Synthesis and Evaluation of a QS-17/18-Based Vaccine Adjuvant

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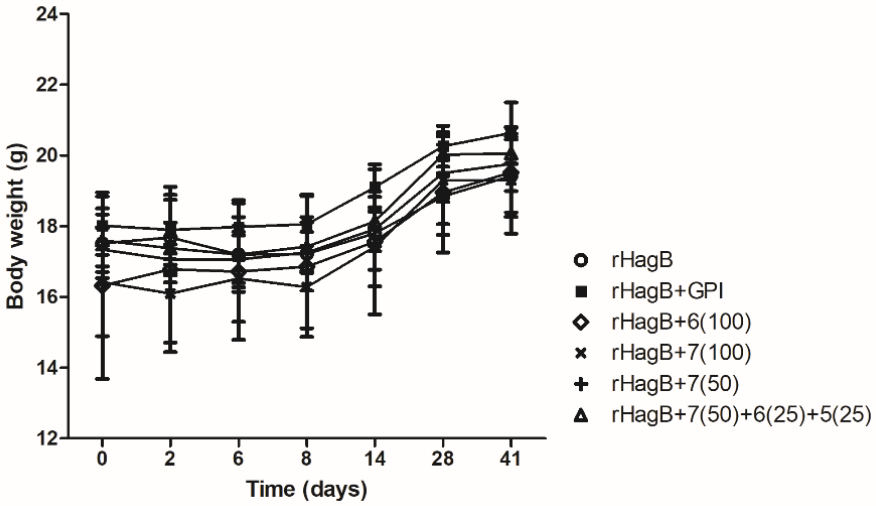
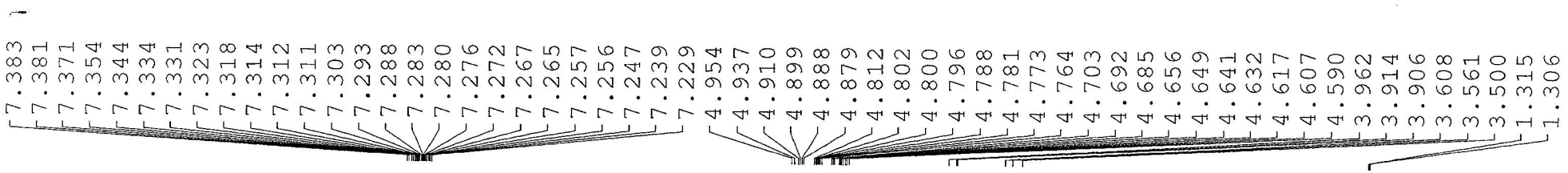


Figure S1. Mice weights at various time points.

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PROCNO                1

F2 - Acquisition Parameters
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Time               9.40
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          14423.077 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                  16
DW               34.667 usec
DE                6.50 usec
TE               298.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                8.00 usec
PL1               1.30 dB
PL1W         6.88972235 W
SFO1        700.0243229 MHz

F2 - Processing parameters
SI                32768
SF          700.0200813 MHz
WDW                  no
SSB       0
LB        0 Hz
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PC                1.00
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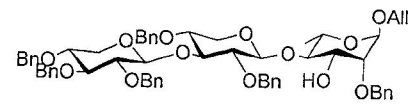
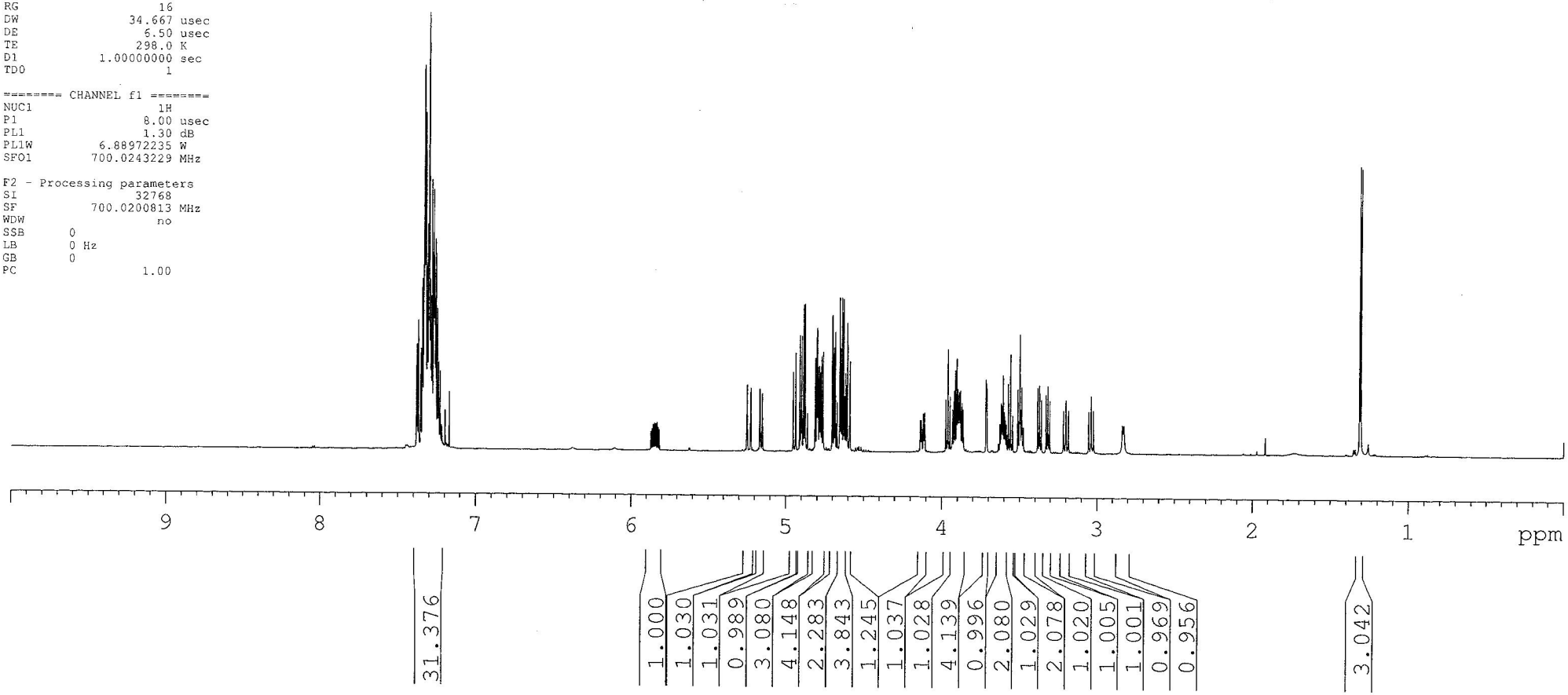
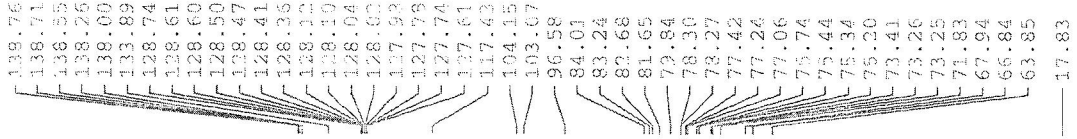
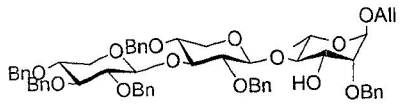


13







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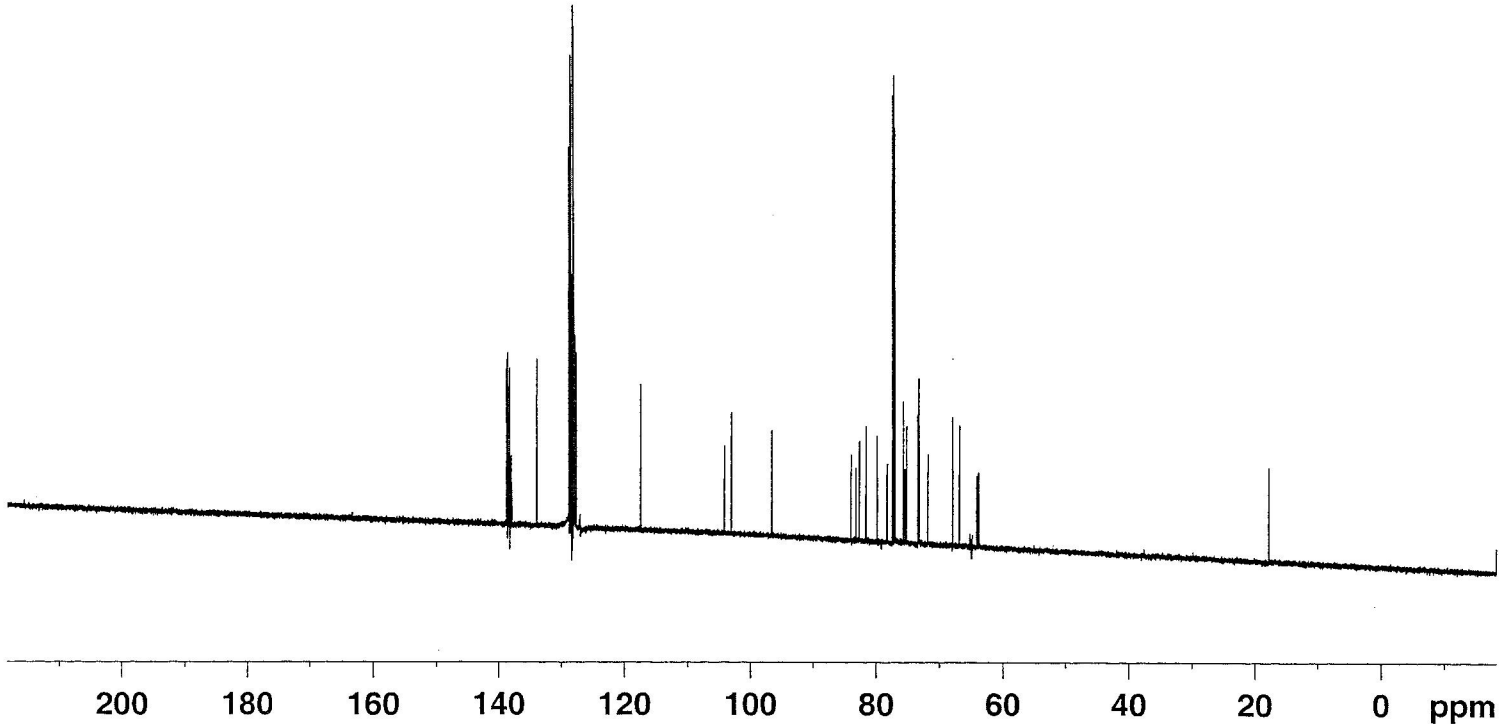
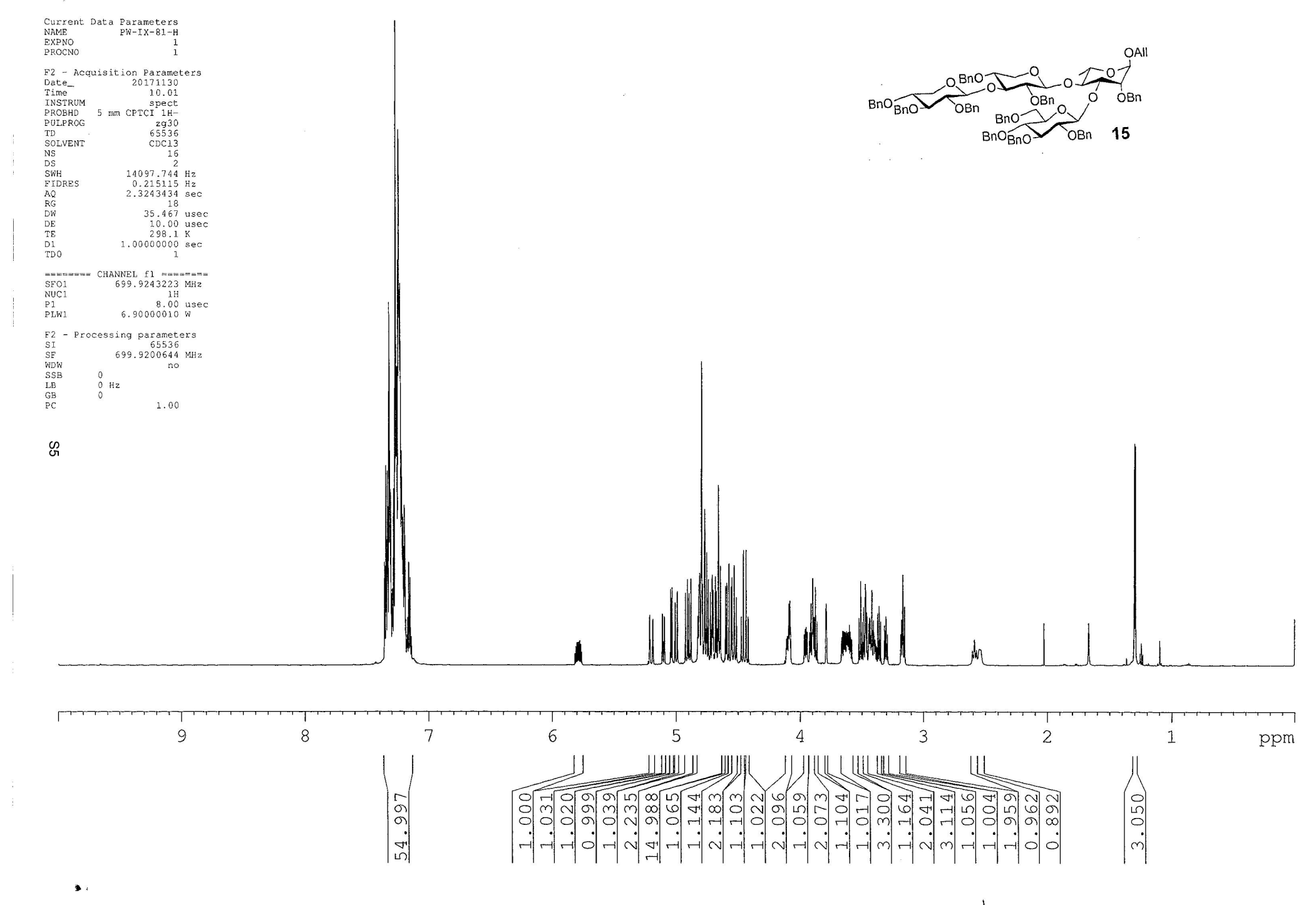


BRUKER

NAME	PW-VIII-50C13
EXPNO	2
PROCNO	1
Date_	20140312
Time	10.37
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	69
DS	4
SWH	41666.668 H
FIDRES	0.635783 H
AQ	0.7864820 s
RG	4
DW	12.000 u
DE	6.50 u
TE	298.0 K
D1	2.00000000 s
D11	0.03000000 s
TD0	1
======== CHANNEL f1 =====	
NUC1	13C
P1	11.00 u
PL1	-1.30 d
PL1W	128.76077271 W
SFO1	176.0377710 M
======== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 u
PL2	1.30 d
PL12	19.50 d
PL13	19.50 d
PL2W	6.88972235 W
PL12W	0.10428017 W
PL13W	0.10428017 W
SFO2	700.0228001 M
SI	32768
SF	176.0201690 M
WDW	no
SSB	0
LB	0.00 H
GB	0
PC	1.40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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 14097.744 Hz
FIDRES 0.215115 Hz
AQ 2.3243434 sec
RG 18
DW 35.467 usec
DE 10.00 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 699.9243223 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.90000010 W
F2 - Processing parameters
SI 65536
SF 699.9200644 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
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BnO
OBn
15
9
8
7
6
5
4
3
2
1
ppm
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1.000
1.031
1.020
0.999
1.039
2.235
14.988
1.065
1.144
2.183
1.103
1.022
2.096
1.059
2.073
1.104
1.017
3.300
1.164
2.041
3.114
1.056
1.004
1.959
0.962
0.892
3.050

138.8 138.7 138.7 138.7 138.6 138.5 138.4 138.1 134.0 128.4 128.4 128.3 128.2 128.2 128.2 128.1 128.1 127.9 127.8 127.7 127.7 127.6 127.5 127.5 127.4 127.4 127.4 127.3 127.3 127.2 127.1 116.6 103.1 101.7 84.4 83.6 82.4 82.3 79.3 78.0 77.8 77.2 77.0 76.8 75.7 75.6 75.4 74.6 74.5 74.3 74.3 73.2 73.1 72.5 68.7 67.5 67.1 17.9

Current Data Parameters
NAME PW-IX-81-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171130
Time 10.31
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2674
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864320 sec
RG 203
DW 12.000 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 176.0126227 MHz
NUC1 13C
P1 14.00 usec
PLW1 95.00000000 W

======== CHANNEL f2 ========
SFO2 699.9227997 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 6.90000010 W
PLW12 0.10452000 W
PLW13 0.04416000 W

F2 - Processing parameters
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WDW no
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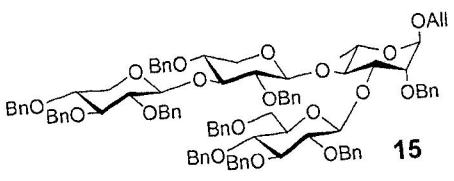
GB 0
PC 1.40



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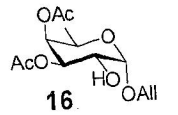

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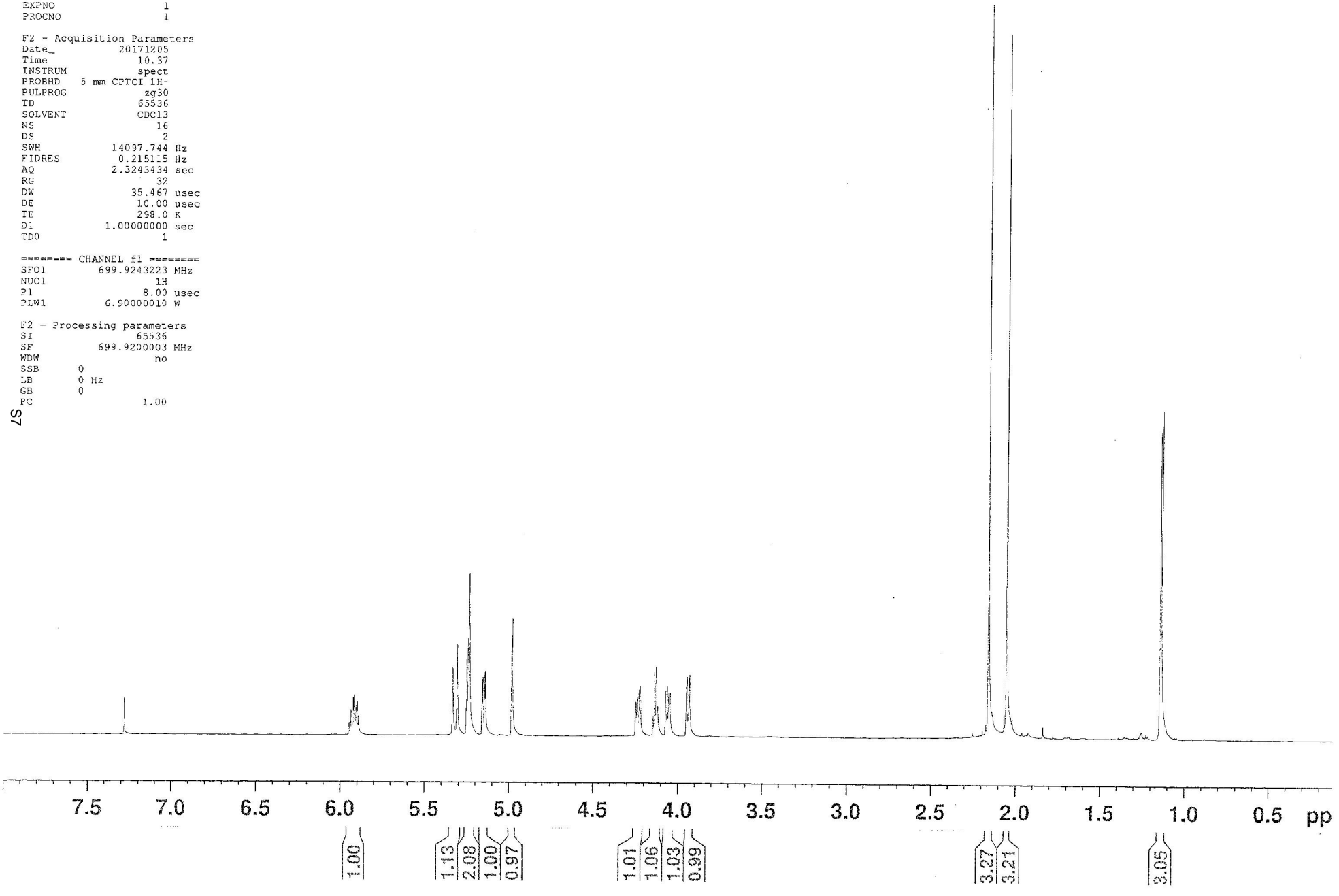
```
Current Data Parameters
NAME        PW-IX-187-SM
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171205
Time               10.37
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            14097.744 Hz
FIDRES         0.215115 Hz
AQ             2.3243434 sec
RG                    32
DW                35.467 usec
DE                10.00 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         699.9243223 MHz
NUC1                  1H
P1                 8.00 usec
PLW1          6.90000010 W

F2 - Processing parameters
SI                 65536
SF           699.9200003 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

S7



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Current Data Parameters
NAME      PW-IX-187-SM-C13
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171205
Time                 10.45
INSTRUM              spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     128
DS                       4
SWH              41666.668 Hz
FIDRES           0.635783 Hz
AQ               0.7864320 sec
RG                     203
DW                12.000 usec
DE                 18.00 usec
TE                 298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          176.0126227 MHz
NUC1                  13C
P1                  14.00 usec
PLW1          95.00000000 W

======== CHANNEL f2 ========
SFO2          699.9227997 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               65.00 usec
PLW2           6.90000010 W
PLW12          0.10452000 W
PLW13          0.04416000 W

F2 - Processing parameters
SI                   32768
SF            175.9950354 MHz
WDW                     no
SSB       0
LB        0 Hz
GB        0
PC                   1.40
```

170.8
170.5
133.3
133.3
118.2
118.2
97.7
77.2
77.0
76.8
71.3
71.2
68.8
66.9
64.9
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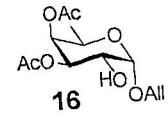
20.8
20.6
15.8



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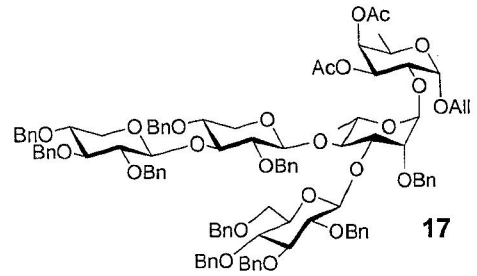
200 180 160 140 120 100 80 60 40 20 0 ppm



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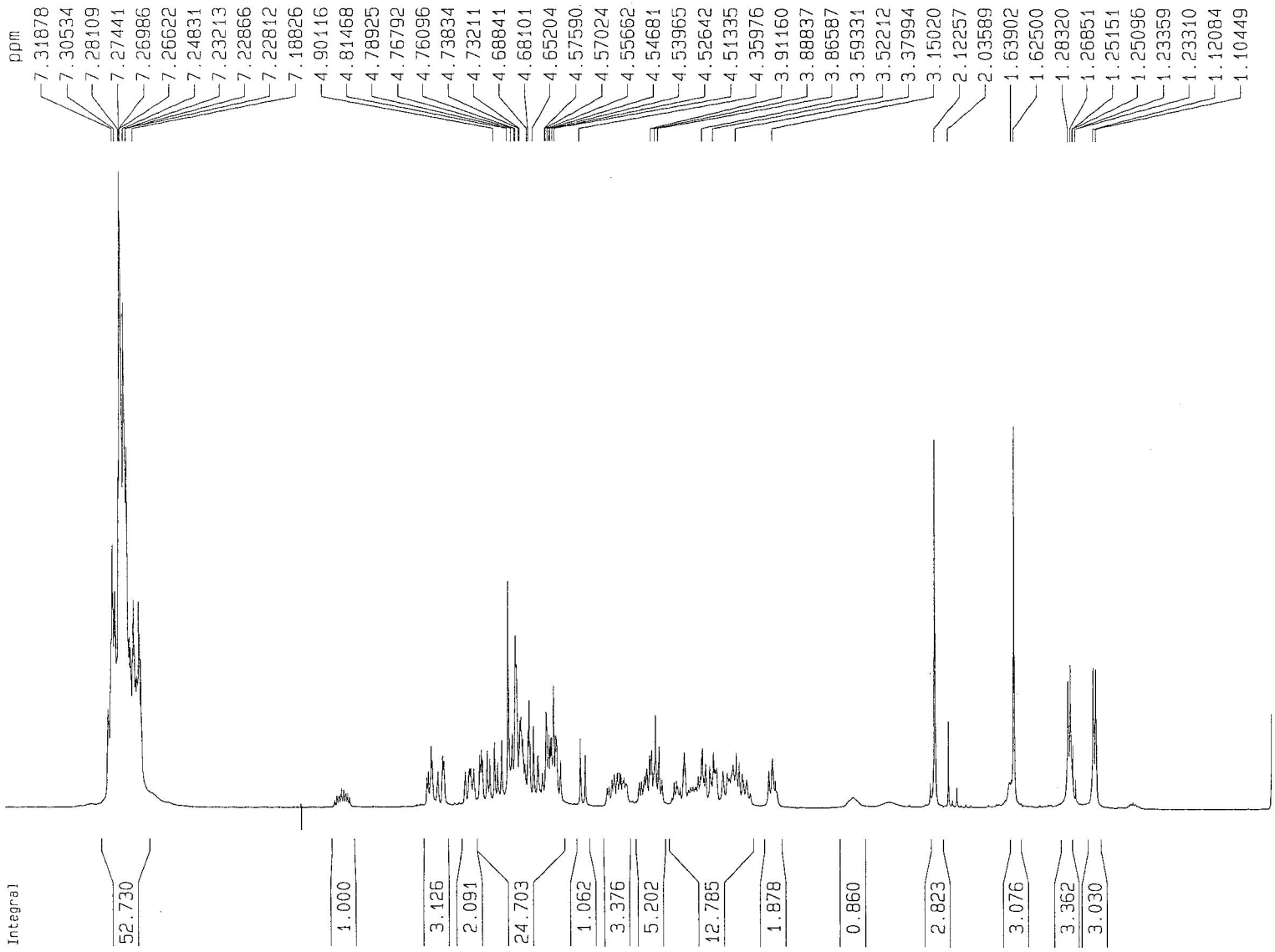


Current Data Parameters

NAME	PW-VIII-63-H
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20160203
Time	9.01
INSTRUM	drx400
PROBHD	5 mm Multinu
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	40.3
DW	60.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

========== CHANNEL f1 ========

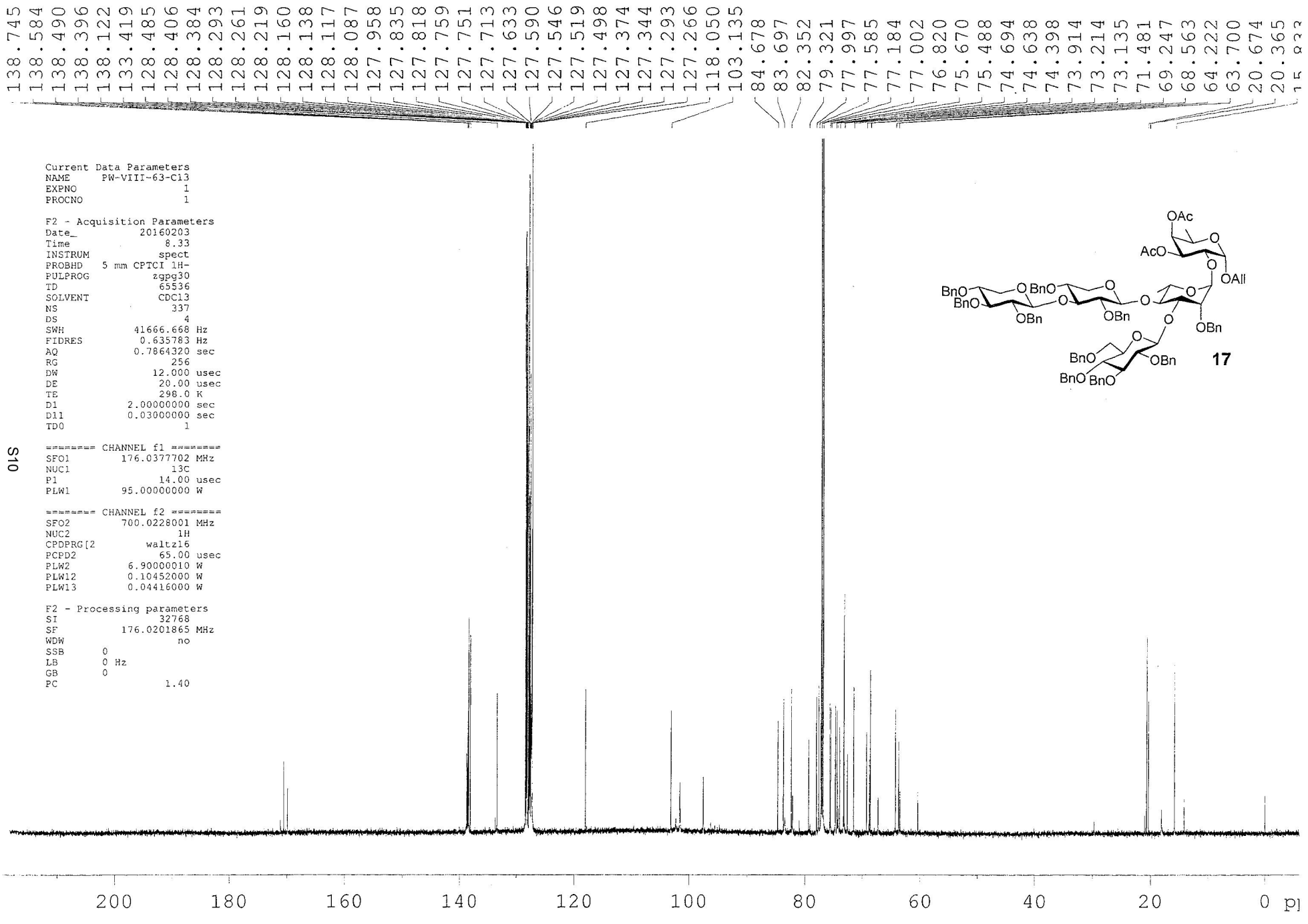
NUC1	1H
P1	6.50 usec
PL1	0.00 dB
SF01	400.1324710 MHz

F2 - Processing parameters

SI	131072
SF	400.1300215 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	8.000 ppm
F1	3201.04 Hz
F2P	0.000 ppm
F2	0.00 Hz
PPMCM	0.40000 ppm/cm
HZCM	160.05202 Hz/cm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Current Data Parameters
NAME PW-VIII-63-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160203
Time 8.33
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 337
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864320 sec
RG 256
DW 12.000 usec
DE 20.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 176.0377702 MHz
NUC1 13C
P1 14.00 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 700.0228001 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 6.90000010 W
PLW12 0.10452000 W
PLW13 0.04416000 W
F2 - Processing parameters
SI 32768
SF 176.0201865 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40
OAc
AcO
OAll
BnO
OBn
17
200 180 160 140 120 100 80 60 40 20 0 pp

```
Current Data Parameters
NAME       PW-IX-103-C2H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170814
Time               9.30
INSTRUM           spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   7
DS                   2
SWH          14097.744 Hz
FIDRES        0.215115 Hz
AQ            2.3243434 sec
RG                22.6
DW               35.467 usec
DE               10.00 usec
TE               298.0 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        700.0243229 MHz
NUC1                1H
P1               8.00 usec
PLW1        6.90000010 W

F2 - Processing parameters
SI                65536
SF          700.0200198 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                1.00
```


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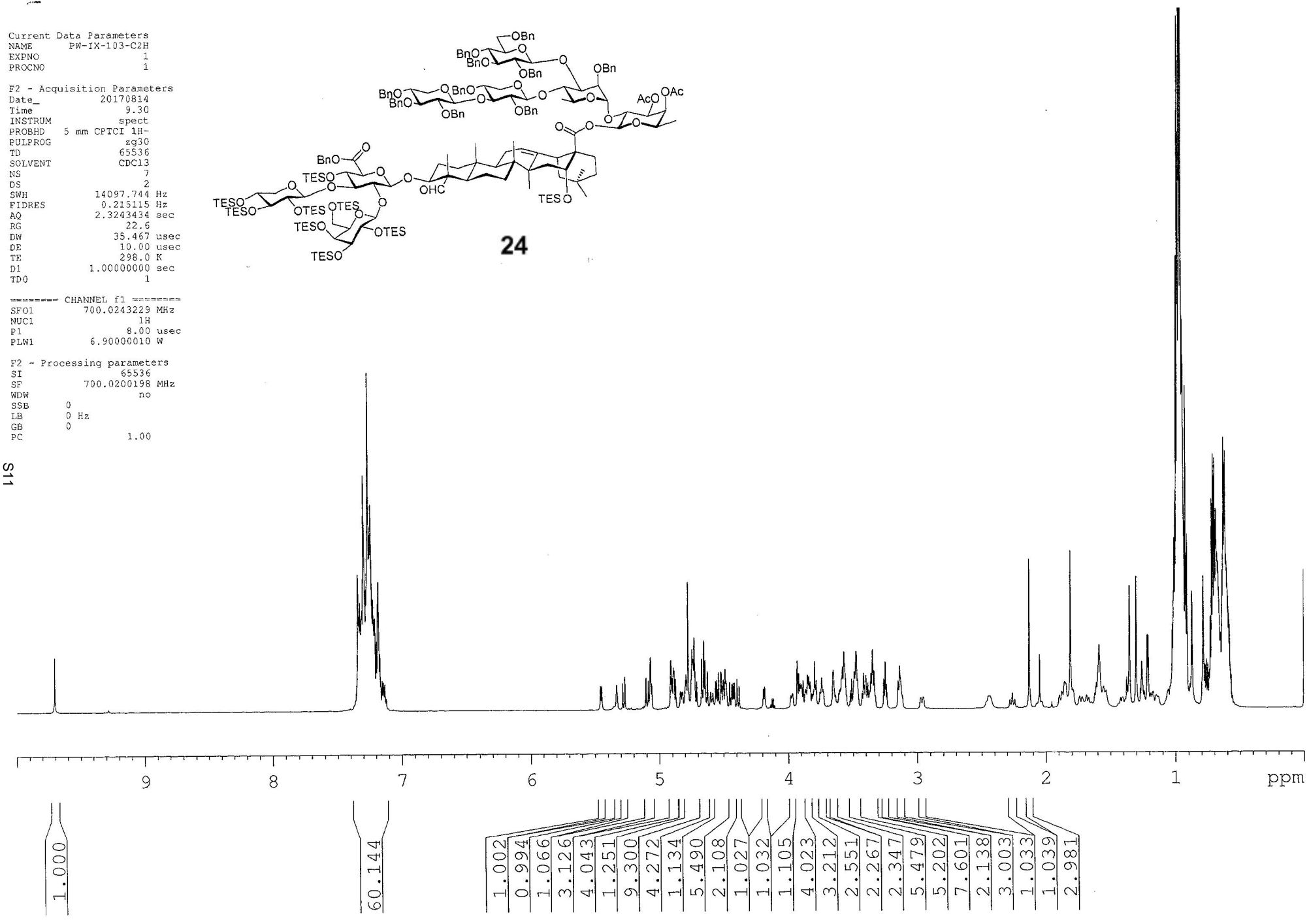

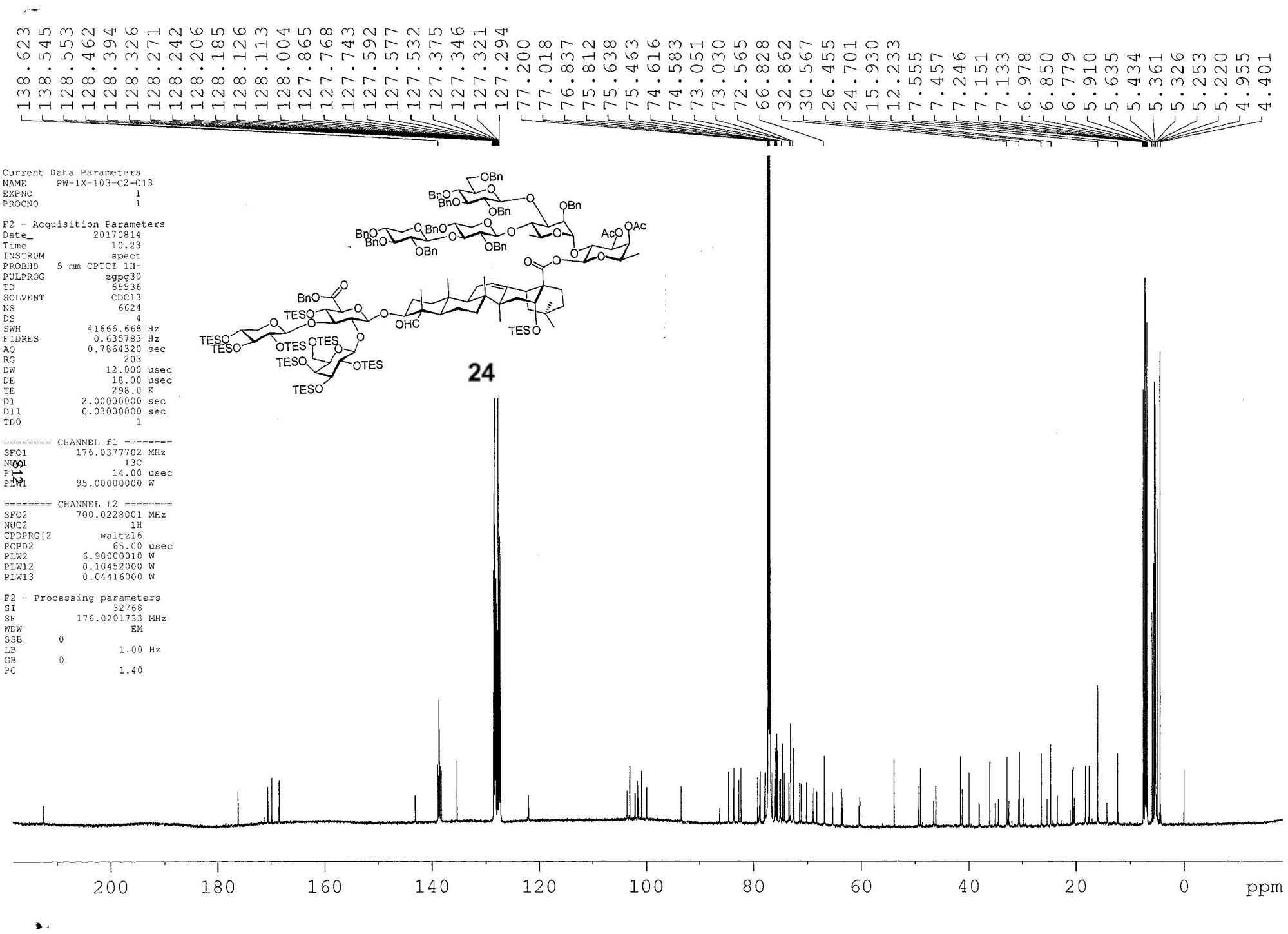
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127.865
127.768
127.743
127.592
127.577
127.532
127.375
127.346
127.321
127.294
77.200
77.018
76.837
75.812
75.638
75.463
74.616
74.583
73.051
73.030
72.565
66.828
32.862
30.567
26.455
24.701
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12.233
7.555
7.457
7.246
7.151
7.133
6.978
6.850
6.779
5.910
5.635
5.434
5.361
5.326
5.253
5.220
4.955
4.401
Current Data Parameters
NAME PW-IX-103-C2-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170814
Time 10.23
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6624
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864320 sec
RG 203
DW 12.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 176.0377702 MHz
NUC1 13C
P1 14.00 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 700.0228001 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 6.90000010 W
PLW12 0.10452000 W
PLW13 0.04416000 W
F2 - Processing parameters
SI 32768
SF 176.0201733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OBn
BnO
AcO
OAc
BnO
TESO
OTES
OHC
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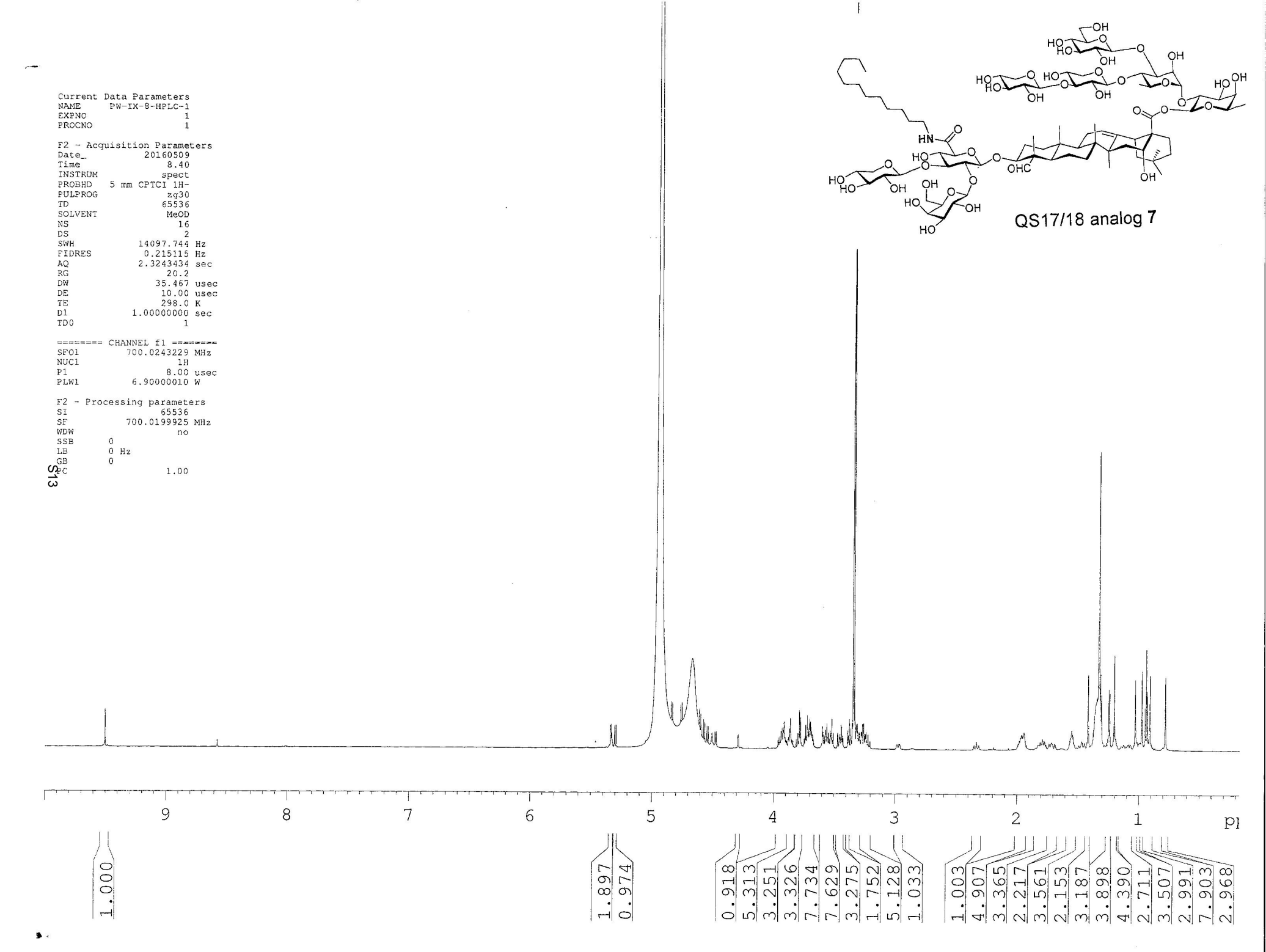
200
180
160
140
120
100
80
60
40
20
0
ppm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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160509
Time 8.40
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 14097.744 Hz
FIDRES 0.215115 Hz
AQ 2.3243434 sec
RG 20.2
DW 35.467 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 700.0243229 MHz
NUC1 1H
P1 8.00 usec
PLW1 6.90000010 W
F2 - Processing parameters
SI 65536
SF 700.0199925 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
QS17/18 analog 7
9
8
7
6
5
4
3
2
1
ppm
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0.918
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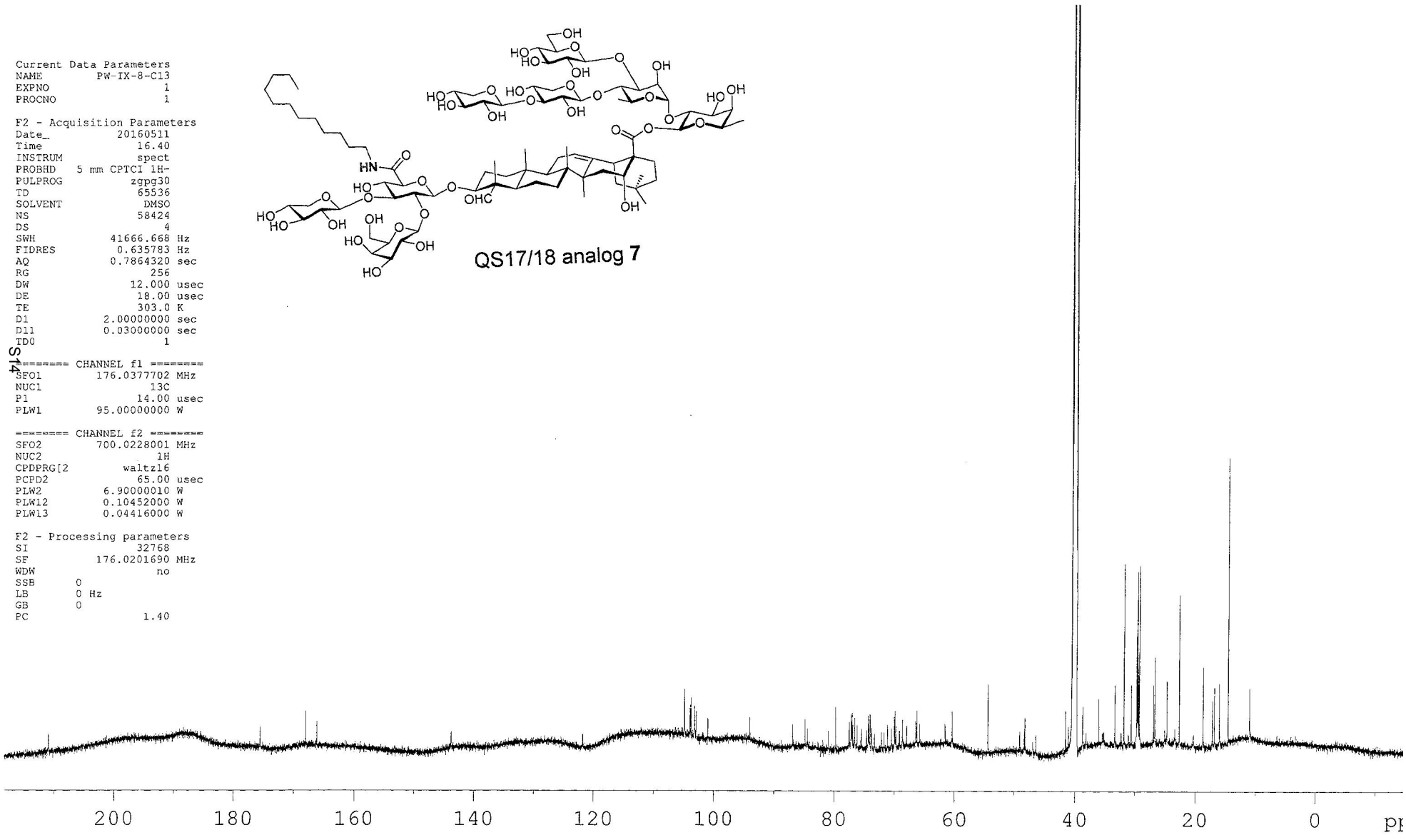
3.326
7.734
7.629
3.275
1.752
5.128
1.033
1.003
4.907
3.365
2.217
3.561
2.153
3.187
3.898
4.390
2.711
3.507
2.991
7.903
2.968

167.861 104.739 103.869 103.707 103.094 103.013 102.810 100.907 93.941 84.793 79.648 77.086 76.921 76.522 74.178 73.927 69.939 69.808 68.542 66.155 60.305 54.351 48.175 41.448 40.494 40.356 40.236 40.117 39.997 39.878 39.822 39.759 39.640 38.634 35.959 33.308 31.791 31.763 30.605 29.709 29.641 29.623 29.595 29.543 29.500 29.436 29.343 29.247 26.899 26.684 24.658 22.600 18.577 17.062 16.718 15.911 14.453 10.930

QS17/18 analog 7

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Current Data Parameters
NAME         PW-IX-8-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160511
Time               16.40
INSTRUM             spect
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                   58424
DS                       4
SWH            41666.668 Hz
FIDRES         0.635783 Hz
AQ             0.7864320 sec
RG                     256
DW                12.000 usec
DE                 18.00 usec
TE                 303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         176.0377702 MHz
NUC1                 13C
P1                 14.00 usec
PLW1         95.00000000 W

======== CHANNEL f2 ========
SFO2         700.0228001 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              65.00 usec
PLW2          6.90000010 W
PLW12         0.10452000 W
PLW13         0.04416000 W

F2 - Processing parameters
SI                   32768
SF           176.0201690 MHz
WDW                     no
SSB       0
LB        0 Hz
GB        0
PC                   1.40
```