHz
FIDRES 199.6367 Hz
SW 199.632 Fm
FNAME Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.360000 MHz
WDW HANN
SSB 0
LB 0 Hz
GB 0
PC 1.00

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



GROUP BM
BM-AC-R80 in CDCl3

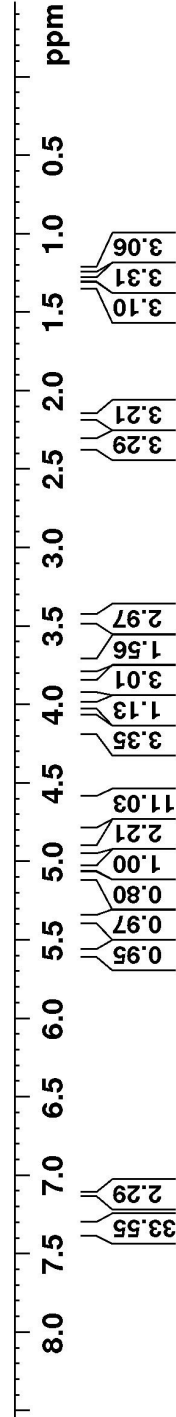
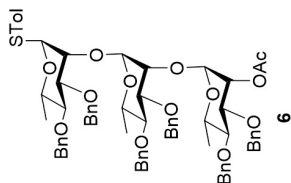
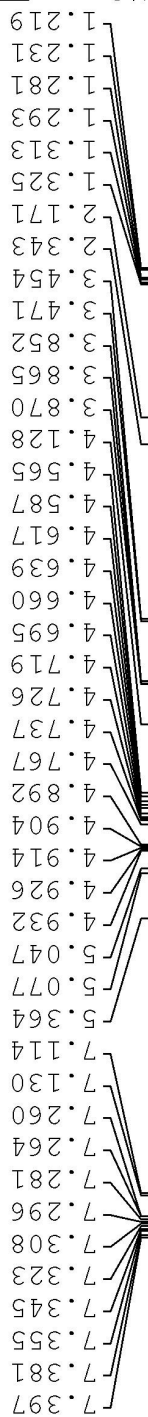


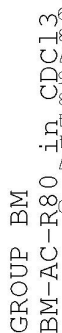
Current Data Parameters
NAME BM-AC-R80
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190426
Time 11:22
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO 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





F2 - Acquisition Parameters	
Date_	20190426
Time	11.27
INSTRUM	Brucker_default_av500
PULPROG	zgpg30
ID	65536
SOLVENT	CDCl3
NS	150
DS	4
SSNH	43859.648 Hz
FIDRES	0.669245 Hz
RG	0.7471104 sec
DW	203
DE	11.400 usec
TE	6.50 usec
D1	300.9 K
D11	2.00000000 sec
D10	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
PLM12     0.47852001 W
PLM13     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



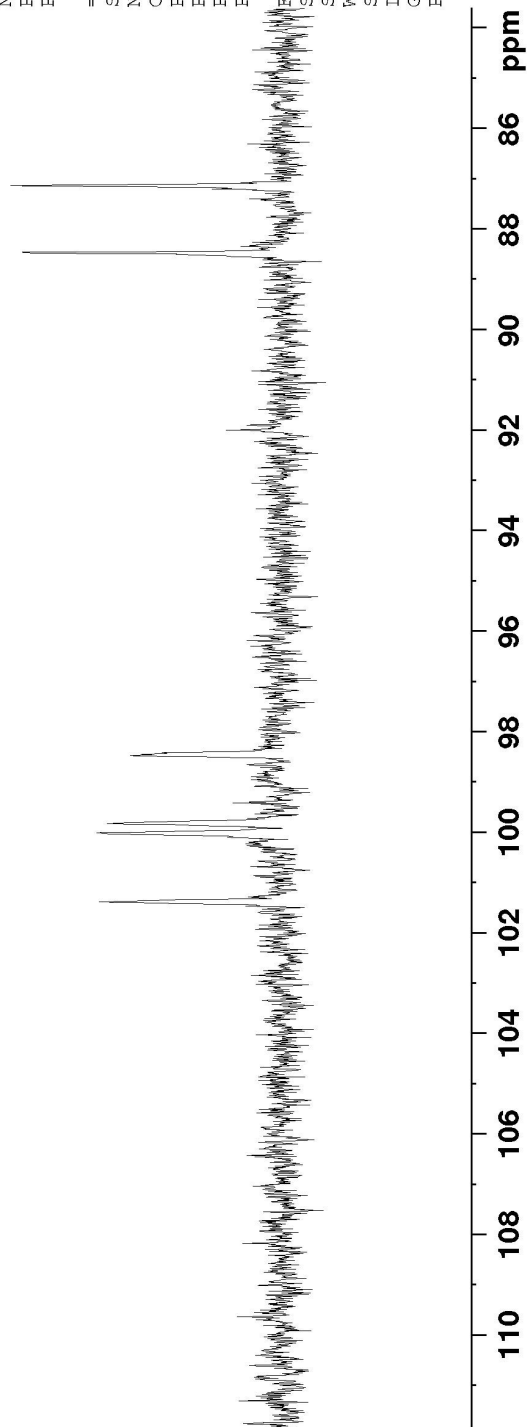
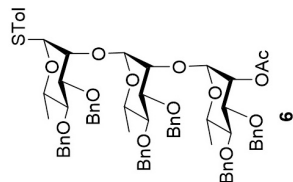
Current Data Parameters
NAME BM-AC-R80
EXPNO 170
PROCNO 1

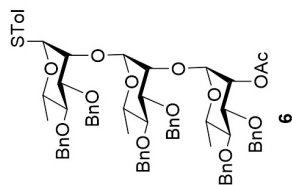
F2 - Acquisition Parameters
Date_ 20191217
Time 20.29
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 16065
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 203
DW 13.200 usec
DE 6.150 usec
TE 276.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG2 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





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 cosygpppqr
 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 0.0000000 sec
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec
 D13 0.0000040 sec
 D16 0.0002000 sec
 INO 0.00019980 sec

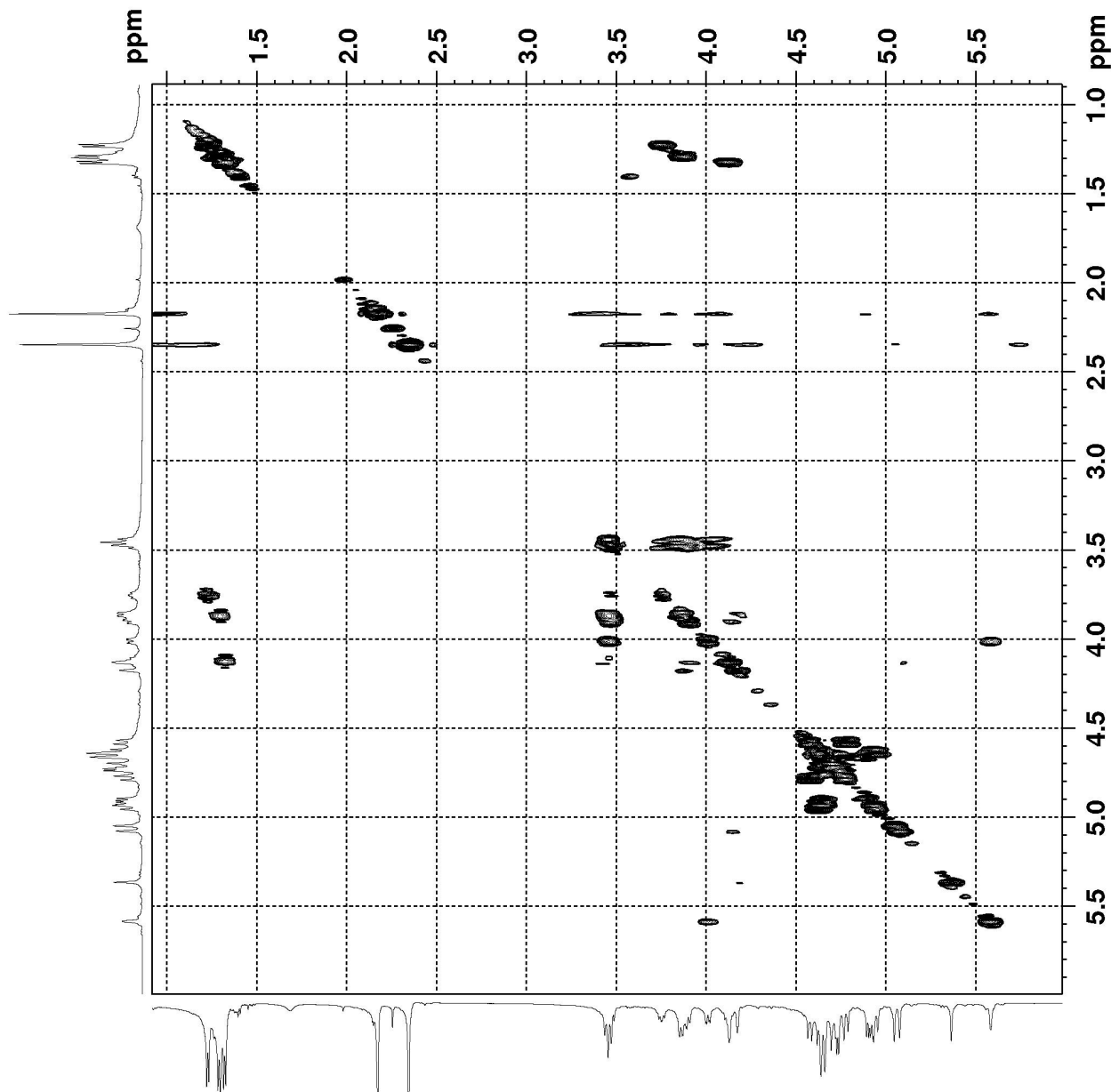
===== CHANNEL f1 =====
 SF01 500.3425017 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.0000000 W
 PLW10 3.40280008 W

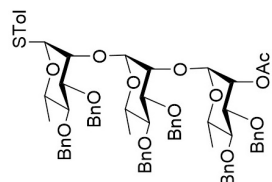
===== GRADIENT CHANNEL =====
 GPMAM[1] SMSQ10.100
 GPZ1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SF01 500.3425 MHz
 FIDRES 78.203201 Hz
 SW 10.003 ppm
 F1MODE QF

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

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

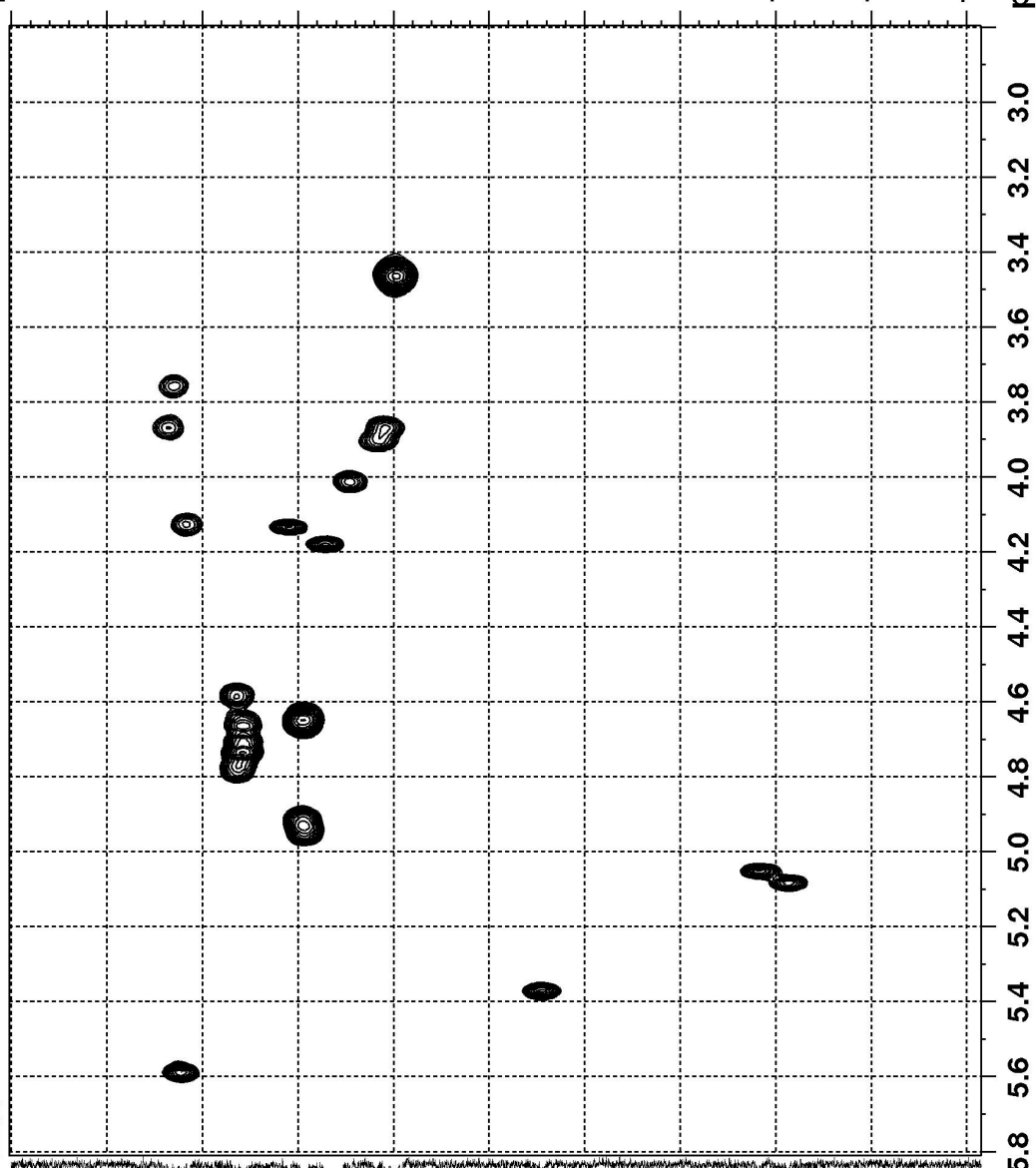




Current Data Parameters
 NAME BM-AC-R80
 EXFO 63
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190426
 Time 11:42
 INSHW Bruker default_av500
 F2PROG zgpg30
 FULPROG hsqcztg32
 TD 1024
 SOLVENT CDCl3
 NS 2
 DS 16
 SW 5000.016 Hz
 FIDRES 4.882813 Hz
 AQ 0.1024000 sec
 RG 50.8
 DM 100.000 usec
 DE 6.50 usec
 TE 300.2 K
 CNUST2 145.0000000
 D0 0.00000300 sec
 D1 1.50000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00000000 sec
 D2 0.0006207 sec
 D3 0.00000000 sec
 INO 0.00001930 sec
 ZGPGTNS

ppm



CHANNEL f1
 SFO1 500.3425017 MHz
 NUC1 13C
 P1 17.50 usec
 P2 35.00 usec
 P28 1000.00 usec
 PLW1 10.00000000 W

CHANNEL f2
 SFO2 125.8231741 MHz
 NUC2 13C
 CPDPRG2 garp
 P3 11.50 usec
 P4 23.00 usec
 P4P2 76.00 usec
 P4M2 66.00000000 W
 P4M12 1.78129995 W

GRADIENT CHANNEL
 GPM1[1] SMSQ10.100
 GPM1[2] SMSQ10.100
 GPM1[3] SMSQ10.100
 GPM1[4] SMSQ10.100
 GP21 80.00 %
 GP22 20.10 %
 GP23 11.00 %
 GP24 5.00 %
 P10 100.00 usec
 P19 600.00 usec

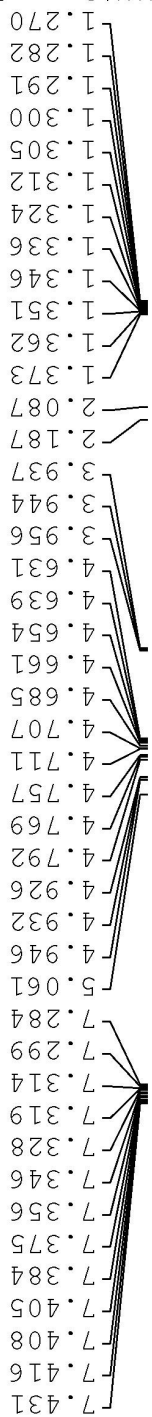
F1 - Acquisition Parameters
 TD 145
 SFO1 125.8232 MHz
 FIDRES 344.862813 Hz
 SW 199.630 Fm
 F2MODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 500.3403113 MHz
 WDW QSI
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

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

ppm

GROUP BM
BM-AC-R176 in CDCl3

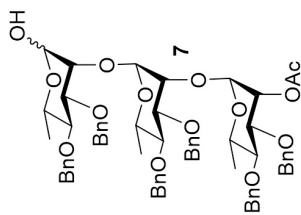


Current Data Parameters
NAME BM-AC-R176
EXPNO 290
PROCNO 1

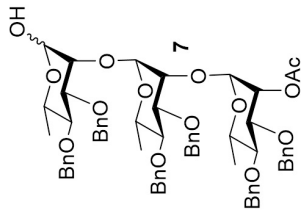
F2 - Acquisition Parameters
Date_ 20191226
Time 18.15
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65560
SOLVENT CDCl3
NS 4
DS 2
SWH 12500.000 Hz
FIDRES 0.187800 Hz
AQ 2.6624000 sec
RG 32
DW 40.000 usec
DE 6.50 usec
TE -2434.5 K
D1 1.00000000 sec
TD0 1

===== 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



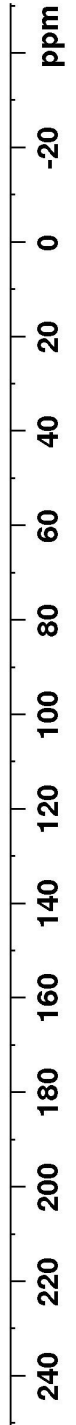
Current Data Parameters
NAME BM-AC-R176
EXPNO 291
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191226
Time 18.20
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO 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
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

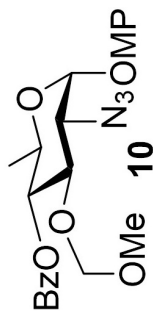
F2 - Processing parameters
SI 32768
SF 125.8156286 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.35



GROUP BM
BM-AC-R61 in CDCl₃



7.605
7.590
7.575
7.479
7.464
7.449
7.260
7.105
7.087
7.079
6.881
6.875
6.857
6.850
5.478
5.471
5.168
5.149
5.130
4.794
4.780
4.758
4.744
4.402
4.383
4.364
4.185
4.173
4.160
4.153
4.140
4.128
3.779
3.456
3.449
3.435
3.428
3.265
1.224
1.211

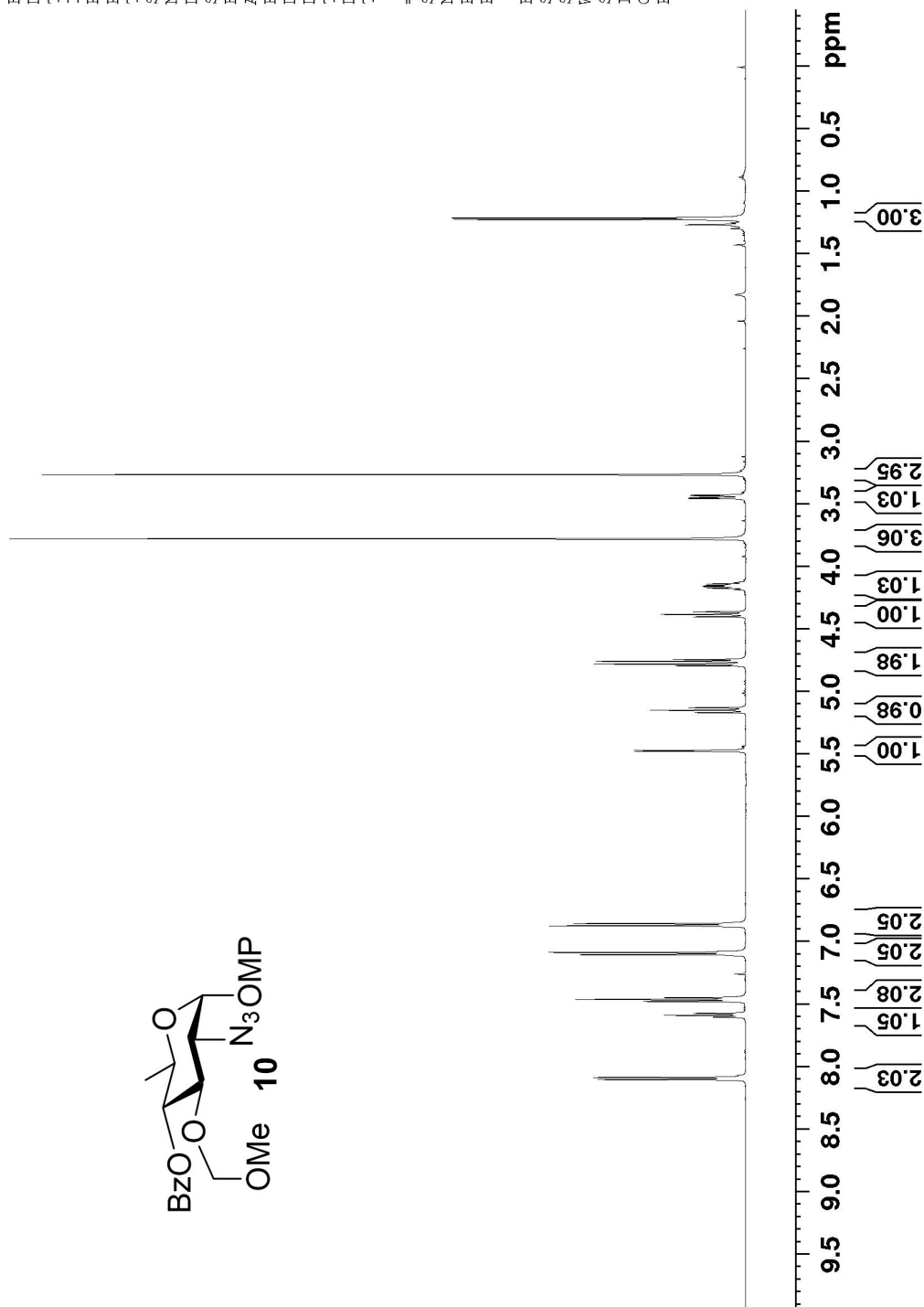


Current Data Parameters
NAME BM-AC-R61
EXPNO 70
PROCNO 1

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



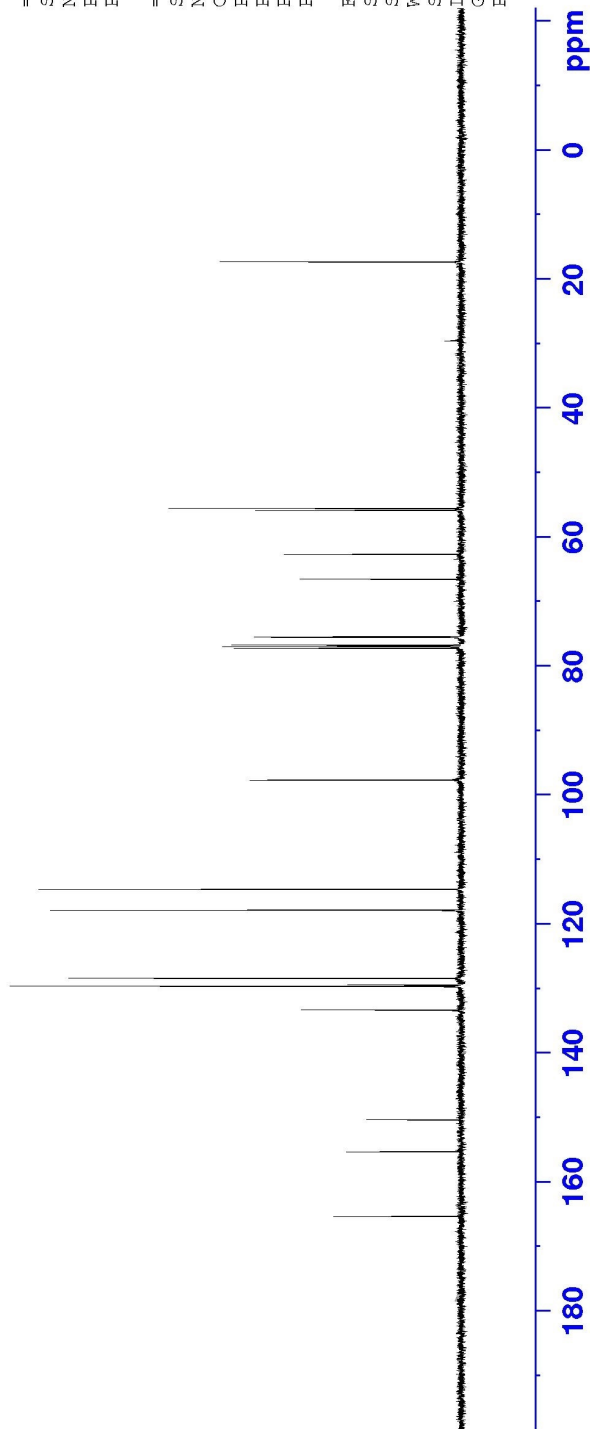
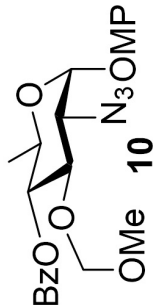
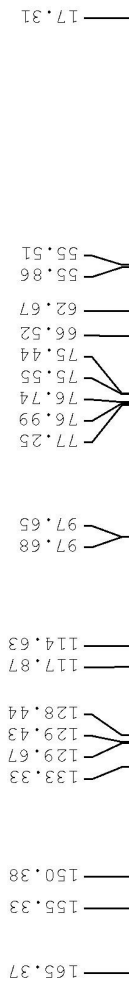
Current Data Parameters
NAME BM-AC-R61
EXPNO 71
PROCNO 1

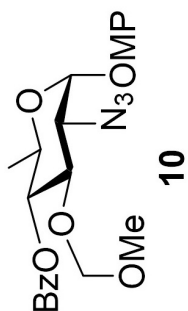
F2 - Acquisition Parameters
Date_ 20180607
Time 15.19
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG2 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 0 1.00 Hz
GB 0
PC 1.40





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 cosygpppqr
 TD 2048
 SOLVENT CDCl3
 NS 1
 DS 8
 SWH 4504.504 Hz
 FIDRES 2.139465 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 0.00020000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00022200 sec

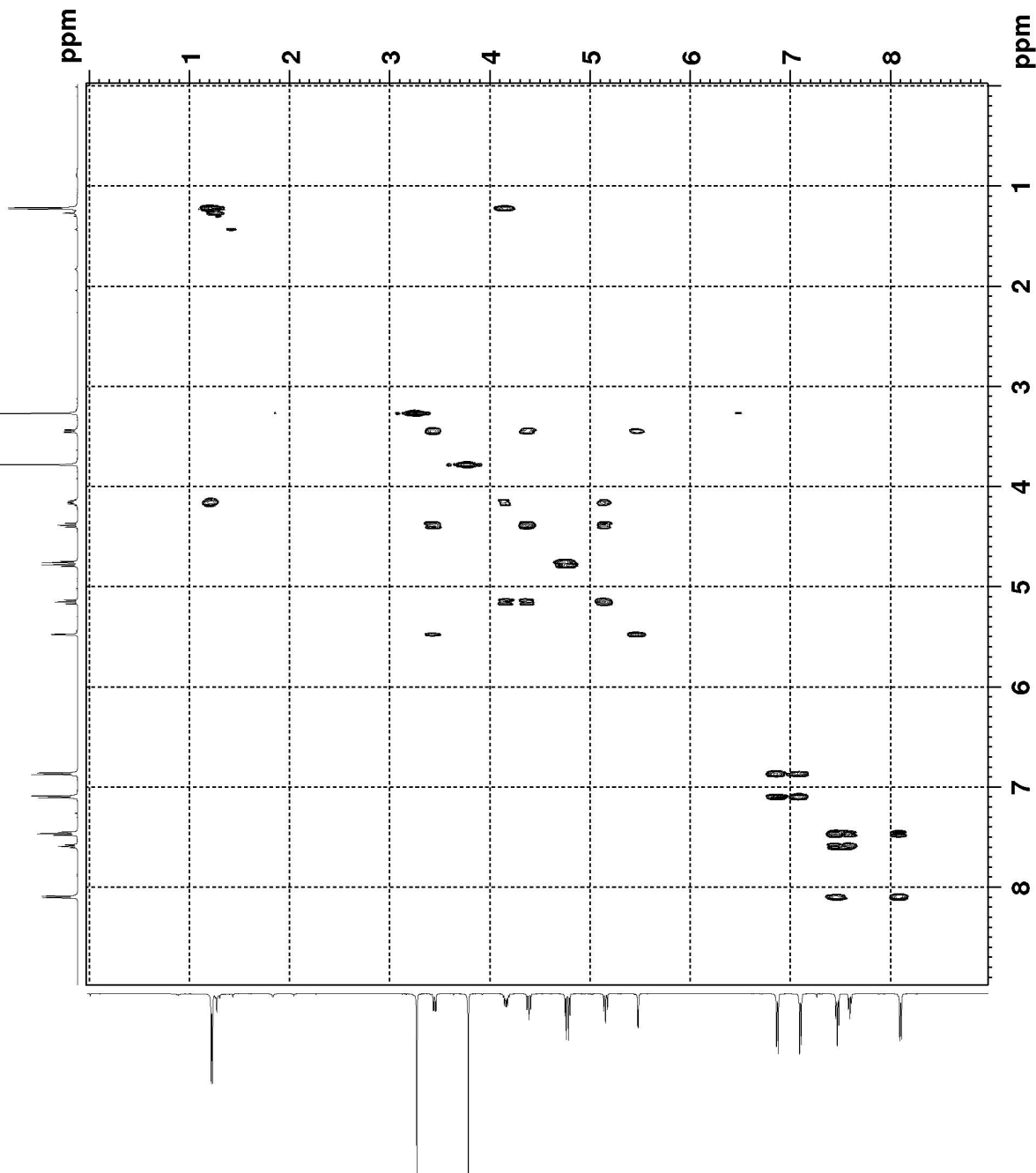
===== CHANNEL f1 =====
 SFO1 500.3422515 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.00000000 W
 PLW10 3.40280008 W

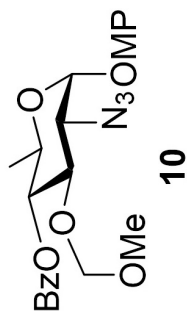
===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPZ1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 87
 SFO1 500.3423 MHz
 FIDRES 103.551826 Hz
 SW 9.003 ppm
 F1MODE QF

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

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





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 QNP 1H/13
PULPROG zgpg30
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 4504.536 Hz
FIDRES 4.336930 Hz
AQ 0.1136640 sec
RG 40.3
DM 111.000 usec
DE 6.50 usec
TE 300.2 K
CNS12 145.000000
DO 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.05000000 sec
D26 0.0086207 sec
ZGPGTNS 0.0000190 sec

===== CHANNEL f1 =====
SFO1 500.3422515 MHz
NUC1 13C
P1 17.50 usec
P2 35.00 usec
P28 1000.00 usec
PLW1 10.00000000 W

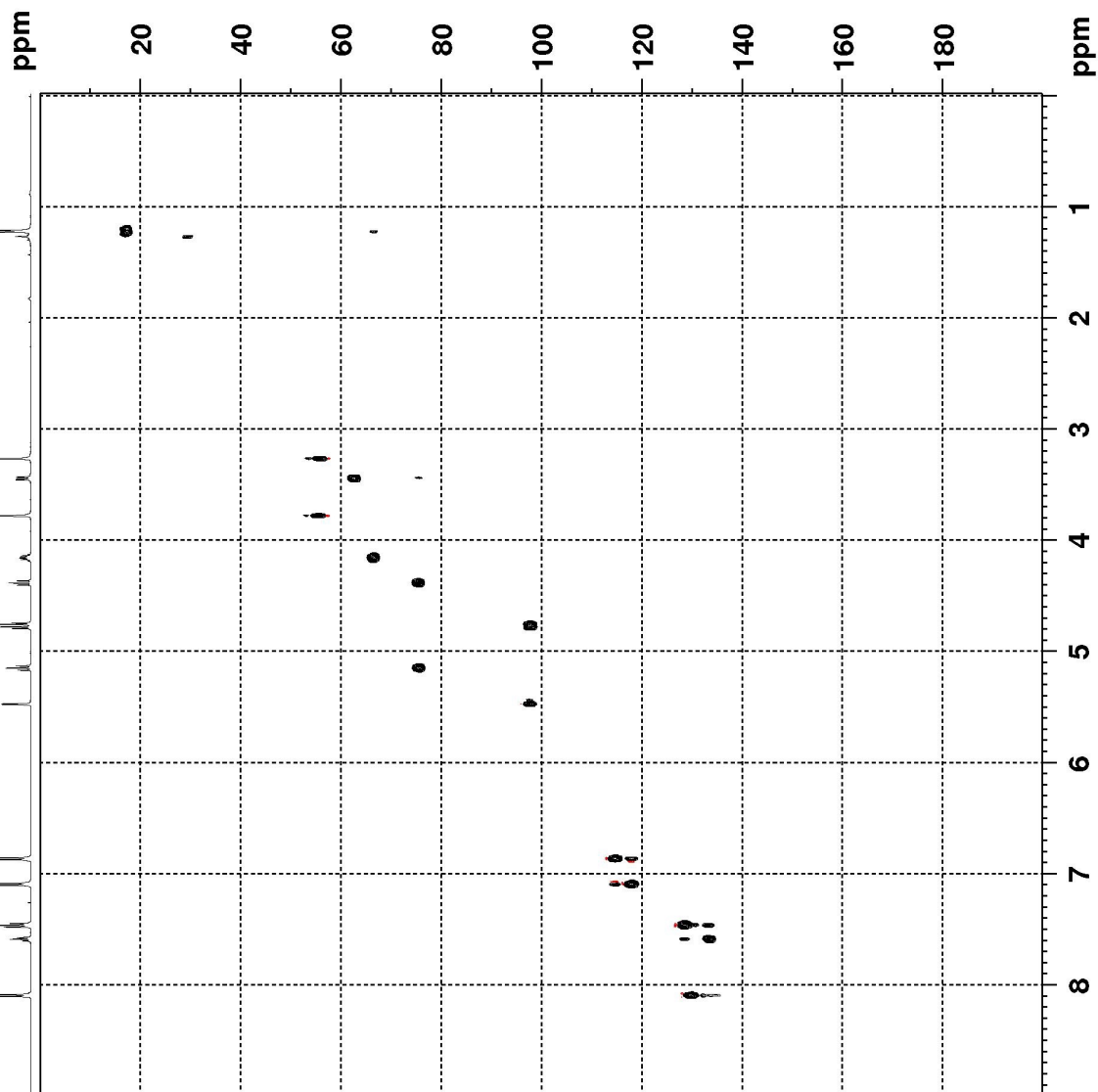
===== CHANNEL f2 =====
SFO2 125.8231741 MHz
NUC2 13C
P1 11.50 usec
P2 23.00 usec
P28 1000.00 usec
PLW2 66.00000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SSGQ10.100
GPNAM[2] SSGQ10.100
GPNAM[3] SSGQ10.100
GPNAM[4] SSGQ10.100
GP21 80.00 %
GP22 20.10 %
GP23 11.00 %
GP24 5.00 %
P1 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 137
SFO1 125.8232 MHz
FIDRES 366.136810 Hz
SW 199.690 Fm
F1MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW QSI
SSB 2
LB 0 Hz
GB 0
PC 1.00

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



GROUP BM
BM-AC-R70 in CDCl3



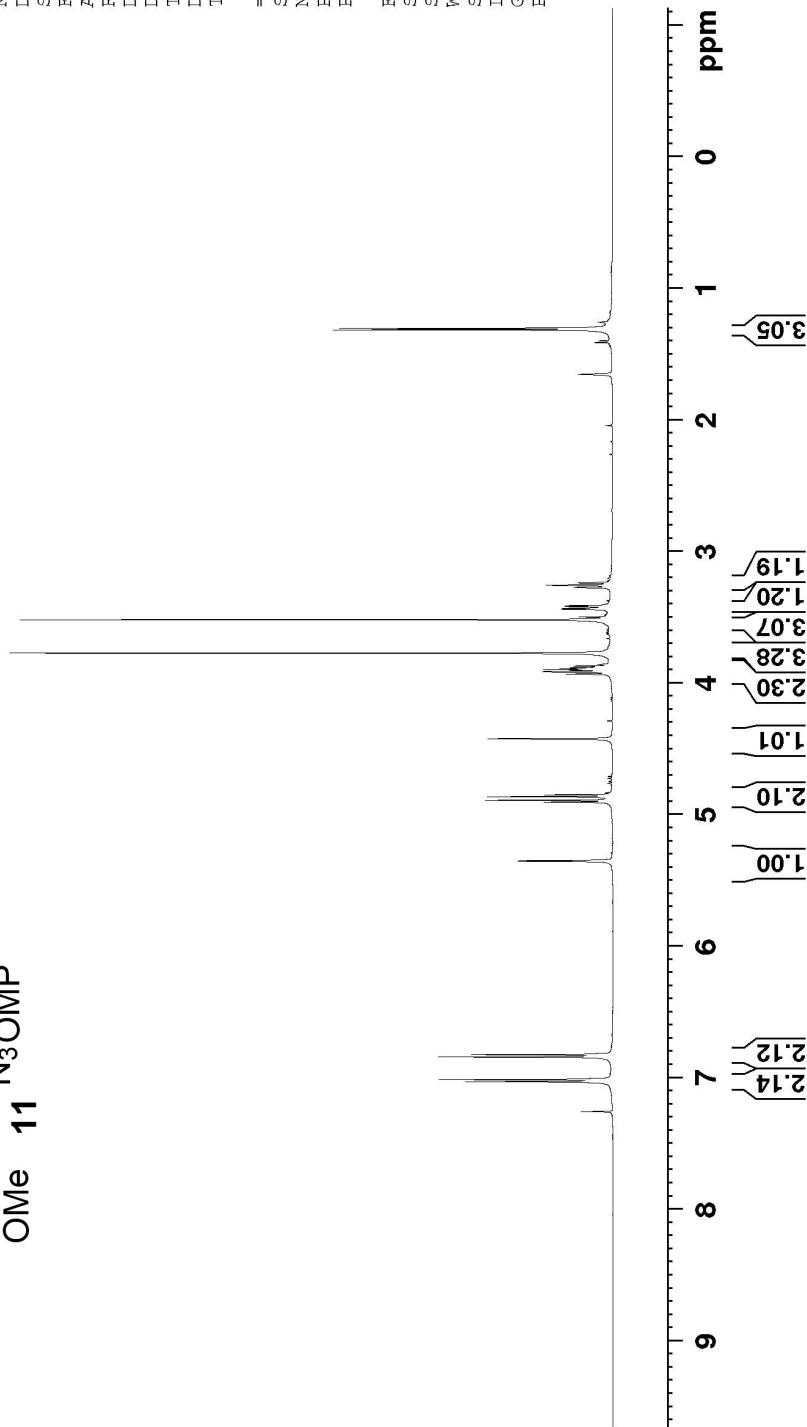
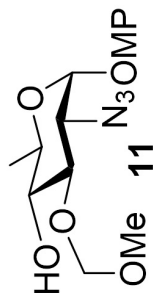
Current Data Parameters
NAME BM-AC-R70
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180720
Time 11.42
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO 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

7.259
7.032
7.014
6.842
6.825
5.356
5.349
4.906
4.892
4.864
4.850
4.423
3.932
3.915
3.912
3.902
3.895
3.889
3.883
3.877
3.870
3.772
3.519
3.439
3.432
3.418
3.411
3.273
3.255
3.237
1.314
1.302



GROUP BM
BM-AC-R70 in CDCl3



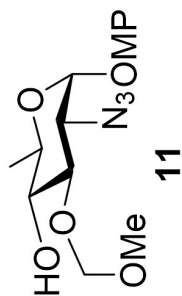
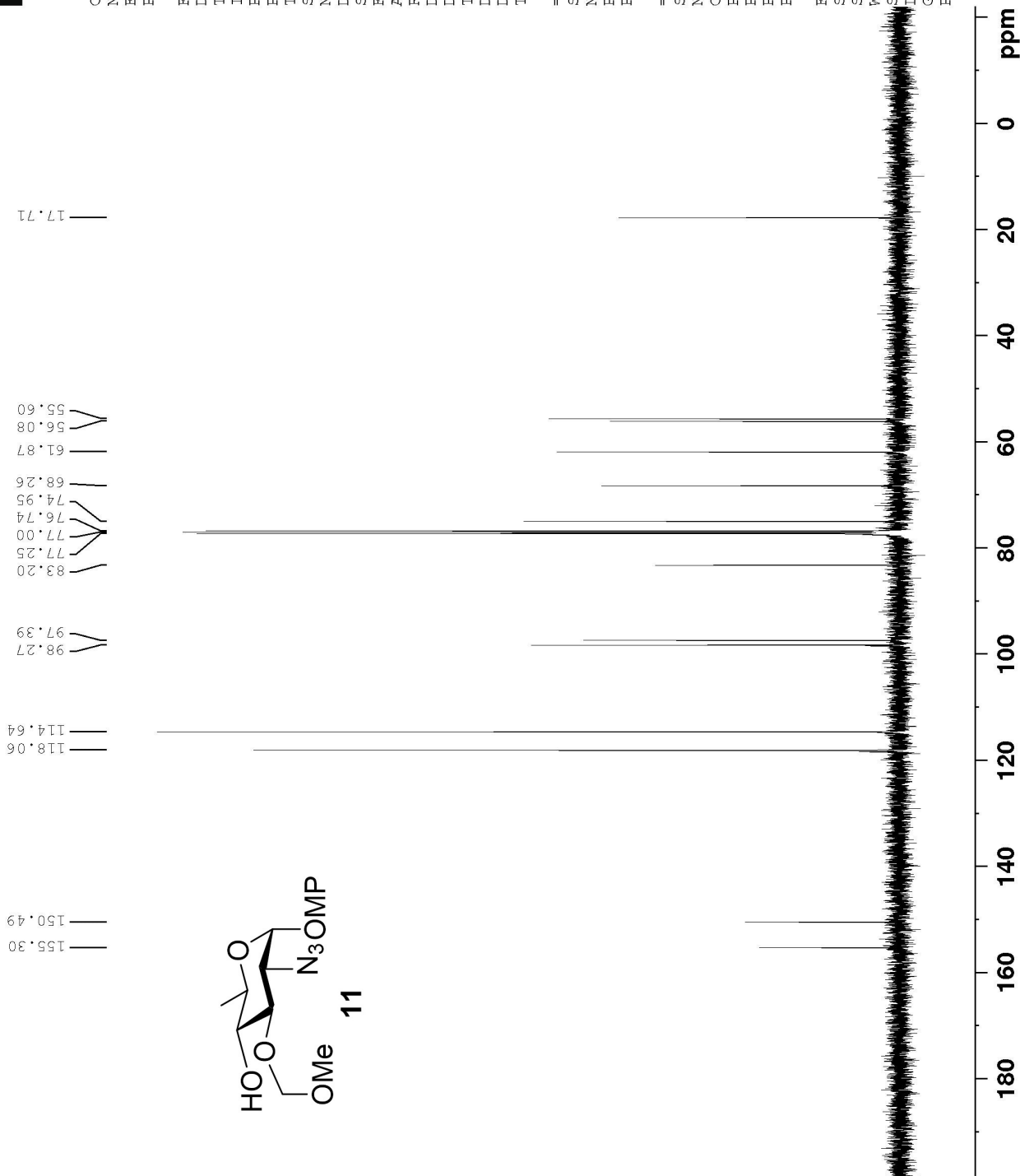
Current Data Parameters
NAME BM-AC-R70
EXPNO 21
PROCNO 1

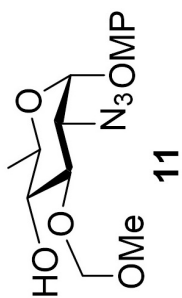
F2 - Acquisition Parameters
Date_ 20180720
Time 11.57
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 77
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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 0
GB 0
PC 1.40





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 cosygpppqr
 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 0.00020000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019980 sec

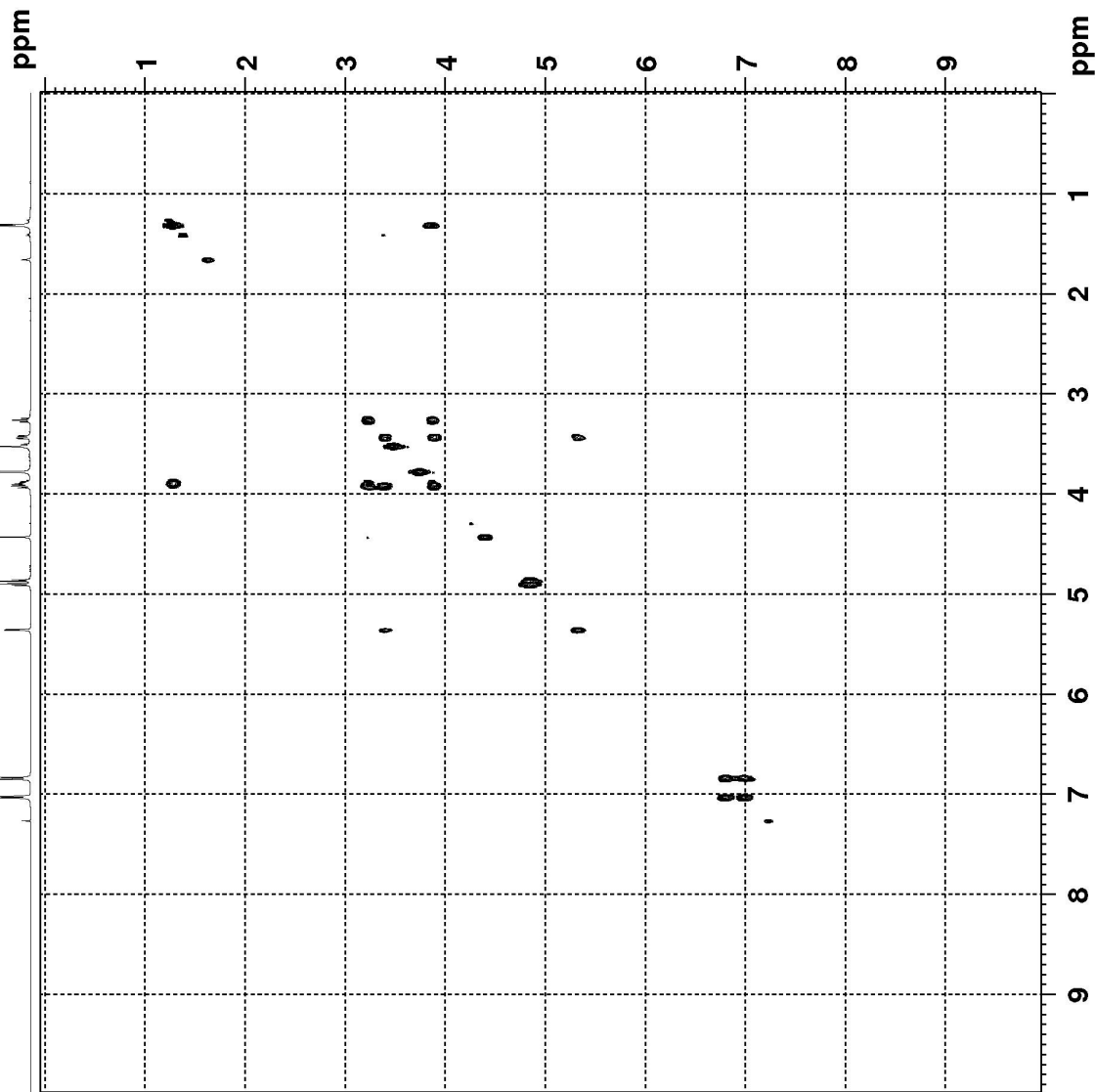
===== CHANNEL f1 =====
 SF01 500.3425017 MHz
 NUC1 1H
 P0 17.50 usec
 PL 17.50 usec
 PL1 2500.00 usec
 PLW1 10.00000000 W
 PLW10 3.40280008 W

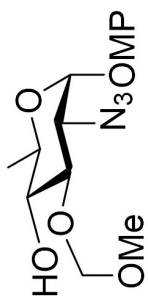
===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GP21 10.00 %
 PL6 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SF01 500.3425 MHz
 FIDRES 78.203201 Hz
 SW 10.003 ppm
 F1MODE QF

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

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

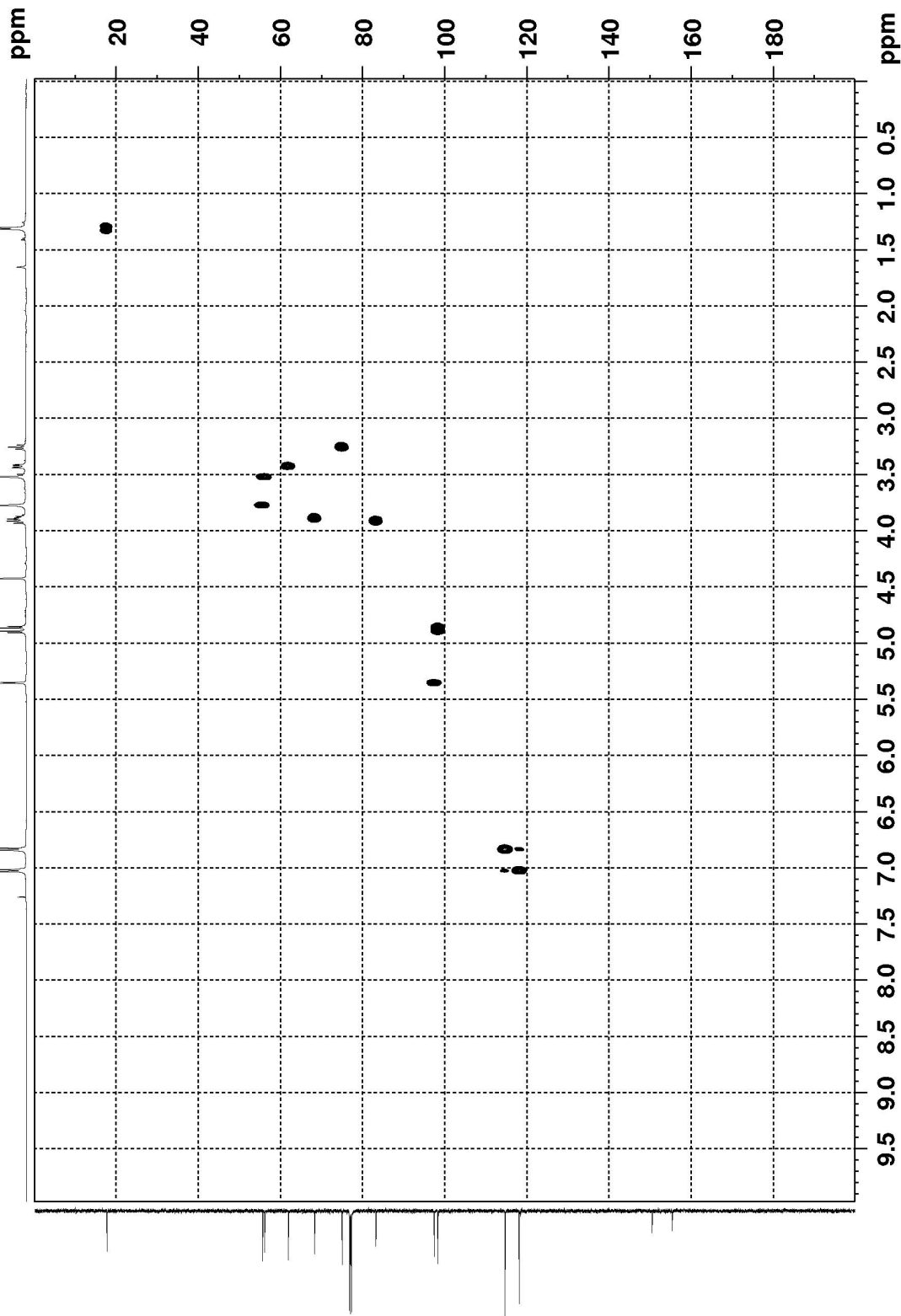




11



Current Data Parameters
NAME BM-AC-R70
EXPNO 23
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080707
Time 11.59
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG hsqcztgpsi2
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 5000.000 Hz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 327.5
DM 100.000 usec
DE 6.50 usec
TE 299.5 K
CNS12 145.0000000
D0 0.0000300 sec
D1 1.0000000 sec
D2 0.0017244 sec
D3 0.0000000 sec
D11 0.0300000 sec
D16 0.0002000 sec
D24 0.00086207 sec
INO 0.00001990 sec
ZGPGFNS
===== CHANNEL f1 =====
SFO1 500.3425017 MHz
NUC1 1H
P1 17.50 usec
F1 175.00 usec
P2 100.00 usec
F2 100.0000000 W
ELW1 10.0000000 W
===== CHANNEL f2 =====
SFO2 125.8231741 MHz
NUC2 13C
P3 17.50 usec
F3 175.00 usec
P4 23.00 usec
F4 23.0000000 W
PCPD2 66.00000000 W
PLW2 70.00 usec
PLW12 1.78129995 W
===== GRADIENT CHANNEL =====
GPNAM[1] SWSQ10.100
GPNAM[2] SWSQ10.100
GPNAM[3] SWSQ10.100
GPNAM[4] SWSQ10.100
GPZ1 20.00 %
GPZ2 20.00 %
GPZ3 11.00 %
GPZ4 -5.00 %
PL6 1000.00 usec
PL9 600.00 usec
F1 - Acquisition Parameters
TD 1024
SFO1 125.8232 MHz
FIDRES 492.659363 Hz
SW 199.690 KHz
FWDWDE Echo-Antiecho
F2 - Processing Parameters
SI 1024
SF 500.3400127 MHz
WDW Q8LINE
SSB 2
LB 0 Hz
GB 0
PC 1.00
F1 - Processing Parameters
SI 1024
WDW echo-antiecho
SF 125.8231741 MHz
WDW Q8LINE
SSB 2
LB 0 Hz
GB 0



GROUP BM
BM-AC-R71 in CDCl3



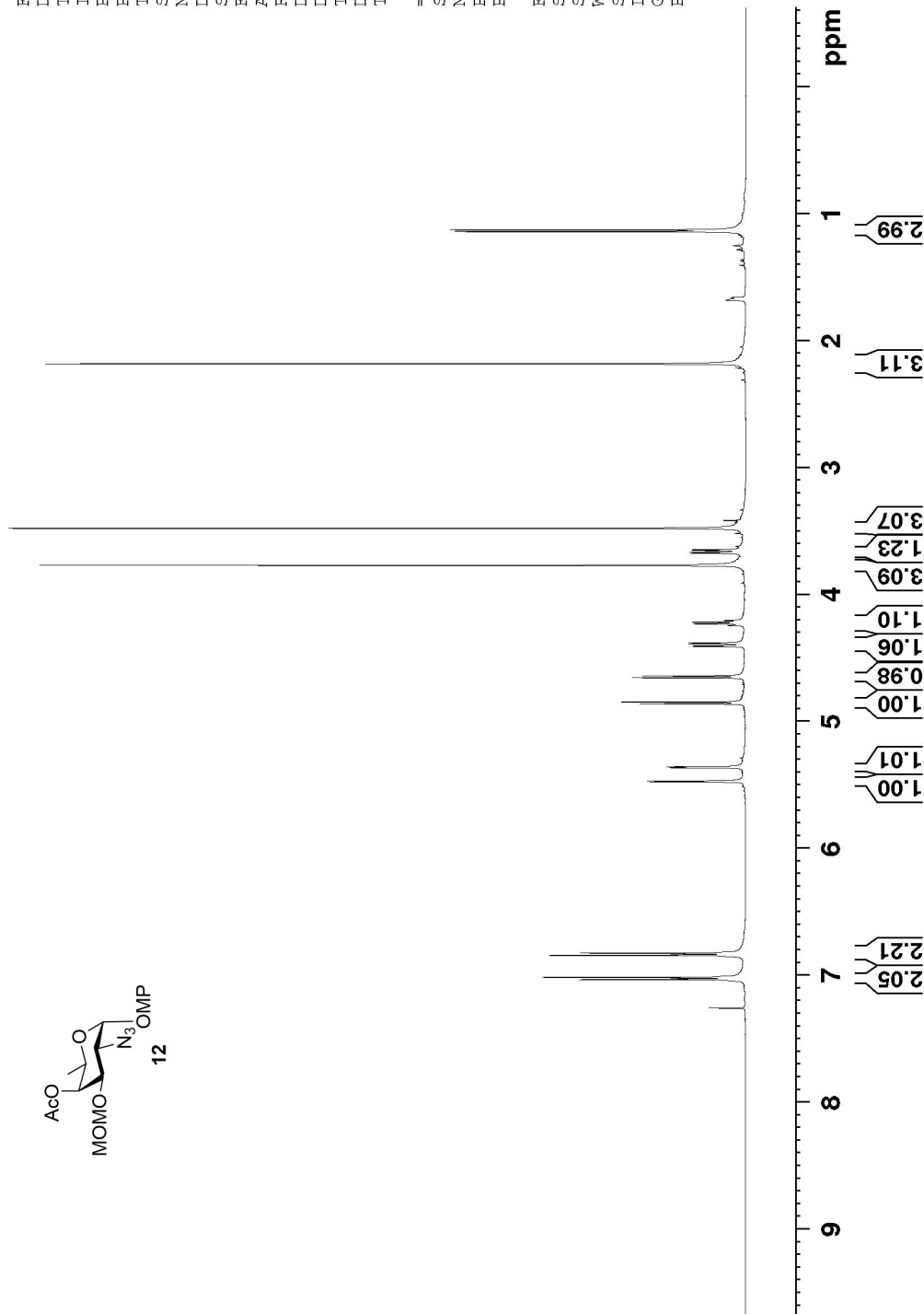
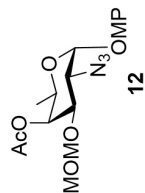
Current Data Parameters
NAME BM-AC-R71
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180725
Time 12.55
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO 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

7.260
7.035
7.031
7.022
7.017
6.845
6.840
6.831
6.827
5.477
5.470
5.364
5.359
4.862
4.848
4.656
4.642
4.409
4.403
4.388
4.381
4.231
4.218
3.769
3.676
3.669
3.654
3.647
3.479
2.182
1.140
1.127



GROUP BM
BM-AC-R71 in CDCl3



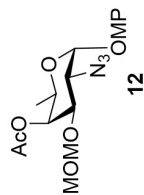
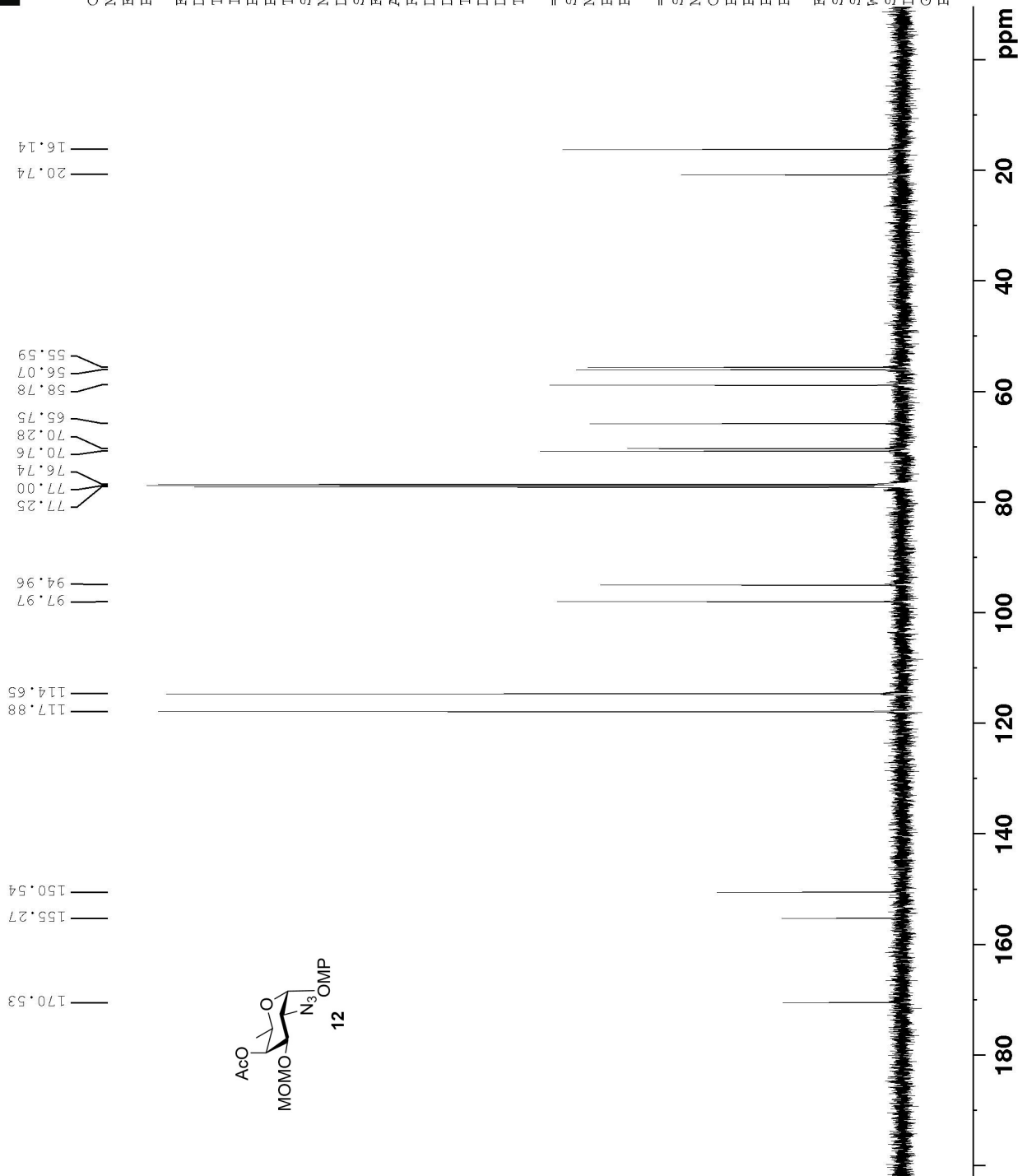
Current Data Parameters
NAME BM-AC-R71
EXPNO 91
PROCNO 1

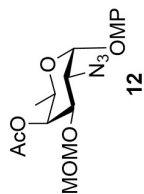
F2 - Acquisition Parameters
Date_ 20180725
Time 12.59
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 89
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG2 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 0
GB 1.00 Hz
PC 1.40





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 FAPBO 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 0.00020000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019980 sec

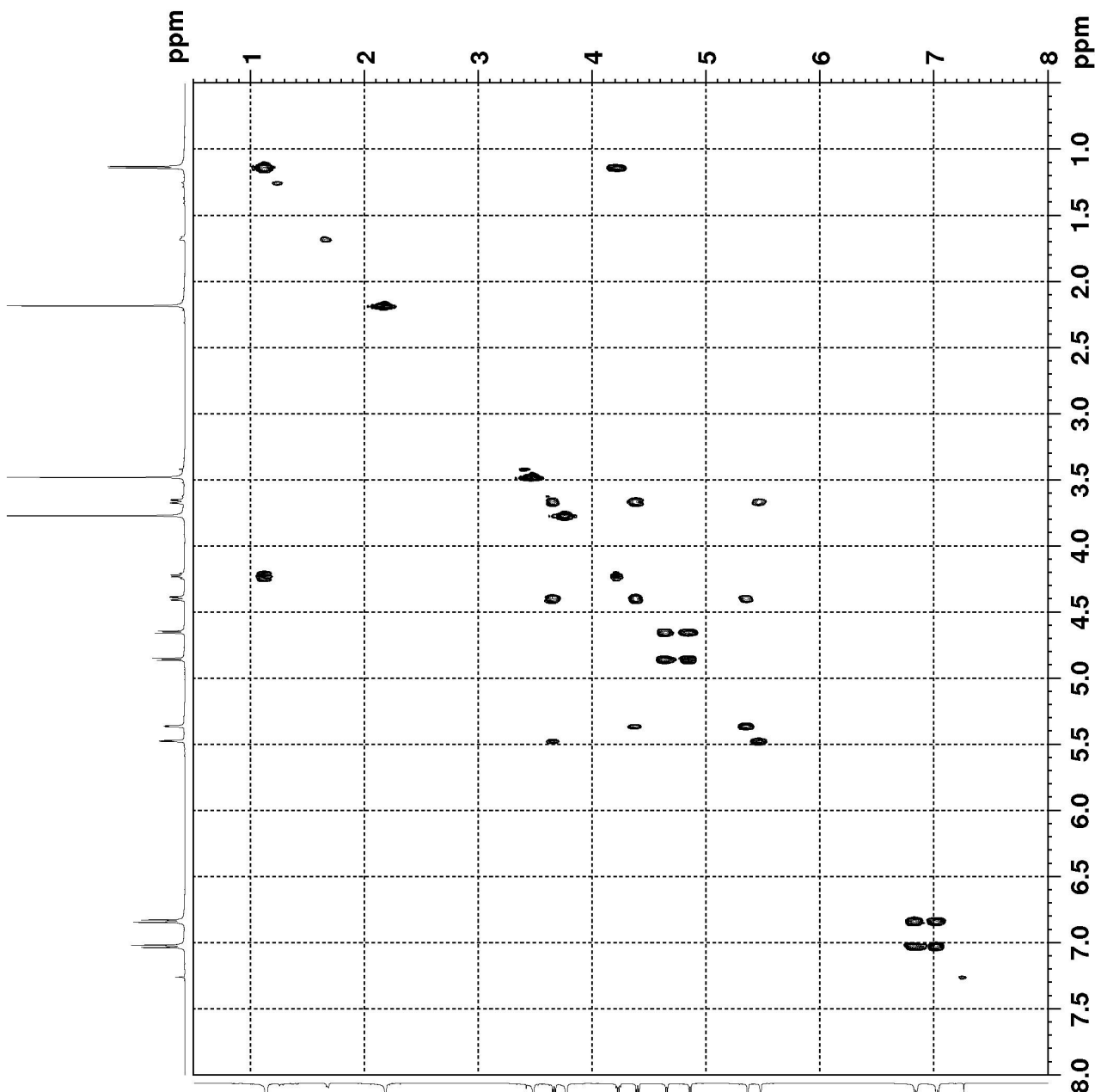
===== CHANNEL f1 =====
 SFO1 500.3425017 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.00000000 W
 PLW10 3.40280008 W

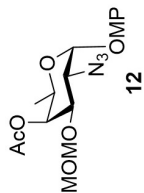
===== GRADIENT CHANNEL =====
 GENAM[1] SMSQ10.100
 GFZ1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 500.3425 MHz
 FIDRES 78.203201 Hz
 SW 10.003 ppm
 F1MODE QF

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

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





Current Data Parameters
 NAME BM-AC-R71
 EXNO 93
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180725
 Time 13.13
 INSHW Bruker-default_av500
 PULPROG zgpg30

TD 1024
 SOLVENT CDCl3
 NS 2
 DS 16
 SWH 5000.016 Hz
 FIDRES 4.882813 Hz
 AQ 0.1024000 sec
 RG 71.8
 DM 100.000 usec
 DE 6.50 usec
 TE 300.2 K
 CNUST2 145.0000000
 D0 0.00000300 sec
 D1 1.50000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00000000 sec
 D26 0.0006207 sec
 INO 0.0000190 sec
 ZGPGTNS

CHANNEL f1
 SFO1 500.3425017 MHz
 NUC1 13C
 P1 17.50 usec
 P2 35.00 usec
 P28 1000.00 usec
 PLW1 10.00000000 W

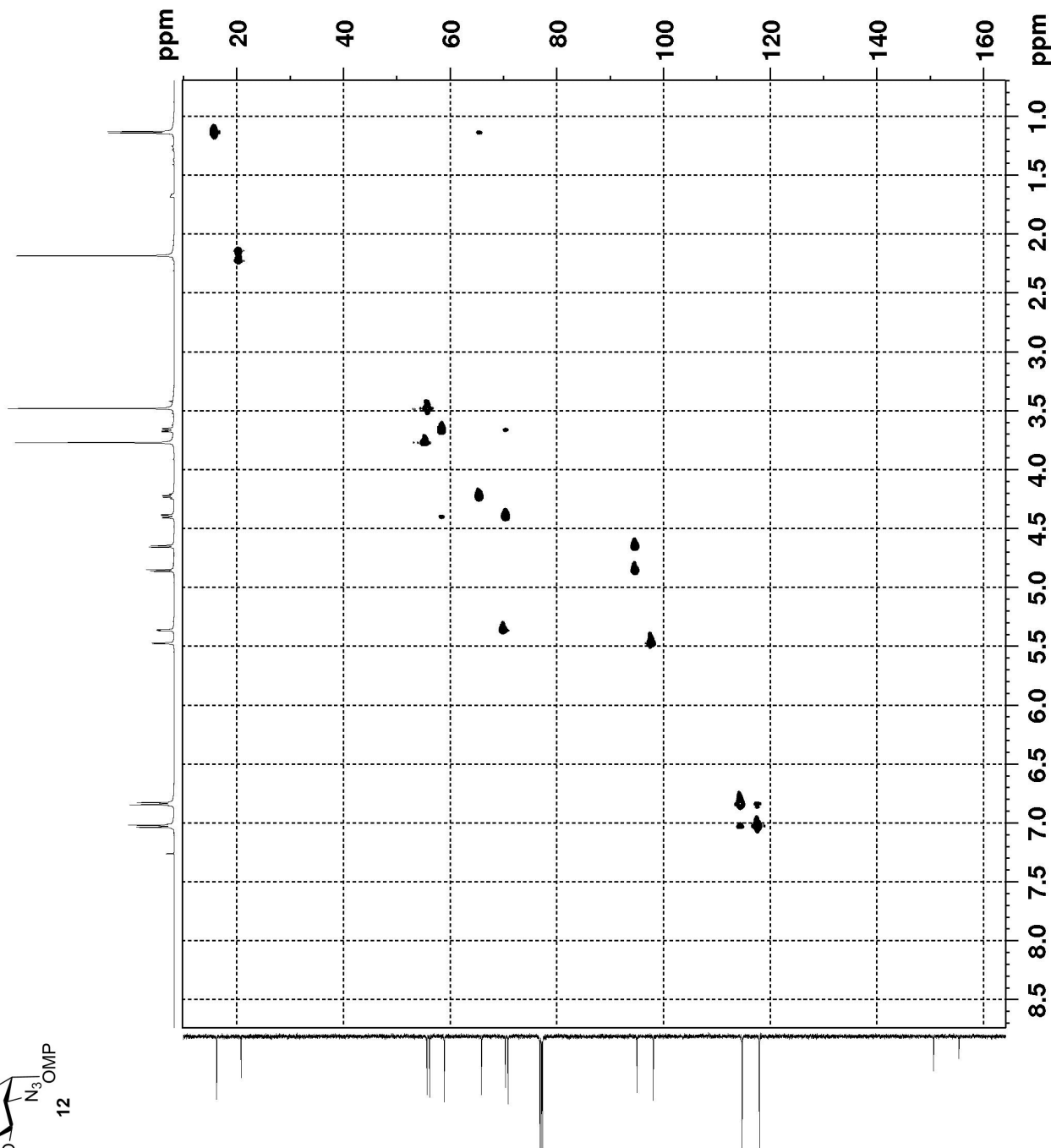
CHANNEL f2
 SFO2 125.8231741 MHz
 NUC2 13C
 P1 11.50 usec
 P2 23.00 usec
 P28 1000.00 usec
 PLW2 66.00000000 W
 PLW12 1.78123995 W

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 %
 P1 100.00 usec
 P19 600.00 usec

F1 - Acquisition Parameters
 ID 256
 SFO1 125.8232 MHz
 NUC1 13C
 P1 199.690 Hz
 SW 199.690 Fm
 F1MODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 125.8106252 MHz
 SSB 0 Hz
 LB 0
 GB 0
 PC 1.00

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



GROUP BM
BM-AC-R78 in CDCl3



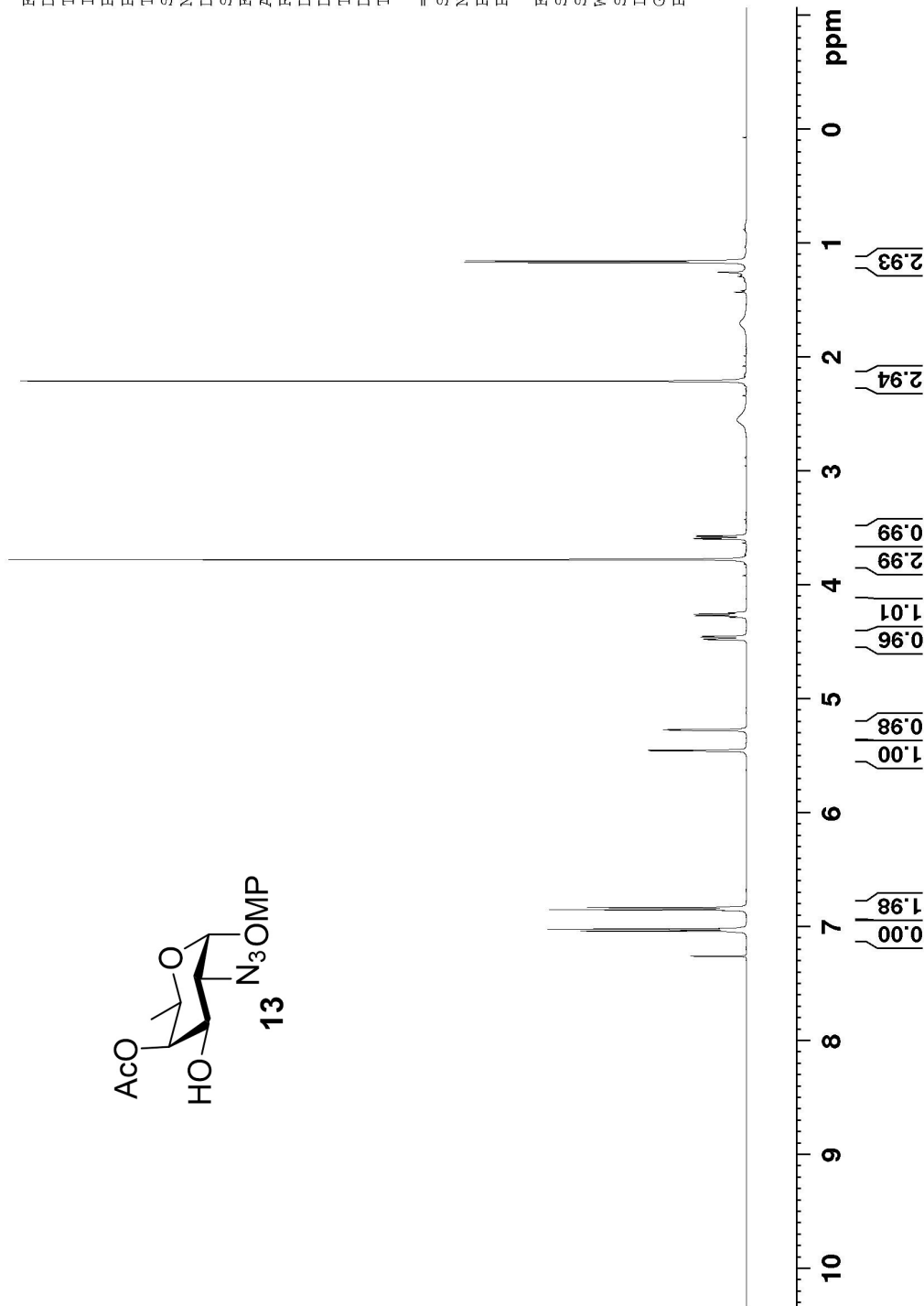
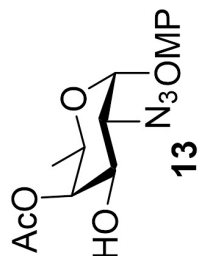
Current Data Parameters
NAME BM-AC-R78
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181002
Time 11.22
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO 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

7.260
7.039
7.021
6.850
6.832
5.457
5.450
5.277
5.275
5.271
4.478
4.472
4.457
4.450
4.283
4.270
4.257
4.244
3.776
3.595
3.589
3.574
3.567
2.209
1.167
1.154



GROUP BM
BM-AC-R78 in CDCl₃



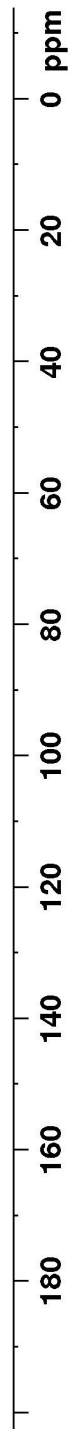
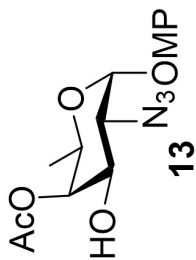
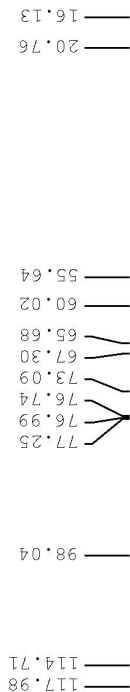
Current Data Parameters
NAME BM-AC-R78
EXPNO 11
PROCNO 1

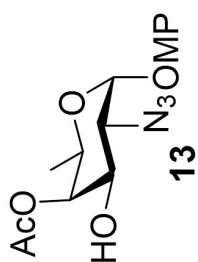
F2 - Acquisition Parameters
Date_ 20181002
Time 11:25
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 70
DS 4
SWH 43859.648 Hz
FIDRES 0.669245 Hz
AQ 0.7471104 sec
RG 203
DW 11.400 usec
DE 6.50 usec
TE 2131.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 500.3420014 MHz
NUC2 1H
CPDPRG2 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 0 1.00 Hz
GB 0
PC 1.10





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 cosygpppqr
 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 0.0000000 sec
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec
 D13 0.0000040 sec
 D16 0.0002000 sec
 INO 0.00019980 sec

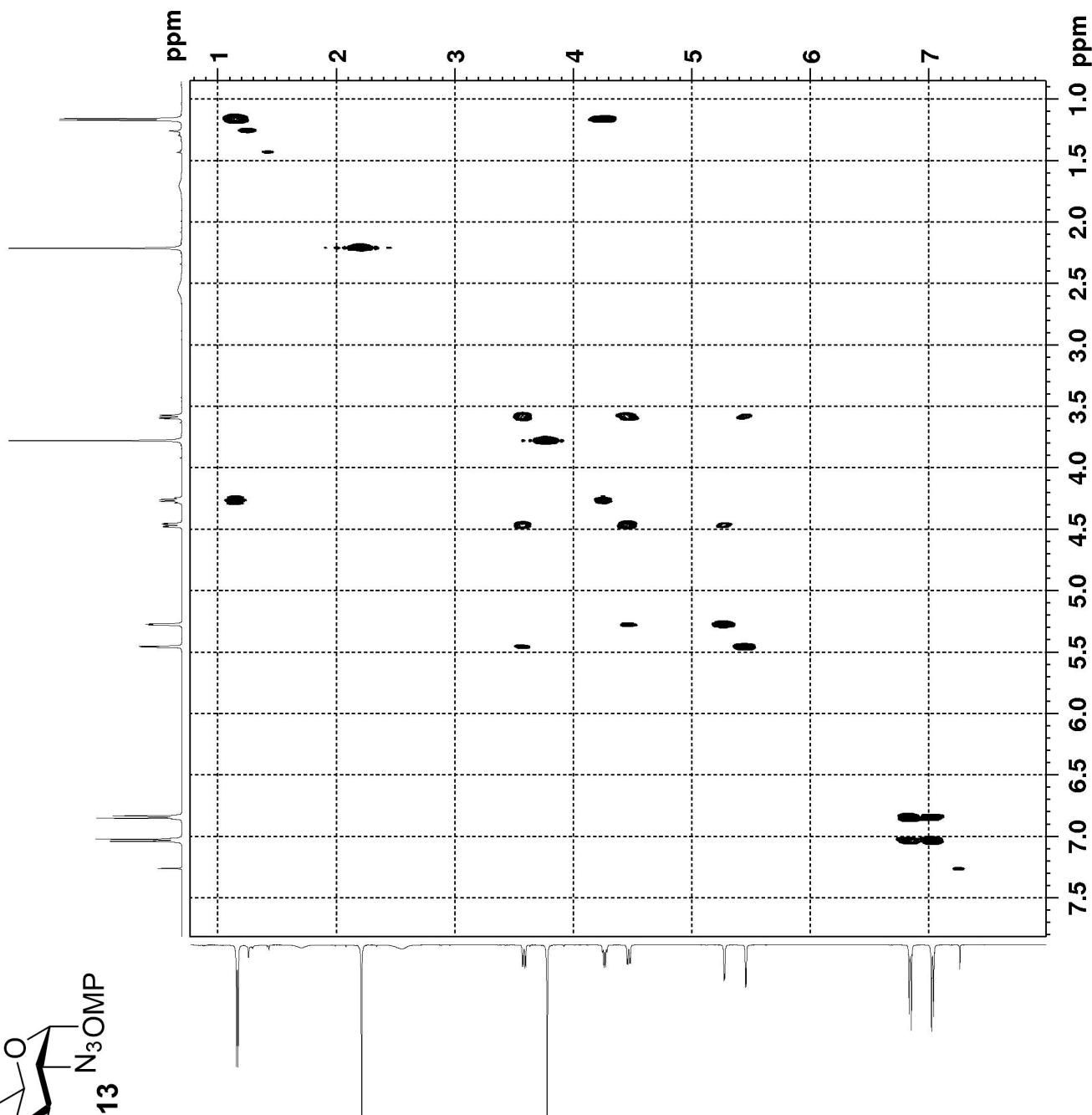
===== CHANNEL f1 =====
 SF01 500.3425017 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.0000000 W
 PLW10 3.40280008 W

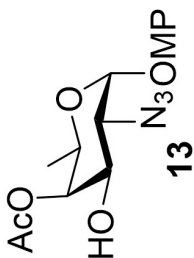
===== GRADIENT CHANNEL =====
 GPM1[1] SMSQ10.100
 GP21 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 91
 SF01 500.3425 MHz
 FIDRES 110.000107 Hz
 SW 10.003 ppm
 FMODE QF

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

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





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 BBO

PULPROG zgpg30

TD 1024

RG 144

DE 100.000 usec

TE 300.2 K

CHST2 145.0000000

DO 0.00000300 sec

D1 1.50000000 sec

D4 0.00172414 sec

D11 0.03000000 sec

D12 0.00000000 sec

D13 0.00000000 sec

IN0 0.00001990 sec

ZGPGFNS

CHANNEL F1

SFO1 500.3425017 MHz

NUC1 13C

P1 17.50 usec

P2 35.00 usec

P28 1000.00 usec

PL1 10.00000000 W

CHANNEL F2

SFO2 125.8231741 MHz

NUC2 13C

CFDPRG[2] garp

P3 11.50 usec

P4 23.00 usec

PL2 66.00000000 W

PL12 1.78129995 W

GRADIENT CHANNEL

GENAM[1] SMSQ10.100

GENAM[2] SMSQ10.100

GENAM[3] SMSQ10.100

GENAM[4] SMSQ10.100

GP21 80.00 %

GP22 20.10 %

GP23 11.00 %

GP24 35.00 %

PL1 1000.00 usec

PL9 600.00 usec

F1 - Acquisition Parameters

TD 76

SFO1 125.8232 MHz

PROBHD 5 mm BBO

SA 199.630 Ppm

FMODE Echo-Antiecho

F2 - Processing parameters

SI 1024

FS 500.3400181 MHz

WDW COSINE

SSB 2

LB 0 Hz

GB 0

FC 1.00

F1 - Processing parameters

SI 1024

MC2 echo-antiecho

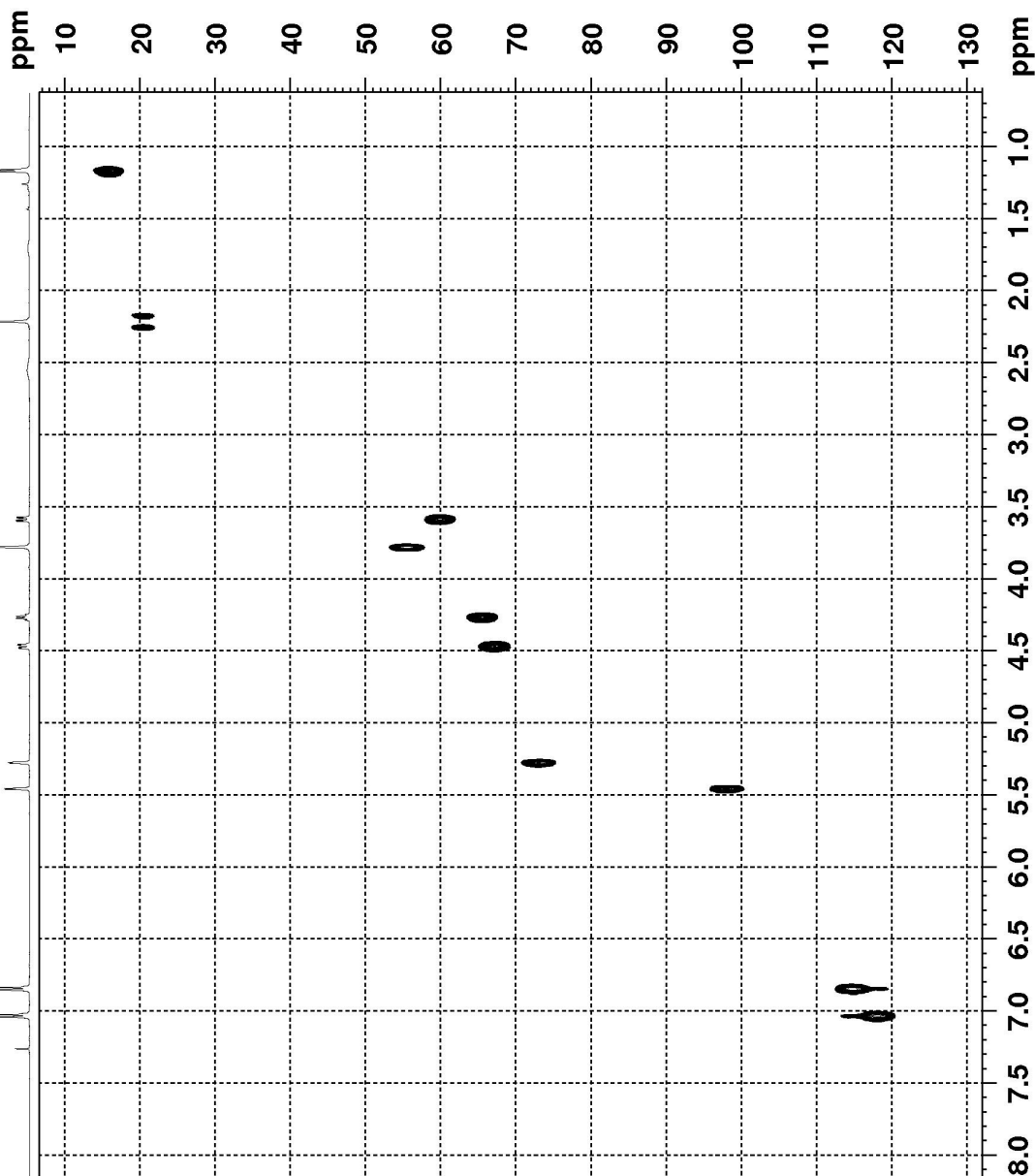
SF 125.8105942 MHz

WDW COSINE

SSB 2

LB 0 Hz

GB 0



GROUP BM
BM-AC-R57SI in CDCl3

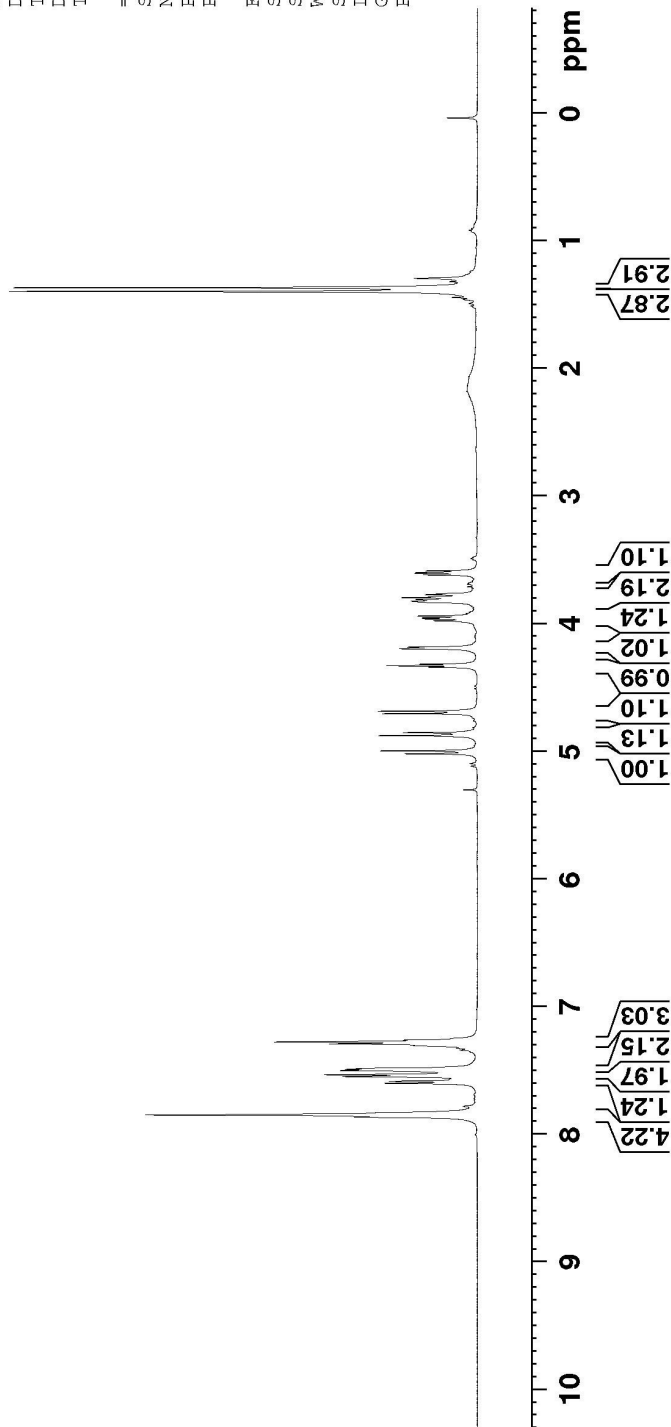
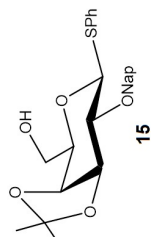
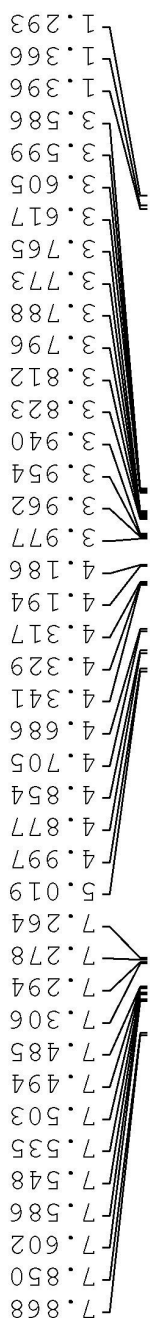


Current Data Parameters
NAME BM-AC-R57SI
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191218
Time 13.11
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65560
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



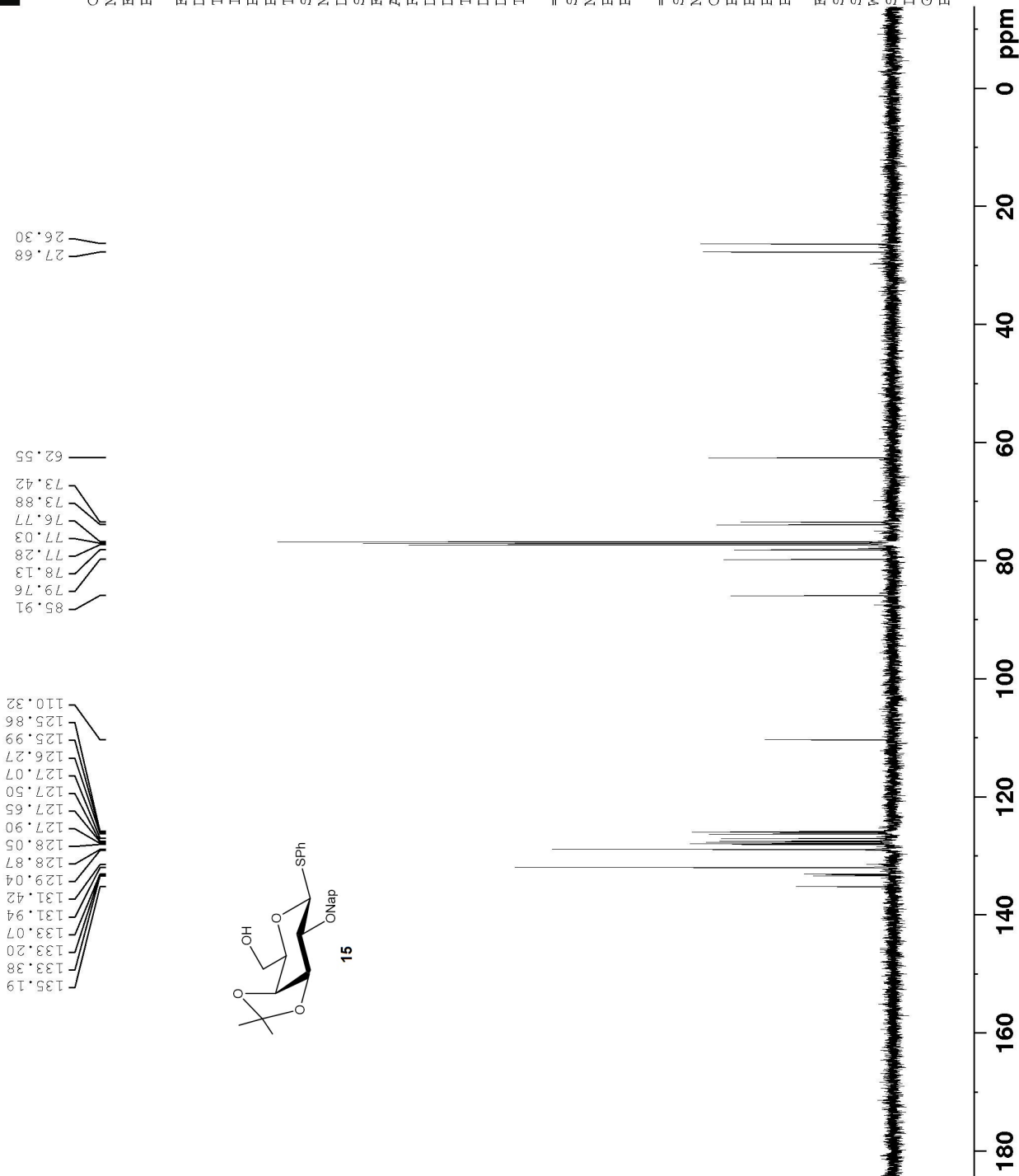
Current Data Parameters
NAME BM-AC-R57SI
EXPNO 71
PROCNO 1

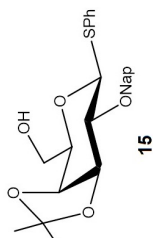
F2 - Acquisition Parameters
Date_ 20191218
Time 13.15
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 53
DS 4
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 203
DW 13.200 usec
DE 6.50 usec
TE 277.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG2 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 0 1.00 Hz
GB 0
PC 1.35





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

F2 - Acquisition Parameters
 Date_ 20191218
 Time 13.18
 INSTRUM Bruker_default_av500
 PROHD 5 mm PABBO BB/
 FULPROG cosygpppqr
 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 0.0000000 sec
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec
 D13 0.0000040 sec
 D16 0.0002000 sec
 INO 0.00019980 sec

===== CHANNEL f1 =====
 SF01 500.3625017 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.0000000 W
 PLW10 3.40280008 W

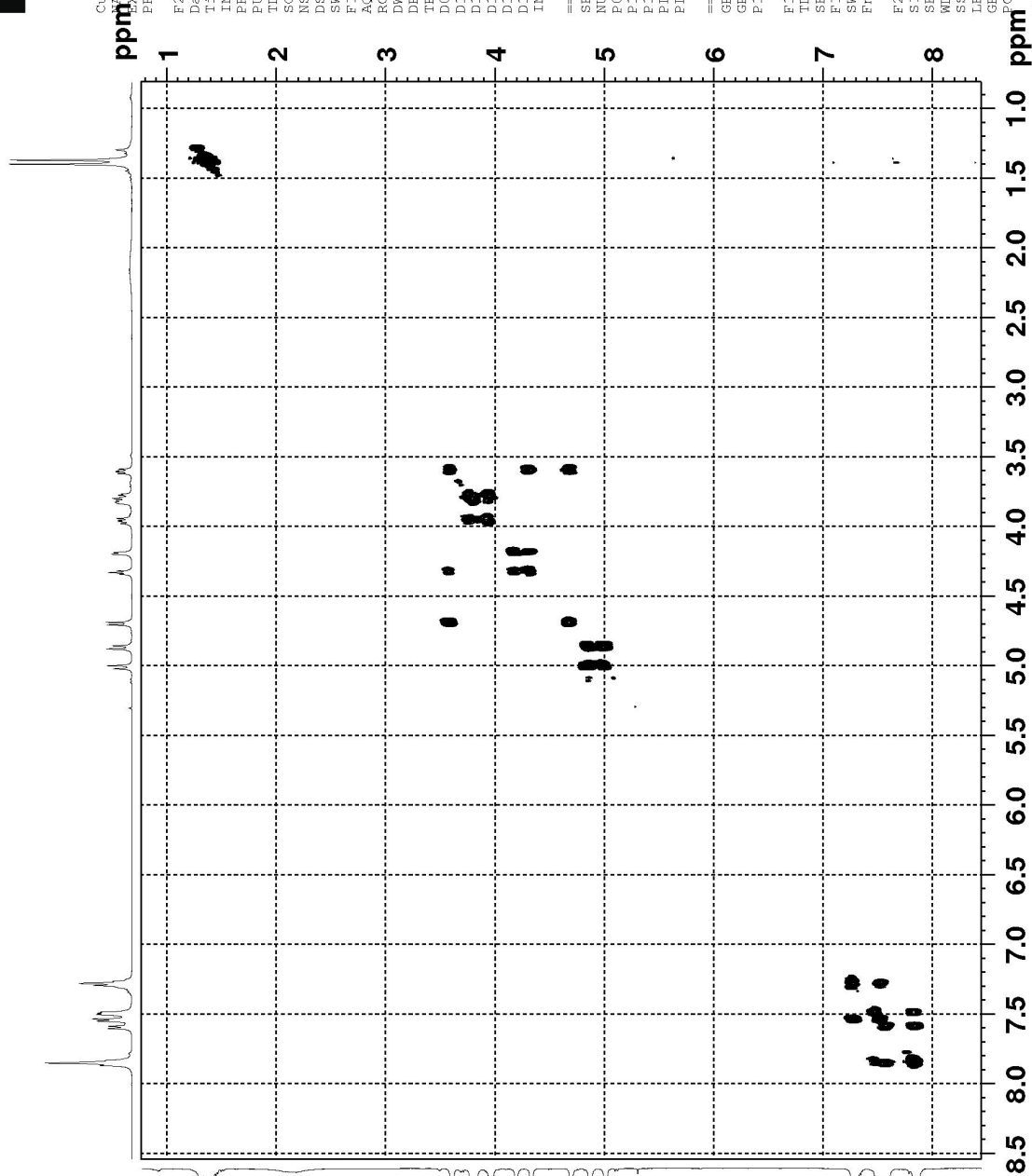
===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPZ1 10.00 %
 P16 1000.00 usec

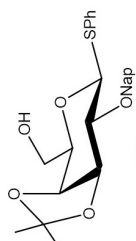
F1 - Acquisition parameters
 TD 128
 SF01 500.3625 MHz
 FIDRES 78.203201 Hz
 SW 10.003 ppm
 F1MODE QF

F2 - Processing parameters
 SI 1024
 SF 500.3600123 MHz
 WDW QSSINE
 SSB 0
 LB 0 Hz
 GB 0

PC 1.00

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





Current Data Parameters
NAME BM-AC-R5751
EXPCO / 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191218
Time_ 13.23

INSTRUM Bruker default_av500
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SH 5000.016 Hz
SF 500.136199 MHz
AQ 0.1024000 sec
RG 144
DM 100.000 usec
DE 6.50 usec
TE 300.2 K
CNS72 145.000000 sec
D0 0.00000000 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00000000 sec
D2 0.00000000 sec
D3 0.00000000 sec
INO 0.00001990 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 500.13625017 MHz
NUC1 13C
P1 17.50 usec
P2 35.00 usec
P8 1000.00 usec
PLW1 10.00000000 W
===== CHANNEL f2 =====
SFO2 125.828031 MHz
NUC2 13C
CPDPRG2 garp
P3 11.50 usec
P4 23.00 usec
P8 1000.00 usec
PLW2 66.00000000 W
PLW12 1.78129995 W

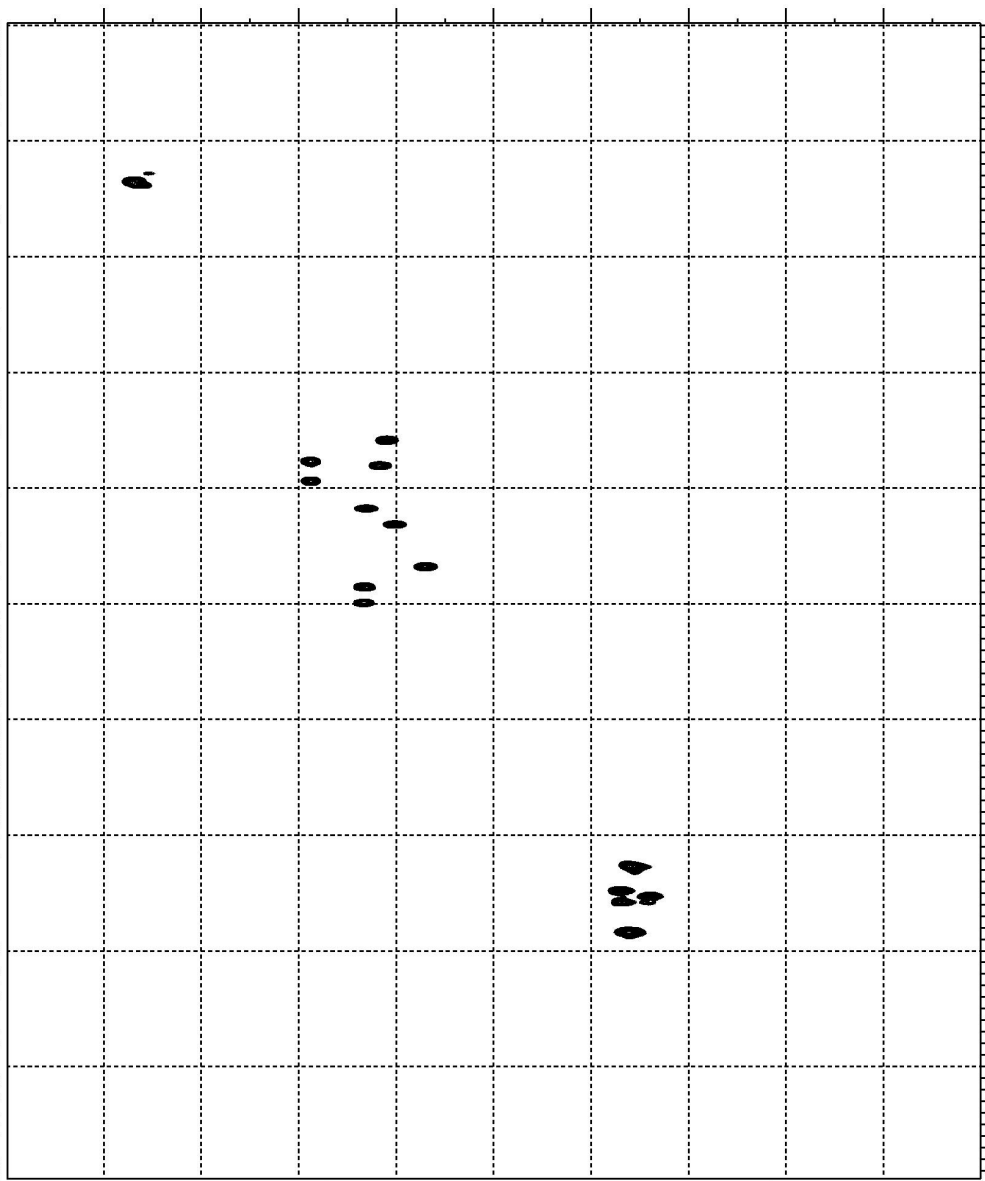
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 5.00 %
P10 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 67
SFO1 125.8282 MHz
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
SM 199.682 F2m
F1MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.13625017 MHz
WDW 500.36000000 Hz
SSB 0 Hz
LB 0
GB 0
PC 1.00

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

ppm 20 40 60 80 100 120 140 160 180 ppm



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



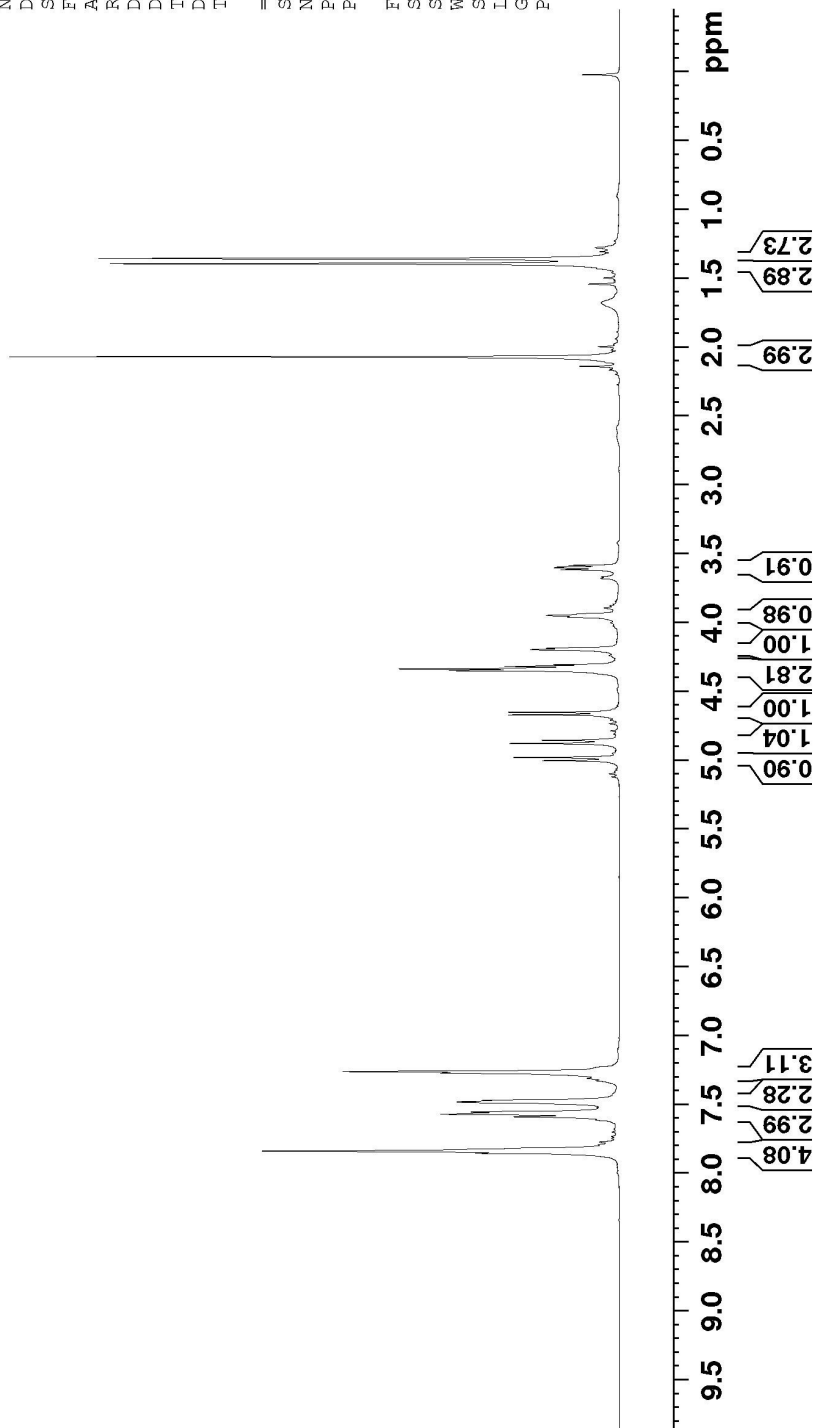
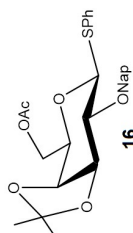
Current Data Parameters
NAME BM-AC-R57 SII
EXPNO 250
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190926
Time 18.24
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65560
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

7.853
7.837
7.827
7.589
7.569
7.553
7.485
7.477
7.468
7.271
7.260
5.001
4.978
4.876
4.853
4.668
4.650
4.346
4.335
4.315
4.303
4.195
4.185
3.946
3.601
3.596
2.067
1.390
1.353



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



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 FAPBO 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 2.0000000 sec
D11 0.0300000 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
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 10.00000000 W
PLW12 0.47852001 W
PLW13 0.24068999 W

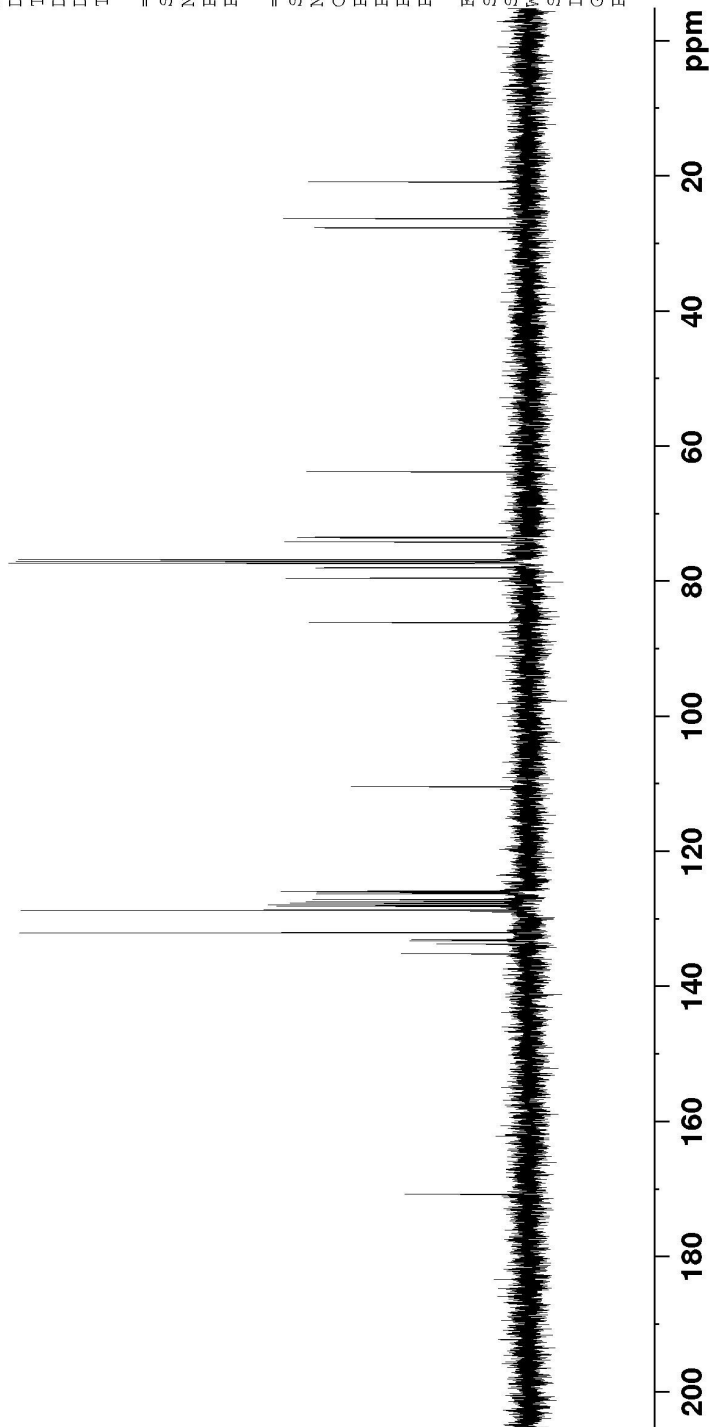
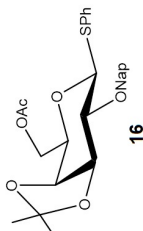
F2 - Processing parameters
SI 32768
SF 125.8156282 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

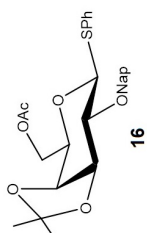
27.62
26.26
20.81

86.08
79.50
77.97
77.28
77.03
76.77
74.12
73.53
73.44
63.74

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

170.75





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

F2 - Acquisition Parameters
Date_ 20130926
Time 16.26
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqr
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
INO 0.00019980 sec

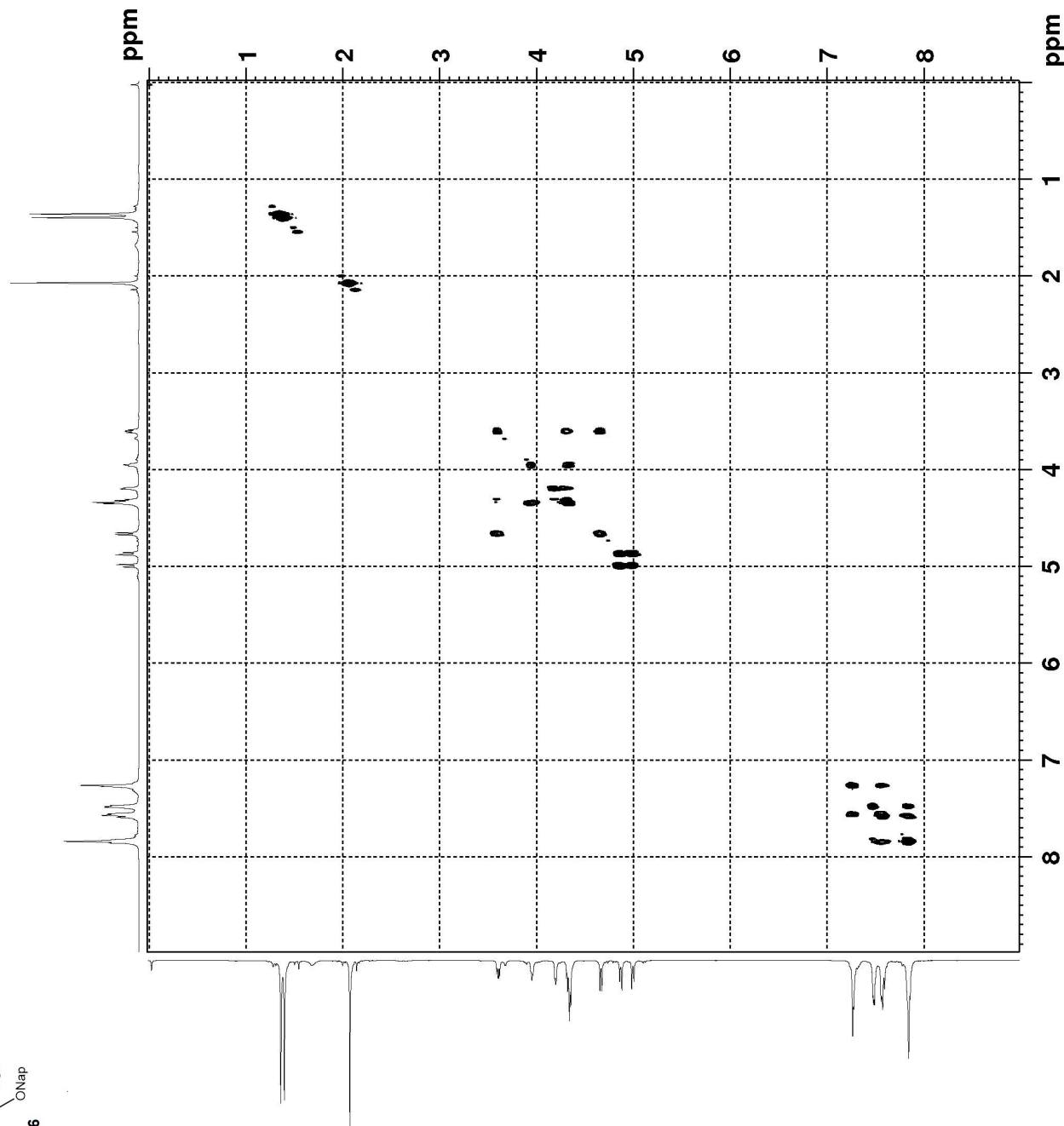
===== CHANNEL f1 =====
SFO1 500.3625017 MHz
NUC1 1H
P0 17.50 usec
P1 17.50 usec
P17 2500.00 usec
PLW1 10.00000000 W
PLW10 3.40280008 W

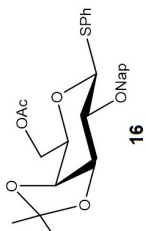
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.3625 MHz
FIDRES 78.203201 Hz
SW 10.003 ppm
F1MODE 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





Current Data Parameters
NAME BM-AC-R57 S11
EXPNO 232
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190926
Time 18.32

PROBHD 5 mm QNP 1H/13
PULPROG zgpg302
TD 1024

SOLVENT DMSO
NS 2
DS 16
SWH 5000.016 Hz

FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 71.8

DM 100.000 usec
DE 6.50 usec
TE 300.2 K

CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec

D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00000000 sec

D22 0.00062007 sec
D37 0.00000000 sec
INO 0.00001930 sec

ZGPGTNS
===== CHANNEL f1 =====
SFO1 500.3625017 MHz

NUC1 13C
P1 17.50 usec
P2 35.00 usec

P28 1000.00 usec
PLW1 10.00000000 W
===== CHANNEL f2 =====

SFO2 125.828031 MHz
NUC2 13C
P3 11.50 usec

CPDPRG2 garp
P4 23.00 usec
P5 60.00 usec

PLW2 66.00000000 W
PLW12 1.78129995 W
===== GRADIENT CHANNEL =====

GPM1[1] SWSQ10.100
GPM1[2] SWSQ10.100
GPM1[3] SWSQ10.100

GPM1[4] SWSQ10.100
GP21 80.00 %
GP22 20.10 %

GP23 11.00 %
GP24 5.00 %
P6 100.00 usec

P19 600.00 usec
F1 - Acquisition parameters
TD 131

SFO1 125.8282 MHz
FIDRES 38.828282 Hz
SW 199.682 Fw

FrMODE Echo-Antiecho
F2 - Processing parameters
SI 1024

SF 125.8156153 MHz
SSB 0 Hz
LB 0

PC 1.00
F1 - Processing parameters
SI 1024

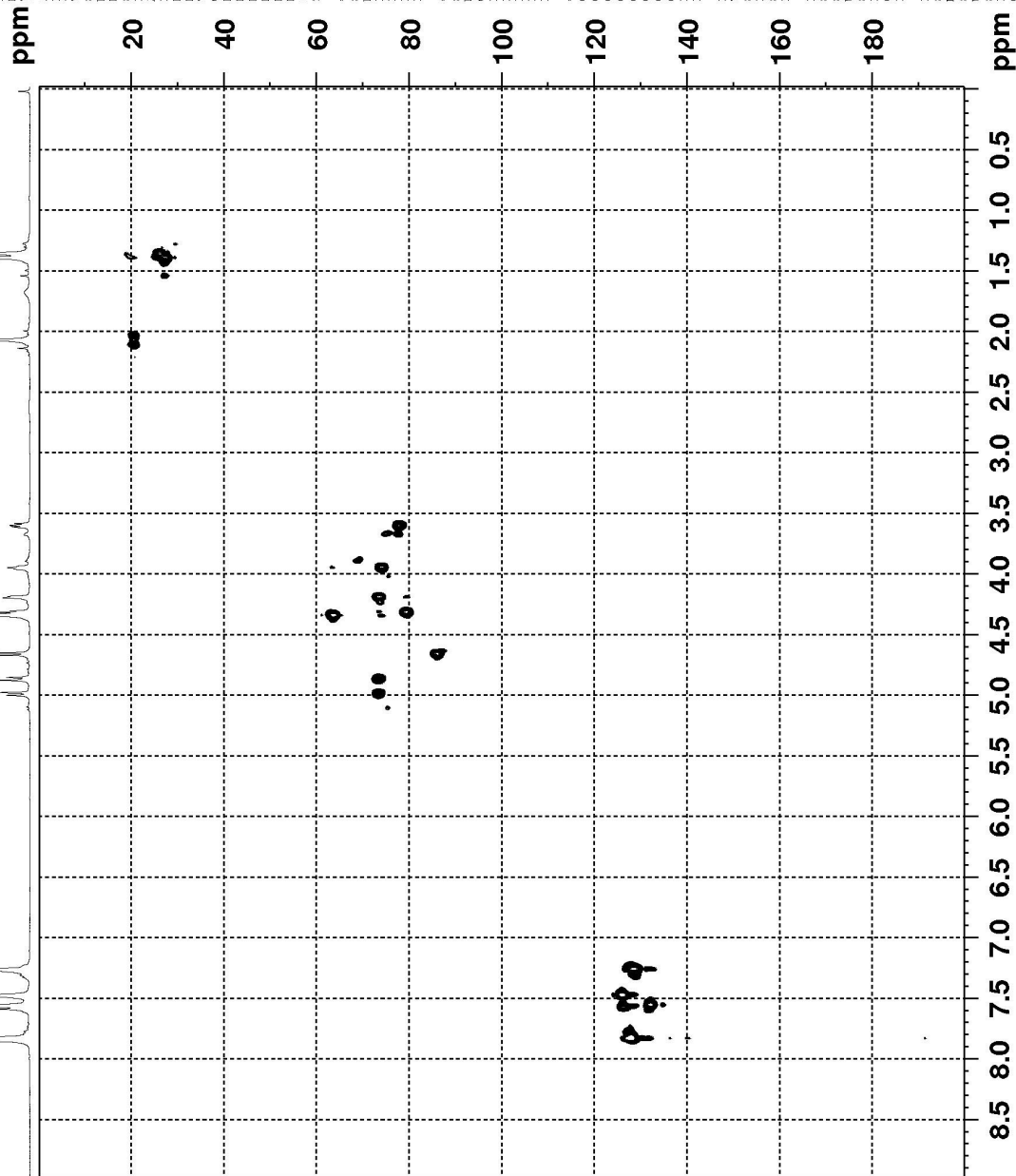
MC2 echo-antiecho
SF 125.8156153 MHz
SSB 0 Hz

LB 0
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho

SF 125.8156153 MHz
SSB 0 Hz
LB 0

GB 0
PC 1.00



GROUP BM
BM-AC-R81 in CDCl3

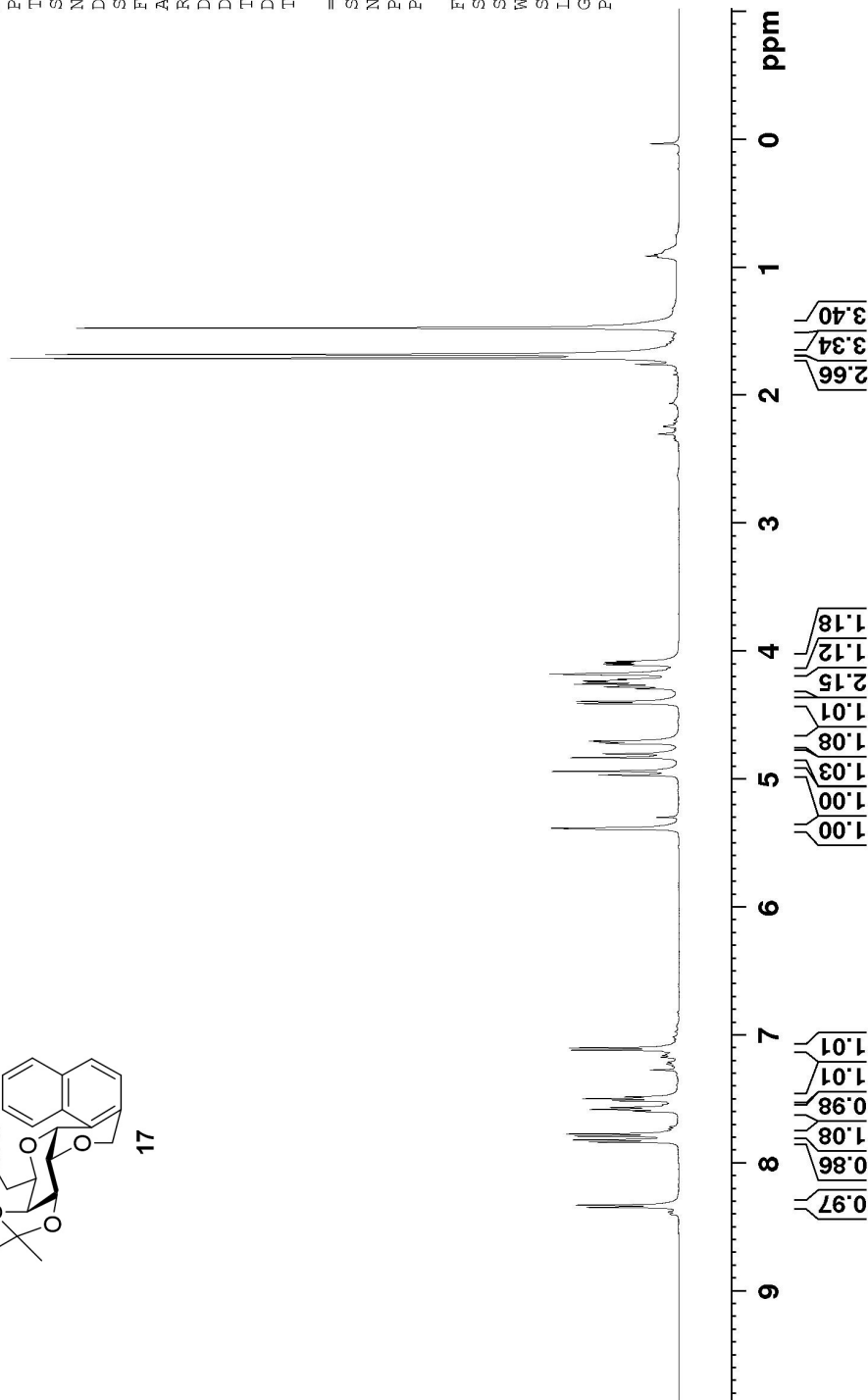
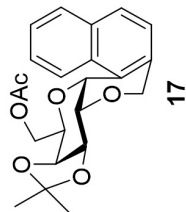
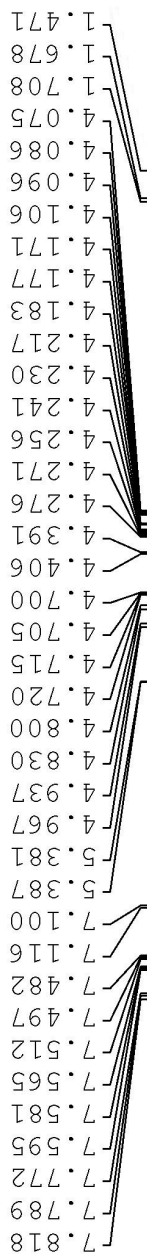


Current Data Parameters
NAME BM-AC-R81
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 17.59
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65560
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/_av500
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

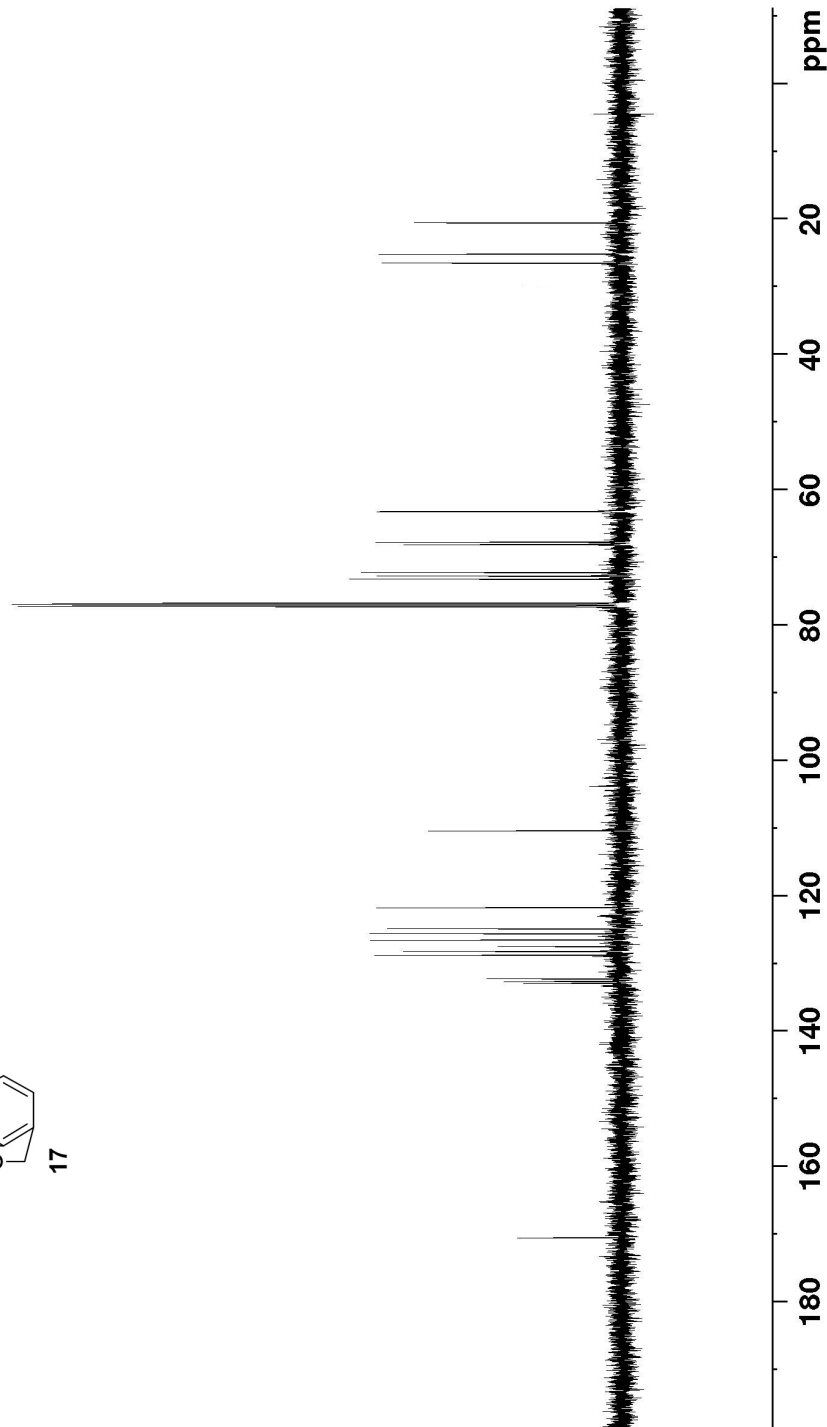
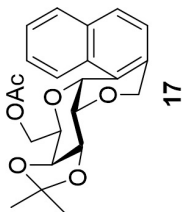
F2 - Processing parameters
SI 32768
SF 125.8156286 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.35

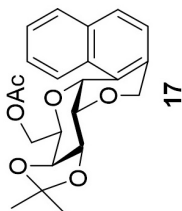
26.49
25.16
20.55

77.26
77.00
76.75
73.19
73.19
72.73
72.19
68.09
67.75
63.25
63.18

132.96
132.71
132.28
128.81
128.22
127.48
126.57
125.60
124.87
121.78
110.41

170.57





Current Data Parameters
NAME BM-AC-R81
EXNO 332
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191219
Time 18.06
INSTRUM Bruker_default_av500
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
ID 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.204800 sec
RG 800
DM 100.000 usec
DE 6.50 usec
TE -1595.9 K
D0 0.0000300 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

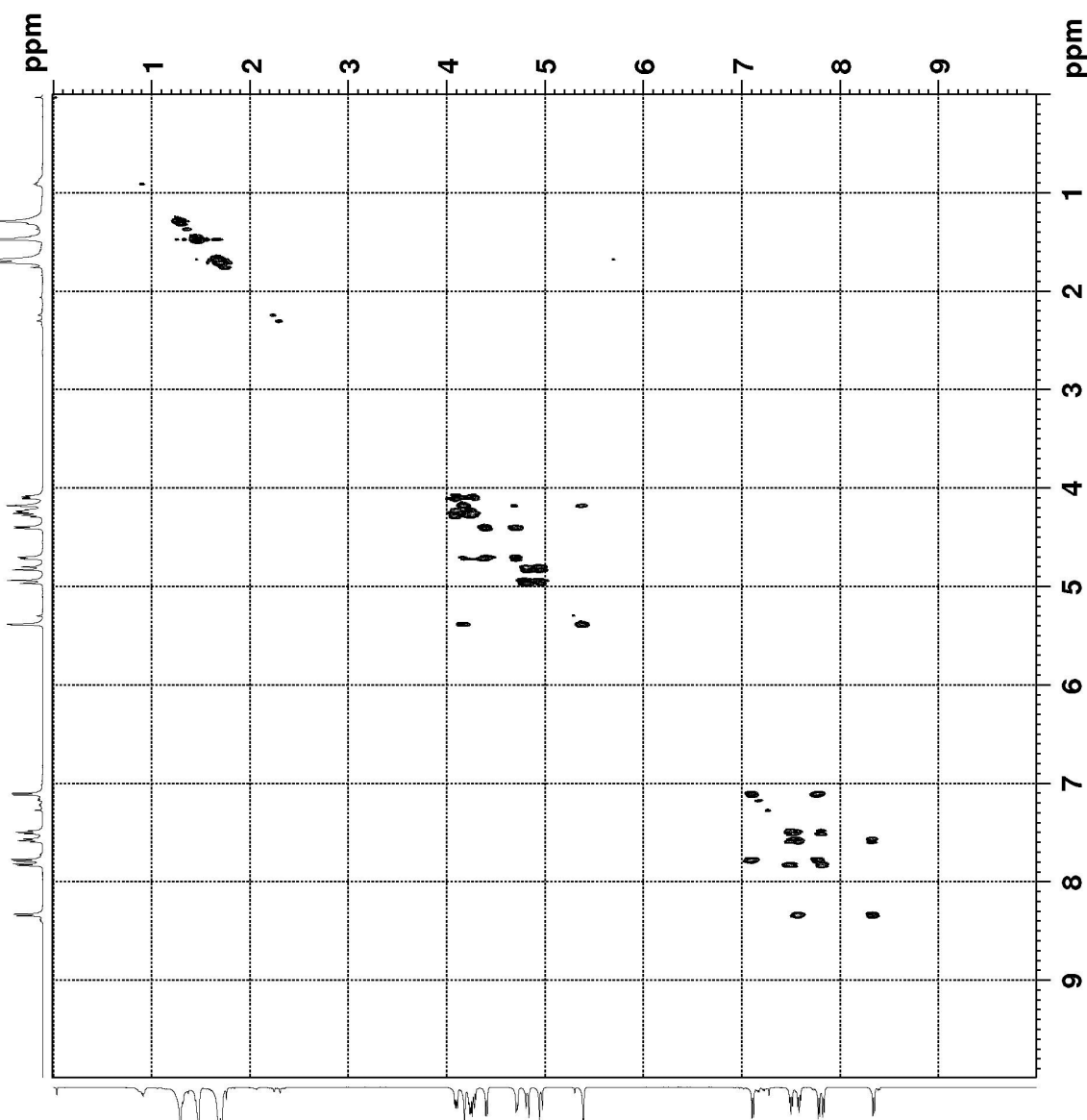
CHANNEL f1
SFO1 500.3625017 MHz
NUC1 1H
P0 17.50 usec
P1 17.50 usec
PL7 2500.00 usec
PLW1 10.0000000 W
PLW10 3.40280008 W

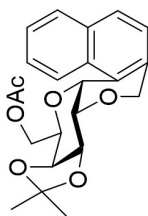
GRADIENT CHANNEL
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

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

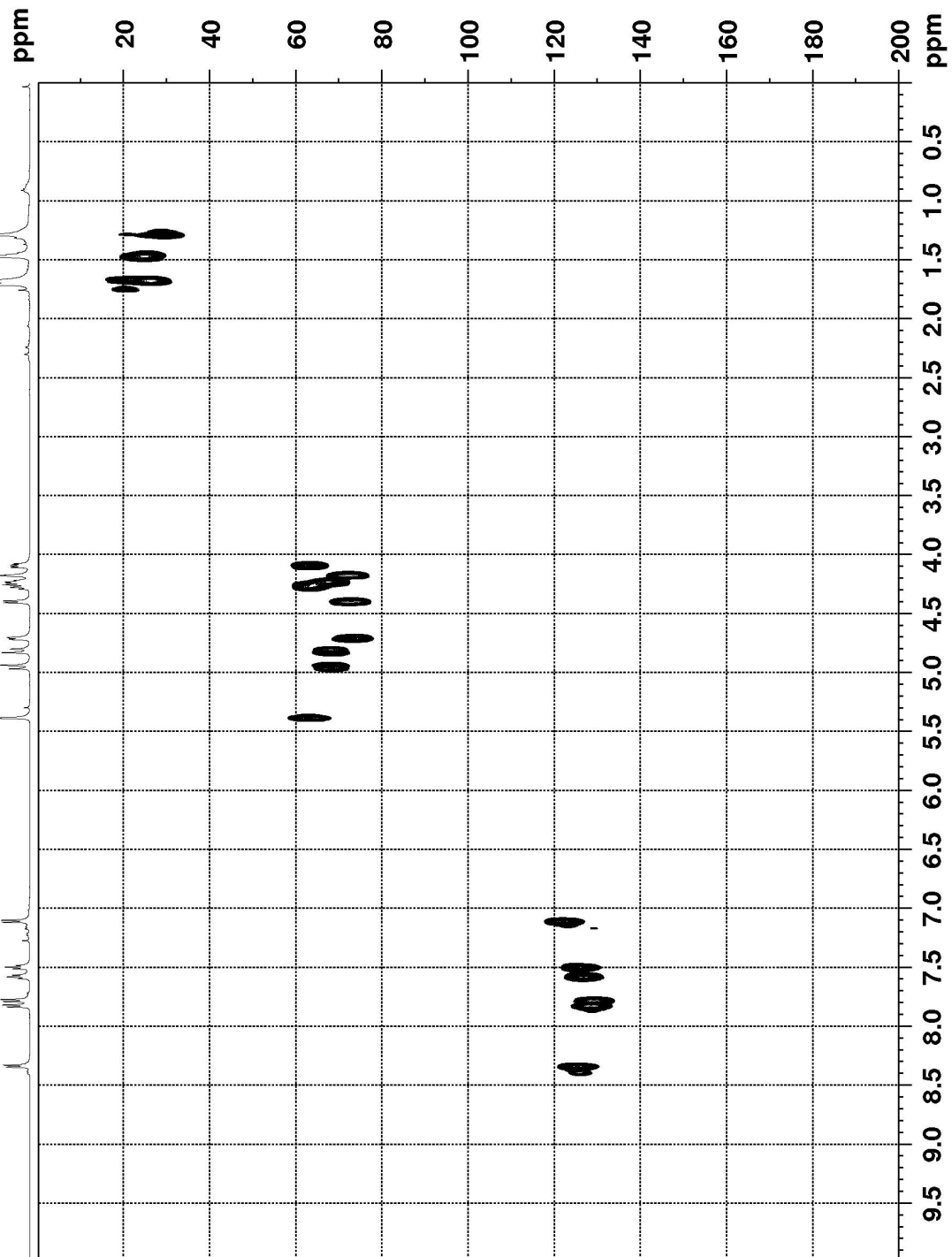
F2 - Processing parameters
SI 1024
SF 500.3600028 MHz
WDW 0
SSB 0 Hz
LB 0 Hz
GB 0
PC 1.00

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





17



Current Data Parameters
 NAME BH-AC-R81
 PROBO 5 mm PABO BH/
 PULPROG hsqcpg2
 SOLVENT CDCl3
 NS 2
 DS 16
 SS 5000.136 Hz
 FIDRES 4.882813 Hz
 AQ 0.1024000 sec
 RG 144
 DE 6.50 usec
 TE -170.6 K
 CNST2 145.000000
 D1 1.5000000 sec
 D4 0.00172414 sec
 D11 0.0300000 sec
 D16 0.0300000 sec
 D24 0.0018207 sec
 INO 0.00001990 sec
 ZGPGTNS
 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 125.822031 MHz
 NUC2 13C
 CPDPRG12 garp
 P3 13.00 usec
 P4 23.00 usec
 PCPD2 70.00 usec
 PLW2 66.00000000 W
 PLW2 1.7822995 W
 GRADIENT CHANNEL
 GPM1(1) SMQ10.100
 GPM1(2) SMQ10.100
 GPM1(3) SMQ10.100
 GPM1(4) SMQ10.100
 GPM2(1) SMQ10.100
 GPM2(2) SMQ10.100
 GPM2(3) SMQ10.100
 GPM2(4) SMQ10.100
 F1 - Acquisition Parameters
 TD 37
 FOS1 135.5352 MHz
 FIDRES 135.5352 MHz
 SW 139.682 Hz
 FIDCODE Echo-Antiecho
 F2 - Processing Parameters
 SI 1024
 SF 500.360028 MHz
 WDW QMINE
 SSB 0 Hz
 LB 0
 GB 0
 PC 1.00
 F1 - Processing Parameters
 SI 1024
 MC2 echo-antiecho
 SF 125.822031 MHz
 WDW QMINE
 SSB 0 Hz
 LB 0
 GB 0

GROUP BM
BM-AC-124 in CDCl3

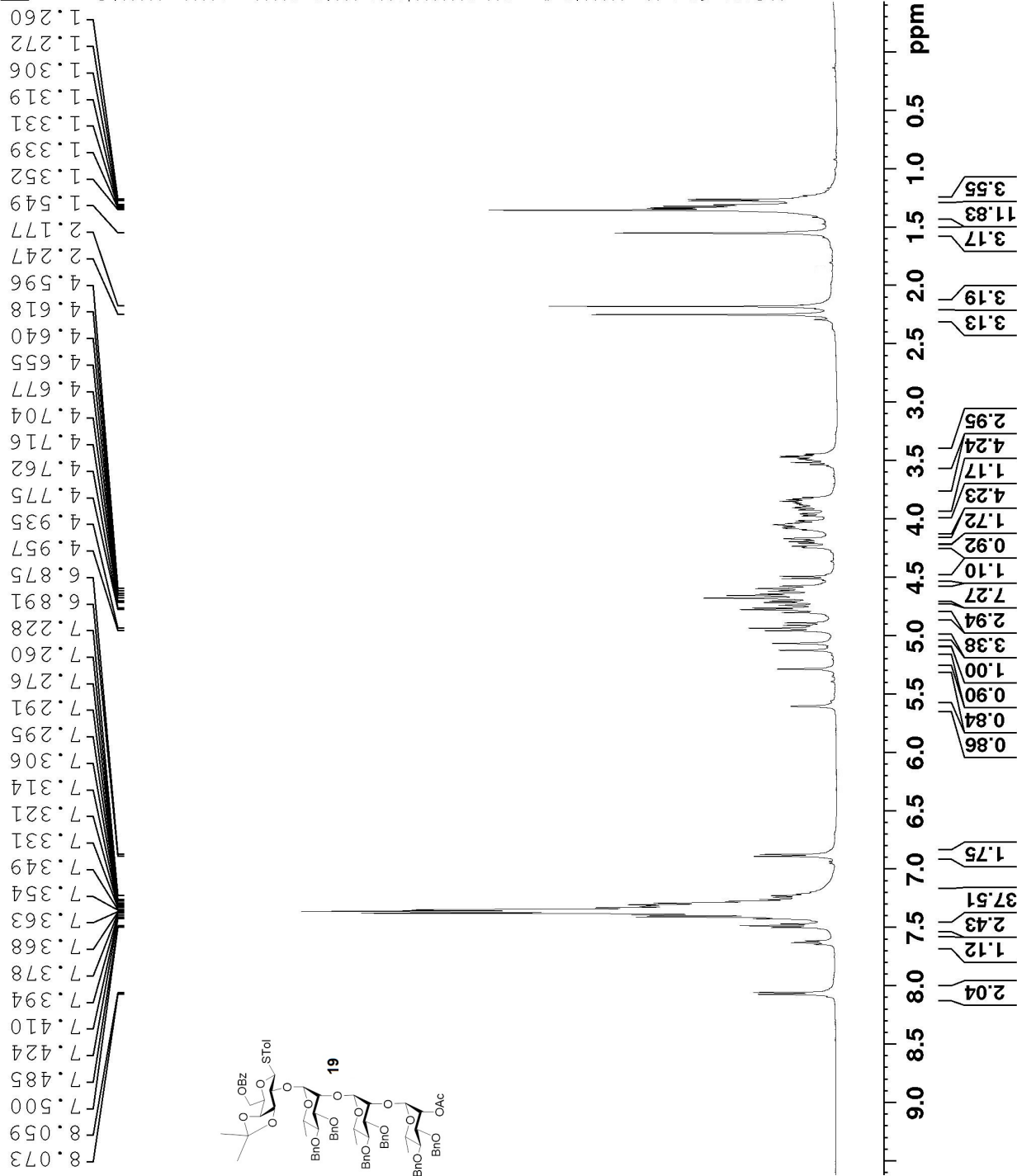
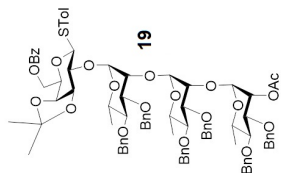


Current Data Parameters
NAME BM-AC-R124
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190516
Time 17.45
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO 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

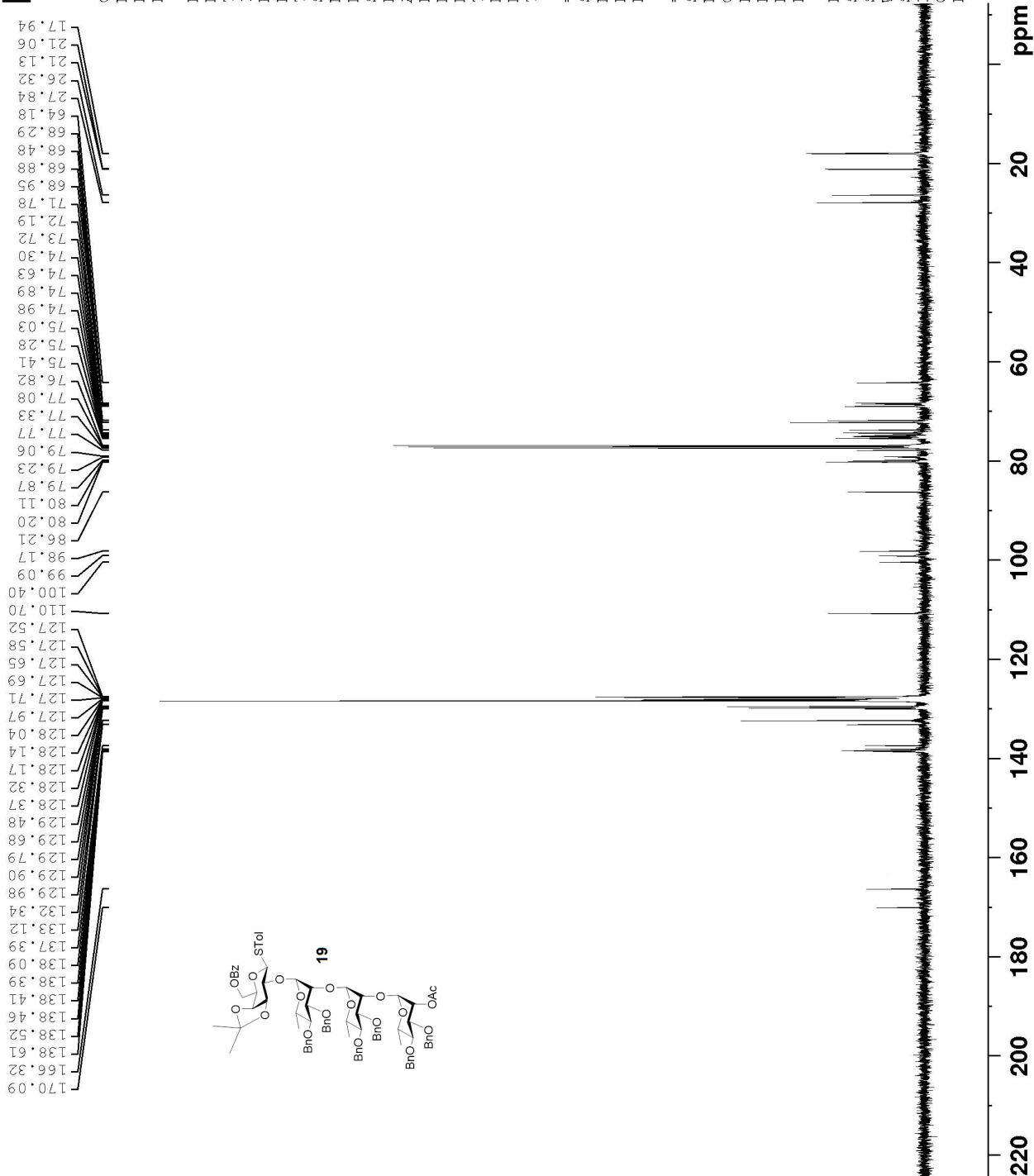
F2 - Processing parameters
SI 131072
SF 500.340013 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

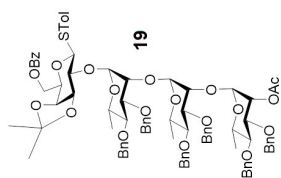


F2 - Acquisition Parameters	
Date_	20190516
Time	18.02
INSTRUM	Bruker_default_av500
PROBHD	5 mm PABO B ⁺
PULPROG	zgpg30
ID	65536
SOLVENT	CDCl ₃
NS	151
DS	4
SSNH	43859.648 Hz
FIDRES	0.669245 Hz
RG	0.7471104 sec
DW	90.5
DE	11.400 usec
TE	6.50 usec
D1	300.9 K
D11	2.00000000 sec
D10	0.03000000 sec
TD0	1

```
===== CHANNEL f2 =====
SFO2      500.3420014 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PFLW2     10.00000000 W
PLM12     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





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 0.00020000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019980 sec

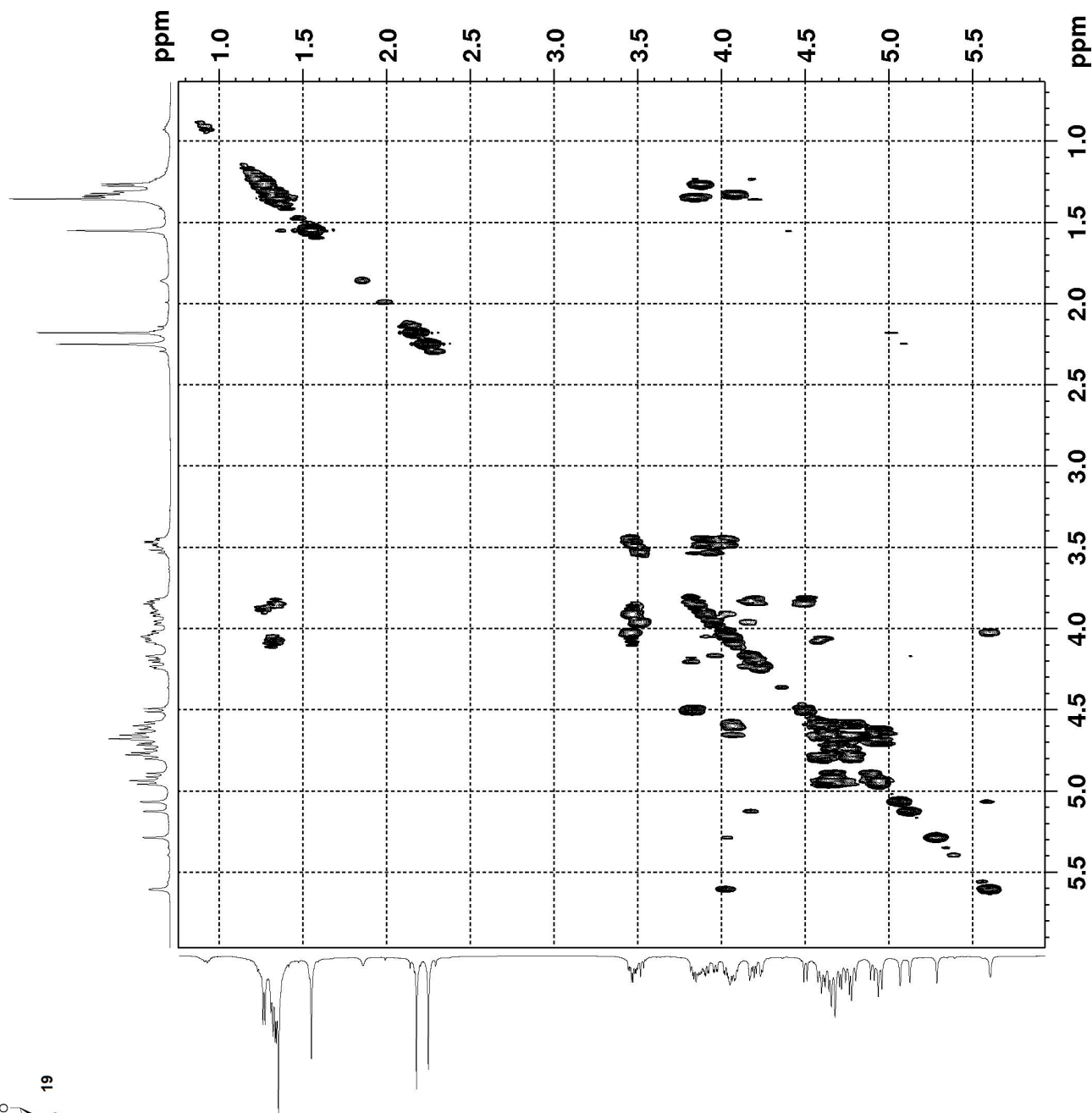
===== CHANNEL f1 =====
 SF01 500.3425017 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.00000000 W
 PLW10 3.40280008 W

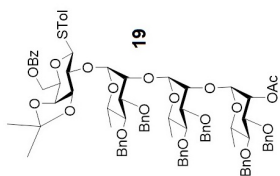
===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GP21 10.00 %
 F16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SF01 500.3425 MHz
 FIDRES 78.203201 Hz
 SW 10.003 ppm
 F1MODE QF

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

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

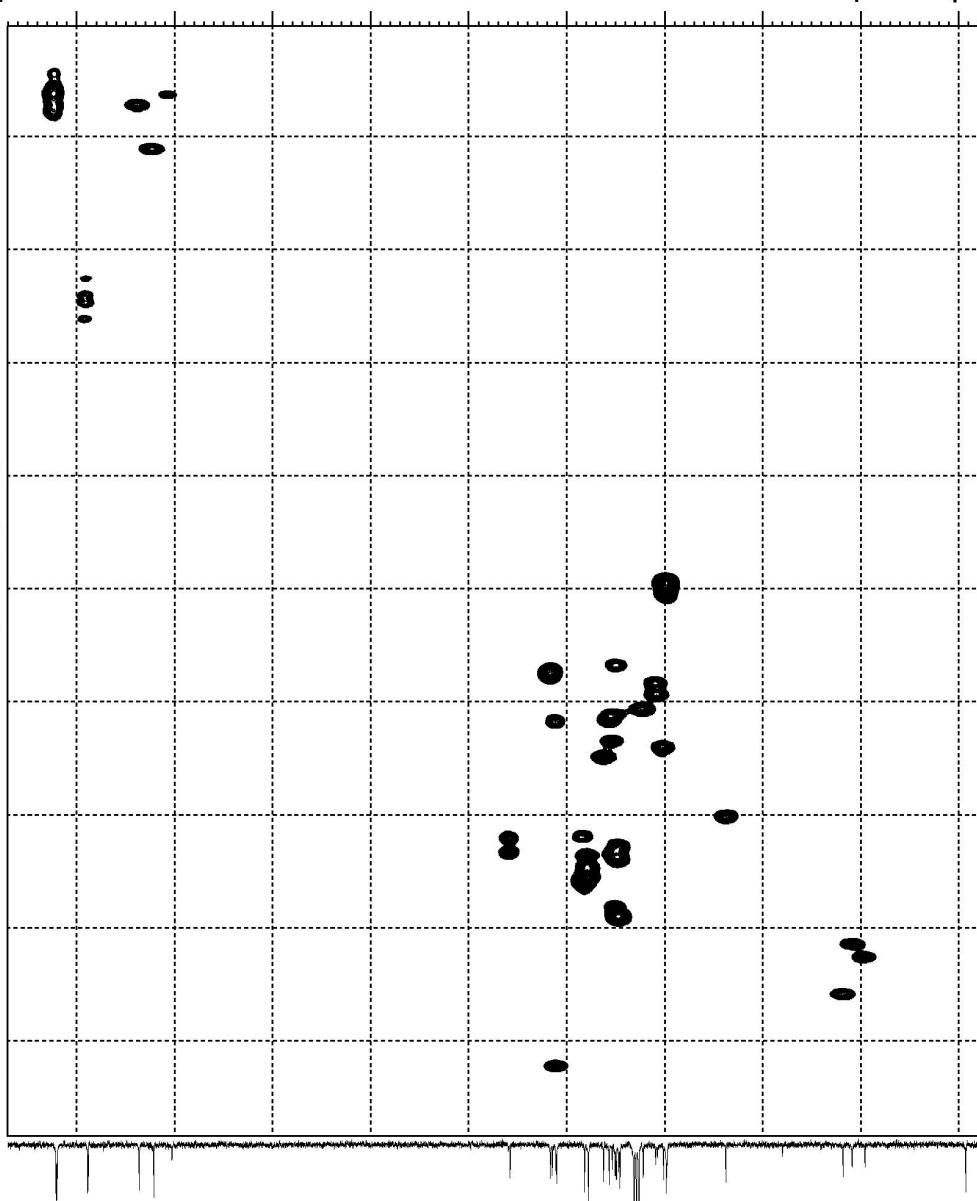




Current Data Parameters
NAME BM-AC-R124
EXPNO 2/2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190516
Time 17.52
INSTRUM Bruker default_av500
PROBHD 5 mm
PULPROG zgpg302
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 5000.016 Hz
SF 500.136133 MHz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 32
DM 100.000 usec
DE 6.50 usec
TE 300.2 K
CNS12 145.000000 K
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00000000 sec
D2 0.0008207 sec
D3 0.00000000 sec
INO 0.00001990 sec
ZGPGTNS

ppm



===== CHANNEL f1 =====
SFO1 500.3425017 MHz
NUC1 13C
P1 17.50 usec
P2 35.00 usec
P28 1000.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 125.8231741 MHz
NUC2 13C
P3 11.50 usec
P4 23.00 usec
P42 66.00000000 sec
PLW2 66.00000000 W
PLW12 1.78129995 W

===== GRADIENT CHANNEL =====
GPM1[1] SWSQ10.100
GPM1[2] SWSQ10.100
GPM1[3] SWSQ10.100
GPM1[4] SWSQ10.100
GP21 80.00 %
GP22 20.10 %
GP23 11.00 %
GP24 5.00 %
P10 100.00 usec
P19 600.00 usec

F1 - Acquisition Parameters
TD 114
SFO1 125.8232 MHz
SF 440.620000 MHz
SW 199.630 Fz
FIDRES 4.882813 Hz
RG 32
DM 100.000 usec
DE 6.50 usec
TE 300.2 K
CNS12 145.000000 K
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00000000 sec
D2 0.0008207 sec
D3 0.00000000 sec
INO 0.00001990 sec
ZGPGTNS

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0
PC 1.00

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

F2 - Processing parameters
SI 1024
SF 500.340000 MHz
WDW 500.340000 MHz
SSB 0 Hz
GB 0

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

ppm

GROUP BM
BM-AC-R125 in CDCl3



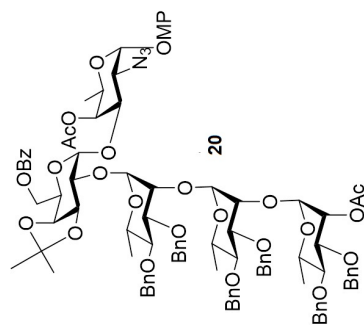
Current Data Parameters
NAME BM-AC-R125US
EXPNO 470
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190527
Time 17.57
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65560
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

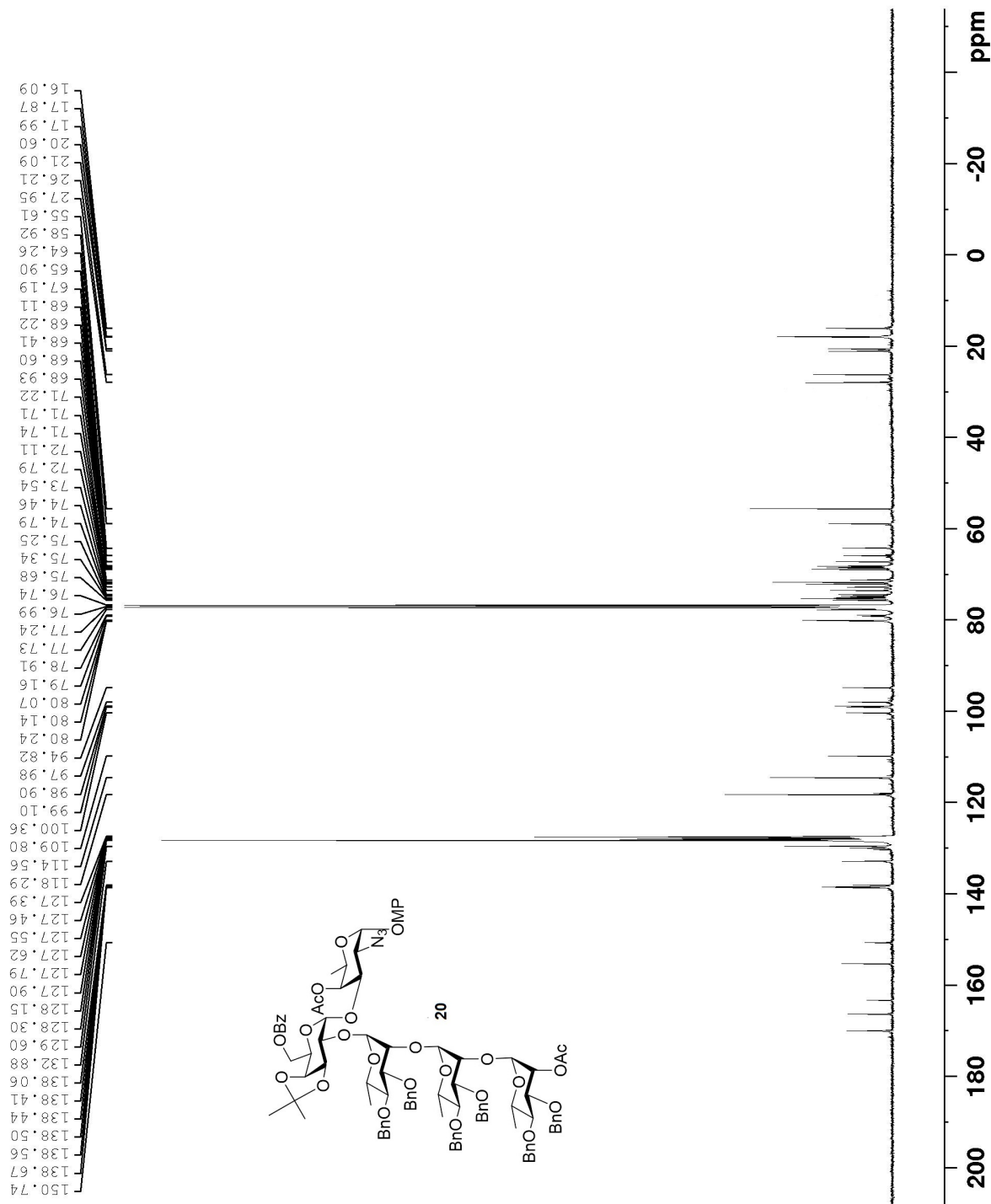
1.0339
1.052
1.219
1.232
1.272
1.281
1.294
1.301
1.314
1.326
1.523
2.037
2.146
2.780
3.786
3.825
4.100
4.105
4.583
4.604
4.610
4.617
4.625
4.633
4.648
4.716
4.731
4.901
4.915
6.770
6.788
6.897
7.236
7.250
7.262
7.275
7.280
7.300
7.311
7.327
7.337
7.346
8.074
8.090

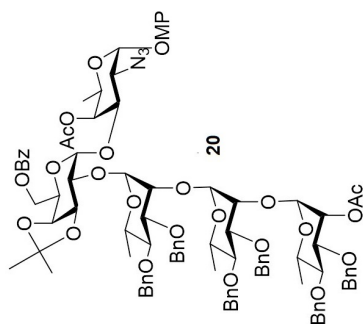


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.96
0.99
33.21
1.80
1.88
1.00
0.81
0.88
1.04
0.81
0.91
3.12
11.08
1.77
0.91
2.92
1.13
2.05
2.90
5.06
0.90
3.21
3.03
2.93
2.94
9.37
3.25
2.70

Current Data Parameters	
NAME	BM-AC-R125US
EXPNO	590
PROCNO	1
F2 - Acquisition Parameters	
Date_	20190603
Time	20.19
INSTRUM	Brucker_default_av500
PROBHD	5 mm PABBO BB/-
PULPROG	zgpg30
ID	65536
SOLVENT	CDC13
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 =====	
SF01	125.8407841 MHz
NUC1	13C
PF1	11.50 usec
PLW1	66.00000000 W
===== CHANNEL f2 =====	
SF02	500.3620014 MHz
NUC2	1H
PCPDPRG[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





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 cosygpppqr
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
INO 0.00019980 sec

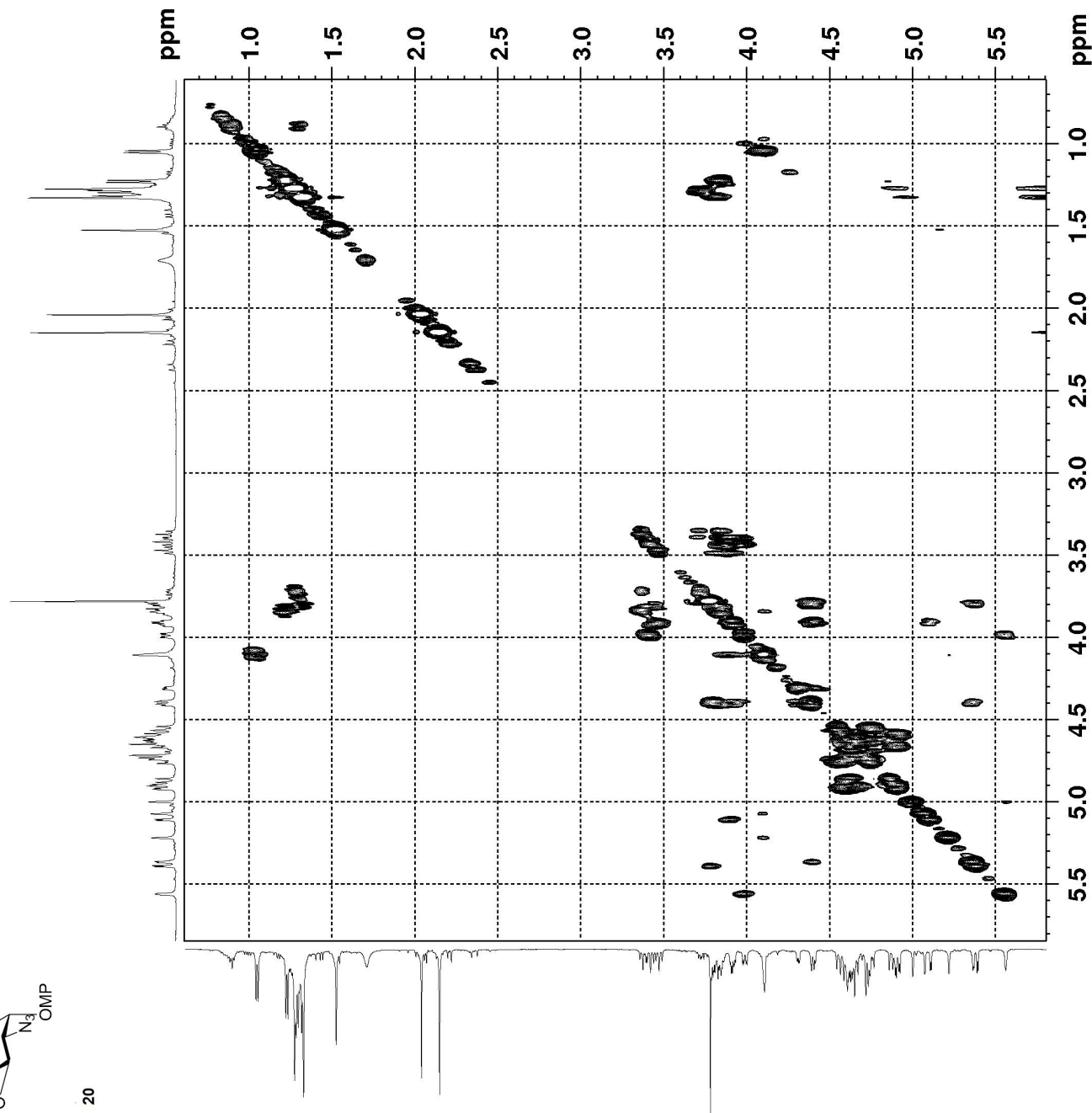
===== CHANNEL f1 =====
SFO1 500.3625017 MHz
NUC1 ¹H
P0 17.50 usec
P1 17.50 usec
P17 2500.00 usec
PLW1 10.00000000 W
PLW10 3.40280008 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
F16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.3625 MHz
FIDRES 78.203201 Hz
SW 10.003 ppm
F1MODE QF

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

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

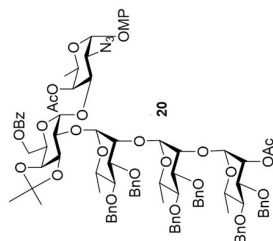
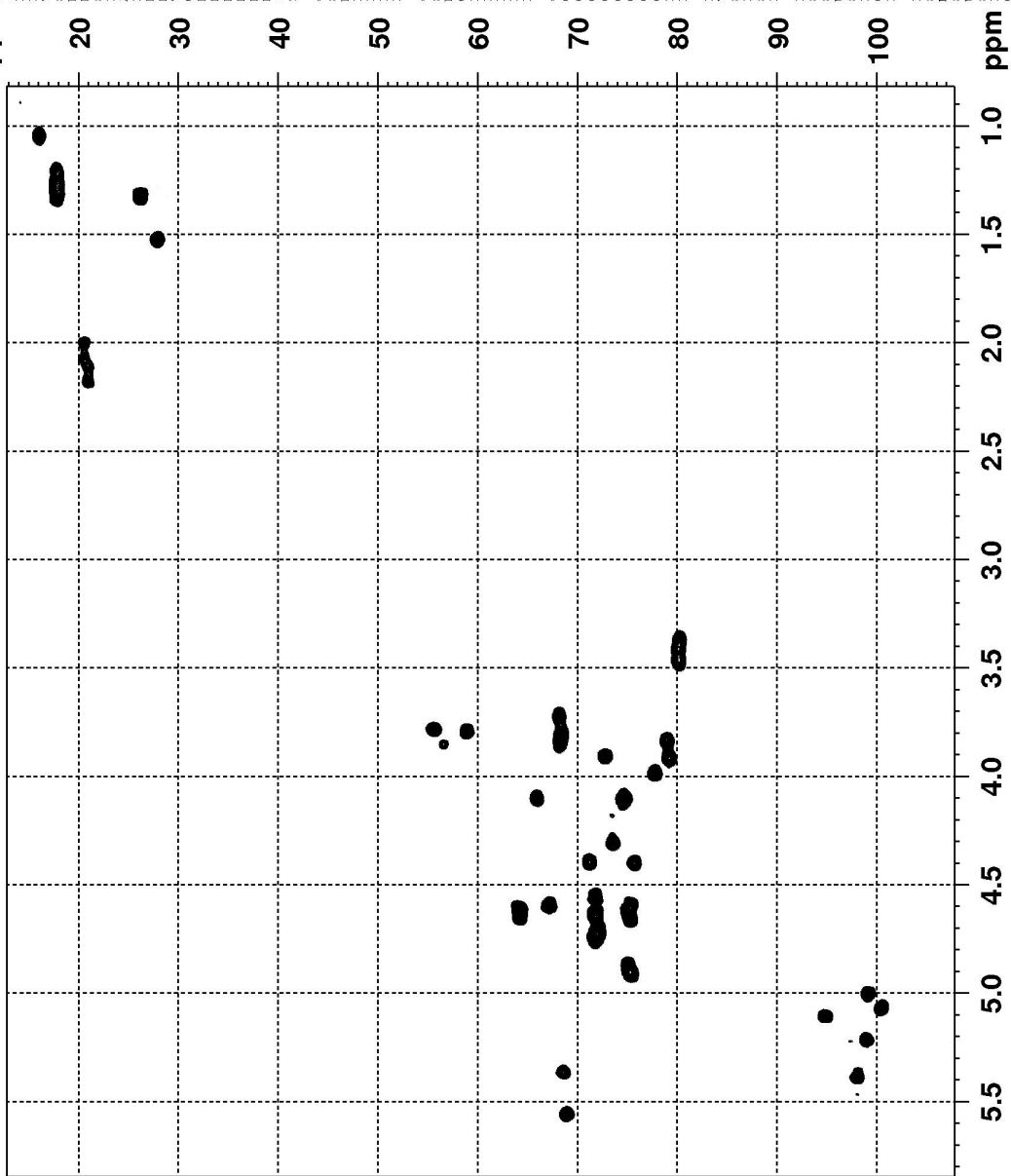




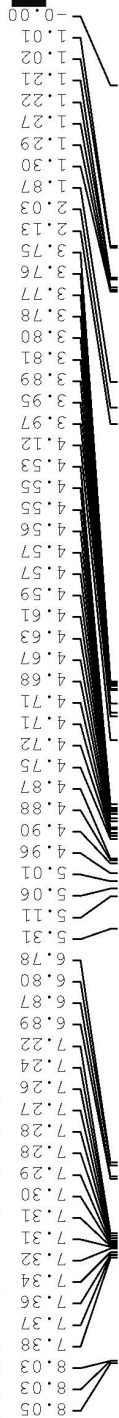
Current Data Parameters
NAME BM-AC-RL250S
EXNO 391
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190528
Time_ 14.33
INSTRUM Bruker default_av500
PROBHD 5 mm QNP 1H/13C
PULPROG zgpg302
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 5000.000 Hz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 161
DM 100.000 usec
DE 6.50 usec
TE 298.2 K
CNS12 145.000000
D0 0.00000000 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.05000000 sec
D22 0.00620000 sec
D36 0.00000000 sec
INO 0.00001900 sec
ZGPGTNS

ppm



GROUP BM
BM-AC-R132 in CDCl3

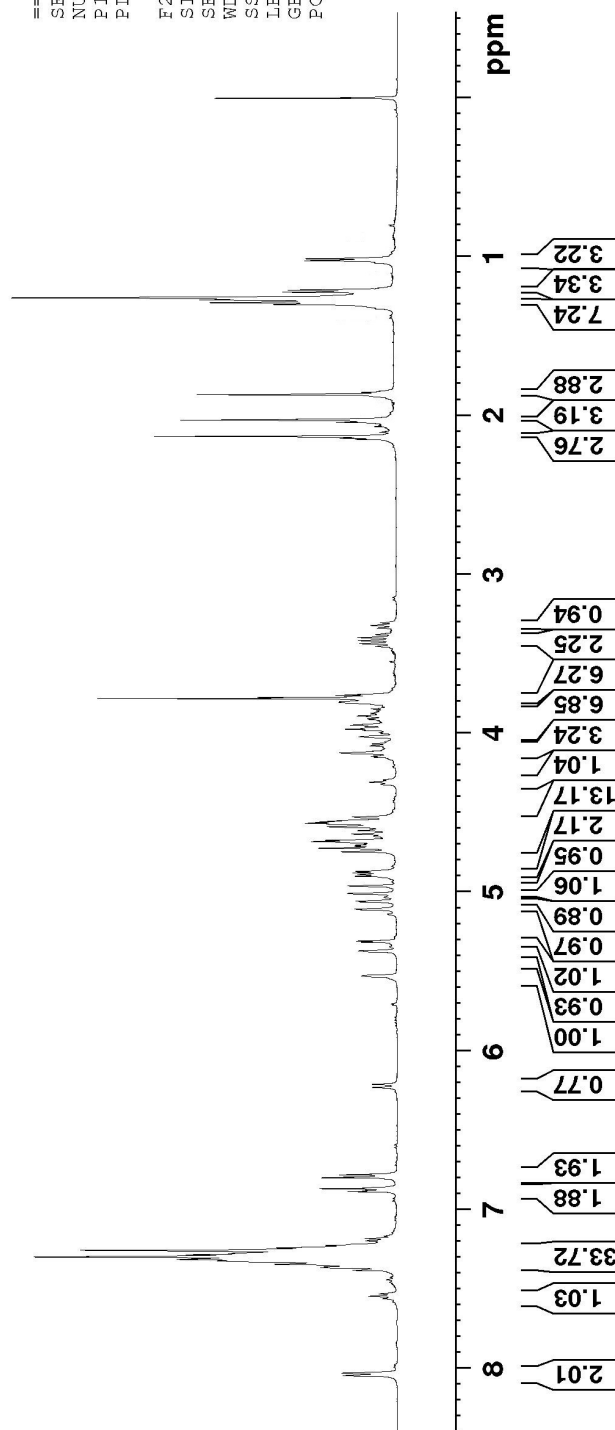
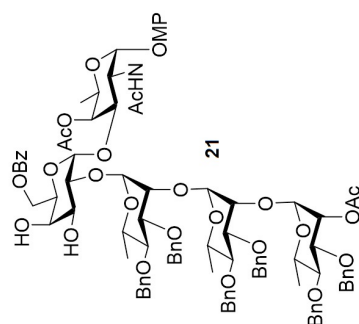


Current Data Parameters
NAME BM-AC-R132
EXPNO 480
PROCNO 1

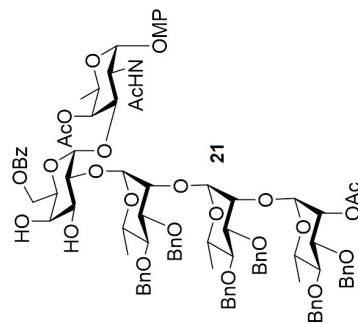
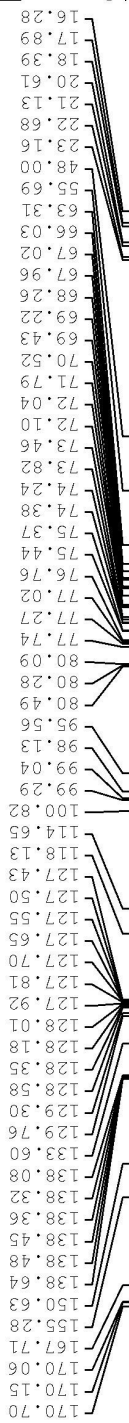
F2 - Acquisition Parameters
Date_ 20190617
Time 20.23
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65560
SOLVENT CDCl3
NS 16
DS 2
SWH 12500.000 Hz
FIDRES 0.187800 Hz
AQ 2.6624000 sec
RG 128
DW 40.000 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1

===== 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

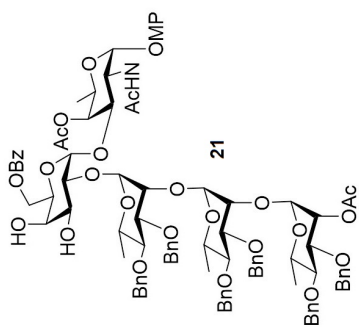
F2 - Acquisition Parameters
Date_ 20190617
Time 20.52
INSTRUM Bruker_default_av500
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 17410
DS 4
SWH 75757.578 Hz
FIDRES 1.155969 Hz
AQ 0.4325376 sec
RG 203
DW 6.600 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 500.3620014 MHz
NUC2 1H
CPDPRG2 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 0
GB 0
PC 1.40

180 160 140 120 100 80 60 40 20 0 ppm



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

F2 - Acquisition Parameters
 Date_ 20130617
 Time 20:25
 INSTRUM Bruker_default_av500
 PROBHD 5 mm PABBO BB/
 PULPROG cosygpppqr
 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 0.00020000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019980 sec

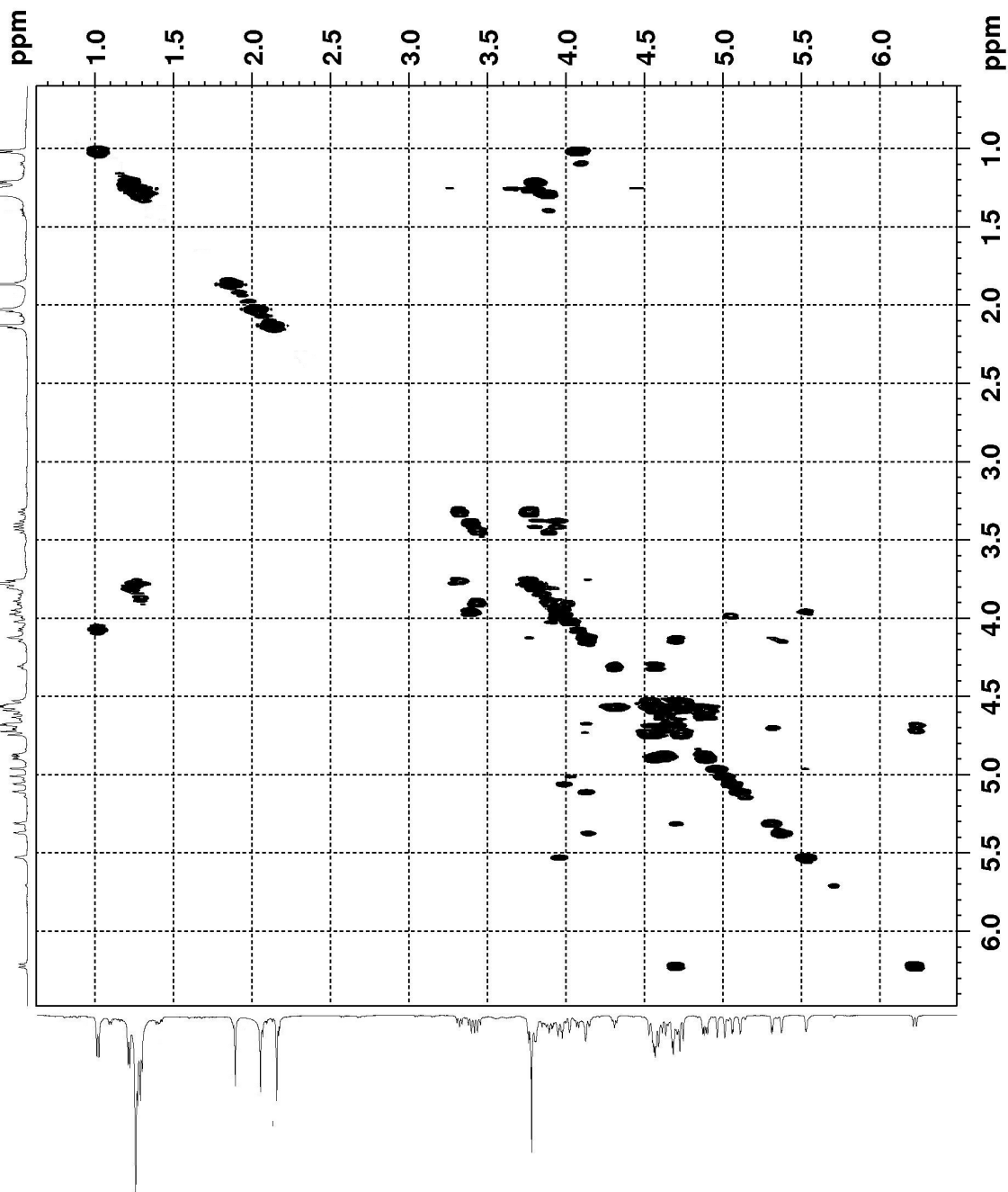
===== CHANNEL f1 =====
 SF01 500.3625017 MHz
 NUC1 1H
 P0 17.50 usec
 P1 17.50 usec
 P17 2500.00 usec
 PLW1 10.0000000 W
 PLW10 3.40280008 W

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

F1 - Acquisition parameters
 TD 128
 SF01 500.3625 MHz
 FIDRES 78.203201 Hz
 SW 10.003 ppm
 F1MODE QF

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

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





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

F2 - Acquisition Parameters
 Date_ 20190617
 Time 20:36
 INSTRUM Bruker_default_av500
 PULPROG 5 mm F4BBO BH/
 TD 65536
 FIDRES 0.1024000 Hz
 TD 65536
 SFO1 500.13625017 MHz
 SOLVENT CDCl3
 NS 16
 DS 16
 SWH 5000.000 Hz
 FIDRES 0.1024000 Hz
 AQ 0.1024000 sec
 RG 128
 DE 100.000 usec
 TE 300.2 K
 TEST2 145.0000000 sec
 D0 0.00000000 sec
 D1 1.50000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 DELTA 0.00000000 sec
 TNO 0.00001990 sec
 ZGPGTNS

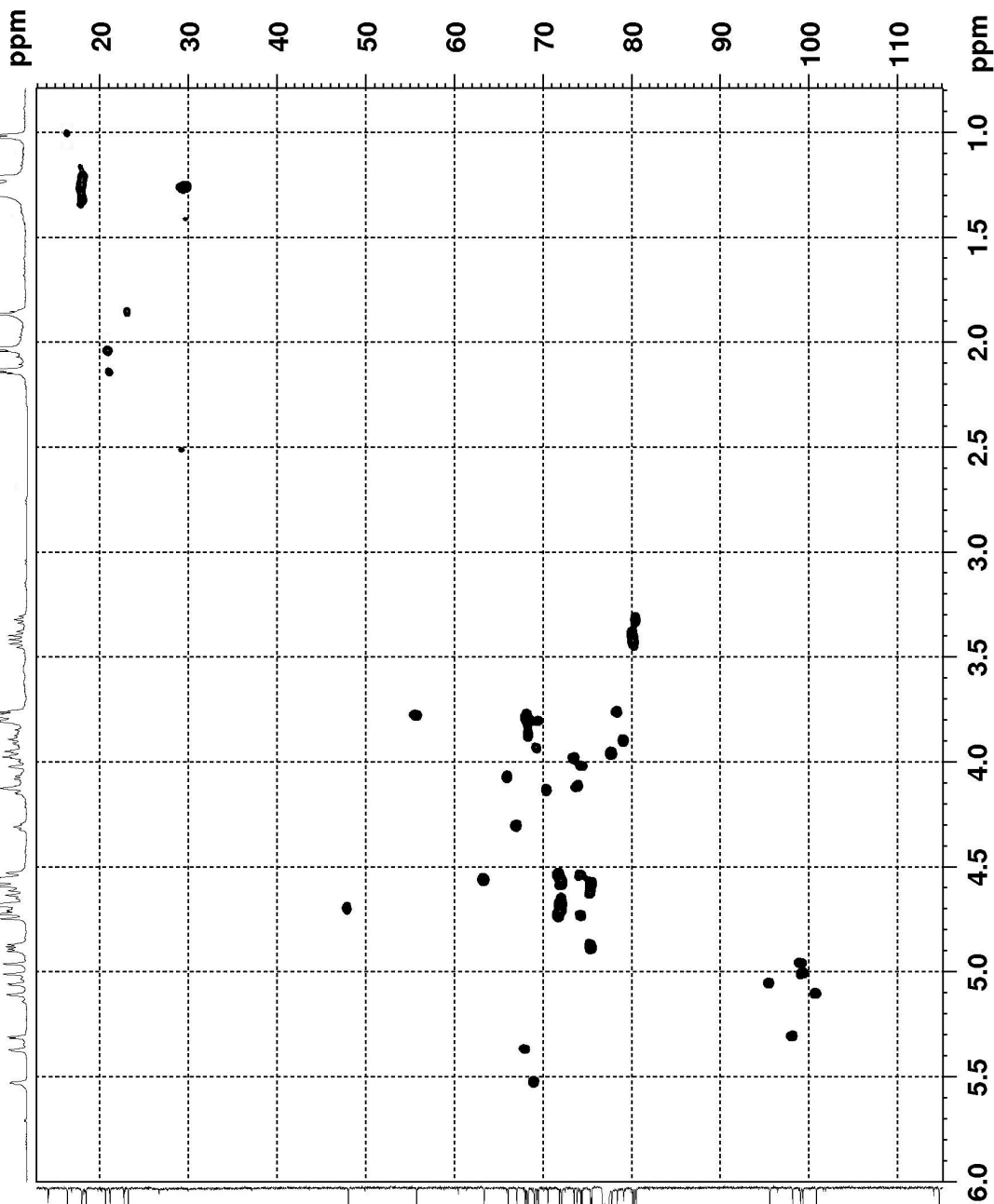
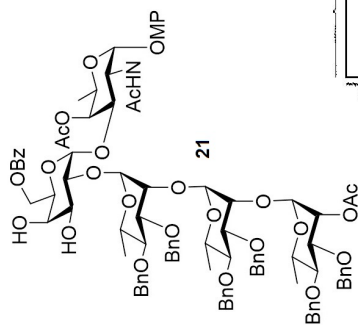
===== CHANNEL f1 =====
 SFO1 500.13625017 MHz
 NUC1 1H
 P1 17.50 usec
 F2 35.00 usec
 P28 1000.00 usec
 PL1 10.00000000 W

===== CHANNEL f2 =====
 SFO2 125.8282000 MHz
 NUC2 13C
 P1 11.50 usec
 F2 23.00 usec
 P4 70.00 usec
 PL12 66.00000000 W
 PL12 1.78129990 W

===== GRADIENT CHANNEL =====
 GENAM[1] SMSQ10.100
 GENAM[2] SMSQ10.100
 GENAM[3] SMSQ10.100
 GENAM[4] SMSQ10.100
 GP21 20.10 %
 GP22 11.00 %
 GP23 -5.00 %
 F16 1000.00 usec
 F19 600.00 usec

F1 - Acquisition Parameters
 TD 256
 SFO1 125.8282000 MHz
 FIDRES 196.293976 Hz
 SFO2 500.13625017 MHz
 F2 - Processing parameters
 SI 1024
 SF 500.13625017 MHz
 SF 125.8282000 MHz
 LB 0 Hz
 GB 0
 FC 1.00

F1 - Processing Parameters
 SI 1024
 SF 125.8282000 MHz
 SF 500.13625017 MHz
 LB 0 Hz
 GB 0



GROUP BM
BM-AC-160C 8 in CD3OD

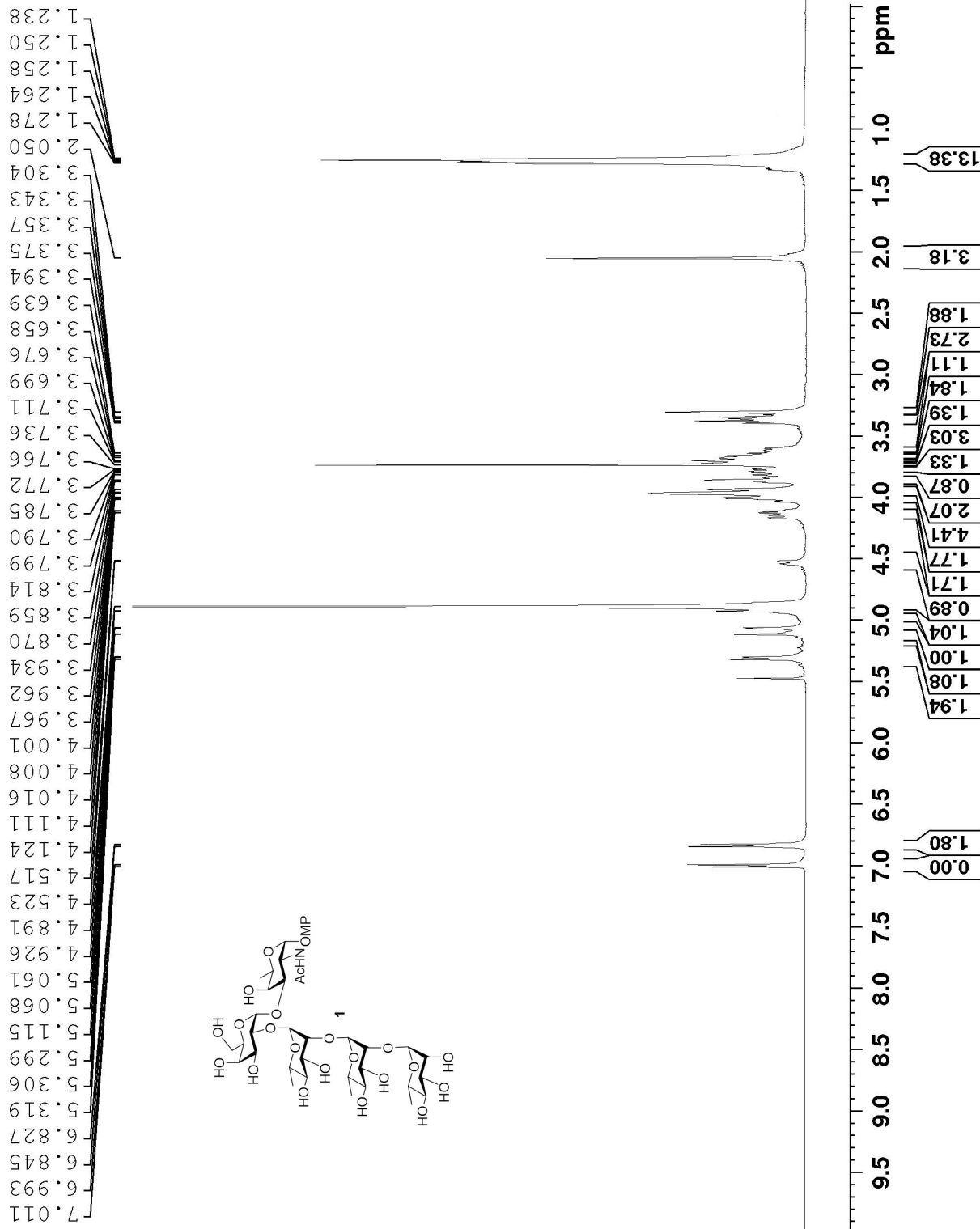


Current Data Parameters
NAME BM-AC-RL160C
EXPNO 481
PROCNO 1

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

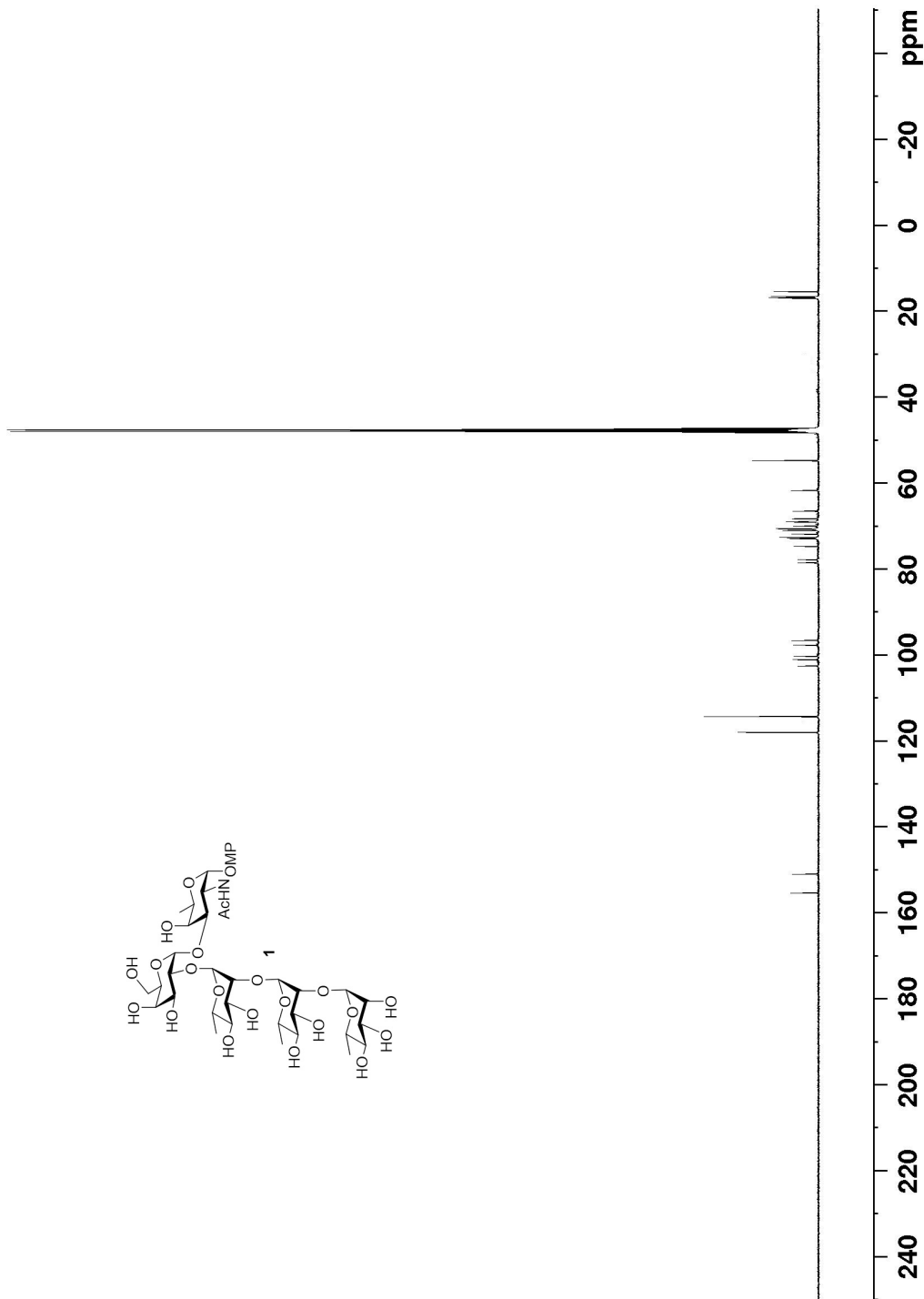
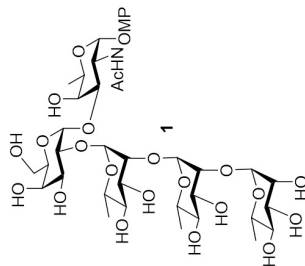
SWH 37878.789 Hz
FIDRES 0.577984 Hz
AQ 0.8650752 sec
RG 90.5
DW 13.200 usec
DE 6.50 usec
TE 730.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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

155.26
150.85
117.88
114.18
102.41
100.95
100.12
97.54
96.49
78.36
77.67
74.57
72.85
72.81
72.61
72.51
71.69
70.85
70.56
70.50
70.42
69.85
68.99
68.90
68.81
68.13
66.37
61.57
54.62
48.13
47.91
47.74
47.57
47.40
47.23
47.06
21.24
16.82
16.59
16.44
15.27



GROUP BM
BM-AC-160C in CDCl3



```

Current Data Parameters
NAME      BM-AC-160C
EXPNO     1.0
PROCNO    1

F2 - Acquisition Parameters
Date_     20190920
Time      6.31
INSTRUM   Bruker_default_av500
PROBHD    5 mm PABBO BB/
PULPROG   cosygpbcf
TD         2048
SOLVENT   MeOD
NS         2
DS         8
SWH        5000.000 Hz
FIDRES     2.441406 Hz
AQ         0.2048000 sec
RG         80.6
DE         100.000 usec
TE         3451.2 K
D0         0.0000000 sec
D1         2.0000000 sec
D11        0.0300000 sec
D12        0.0002000 sec
D13        0.0000040 sec
D16        0.0002000 sec
IN0        0.00019980 sec

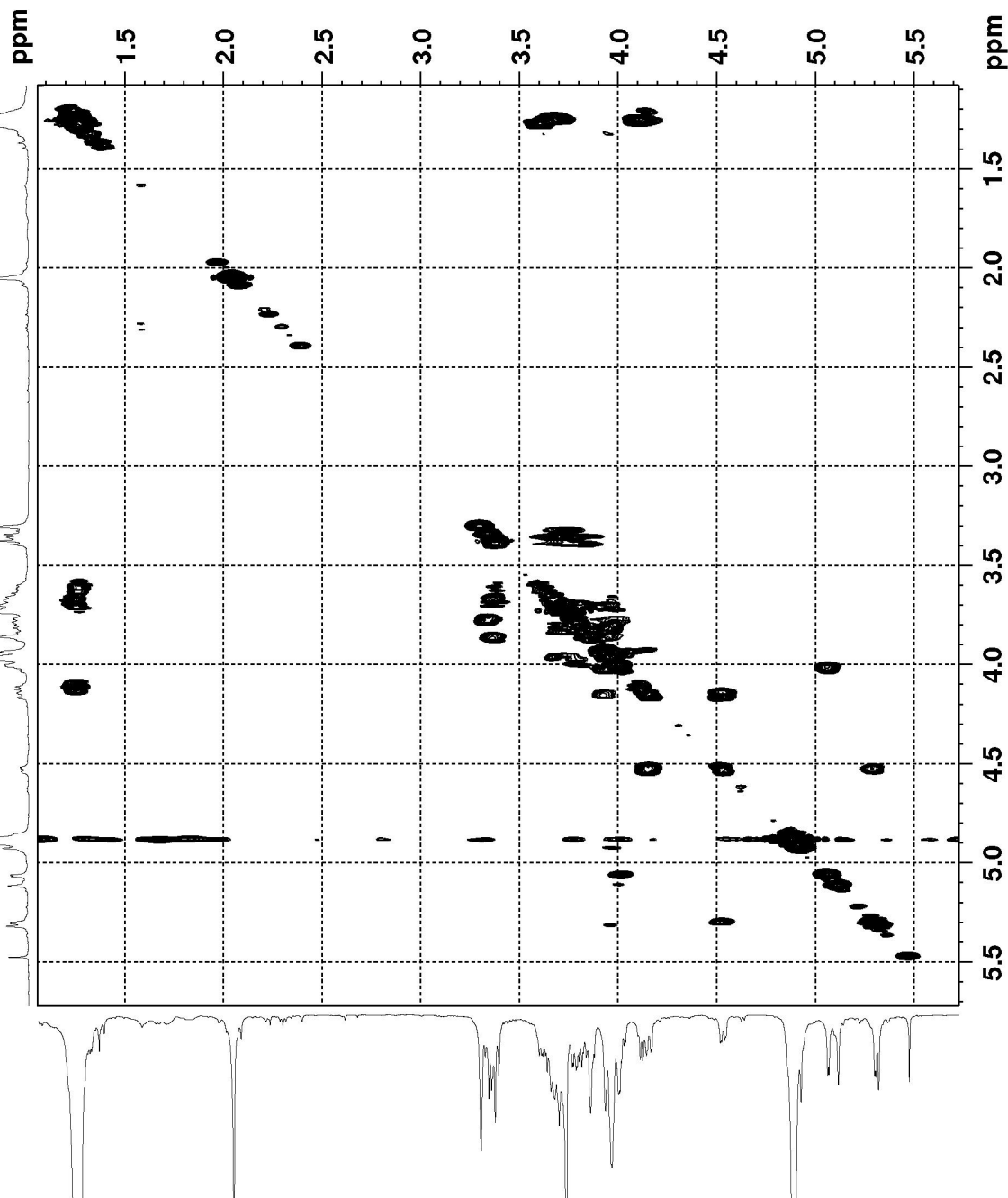
===== CHANNEL f1 =====
SF01      500.3625017 MHz
NUC1      1H
P0         17.50 usec
PL1        17.50 usec
PL17       2500.00 usec
PLW1       10.0000000 W
PLW10      3.40280008 W

===== GRADIENT CHANNEL =====
GPNAM[1]  SMSQ10.100
GP21      10.00 %
PL6        1000.00 usec

F1 - Acquisition parameters
TD         128
SF01      500.3625 MHz
FIDRES     78.203201 Hz
SW         10.003 ppm
F1MODE     QF

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

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



GROUP BM
BM-AB-160C in CD3OD
HSQC



Current Data Parameters
NAME BM-AC-160C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190920
Time 6.44
INSTRUM Bruker-default_av500
PULPROG zgpg30
TD 1024
SOLVENT MeOD
NS 4
DS 16
SW 5000.016 Hz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 80.6
DM 100.000 usec
DE 6.50 usec
TE 300.2 K
CNS12 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.03000000 sec
D2 0.0086207 sec
D3 0.0086207 sec
INO 0.00001930 sec
ZGPGTNS

===== CHANNEL f1 =====
SFO1 500.3625014 MHz
NUC1 13C
P1 17.50 usec
P2 35.00 usec
P28 1000.00 usec
PLW1 10.00000000 W

===== CHANNEL f2 =====
SFO2 125.828031 MHz
NUC2 13C
P2 11.50 usec
P3 23.00 usec
P4 76.00 usec
PLW2 66.00000000 W
PLW12 1.78129995 W

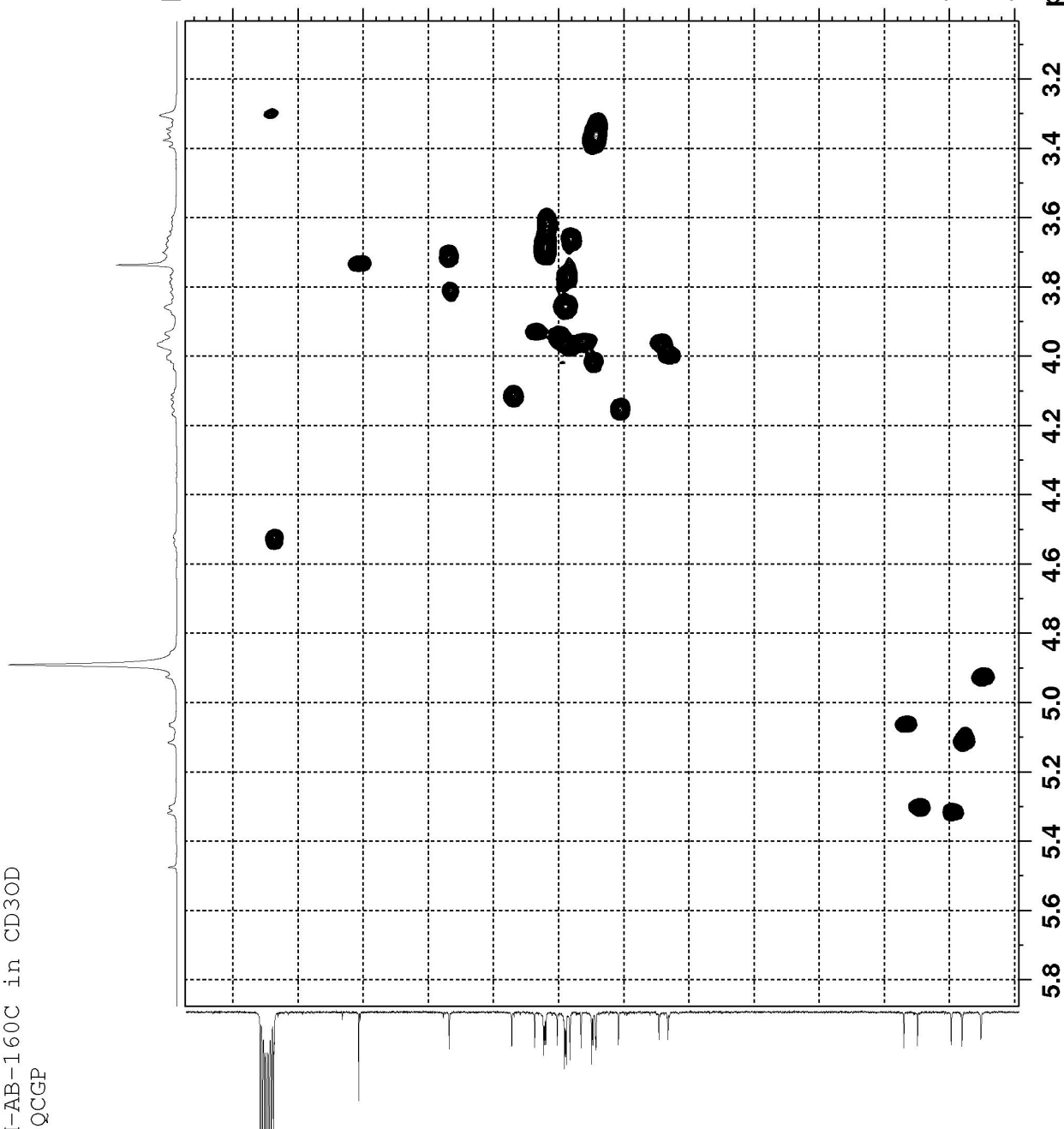
===== GRADIENT CHANNEL =====
GPNAM[1] SWSQ10.100
GPNAM[2] SWSQ10.100
GPNAM[3] SWSQ10.100
GPNAM[4] SWSQ10.100
GP21 80.00 %
GP22 20.10 %
GP23 11.00 %
GP24 5.00 %
P1 100.00 usec
P19 600.00 usec

F1 - Acquisition Parameters
TD 195
SFO1 125.8282 MHz
SFO2 251.561611 Hz
SW 199.682 Fm
FIDRES
F1MODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.360000 MHz
WDW 500.360000 MHz
SSB 0 Hz
LB 0
GB 0
PC 1.00

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

ppm 45 50 55 60 65 70 75 80 85 90 95 100 105 ppm



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

Display Report

Analysis Info

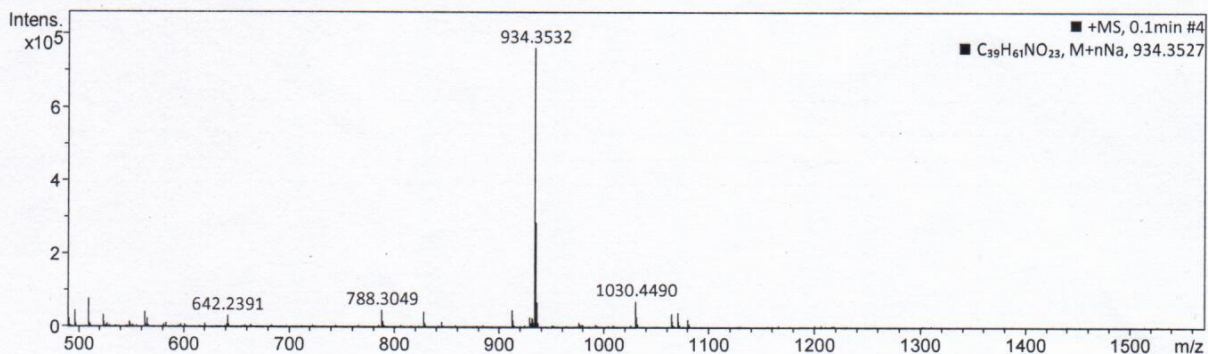
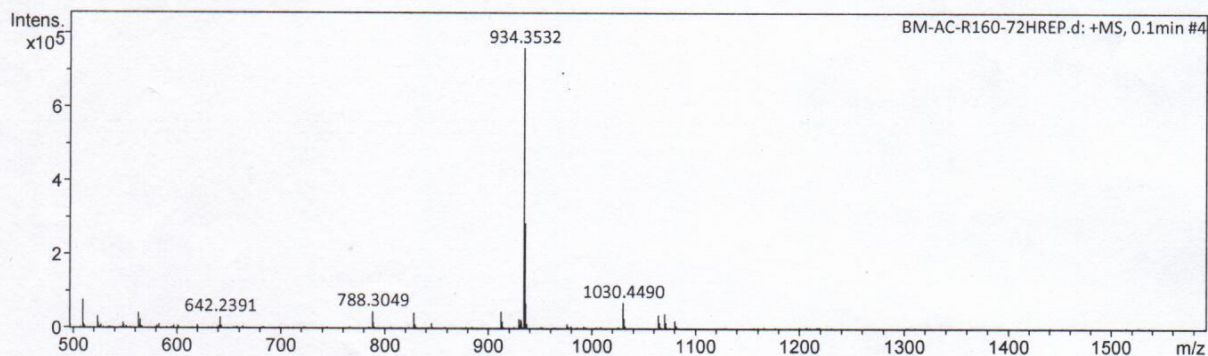
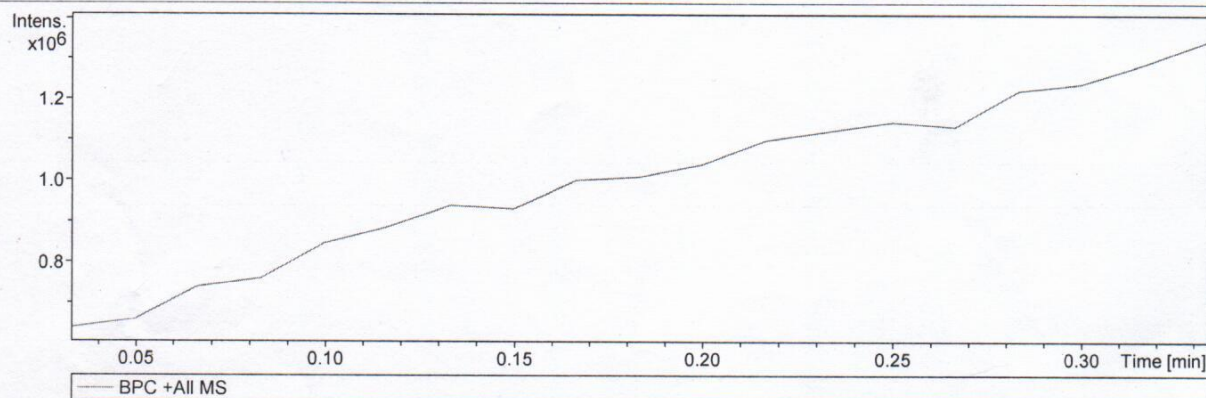
Analysis Name D:\Data\User data\2019\SEP\BM-AC-R160-72HREP.d
 Method Tune_pos_Mid.m
 Sample Name BM-AC-R160-72HREP
 Comment

Acquisition Date 9/24/2019 3:37:12 PM

Operator IISER Kalyani
 Instrument maXis impact 8282001.00127

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-R160-72HREP.d

Bruker Compass DataAnalysis 4.1

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by: IISER Kalyani

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Display Report

Analysis Info

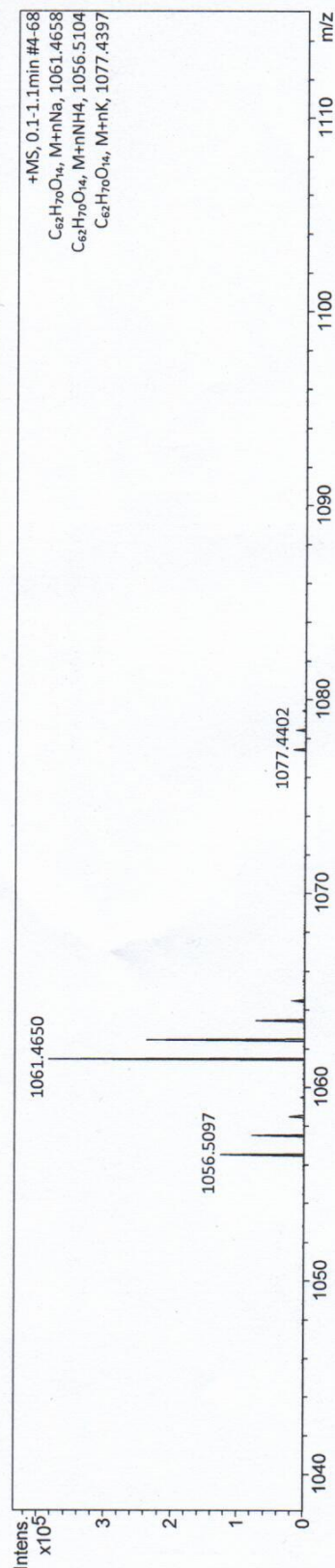
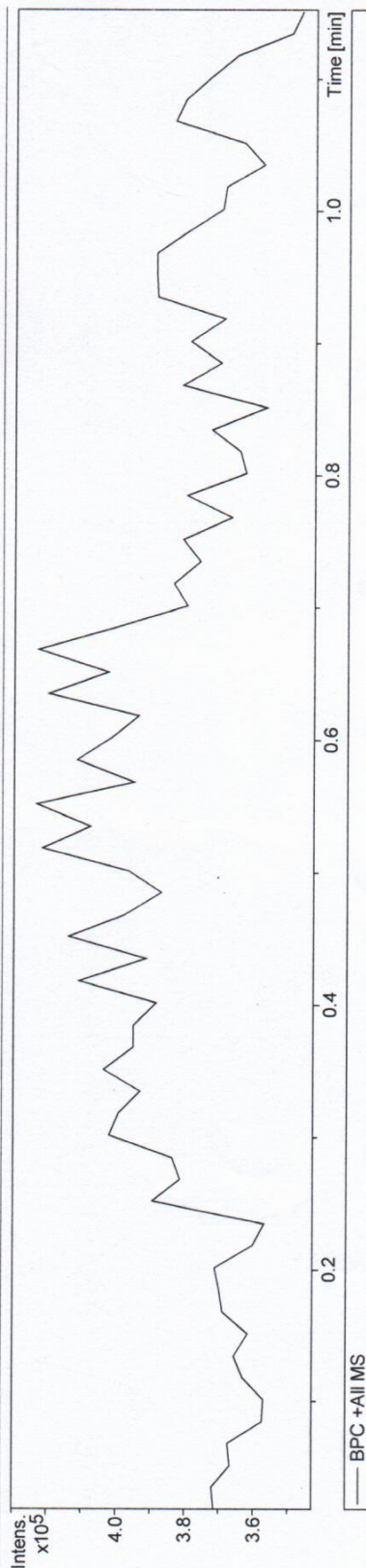
Analysis Name D:\Data\User data\2019\DEC\BM-AC-TRIOH.d
 Method Tune_pos_Mid.m
 Sample Name BM-AC-TRIOH
 Comment pyrrole -COOH and -COOET

Acquisition Date 12/24/2019 12:54:04 PM

Operator IISER Kalyani
 Instrument maxIs impact 8282001.00127

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

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