

SUPPORTING INFORMATION

An organocatalytic strategy for the stereoselective synthesis of C-galactosides with fluorine at the pseudoanomeric carbon

Ahmad S. Altit, ^a S. Bachan, ^a W. Alrowhani ^a and D. R. Mootoo ^a

Department of Chemistry, Hunter College, 695 Park Avenue New York, NY 10065,
USA. E-mail: dmootoo@hunter.cuny.edu

Table of Contents

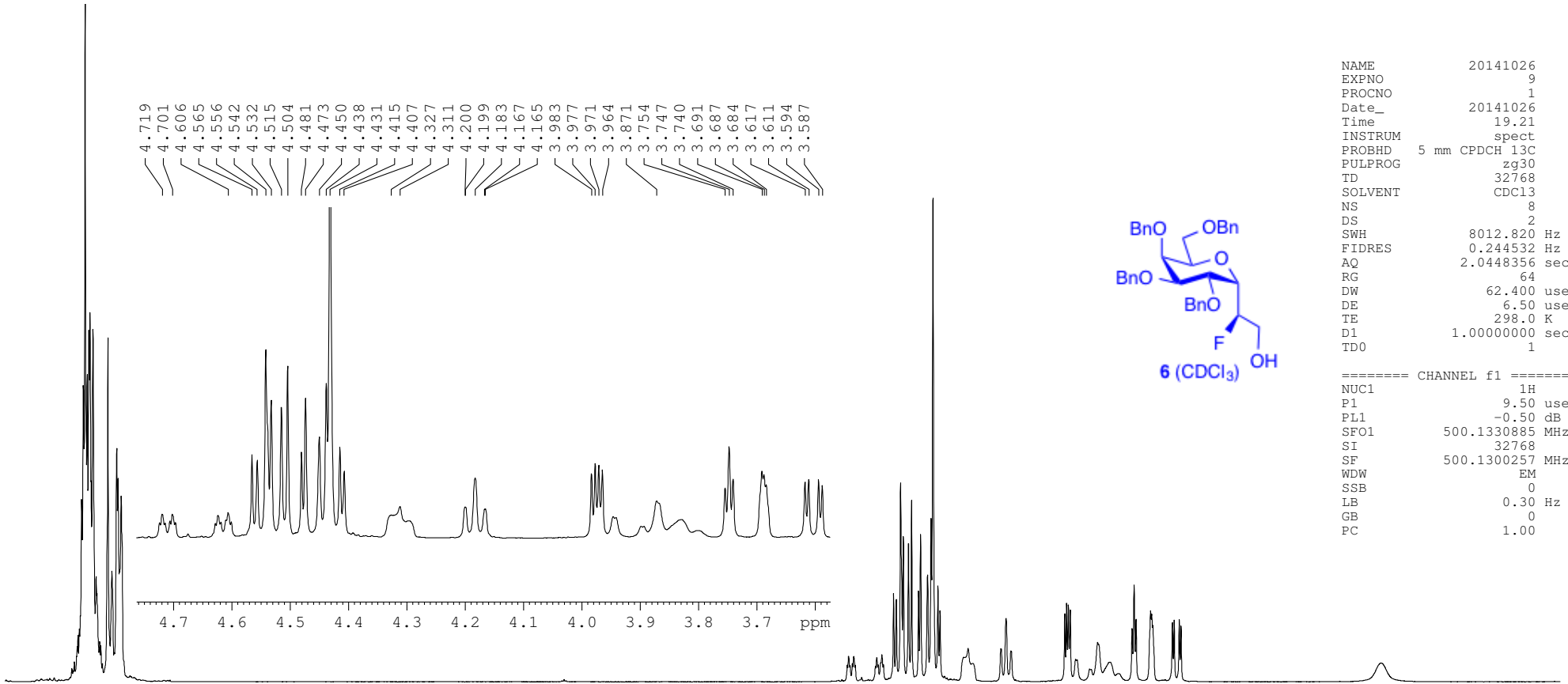
Table of NMR assignments for fluorinated derivatives	S2
NMR spectral charts for fluorinated materials	S3 – S64

NMR assignments for fluorinated derivatives [δ /ppm (multiplicity, J/Hz)]

	6 (CDCl ₃)	7 (CDCl ₃)	8 (CDCl ₃)	9 (C ₆ D ₆)	10 (C ₆ D ₆)	15 (C ₆ D ₆)	11 (CDCl ₃)	12 (CDCl ₃)	13 (CDCl ₃)	14 (C ₆ D ₆)
H1	4.20 (t, 8.1)	3.43 (dd, 9.2, 28.4)	3.97 (ddd, 3.0, 5.9, 34.1)	3.70 (ddd, 1.8, 10.0, 11.8)	4.62 (ddd, 2.1, 8.9, 18.0)	3.78 (m)	3.84 (dd, 2.4, 7.0)	3.20 (ddd, 1.7, 9.7, 27.7)	3.82 (dt, 4.5, 29.0)	4.43 (m, buried)
C1	65.2 (d, 32)	79.2 (d, 19)	73.5 (d, 35)	80.5 (d, 21)	68.3 (dd, 25, 34)	78.2 (t, 28)	69.6 (d, 29)	80.9 (d, 20)	73.3(d, 14)	72.3 (t, 31)
H2	3.75 (t, 3.5)	4.19 (t, 9.6)	3.84 (t, 2.6)	4.08 (t, 9.6)	4.47 (m)	4.45 (t, 9.4)	3.72 (m)	4.08 (t, 9.5)	3.92 (m)	3.82 (dd, 2.8, 4.4)
H3	3.69 (m)	3.66 (dd, 2.2, 9.5)	3.96 (dd, 9.5)	3.33 (dd, 2.7, 8.2)	3.99 (dd, 3.1, 5.3)	3.34 (dd, 2.8, 9.3)	3.99 (dd, 2.4, 7.0)	3.53 (m)	3.92 (m)	4.00 (m)
H4	3.98 (dd, 3.2, 6.3)	3.97 (bs)	4.05 (bt, 7.1)	3.85 (m)	4.05 (dd, 2.2, 5.0)	3.70 (d, 1.9)	3.72 (m)	3.90 (d, 2.0)	3.92 (m)	4.06 (dd, 2.4, 5.3)
H5	4.33 (m)	3.58 (t, 6.1)	4.14 (m)	3.36 (m)	3.80 (dd, 3.1, 5.0)	3.30 (t, 6.5)	4.33 (t, 7.2)	3.46 (t, 6.3)	4.19 (m)	4.57 (m)
H6	4.43 (m) 3.60 (dd, 3.1, 11.6)	3.61 (dd, 6.3, 8.7) 3.48 (dd, 5.8, 8.8)	3.59 (t, 9.5) 3.31 (dd, 4.4, 10.2)	3.63 (t, 8.1) 3.52 (dd, 5.4, 8.9)	4.38 (m) 3.71 (dd, 2.9, 11.2)	3.52 (dd, 6.3, 9.2) 3.47 (dd, 6.6, 9.2)	4.07 (dd, 8.5, 11.5) 3.72 (m)	3.53 (m)	3.70 (dd, 7.2, 10.3) 3.52 (dd, 5.1, 10.3)	4.20 (dd, 7.9, 11.3) 3.97 (dd, 3.5, 11.3)
H1'	4.65 (ddt, 2.8, 8.9, 48.0)	4.91 (dt, 3.8, 51.7)	4.87 (dq, 4.3, 46.7)	4.88 (dt, 4.5, 45)	--	--	5.02 (ddd, 5.5, 7.0, 46.8)	5.09 (dd, 8.0, 47.0)	5.19 (dt, 5.0, 47.8)	--
C1'	90.4 (d, 169)	90.0 (d, 178)	93.5 (d, 178)	93.4 (d, 174)	123.6 (t, 243)	121.9 (t, 245)	90.2 (d, 168)	90.7 (d, 174)	94.1 (d, 174)	120.9 (t, 242)
H2'	3.80 (bm)	4.05 (ddd, 6.2, 12.6, 19.6)	3.78 (bm)	3.85 (bm)	4.10 (bm) 3.93 (bm)	3.91 (bm) 3.78 (bm)	6.05 (m)	6.01 (m)	5.82 (m)	6.36 (m)
C2'	63.1 (d, 21)	3.85 (m) 62.9 (d, 23)	63.1 (d, 25)	62.3 (d, 25)	64.1 (dd, 28, 34)	64.2 (t, 32)	134.8 (d, 17)	133.6 (d, 20)	133.2 (d, 19)	132.9 (t, 24)
H3'	--	--	--	--	--	--	5.43 (bd, 17.5)	5.32 (ddd, 1.0, 2.5, 17.0)	5.30 (dt, 1.6, 18.6) 5.20 (d, 10.7)	5.71 (bd, 17.5) 5.10 (d, 11.2)
C3'							5.28 (d, 11.0) 118.0 (d, 13)	5.21 (d, 10.5) 118.9 (d, 12)	119.3 (d, 11)	119.3 (t, 10)
¹⁹ F (CDCl ₃)	-198.5 (s)	-206.9 (s)	-198.5 (s)	-196.5 (s)	-114.6 (ABq, 256 Hz, $\Delta\delta$ = 9.8 ppm)	114.3 (ABq, 264 Hz, $\Delta\delta$ = 6.6 ppm)	-190.5 (s)	-193.7 (s)	-184.7 (s)	-103.2 (ABq, 264 Hz, $\Delta\delta$ = 7.3 ppm)

AAACRYOPROTON CDCl3 /opt/topspin aaltiti 12

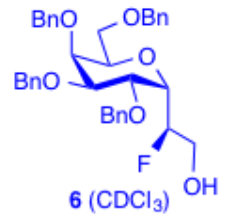
7.323
7.317
7.309
7.304
7.301
7.297
7.290
7.279
7.277
7.267
7.263
7.239
7.226
7.217
7.209
7.205
7.200
7.194
4.719
4.701
4.623
4.606
4.565
4.556
4.542
4.532
4.515
4.504
4.481
4.473
4.450
4.438
4.431
4.415
4.407
4.327
4.311
4.200
4.199
4.183
4.165
3.977
3.971
3.964
3.946
3.871
3.754
3.747
3.740
3.691
3.687
3.684
3.617
3.611
3.594
3.587



```

NAME          20141026
EXPNO         9
PROCNO        1
Date_         20141026
Time          19.21
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            8
DS            2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            2.0448356 sec
RG            64
DW            62.400 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

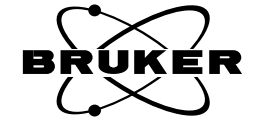
===== CHANNEL f1 =====
NUC1          1H
P1            9.50 usec
PL1          -0.50 dB
SF01         500.1330885 MHz
SI           32768
SF           500.1300257 MHz
WDW           EM
SSB           0
LB           0.30 Hz
GB            0
PC            1.00
    
```



7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm

19.85
0.51
0.52
8.88
1.00
1.00
1.13
1.95
0.97
0.96
0.96
0.87

AAACRYOCOSY CDC13 /opt/topspin aaltiti 12



```

NAME          20141026
EXPNO         10
PROCNO        1
Date_         20141026
Time          19.22
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       cosygpgqf
TD            2048
SOLVENT       CDC13
NS            1
DS            8
SWH           6666.667 Hz
FIDRES        3.255208 Hz
AQ            0.1537250 sec
RG            40.3
DW            75.000 usec
DE            6.00 usec
TE            298.0 K
d0            0.00000300 sec
D1            1.48689198 sec
d13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00015000 sec

```

```

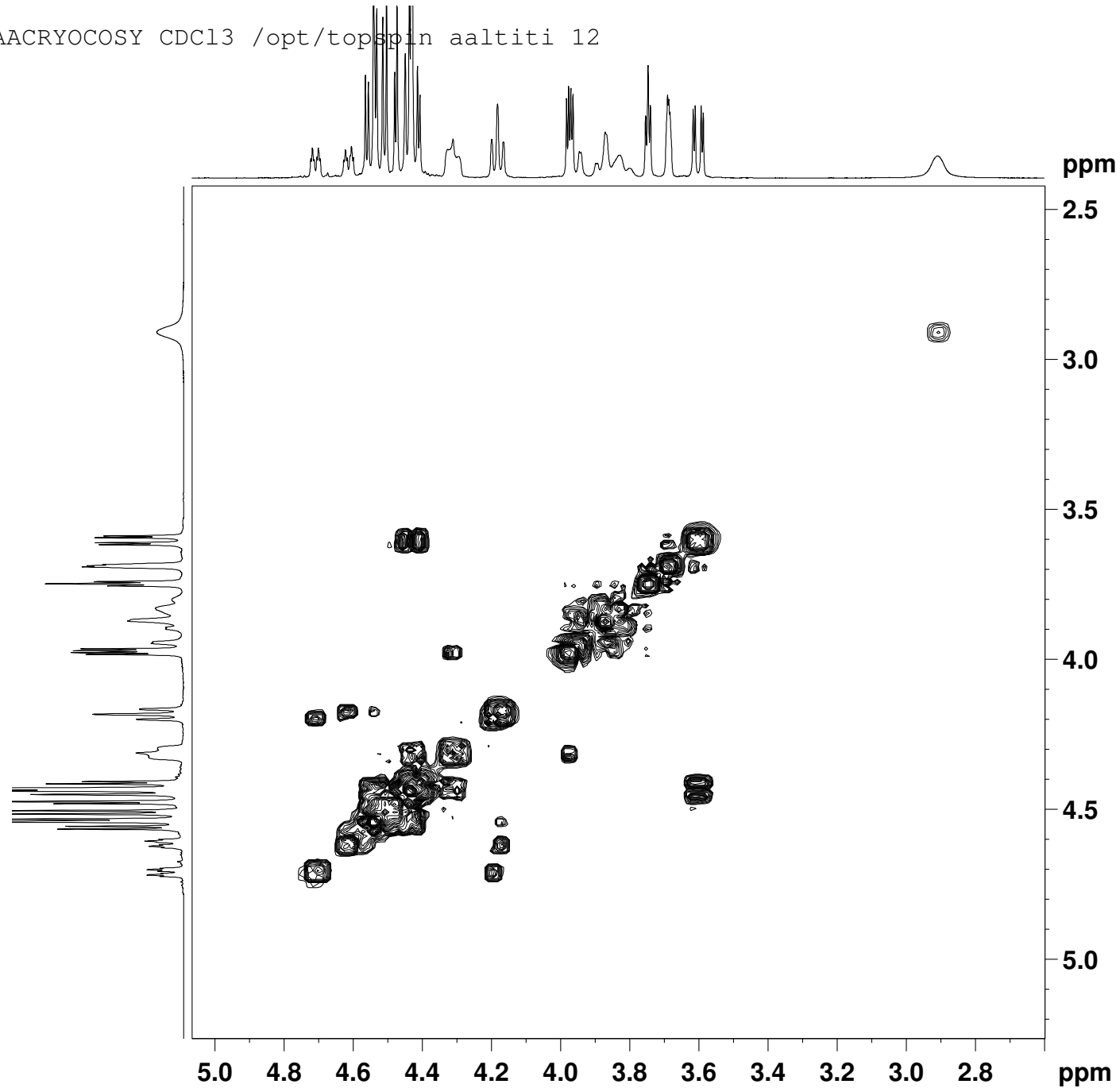
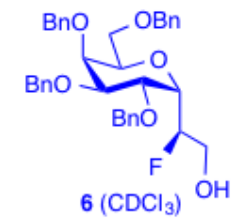
===== CHANNEL f1 =====
NUC1          1H
P0            9.50 usec
P1            9.50 usec
PL1          -0.50 dB
SFO1         500.1330069 MHz

```

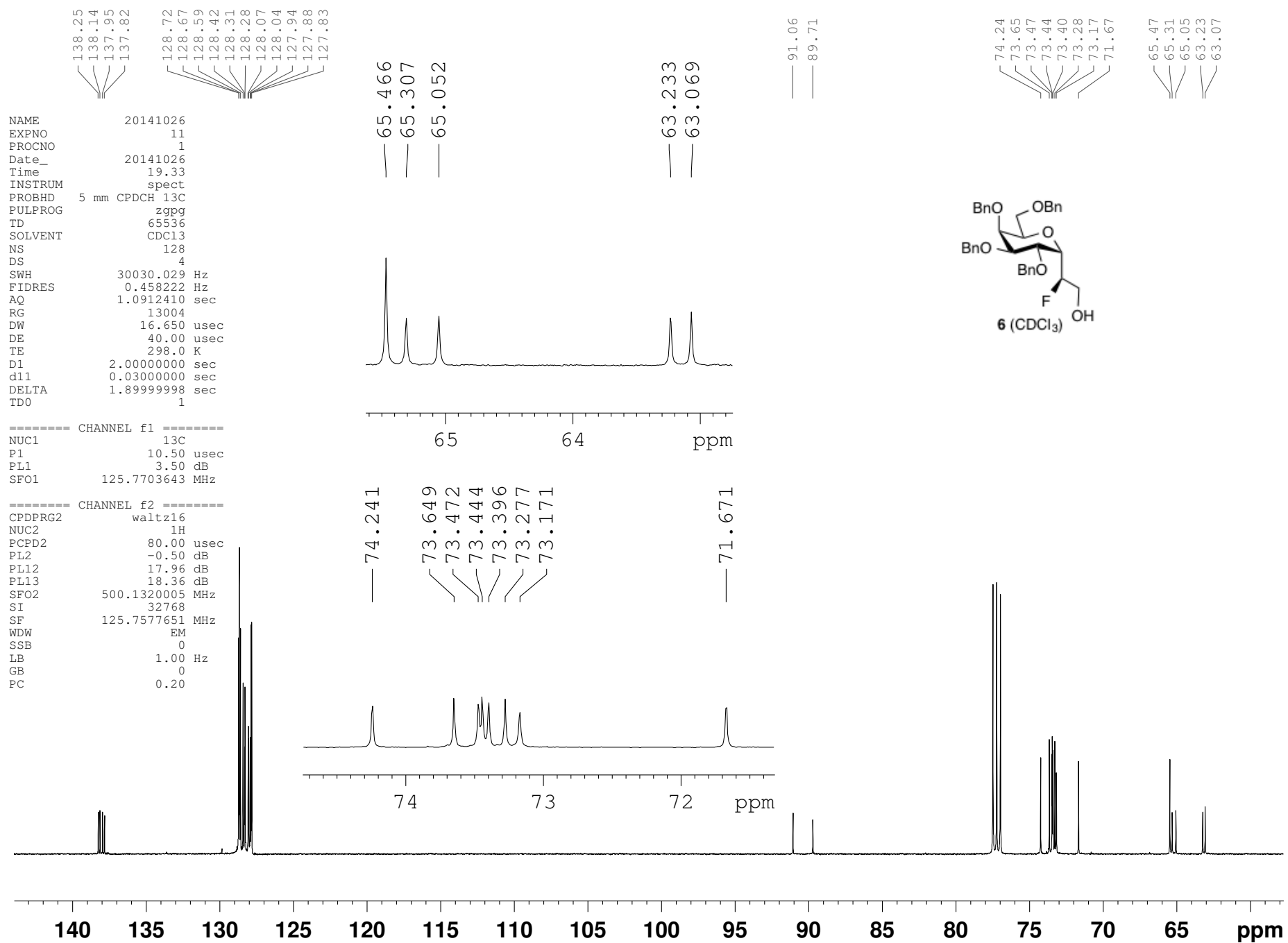
```

===== GRADIENT CHANNEL =====
GPNAME1      SINE.100
GPZ1         10.00 %
P16          1000.00 usec
ND0          1
TD           128
SFO1         500.133 MHz
FIDRES       52.083332 Hz
SW           13.330 ppm
FnMODE       QF
SI           1024
SF           500.1300273 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40
SI           1024
MC2          QF
SF           500.1300256 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0

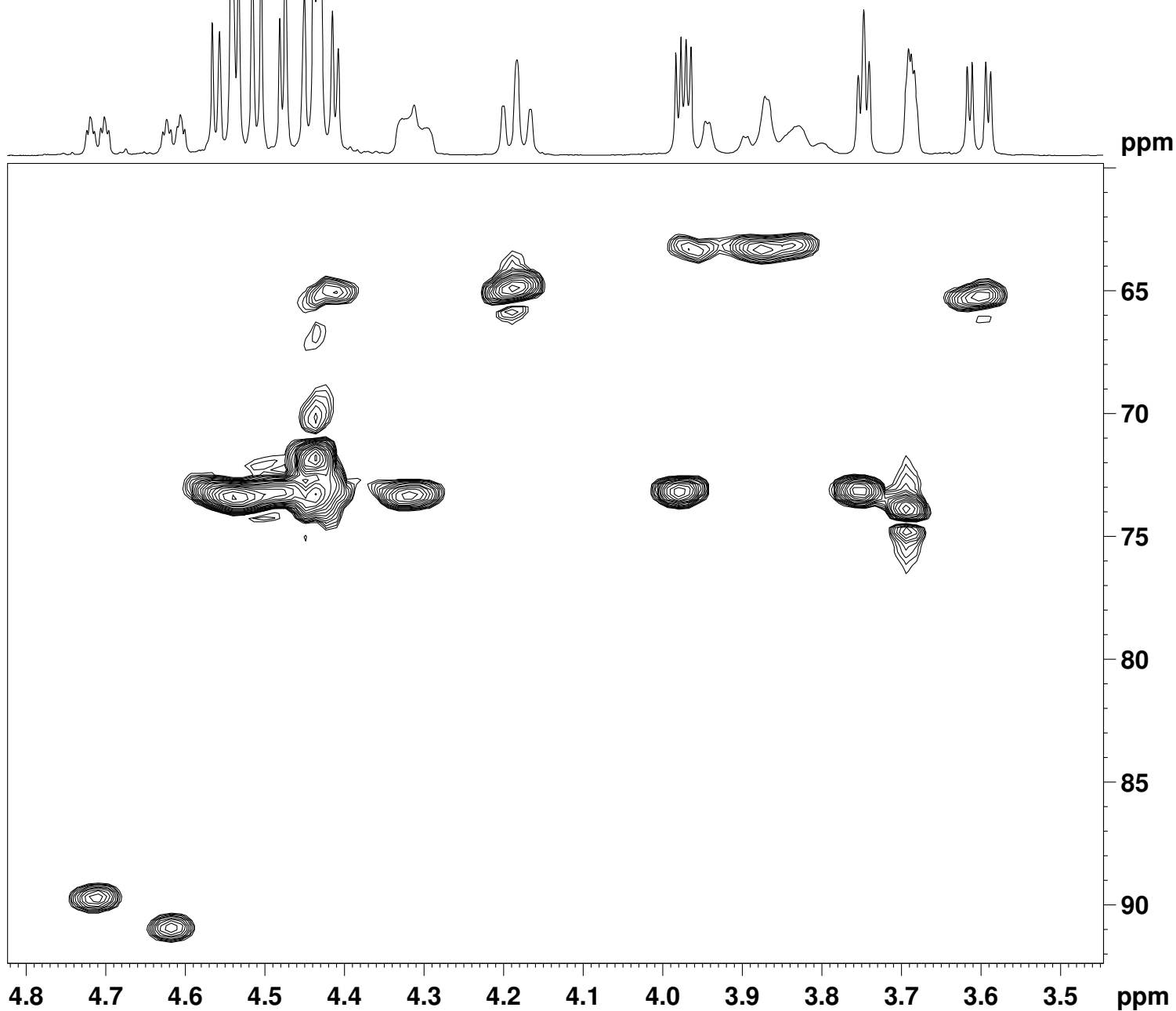
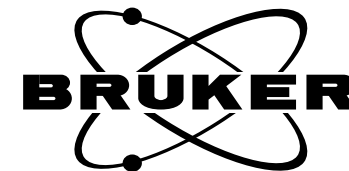
```



AAACRYOCARBON CDC13 /opt/topspin aaltiti 12



AAACRYOHSQC CDC13 /opt/topspin aaltiti 12



```

NAME          20141026
EXPNO         12
PROCNO        1
Date_         20141026
Time          19.33
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       hsqcetgp
TD            1024
SOLVENT       CDC13
NS            2
DS            16
SWH           6666.667 Hz
FIDRES        6.510417 Hz
AQ            0.0769250 sec
RG            46391
DW            75.000 usec
DE            6.00 usec
TE            298.0 K
CNST2         145.0000000
d0            0.00000300 sec
d1            1.20000005 sec
d4            0.00172414 sec
d11           0.03000000 sec
d13           0.00000400 sec
D16           0.00020000 sec
DELTA         0.00122500 sec
DELTA1        0.00071614 sec
IN0           0.00001990 sec
STICNT        0
ZGOPTNS

```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.50 usec
p2            19.00 usec
P28           2000.00 usec
PL1           -0.50 dB
SFO1          500.1330069 MHz

```

```

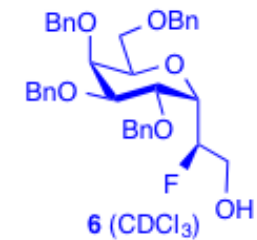
===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            10.50 usec
p4            21.00 usec
PCPD2         70.00 usec
PL2           3.50 dB
PL12          19.98 dB
SFO2          125.7678496 MHz

```

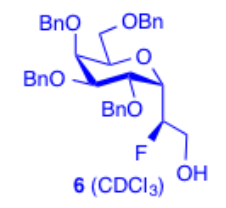
```

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec
ND0           2
TD            128
SFO1          125.7678 MHz
FIDRES        196.293976 Hz
SW            199.778 ppm
FnmODE        Echo-Antiecho
SI            1024
SF            500.1300237 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            125.7577644 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0

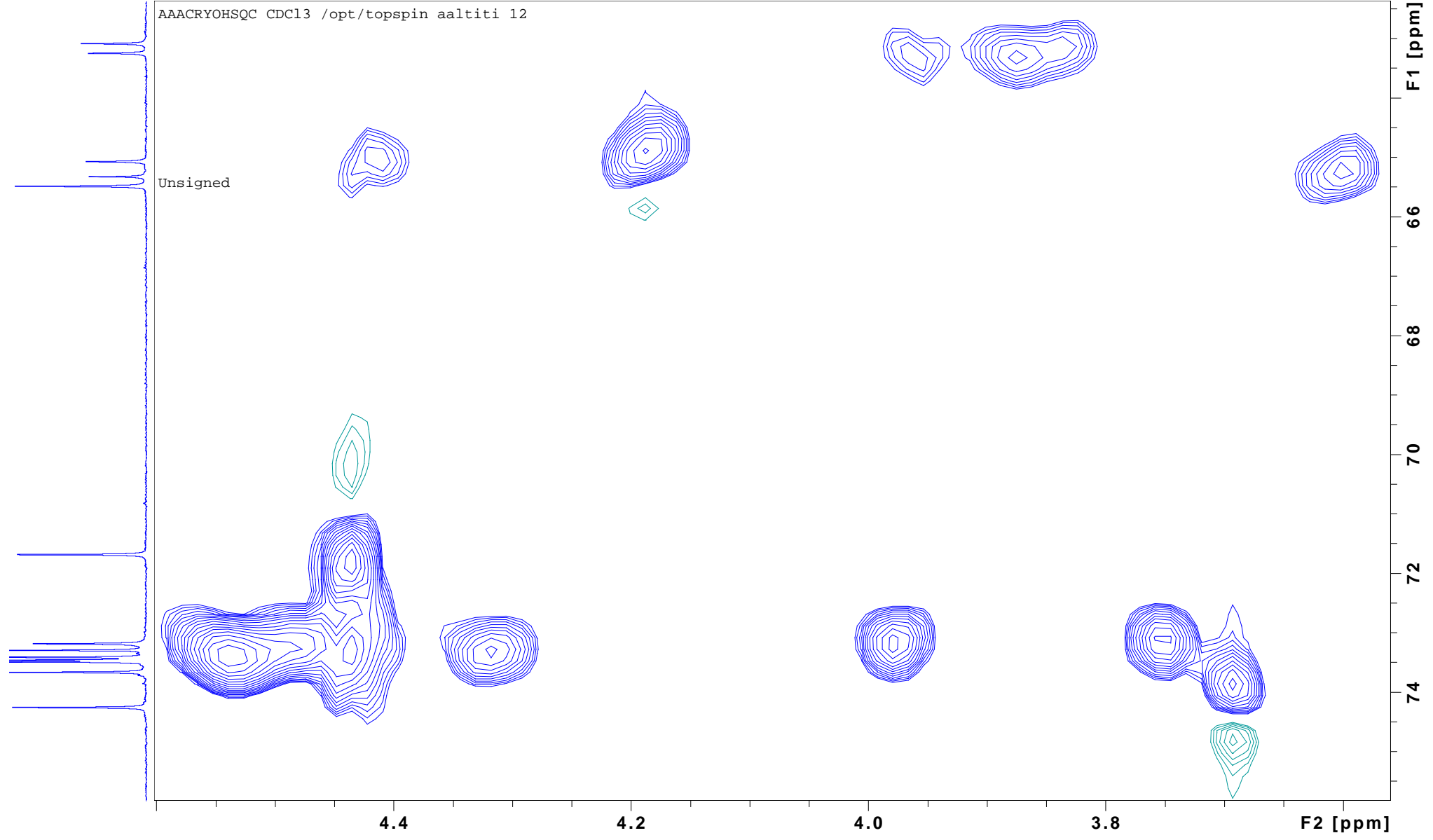
```



20141026 12 1 /export/bruker500 aaltiti



AAACRYOHSQC CDCl₃ /opt/topspin aaltiti 12



AAACRYOPROTON C6D6 /opt/topspin aaltiti 11

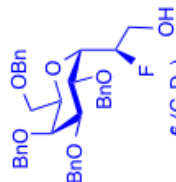
7.322
7.307
7.205
7.202
7.188
7.180
7.144
7.140
7.137
7.133
7.130
7.120
7.107
7.098
7.093
7.087
7.081
7.067
4.664
4.643
4.620
4.615
4.613
4.597
4.459
4.435
4.417
4.392
4.326
4.302
4.293
4.270
4.160
4.136
4.109
4.086
4.071
4.064
4.058
4.052
3.996
3.993
3.870
3.866
3.863
3.830
3.823
3.816
3.804
3.797
3.781
3.775

```

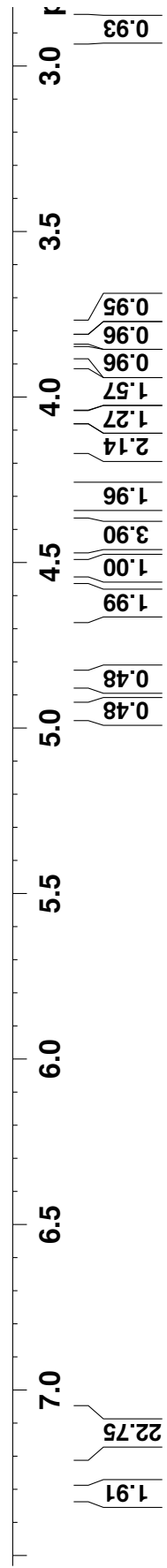
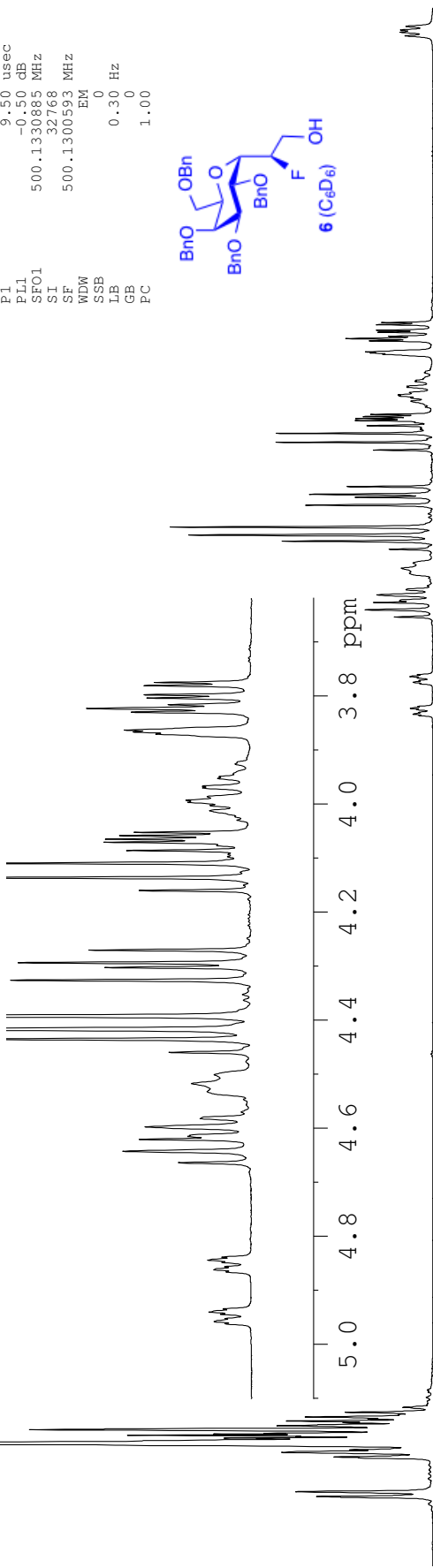
NAME      20141026
EXPNO     1
PROCNO    1
Date_     20141026
Time      18.04
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zg30
TD         32768
SOLVENT   C6D6
NS         8
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0448356 sec
RG         40.3
DW         62.400 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        9.50 usec
PL1       -0.50 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300593 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```



4.643
4.620
4.597
4.435
4.417
4.392
4.326
4.302
4.293
4.270
4.160
4.136
4.109
4.086
4.071
4.064
4.058
4.052
3.866
3.863
3.830
3.823
3.804
3.797
3.781
3.775



NAME 20141026
 EXPNO 3
 PROCNO 1
 Date_ 20141026
 Time 18.16
 INSTRUM spect
 PROBHD 5 mm CPDCH 13C
 PULPROG zgpg
 TD 65536
 SOLVENT C6D6
 NS 125
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 10321.3
 DW 16.650 usec
 DE 40.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 3.50 dB
 SFO1 125.7703643 MHz

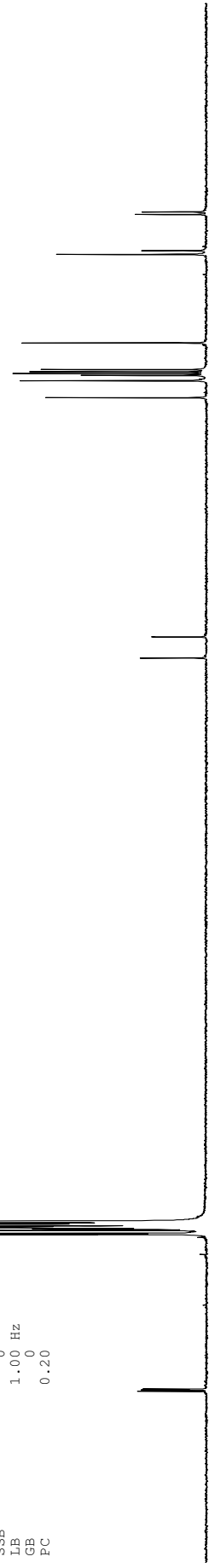
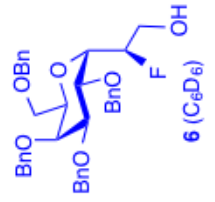
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCFD2 80.00 usec
 PL2 -0.50 dB
 PL12 17.96 dB
 PL13 18.36 dB
 SFO2 500.1320005 MHz
 SI 32768
 SF 125.7577170 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 0.20

139.06
 138.98
 138.95
 138.95
 139.06
 129.01
 128.97
 128.95
 128.77
 128.68
 128.52
 128.32
 128.25

 92.11
 90.76

 75.44
 74.35
 74.34
 74.01
 73.89
 73.78
 73.63
 71.93

 66.26
 66.02
 63.70
 63.54



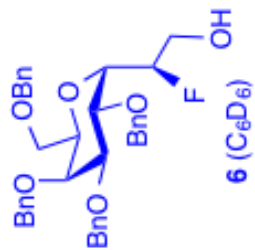
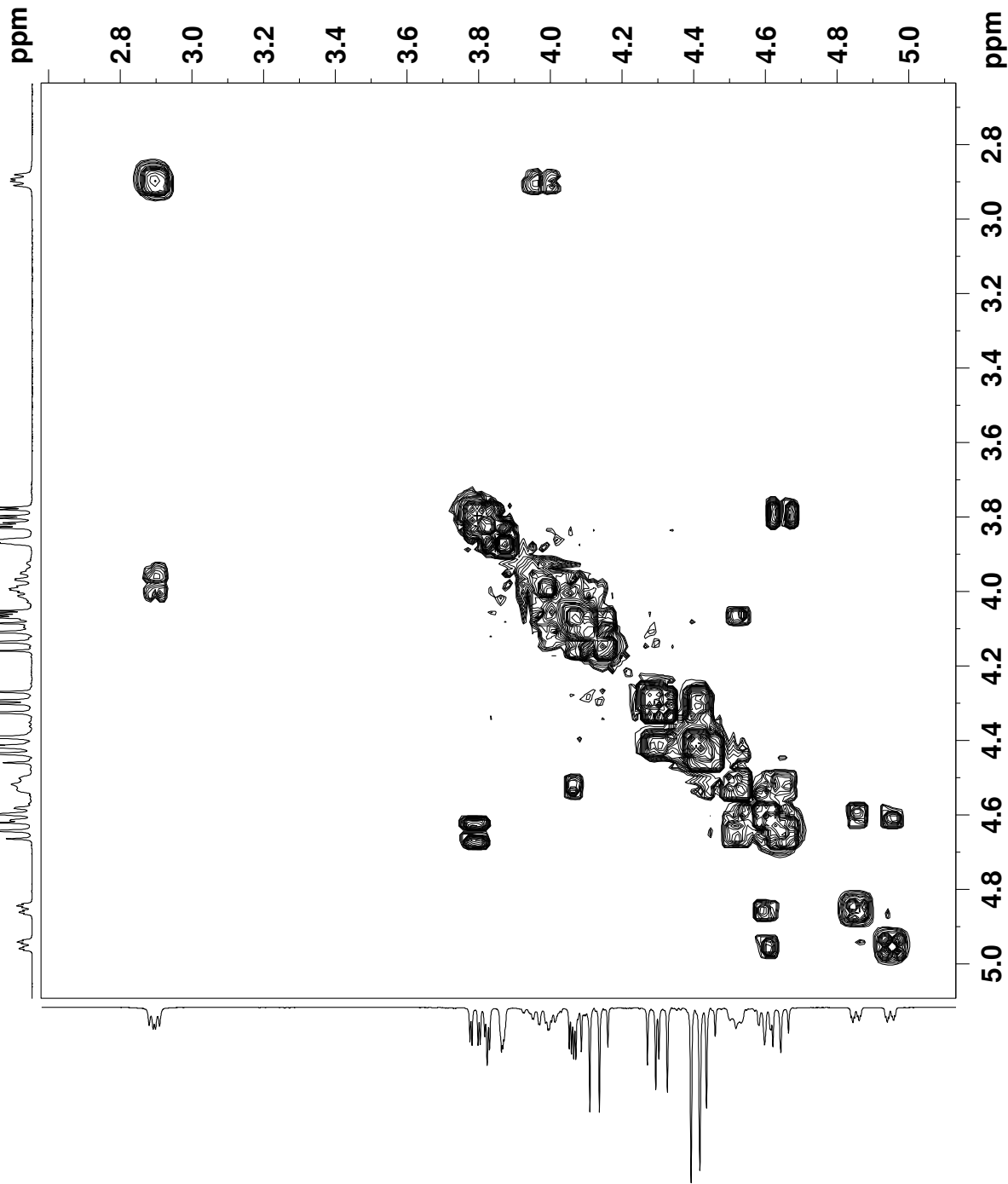


```

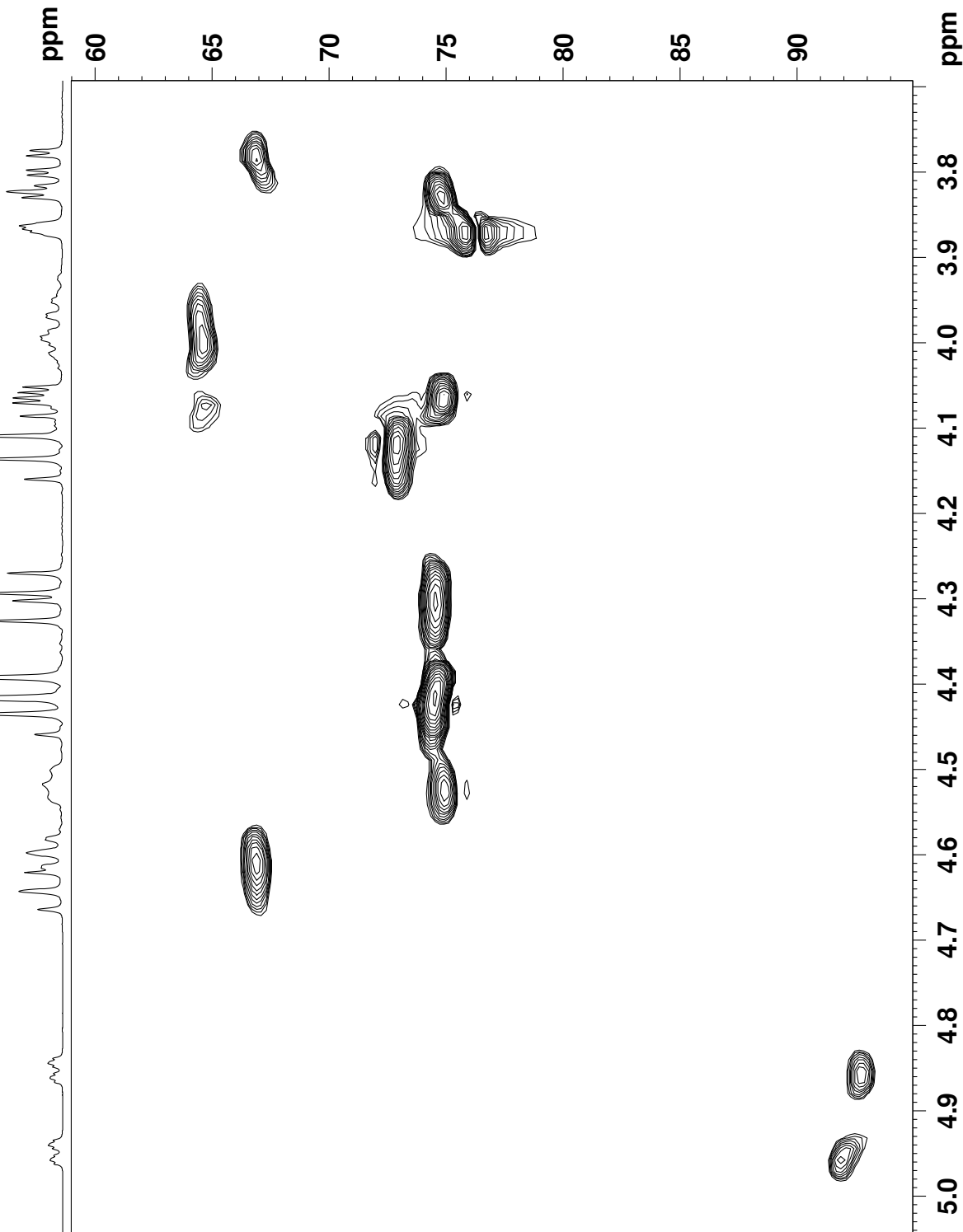
NAME      20141026
EXPNO     2
PROCNO    1
Date_     20141026
Time      18.05
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   cosygpscf
TD         2048
SOLVENT   C6D6
NS         1
DS         8
SMH       6666.667 Hz
FIDRES    3.255208 Hz
AQ         0.1537250 sec
RG         25.4
DM         75.000 usec
DE         6.00 usec
HE         9.00 usec
DI         0.0000000 K
DQ         1.48689198 sec
G13       0.0000400 sec
D16       0.0002000 sec
IN0       0.00015000 sec

===== CHANNEL f1 =====
NUC1      1H
P0        9.50 usec
P1        9.50 usec
PL1       -0.50 dB
SFO1      500.1330069 MHz

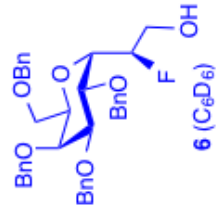
===== GRADIENT CHANNEL =====
GPNAMI    SINE.100
GPZ1      10.00 %
FL6       1000.00 usec
ND0       1
LD0       12
SFO1      500.133 MHz
FIDRES    52.08332 Hz
SM         13.330 Ppm
F0MODE    OF
SI         1024
SF         500.1300581 MHz
WDW        SINE
LB         0
SSB        0
GB         0
FC         1.40
SI         1024
MC2       OF
SF         500.1300583 MHz
WDW        SINE
LB         0
SSB        0
GB         0
    
```

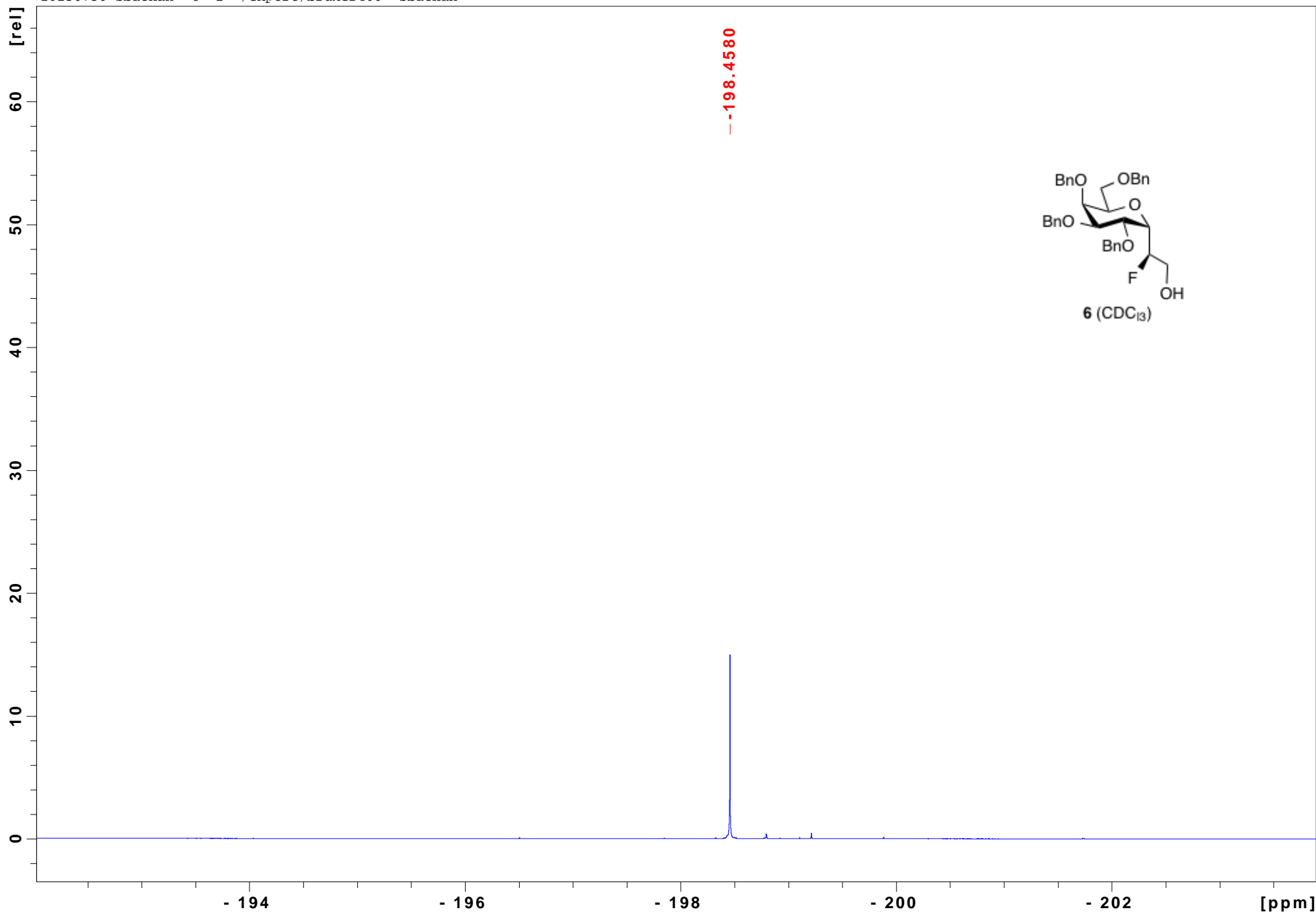


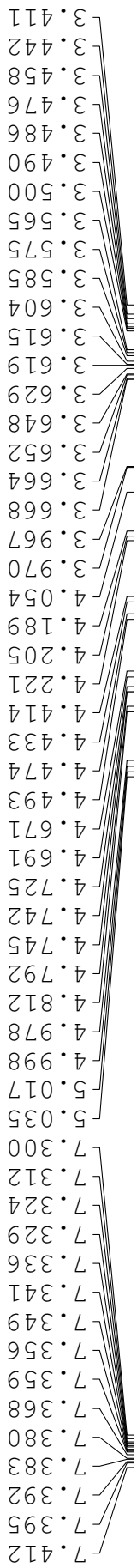
AAACRYOHSQC C6D6 /opt/topspin aaltiti 11



```
NAME 20141026
EXPNO 1
PROCNO 1
Date_ 20141026
Time 11:28:32
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 2
DS 2
SWH 6666.467 Hz
FIDRES 6.510417 Hz
AQ 0.0772953 sec
RG 320
DE 75.000 usec
TE 300.2
CNS1 145.0000000 K
CNS2 0.0000000 sec
d0 0.0000000 sec
d1 0.0000000 sec
d2 0.0000000 sec
d3 0.0000000 sec
DELTA 0.0012500 sec
DELTA1 0.00071614 sec
DELTA2 0.0000000 sec
DELTA3 0.0000000 sec
NUC1 13C
NUC2 1H
SFO1 500.1330065 MHz
SFO2 125.7678496 MHz
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PC 1.00 usec
PD 1.00 usec
PF 2000.00 usec
PL1 -0.50 dB
PL2 -0.50 dB
SFO1 500.1330065 MHz
===== CHANNEL f2 =====
P2 10.50 usec
PC 1.00 usec
PD 1.00 usec
PF 2000.00 usec
PL1 -0.50 dB
PL2 -0.50 dB
SFO2 125.7678496 MHz
===== GRADIENT CHANNEL =====
GPM1 SINE 100
GPM2 SINE 100
GPR1 20.10 %
GPR2 20.10 %
P16 1000.00 usec
ND0 12
ND1 12
ND2 12
SFO1 125.7678 MHz
FIDRES 196.283976 Hz
AQ 0.0772953 sec
RG 320
PROBHD Echo-AntiEcho Pfm
SI 1024
SF 500.1300558 MHz
SSB 2
KSH2 2
LB 0.00 Hz
PC 0
PD 0
PF 0
PL 0
SI 1024
MC2 echo-antiEcho
RG 320
WDW COSY
SSB 2
GB 0.00 Hz
GB 0
```

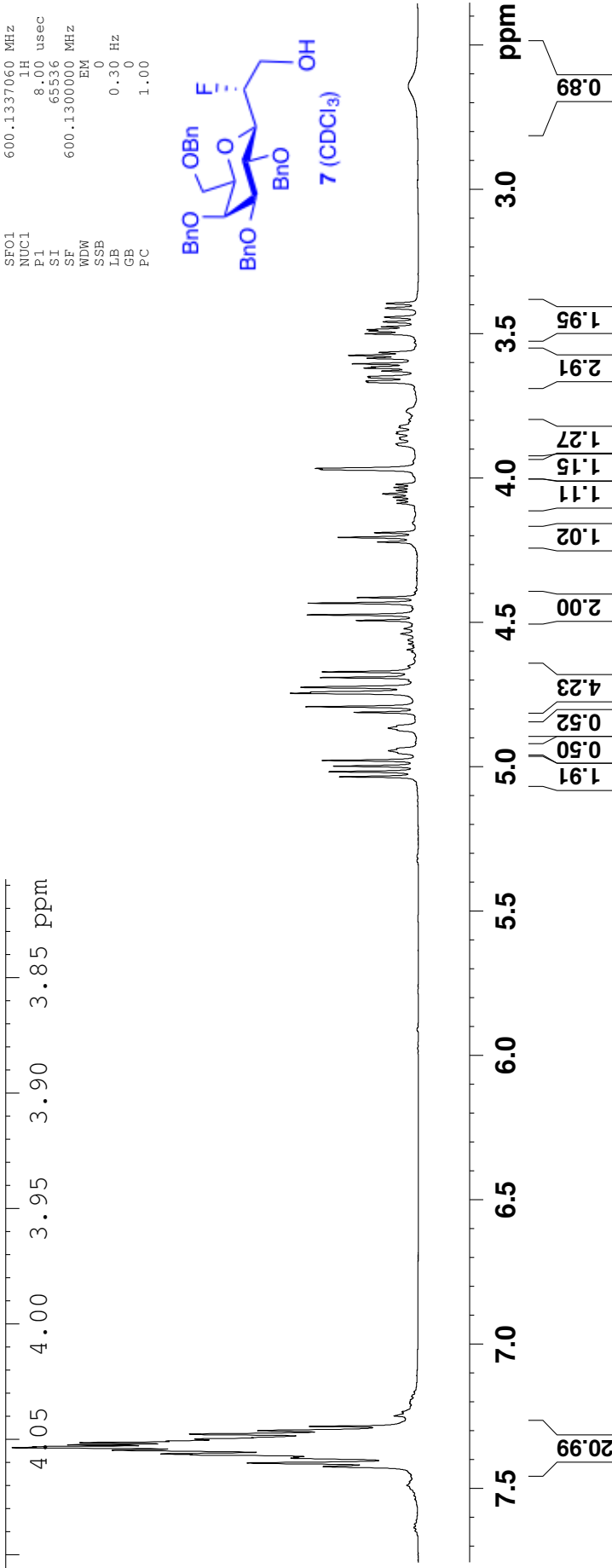
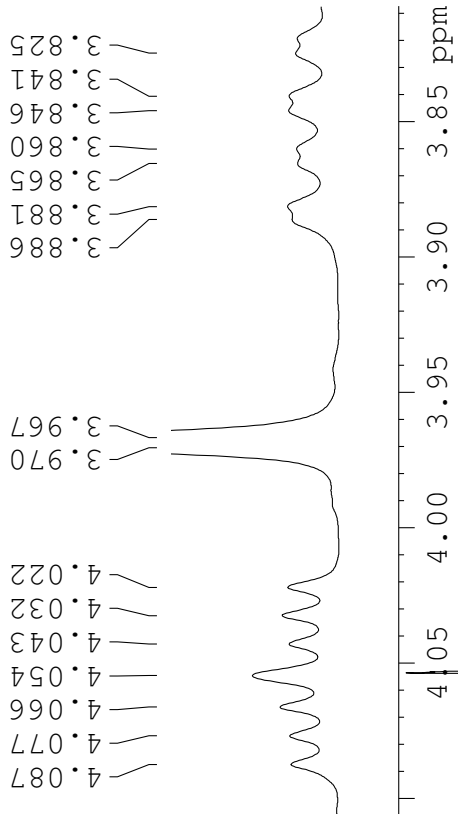


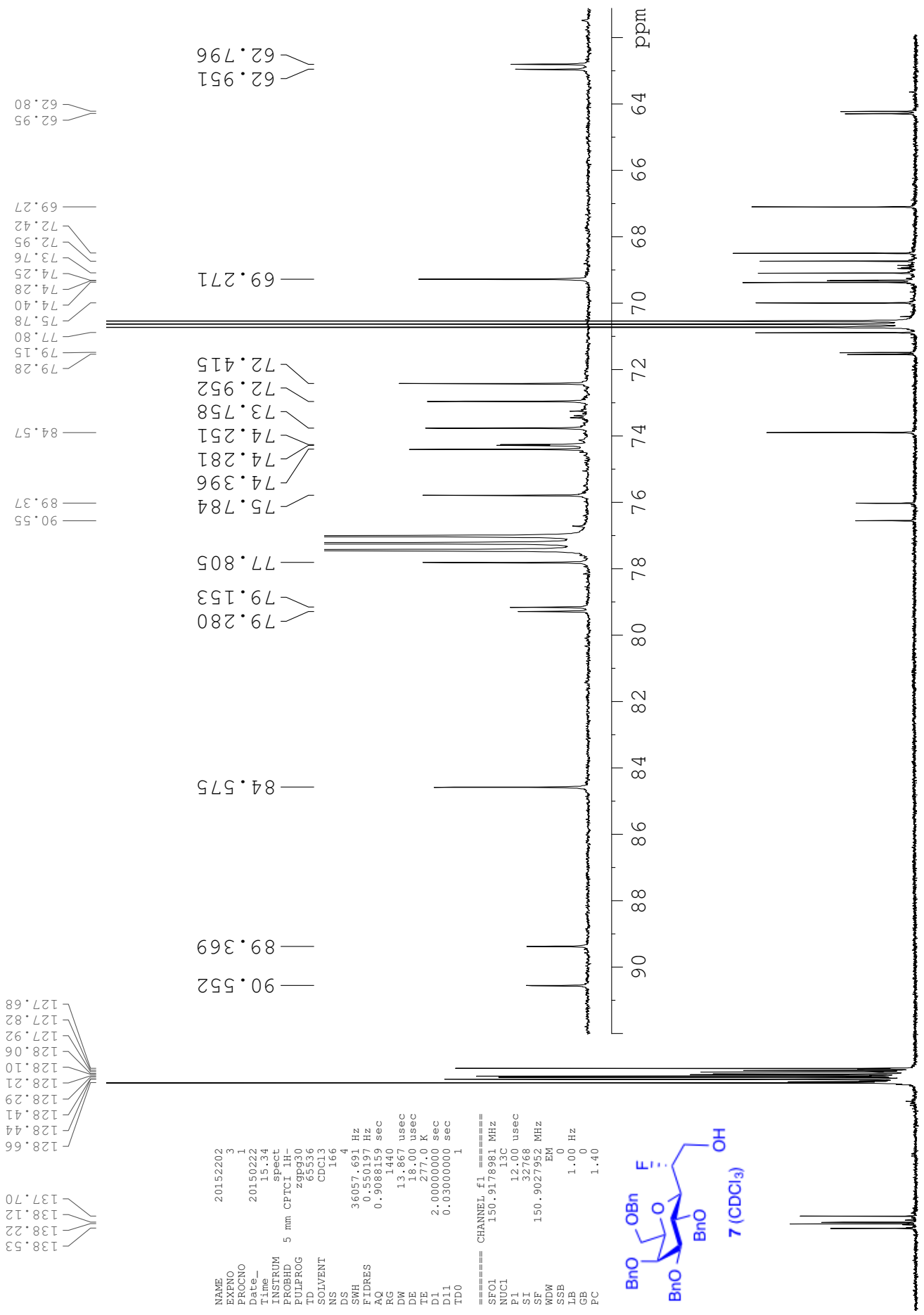




```

NAME      20152202
EXPNO    1
PROCNO   1
Date_    20150222
Time     15.20
INSTRUM  spect
PROBHD   5 mm CPTCI 1H-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       12019.230 Hz
FIDRES    0.183399 Hz
AQ        2.7263477 sec
RG        7.12
DW        41.600 usec
DE        10.00 usec
TE        277.0 K
D1        1.00000000 sec
TD0       1
===== CHANNEL f1 =====
SFO1     600.1337060 MHz
NUC1     1H
P1       8.00 usec
SI       65536
SF       600.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```





```

===== CHANNEL f1 =====
SFO1 150.9178981 MHz
NUC1 13C
P1 12.00 usec
SI 32768
SF 150.9027952 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
=====
NAME 20152202
EXPNO 3
PROCNO 1
Date_ 20150222
Time 15.34
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 166
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 1440
DW 13.867 usec
DE 18.00 usec
TE 277.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

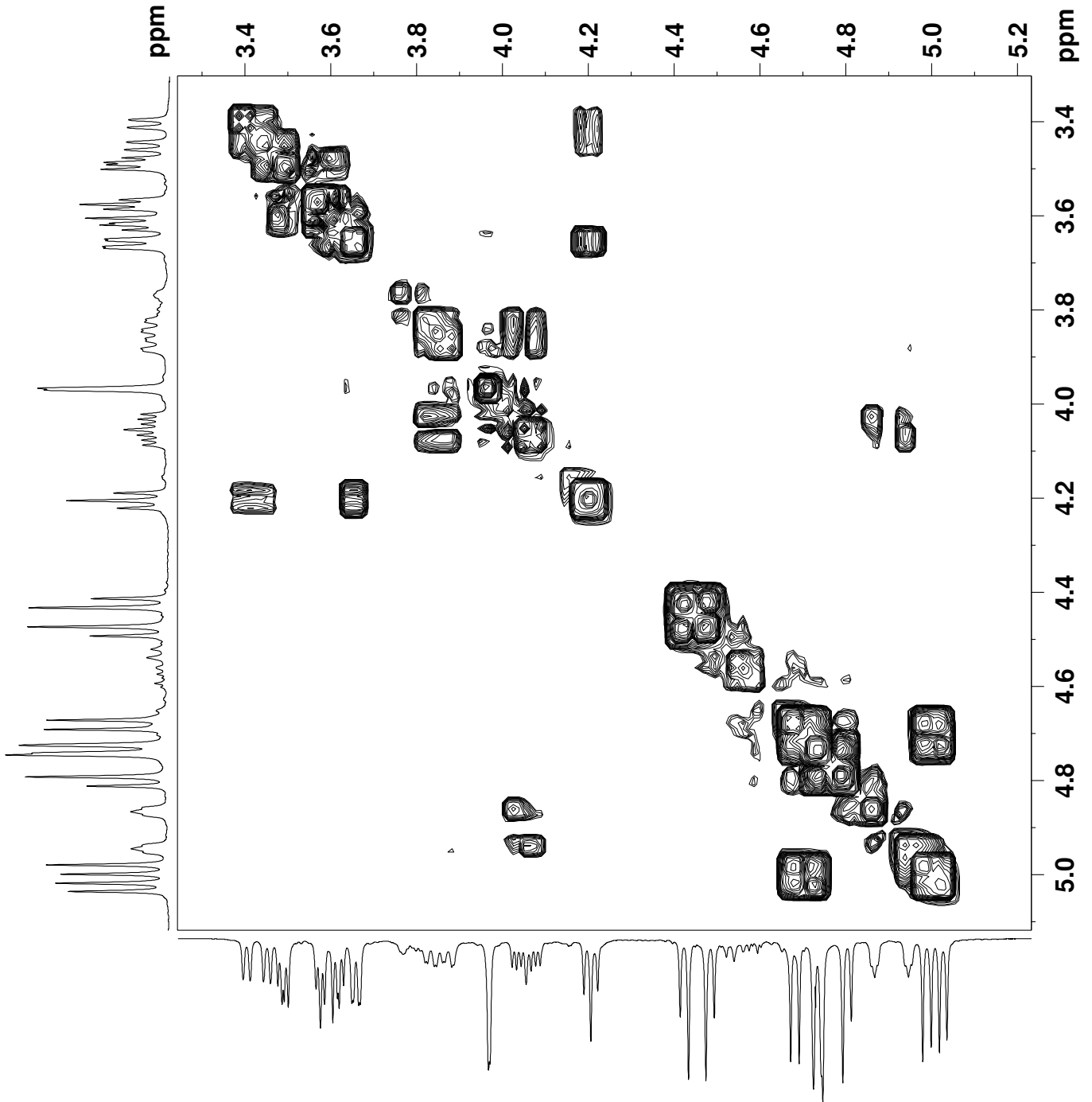
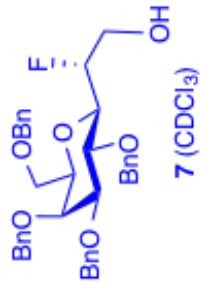
```

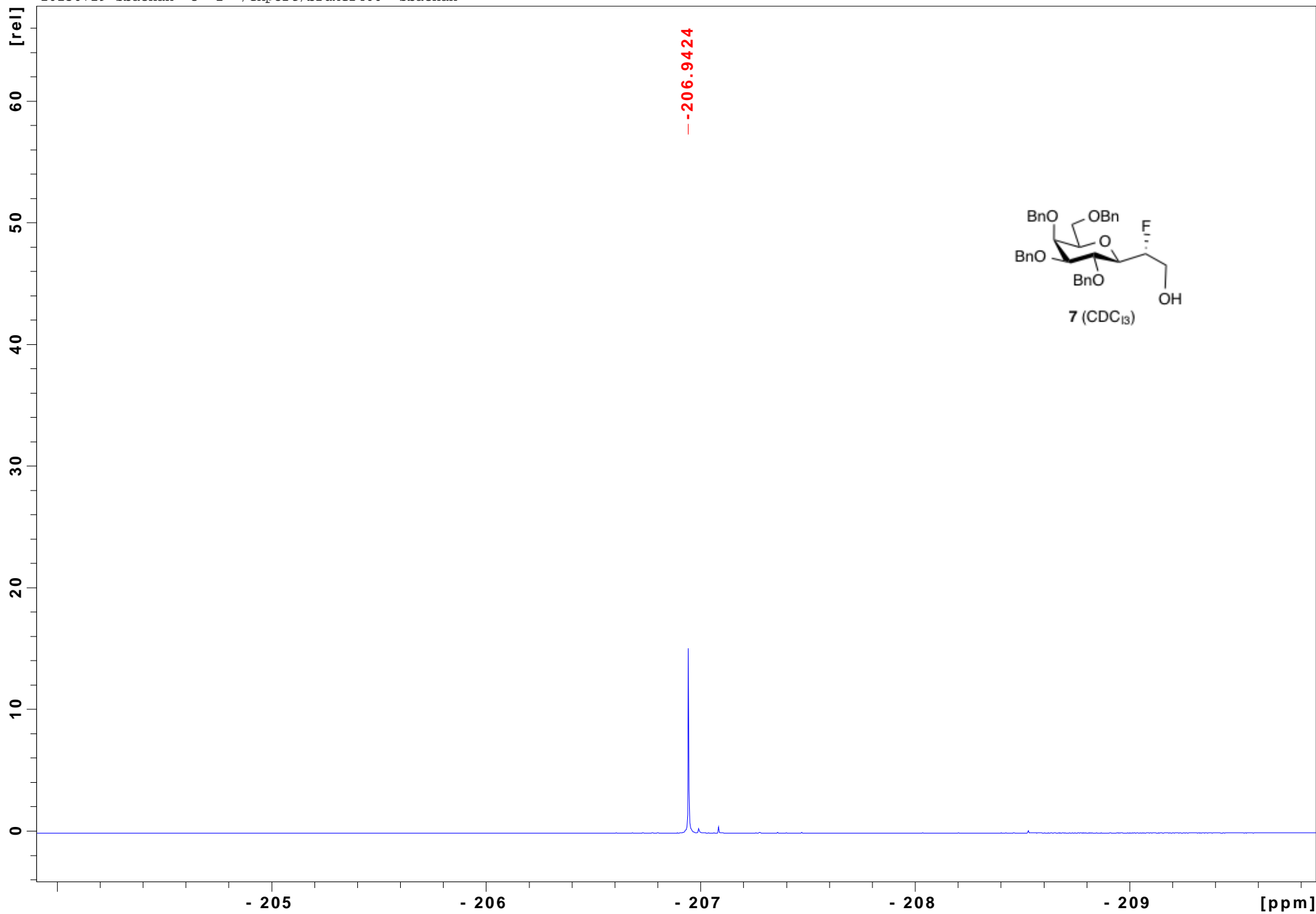


```

20152202
NAME 2
EXPNO 2
PROCNO 1
Date_ 20150222
Time_ 15.20
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG cosygpgf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 8012.820 Hz
FIDRES 3.912510 Hz
AQ 0.1278452 sec
RG 64
DW 62.400 usec
DE 10.00 usec
TE 277.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012480 sec

===== CHANNEL f1 =====
SFO1 600.1336081 MHz
NUC1 1H
P1 8.00 usec
PD 8.00 usec
RF0 1
TD 128
SFO1 600.1336 MHz
FIDRES 62.600159 Hz
SA 13.352 ppm
FAMODE
SI 1024
SF 600.1300000 MHz
SSB QSIGN
MDW 0.00 Hz
LB 0
GB 0
PC 1.40
SI 1024
MC2 QF
SF 600.1300000 MHz
SSB QSIGN
MDW 0.00 Hz
LB 0
GB 0
    
```

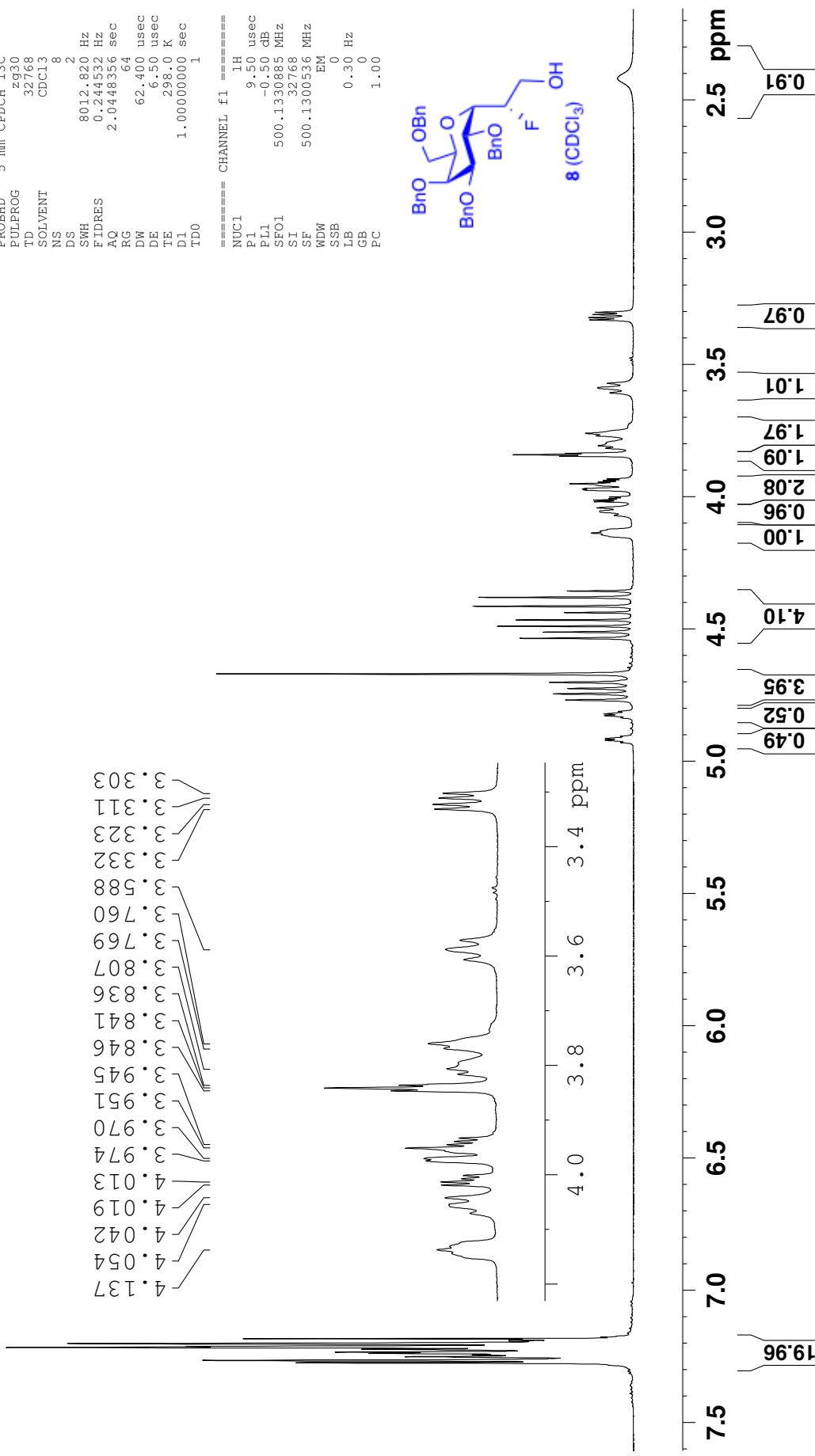
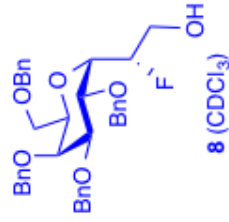




7.274
7.265
7.251
7.239
7.234
7.223
7.216
7.212
7.201
7.183
4.921
4.914
4.827
4.821
4.769
4.745
4.725
4.702
4.670
4.535
4.512
4.489
4.466
4.438
4.414
4.381
4.357
4.144
4.137
4.131
4.054
4.042
4.019
4.013
3.974
3.970
3.951
3.945
3.939
3.933
3.846
3.841
3.836
3.817
3.807
3.796
3.769
3.760
3.588
3.332
3.323
3.311
3.303

```

NAME      20141105
EXPNO     23
PROCNO    1
Date_     20141105
Time_     23.58
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         8
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         2.0448356 sec
RG         64
DW         62.400 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
TD0        1
===== CHANNEL f1 =====
NUC1       1H
P1         9.50 usec
PL1        -0.50 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300536 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



AAACRYOCARBON CDCl3 /opt/topspin aaltiti 1

127.79
127.84
127.98
128.11
128.55
128.91
128.98
128.92
128.97
129.67
130.72
130.81
130.89
130.91
130.95

79.15
79.09
75.71
74.97
74.94
74.59
74.20
73.57
73.30
69.18
63.25
63.07

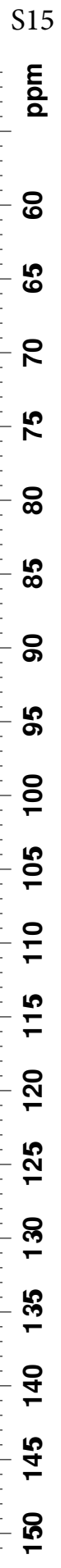
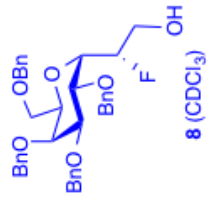
```

NAME      20141105
EXPNO     25
PROCNO    1
Date_     20141106
Time      0.08
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         91
DS         4
SWH        50050.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         1496.5
DE         16.650 usec
TE         40.00 usec
TE        298.0 K
D1         2.00000000 sec
d11        0.05000000 sec
DELTA     1.89999998 sec
TD0        1
    
```

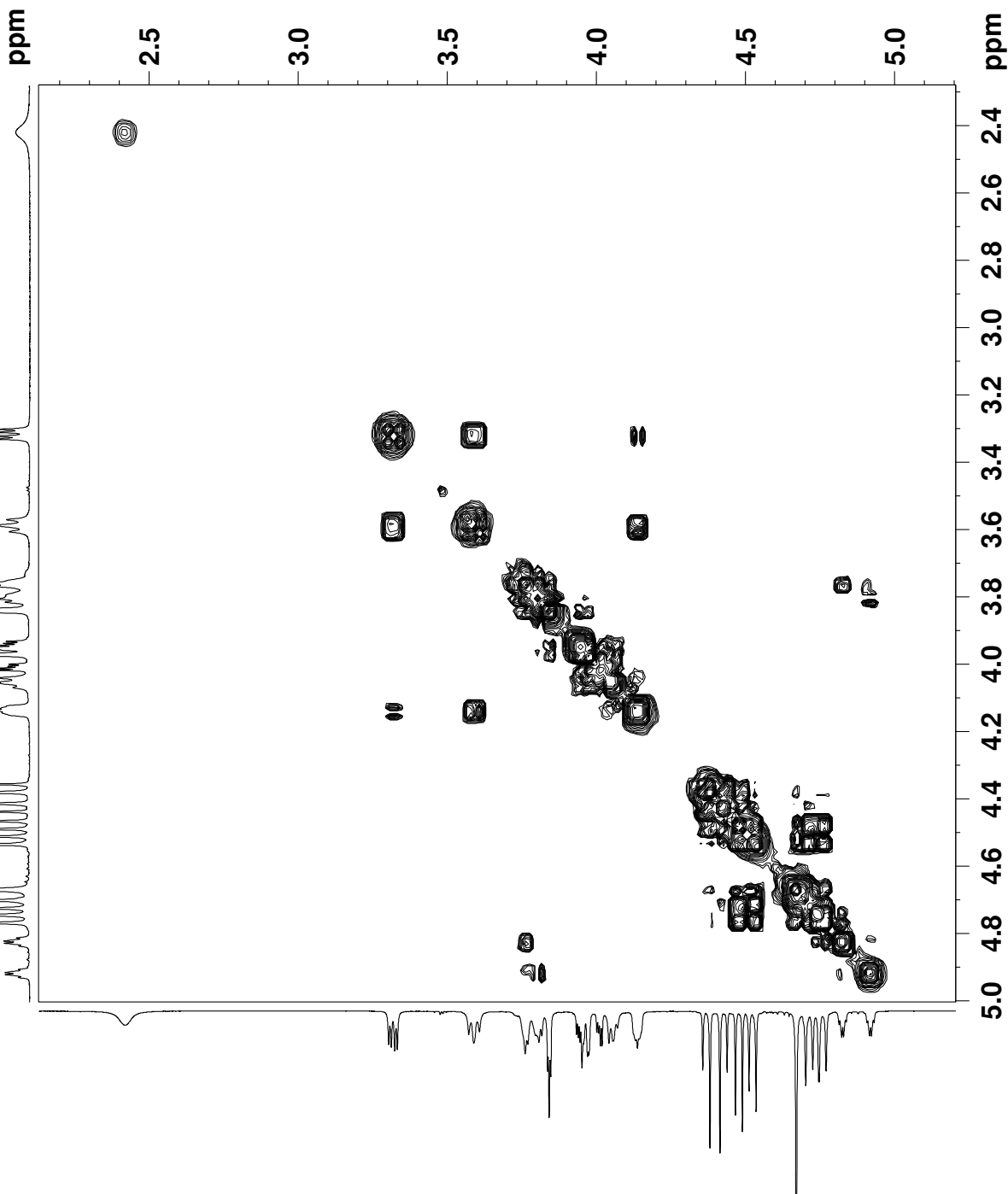
```

===== CHANNEL f1 =====
NUC1      13C
P1        10.50 usec
PL1       5.50 dB
SFO1     125.7703645 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -0.50 dB
PL12     17.96 dB
PL13     18.36 dB
SFO2     500.1520005 MHz
SF        527.68 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.20
    
```



AAACRYCOSY CDCl3 /opt/topspin aaltiti 1

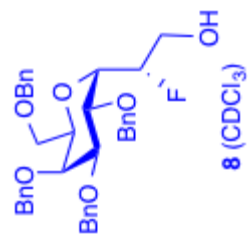


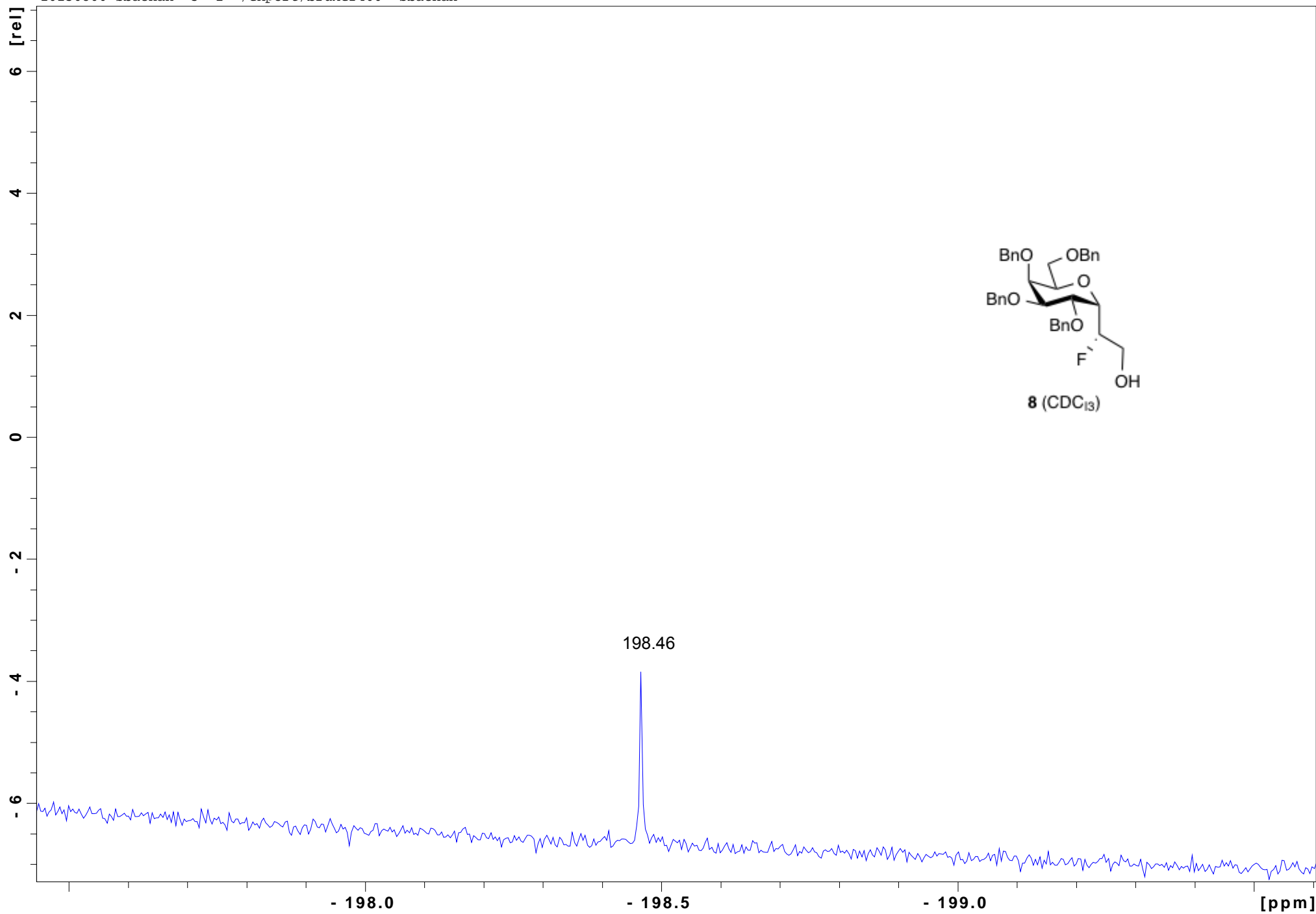
```

NAME      20141105
EXPNO     24
PROCNO    1
Date_     20141105
Time      23.59
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   cosy90
SOLVENT   CDCl3
NS         1
DS         8
SWH        6666.667 Hz
FIDRES    3.255208 Hz
AQ         0.1537250 sec
RG         655
DE         75.000 usec
TE         298.0 K
d0         0.10000300 sec
d1         1.48689198 sec
d13        0.00000400 sec
d16        0.00020000 sec
IN0        0.100015000 sec

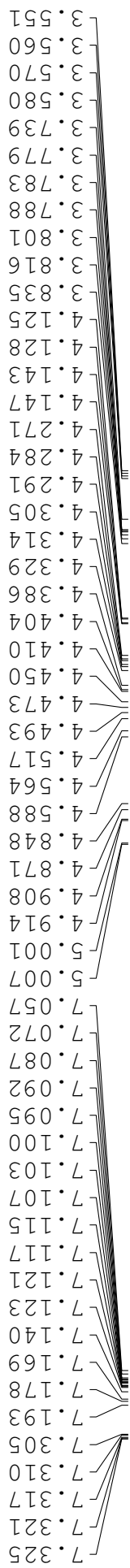
===== CHANNEL f1 =====
NUC1       1H
P0         9.50 usec
P1         9.50 usec
PL1        -0.50 dB
SFO1       500.1330069 MHz

===== GRADIENT CHANNEL =====
GPNAM1
GEZ1       10.00 %
P16        1000.00 usec
NDO        1
TD         128
FIDRES    52.083332 Hz
SW         13.330 ppm
FQMODE     QF
SI         1024
SF         500.1300541 MHz
WDW        SINE
SSB        0
GB         0
PC         1.40
SI         1024
MC2        QF
SF         500.1300545 MHz
WDW        SINE
SSB        0
GB         0
    
```





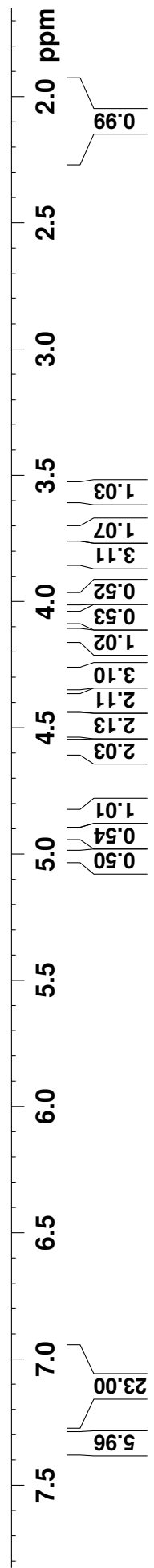
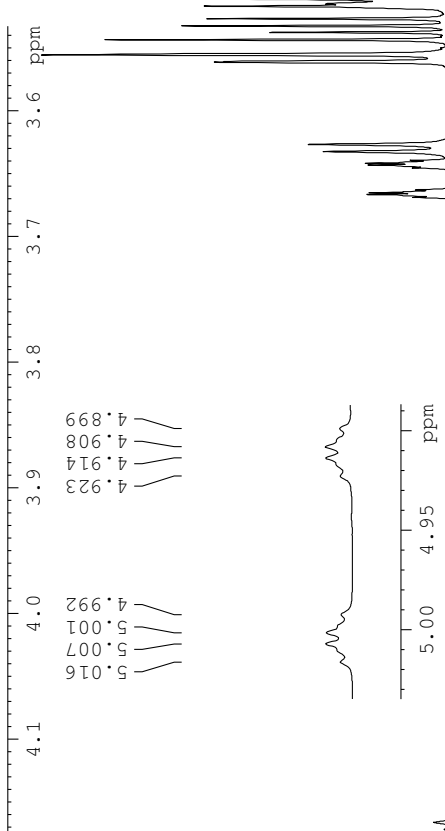
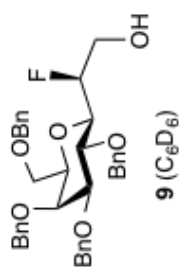
AAACRYOPROTON C6D6 /opt/topspin aaltiti 5



4.147
4.143
4.128
4.125
4.068
4.063
4.055
4.050
3.996
3.991
3.984
3.978
7.087
7.072
7.057
3.835
3.816
3.801
3.788
3.783
3.779
3.739
4.914
4.908
4.871
4.848
4.588
4.564
4.517
3.580
3.570
3.560

NAME 20141107
EXPNO 1
PROCNO 1
Date_ 20141107
Time 13.19
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 32768
SOLVENT C6D6
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0448356 sec
RG 40.3
DM 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
PL 9.50 usec
PL1 -0.50 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300622 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AAACRYOCARBON C6D6 /opt/topspin aaltiti 5

NAME 20141107
 EXPNO 3
 PROCNO 1
 Date_ 20141107
 Time 13.29
 INSTRUM spect
 PROBHD 5 mm CPDCH-13C
 PULPROG zgpg30
 TD 65536
 ID C6D6
 SOLVENT C6D6
 NS 92
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 10321.3
 DW 16.650 usec
 DE 40.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

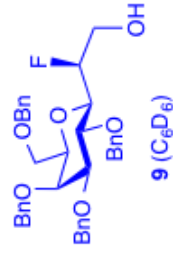
128.97
128.94
128.87
128.68
128.49
128.30
128.24
128.13
128.10

80.390
76.674
76.674
75.871
75.634
75.600
75.600
75.057
74.448
74.260
74.130
73.890
73.372

95.08
93.66
70.336
63.507
63.319

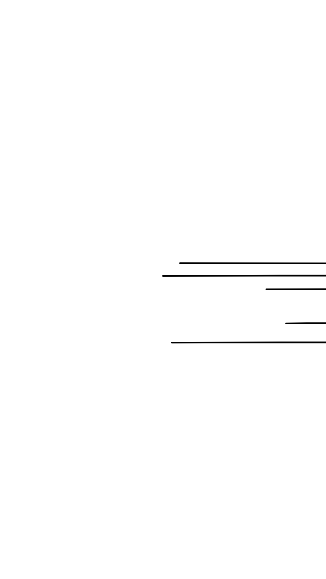
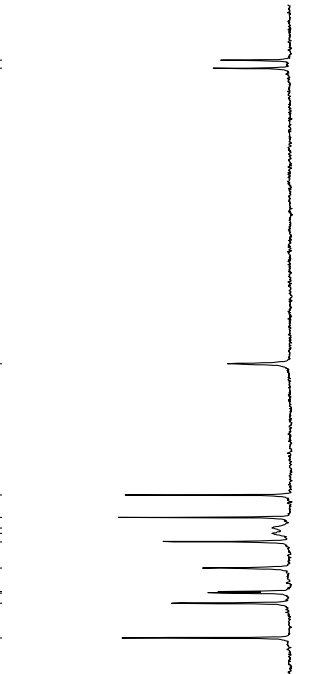
80.39
76.67
75.87
75.63
75.60
75.06
74.45
74.26
74.13
73.89
73.37
70.34

63.51
63.32

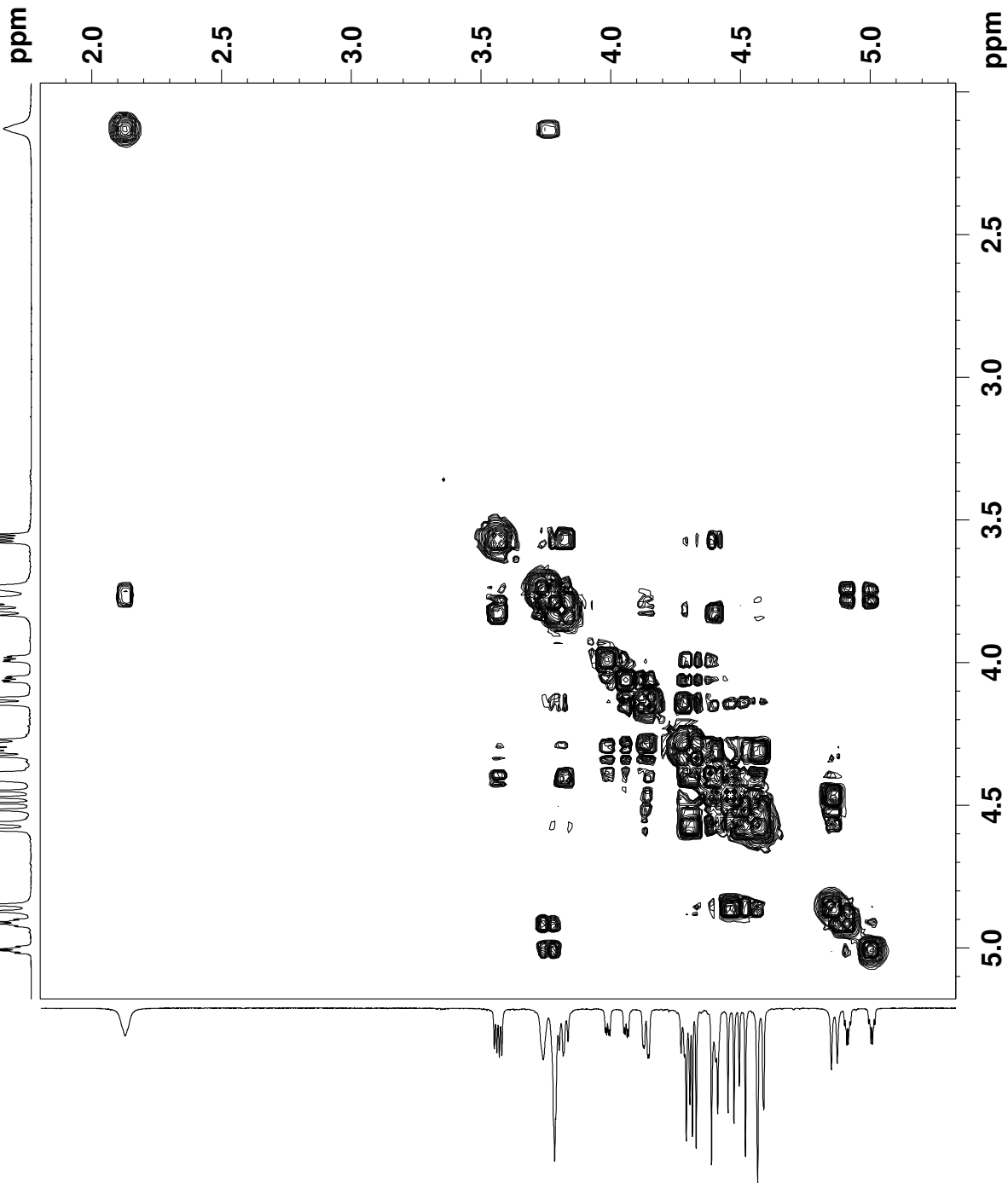


==== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 3.50 dB
 SF01 125.7703643 MHz
 =====
 CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -0.50 dB
 PL12 17.96 dB
 PL13 18.36 dB
 SF02 500.1320005 MHz
 SI 32768
 SF 125.7577173 MHz
 EM
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 0.20

83 82 81 80 79 78 77 76 75 74 73 72 71 70 69 68 67 66 65 64 ppm

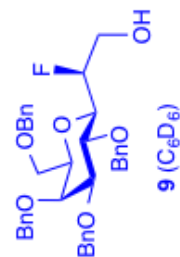


AAACRYOCOSY C6D6 /opt/topspin aaliti 5

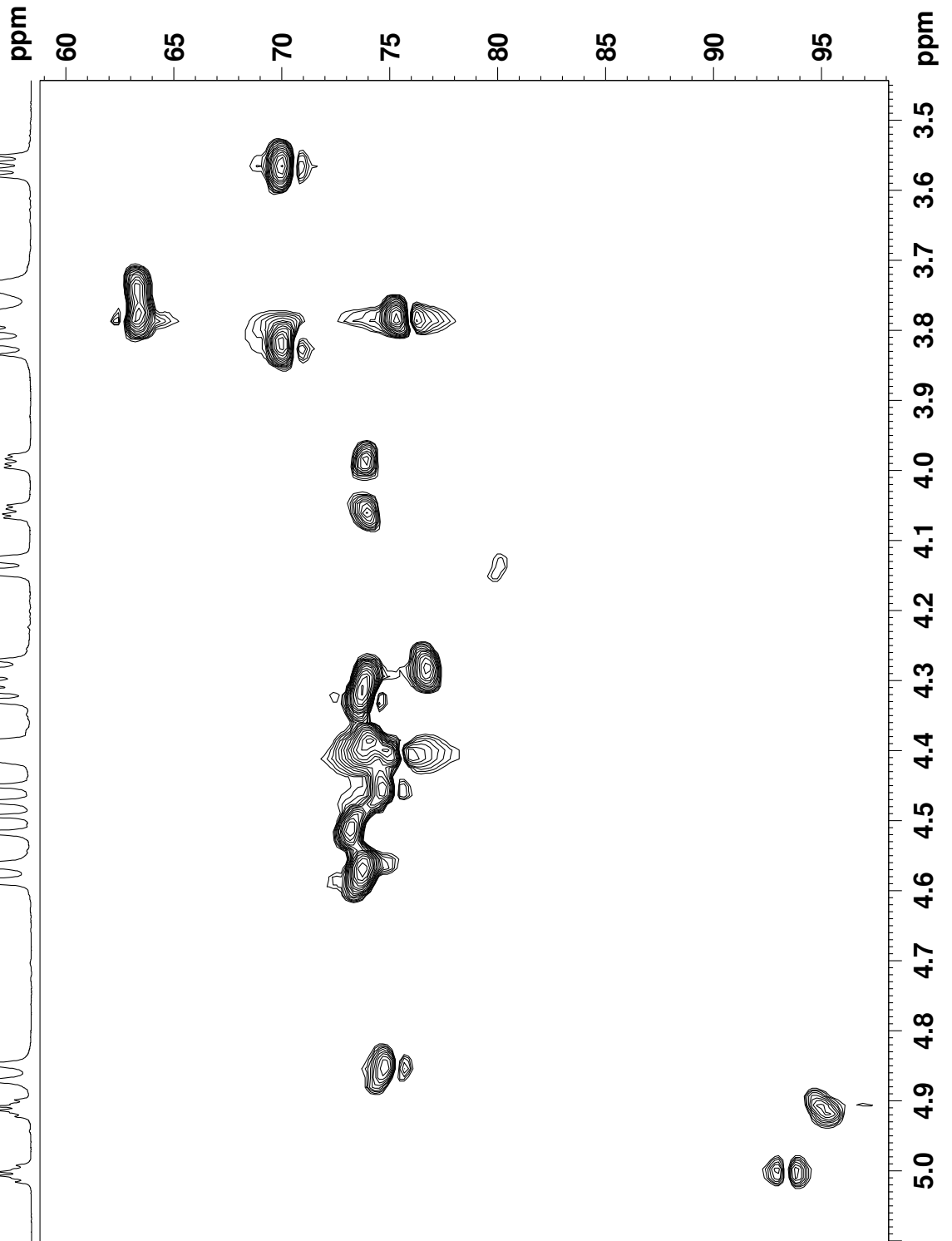
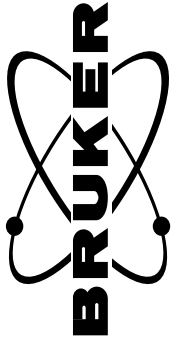


```

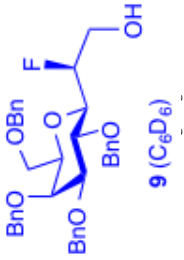
NAME                20141107
EXPNO                2
PROCNO              1
File_               20141107
File_               13_19
INSTRUM             spect
PROBHD              5 mm CPDCH 13C
PULPROG             cosygpcfg
TD                  2048
SOLVENT             C6D6
NS                   1
DS                   8
SWH                 6666.667 Hz
FIDRES              3.255208 Hz
AQ                  0.1537250 sec
RG                   32
DW                  75.000 usec
DE                   6.00 usec
TE                  298.0 K
DO                  0.0000300 sec
d1                  1.4600400 sec
d13                 0.0000000 sec
d16                 0.0002000 sec
IN0                 0.00015000 SEC
===== CHANNEL f1 =====
NUC1                 1H
P0                   9.50 usec
PL                   9.50 usec
PL1                  -0.50 dB
SFO1                 500.1330069 MHz
===== GRADIENT CHANNEL =====
GFNAM1              SINE.100
GFZ1                 10.00 %
PL6                  1000.00 usec
ND0                  1
ND1                  12
SFO1                 500.133 MHz
FIDRES              52.08332 Hz
SWH                 13.330 Ppm
FQMODE              OF
SI                   1024
SF                   500.1300622 MHz
WDW                  SINE
SSB                   0
LB                   0.00 Hz
GB                   0
PC                   1.40
SI                   1024
MC2                 OF
SF                   500.1300631 MHz
WDW                  SINE
SSB                   0
LB                   0.00 Hz
GB
  
```



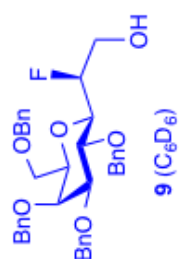
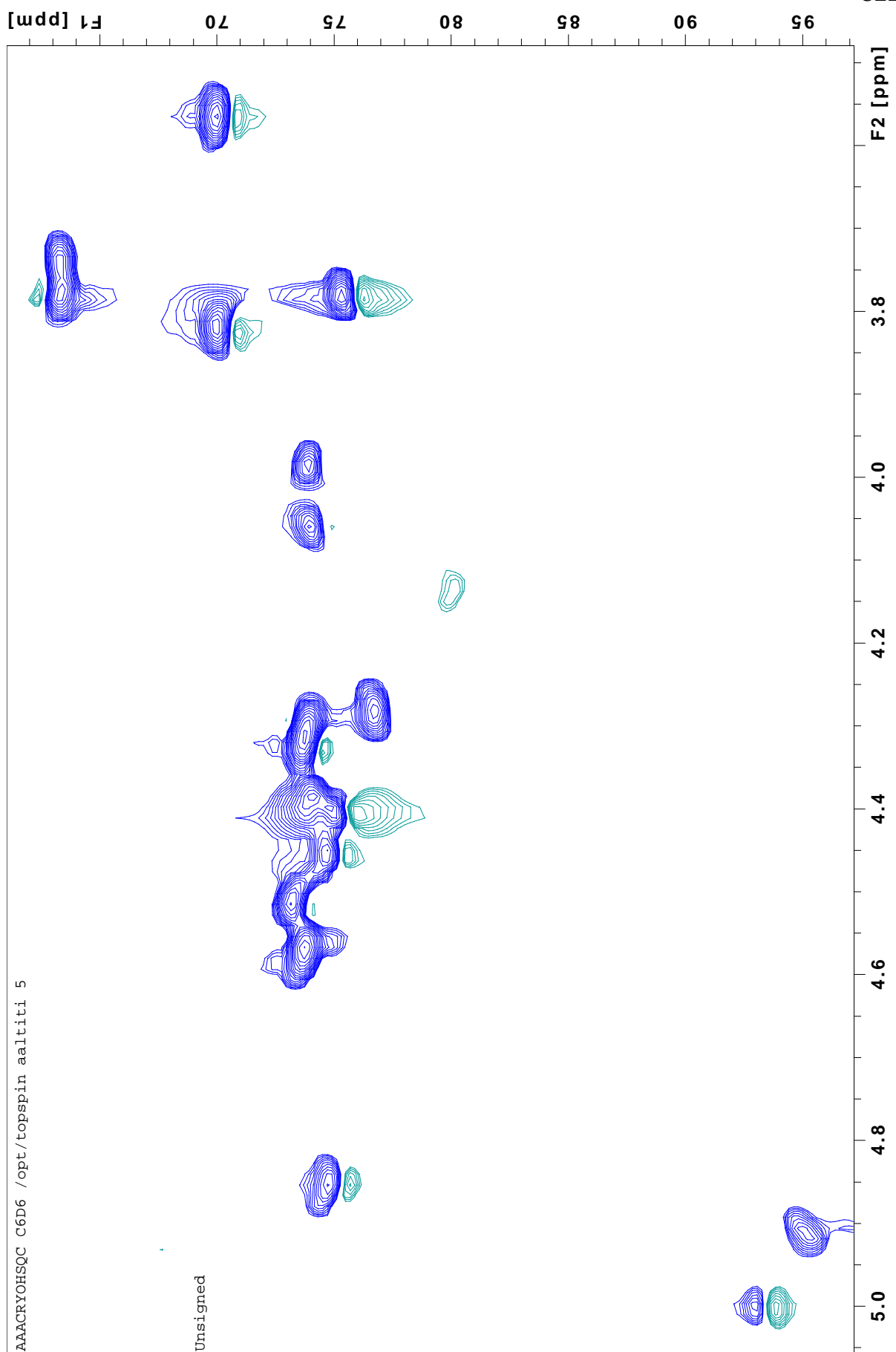
AAACRYOHSQC C6D6 /opt/topspin aaltiti 5



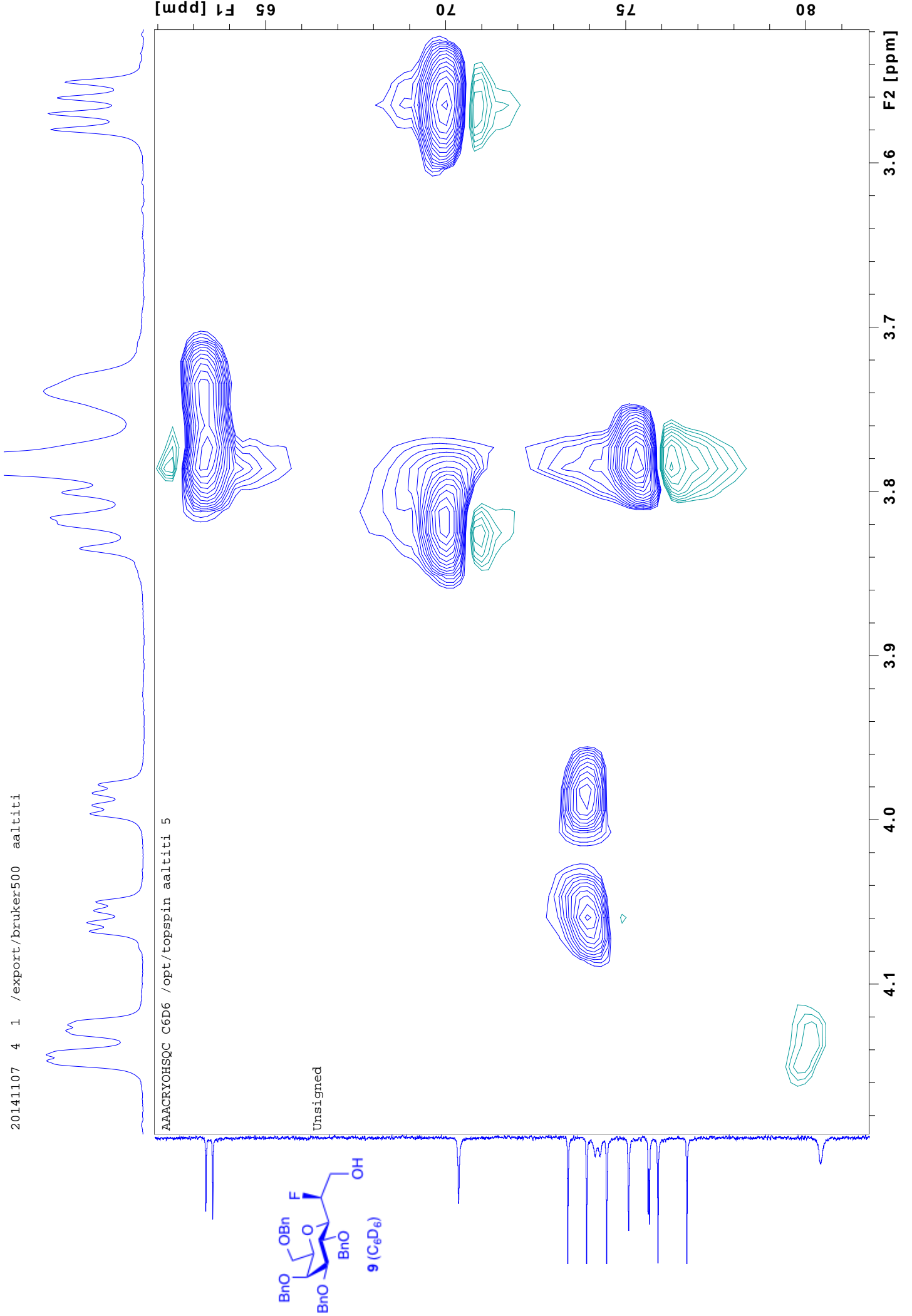
```
NAME 20141107
EXPNO 4
PROCNO 1
Date_ 20141107
Time 13.29
PROBHD 5 mm CPDQX 13C
PULPROG hsqcqtpp
SOLVENT CDCl3
NS 2
DS 1
SWH 6666.657 Hz
FIDRES 6.510417 Hz
AQ 0.946341 sec
RG 640
DM 75.000 usec
TE 298.0 K
CSTZ 145.000000 sec
D1 1.20000000 sec
d11 1.20000005 sec
d4 0.00172418 sec
d13 0.00000000 sec
d16 0.00020000 sec
DELTA 0.00000000 sec
DELTA1 0.00016184 sec
INSTRUM spect
ZCOPTNS 0
===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
P2 2000.00 usec
PL2 -0.50 dB
SFO1 500.135069 MHz
===== CHANNEL f2 =====
NUC2 13C
P3 10.50 usec
PL3 0.00 dB
P4 70.00 usec
PL4 3.50 dB
SFO2 125.767849 MHz
===== GRADIENT CHANNEL =====
GPMAX1 SINE,100
GPMAX2 SINE,100
P16 20.10 usec
PL16 0.00 dB
P17 1000.00 usec
TD 128
SFO1 125.7678 MHz
SFO2 500.135069 MHz
SWHRES 199.775775 ppm
F2F2D2 Echo-AntiEcho
SF 500.1305619 MHz
WDW COSINE
GB 0.00 Hz
SI 1
SF 1.024
MC2 echo-antlecho MHz
WDW COSINE
GB 0.00 Hz
```



20141107 4 1 /export/bruker500 aaltiti



20141107 4 1 /export/bruker500 aaltiti



AAACRYOPROTON CDCl3 /opt/topspin aaltiti 7

7.280
7.277
7.264
7.260
7.246
7.235
7.230
7.220
7.217
7.210
7.207
7.204
7.187
7.187
4.898
4.877
4.855
4.705
4.700
4.681
4.609
4.602
4.594
4.586
4.572
4.531
4.508
4.403
4.379
4.363
4.339
3.929
3.924
3.866
3.847
3.828
3.779
3.767
3.620
3.616
3.600
3.596
3.584
3.578
3.573
3.564
3.560
3.554
3.505
3.497
3.486
3.477
3.457

```

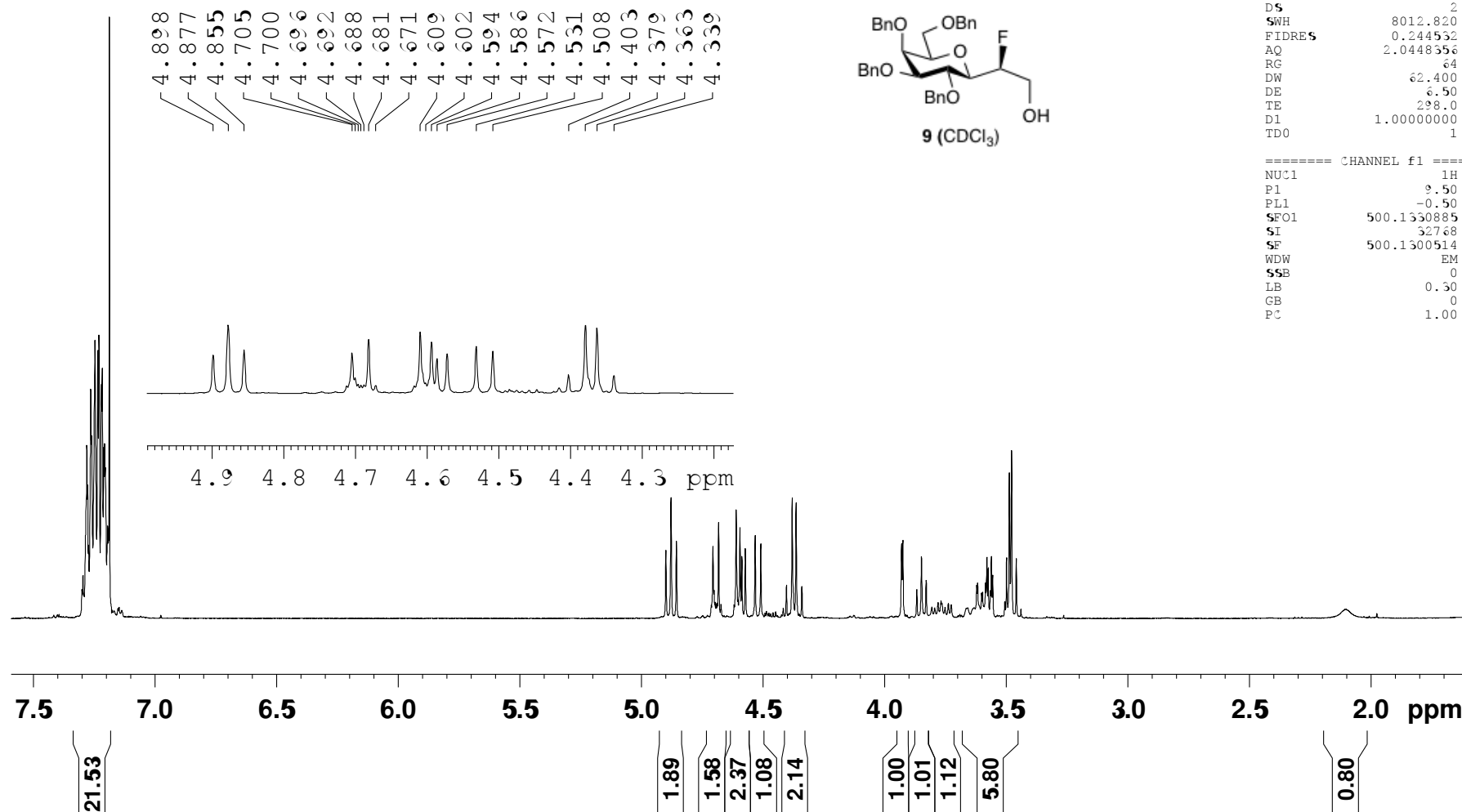
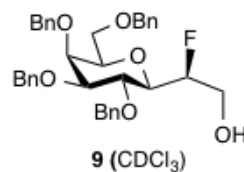
NAME          20141105
EXPNO         19
PROCNO        1
Date_         20141105
Time          23.36
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            8
DS            2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ           2.0448356 sec
RG            64
DW           62.400 usec
DE           6.50 usec
TE           298.0 K
D1           1.00000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1           1H
P1            9.50 usec
PL1           -0.50 dB
SFO1          500.1330885 MHz
SI            32768
SF           500.1300514 MHz
WDW           EM
SSB           0
LB            0.50 Hz
GB            0
PC            1.00

```



AAACRYOCOSY CDCl₃ /opt/topspin aaltiti 7

```

NAME          20141105
EXPNO         20
PROCNO        1
Date_         20141105
Time         23.37
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       cosygpgf
TD            2048
SOLVENT       CDCl3
NS            1
DS            8
SWH           6666.467 Hz
FIDRES        3.255208 Hz
AQ            0.1537250 sec
RG            57
DW            75.000 usec
DE            6.00 usec
TE            298.0 K
d0            0.00000500 sec
d1            1.4848198 sec
d13           0.00000400 sec
d16           0.00020000 sec
INO           0.00015000 sec

```

```

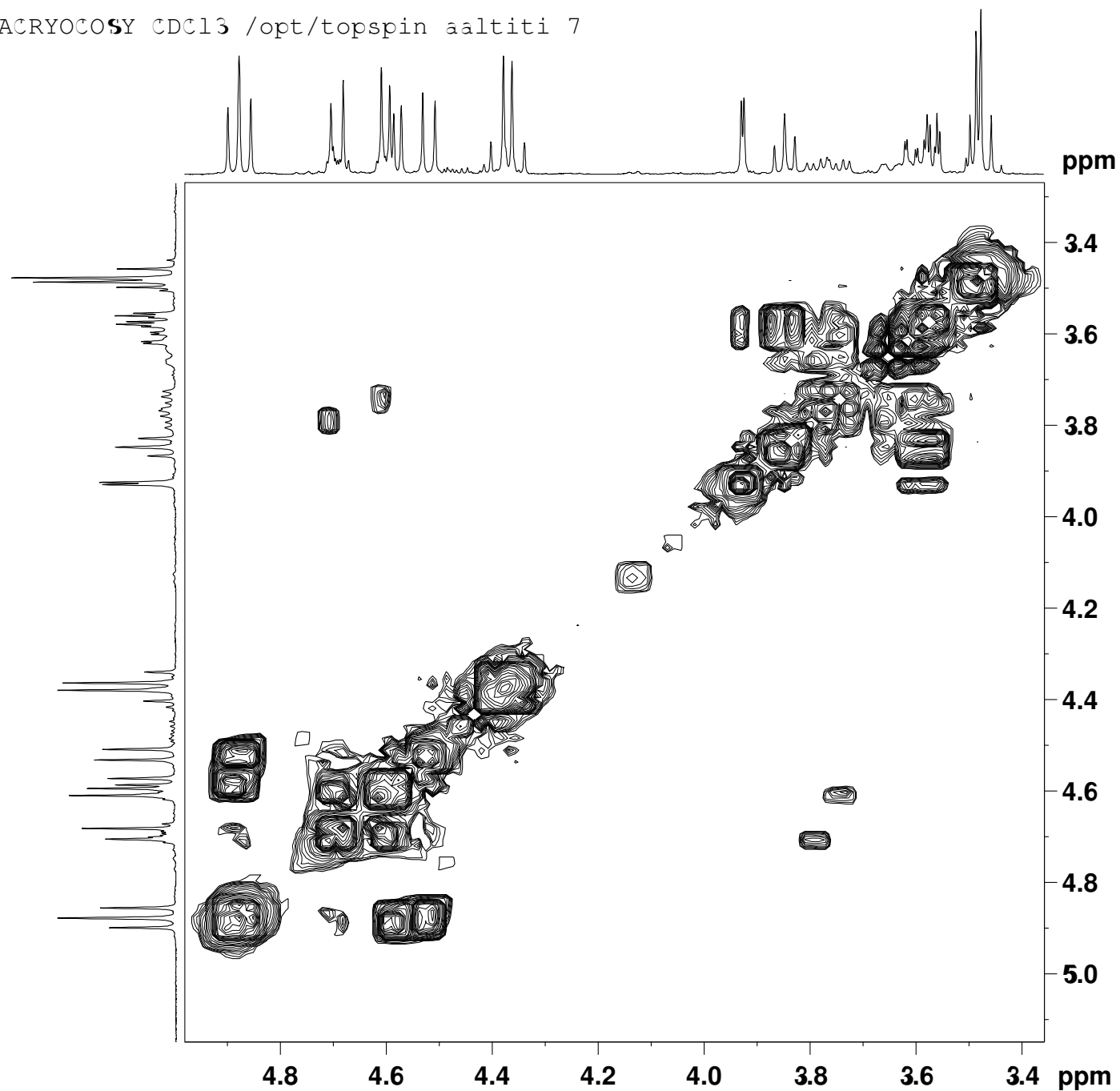
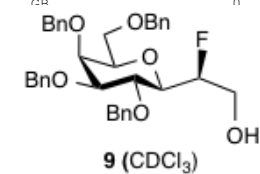
===== CHANNEL f1 =====
NUC1          1H
P0            9.50 usec
P1            9.50 usec
PL1           -0.50 dB
SFO1          500.1530069 MHz

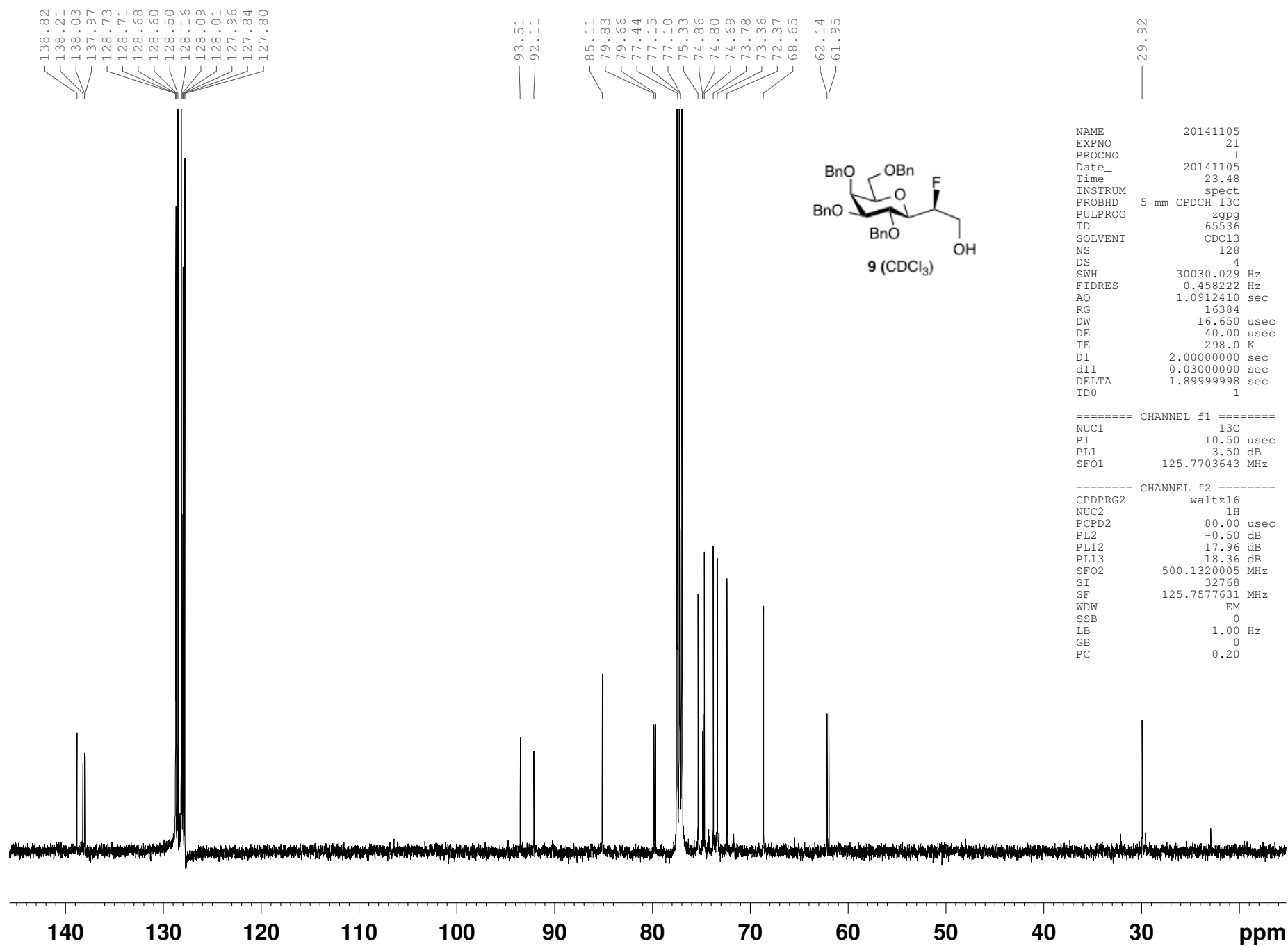
```

```

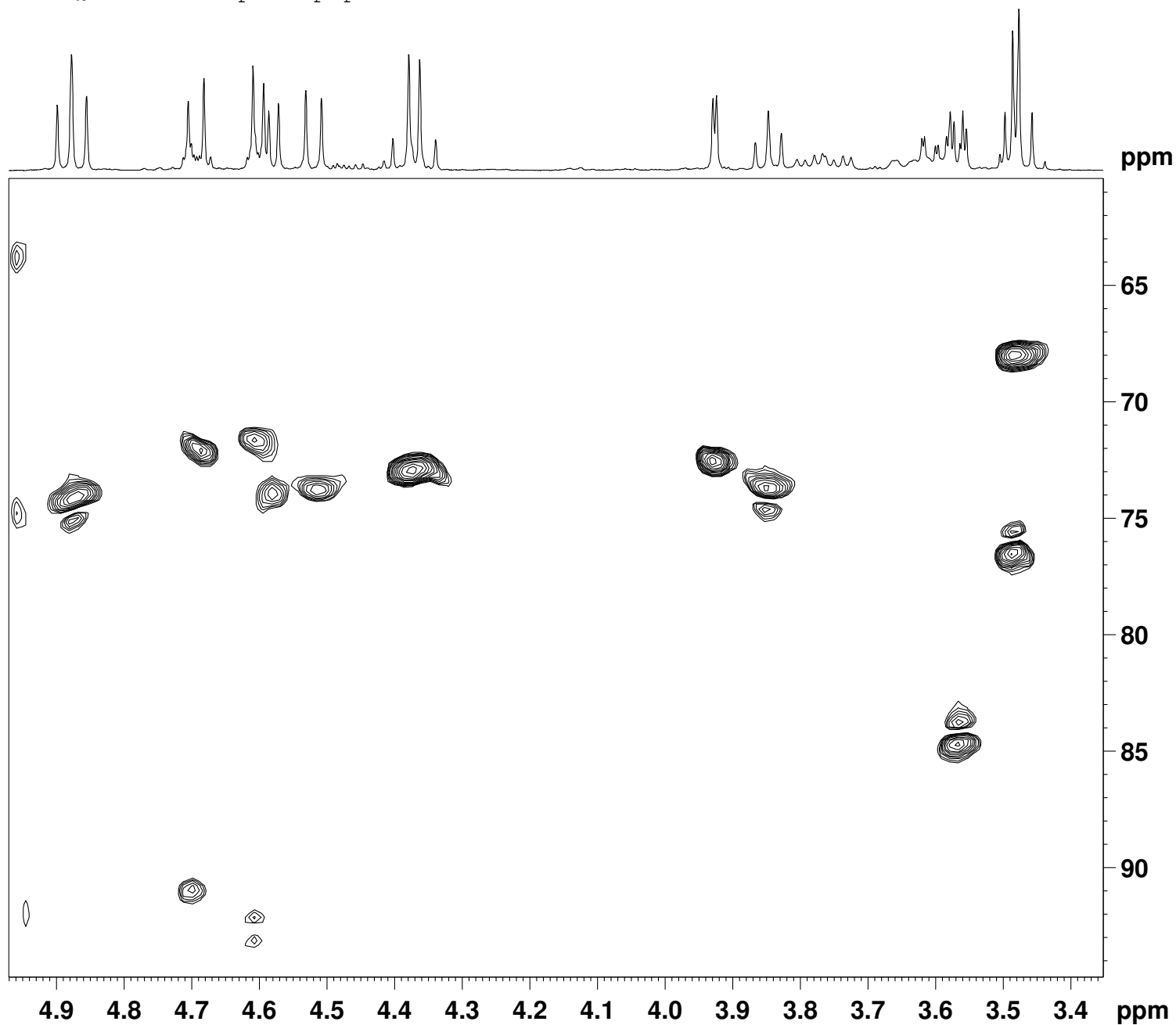
===== GRADIENT CHANNEL =====
GPNAME1       SINE.100
GPZ1          10.00 %
P16           1000.00 usec
ND0           1
TD            128
SFO1          500.133 MHz
FIDRES        52.083332 Hz
SW            13.330 ppm
FRMODE        QF
SI            1024
SF            500.1300509 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            500.1300515 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
CR            0

```





AAACRYOHSQC CDC13 /opt/topspin aaltiti 7



```

NAME          20141105
EXPNO         22
PROCNO        1
Date_         20141105
Time          23.48
INSTRUM       spect
PROBHD        5 mm CPDCH-13C
PULPROG       hsqcetgp
TD            1024
SOLVENT       CDC13
NS            2
DS            16
SWH           6666.667 Hz
FIDRES        6.510417 Hz
AQ            0.0769250 sec
RG            20642.5
DW            75.000 usec
DE            6.00 usec
TE            298.0 K
CNST2         145.0000000
d0            0.00000300 sec
d1            1.20000005 sec
d4            0.00172414 sec
d11           0.03000000 sec
d13           0.00000400 sec
d16           0.00020000 sec
DELTA         0.00122500 sec
DELTA1        0.00071614 sec
IN0           0.00001930 sec
ST1CNT        0
ZGOPTNS

```

```

----- CHANNEL f1 -----
NUC1          1H
P1            9.50 usec
P2            19.00 usec
P28           2000.00 usec
PL1           -0.50 dB
SFO1          500.1330069 MHz

```

```

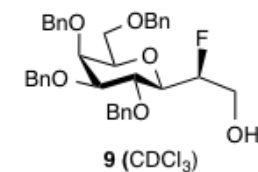
----- CHANNEL f2 -----
CPDPRG2       garp
NUC2          13C
P3            10.50 usec
P4            21.00 usec
PCPD2         70.00 usec
PL2           3.50 dB
PL12          19.98 dB
SFO2          125.7678496 MHz

```

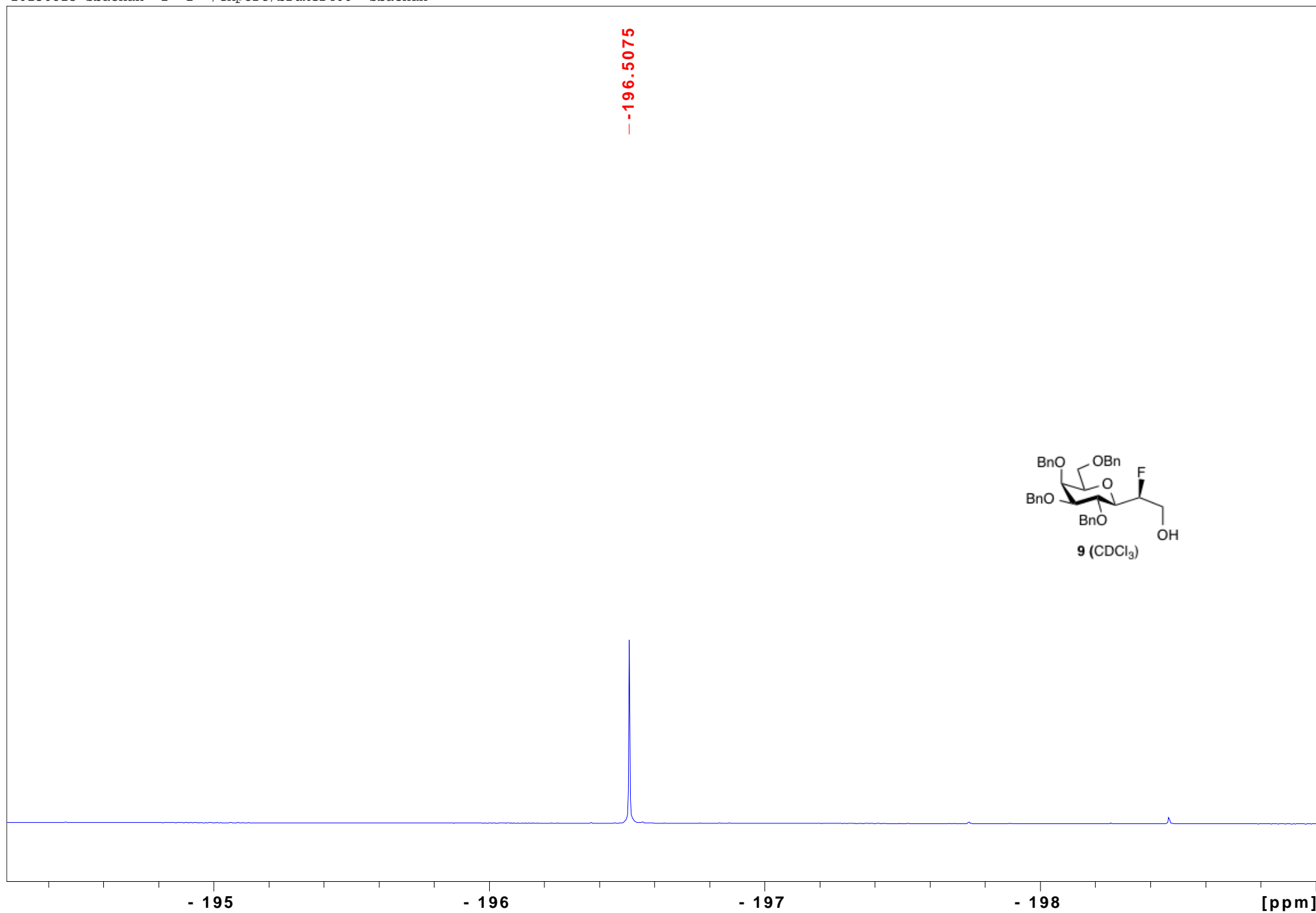
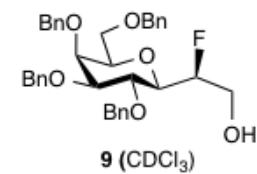
```

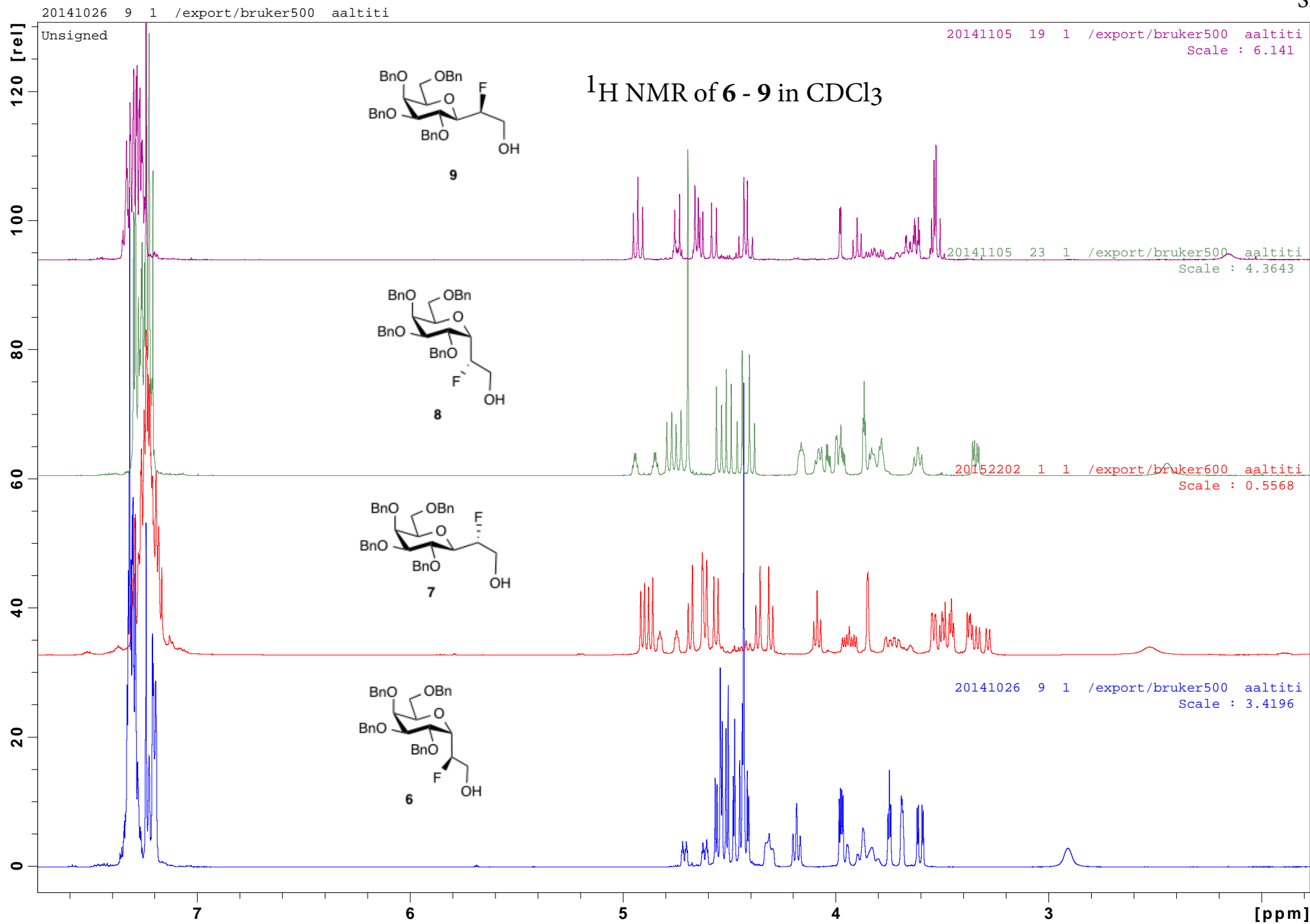
----- GRADIENT CHANNEL -----
GFNAM1        SINE.100
GFNAM2        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec
ND0           2
TD            115
SFO1          125.7678 MHz
FIDRES        218.483719 Hz
SW            199.778 ppm
FIRMODE       Echo-Antiecho
SI            1024
SF            500.1300487 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
NUC2          echo-antiecho
SF            125.7578451 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0

```



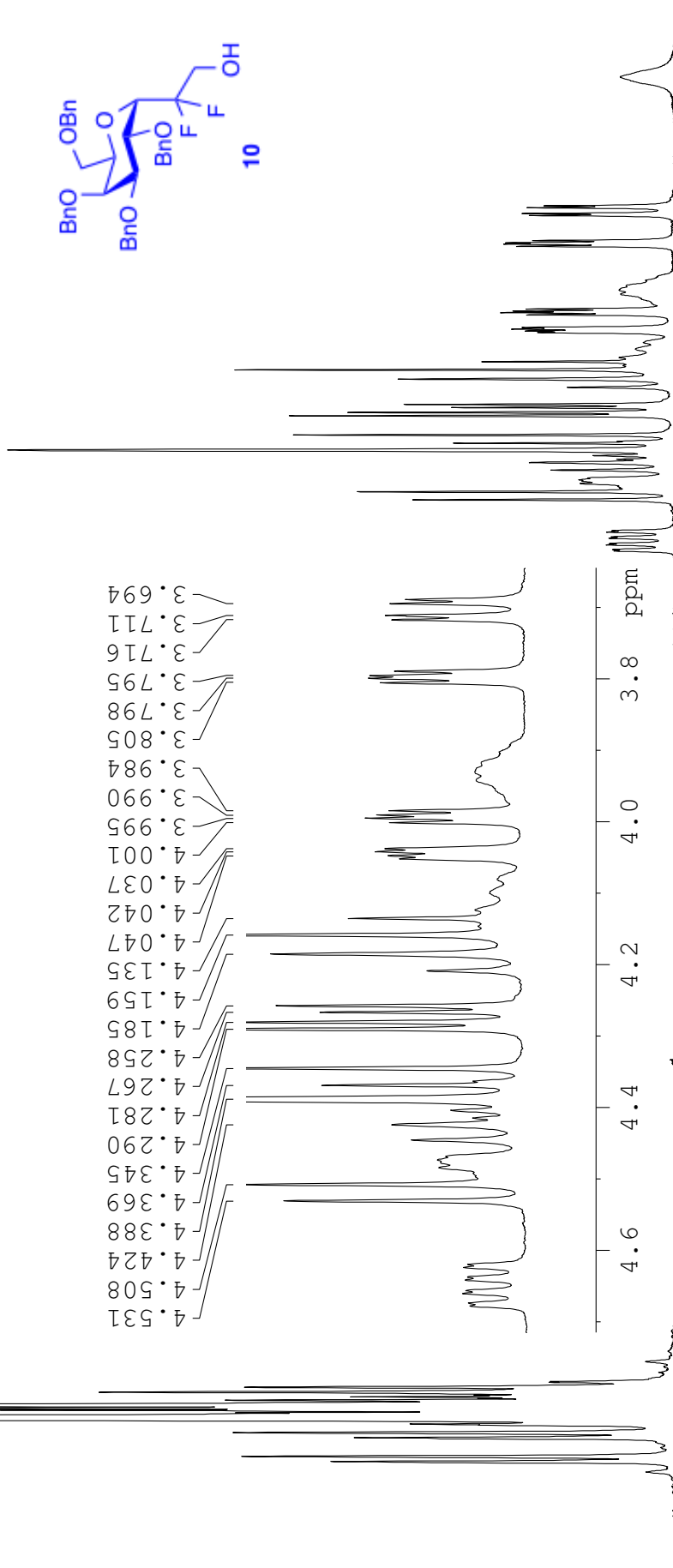
--196.5075



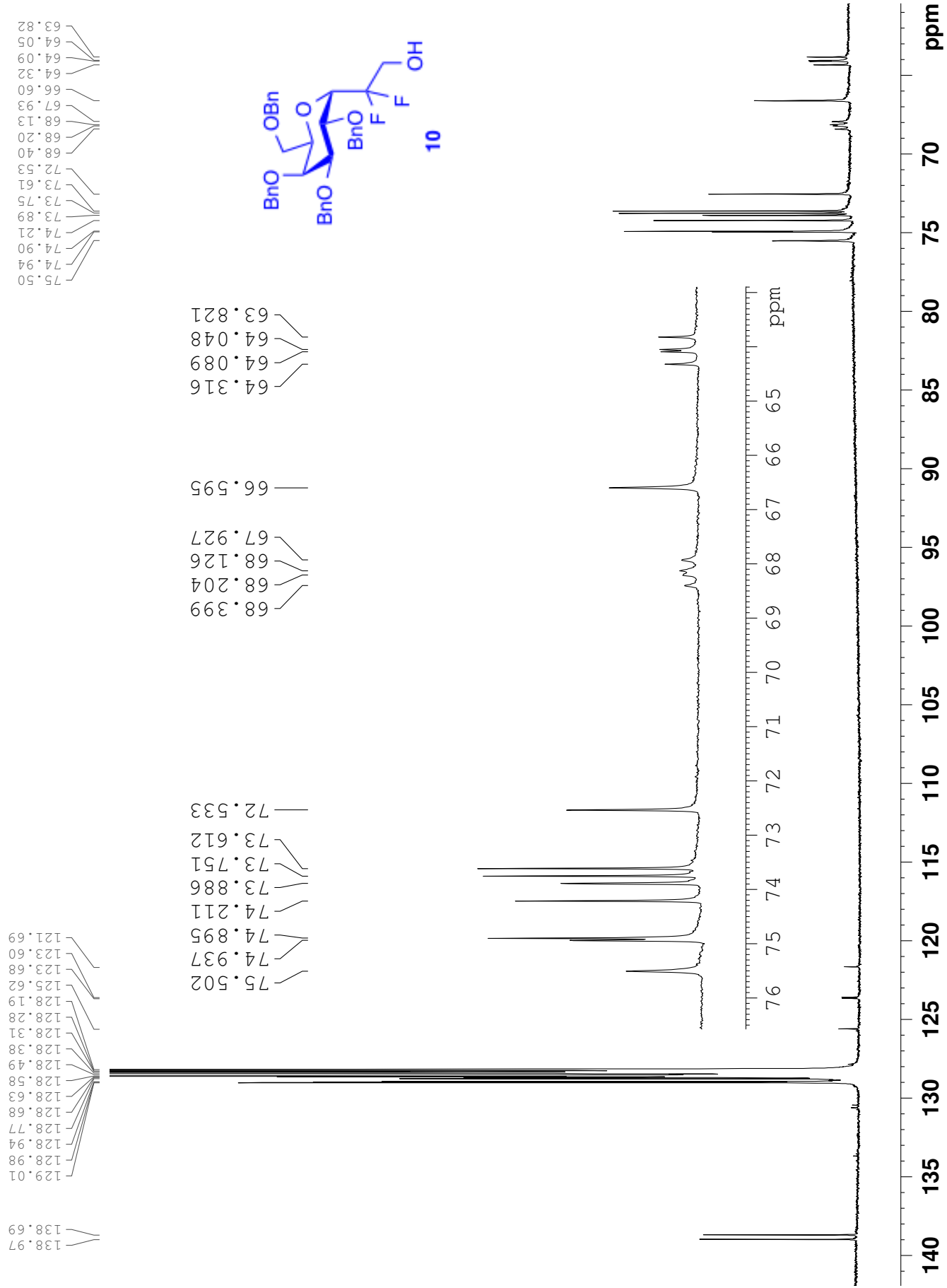


AAACRYOPROTON C6D6 /opt/topspin aaltiti 9

7.285
7.271
7.217
7.203
7.181
7.178
7.149
7.146
7.138
7.109
7.104
7.100
7.095
7.087
7.072
7.059
7.056
4.623
4.531
4.508
4.484
4.473
4.468
4.446
4.424
4.404
4.388
4.369
4.345
4.290
4.281
4.267
4.258
4.209
4.185
4.159
4.135
4.052
4.047
4.042
4.037
4.001
3.995
3.990
3.984
3.805
3.798
3.795
3.788
3.716
3.711
3.694

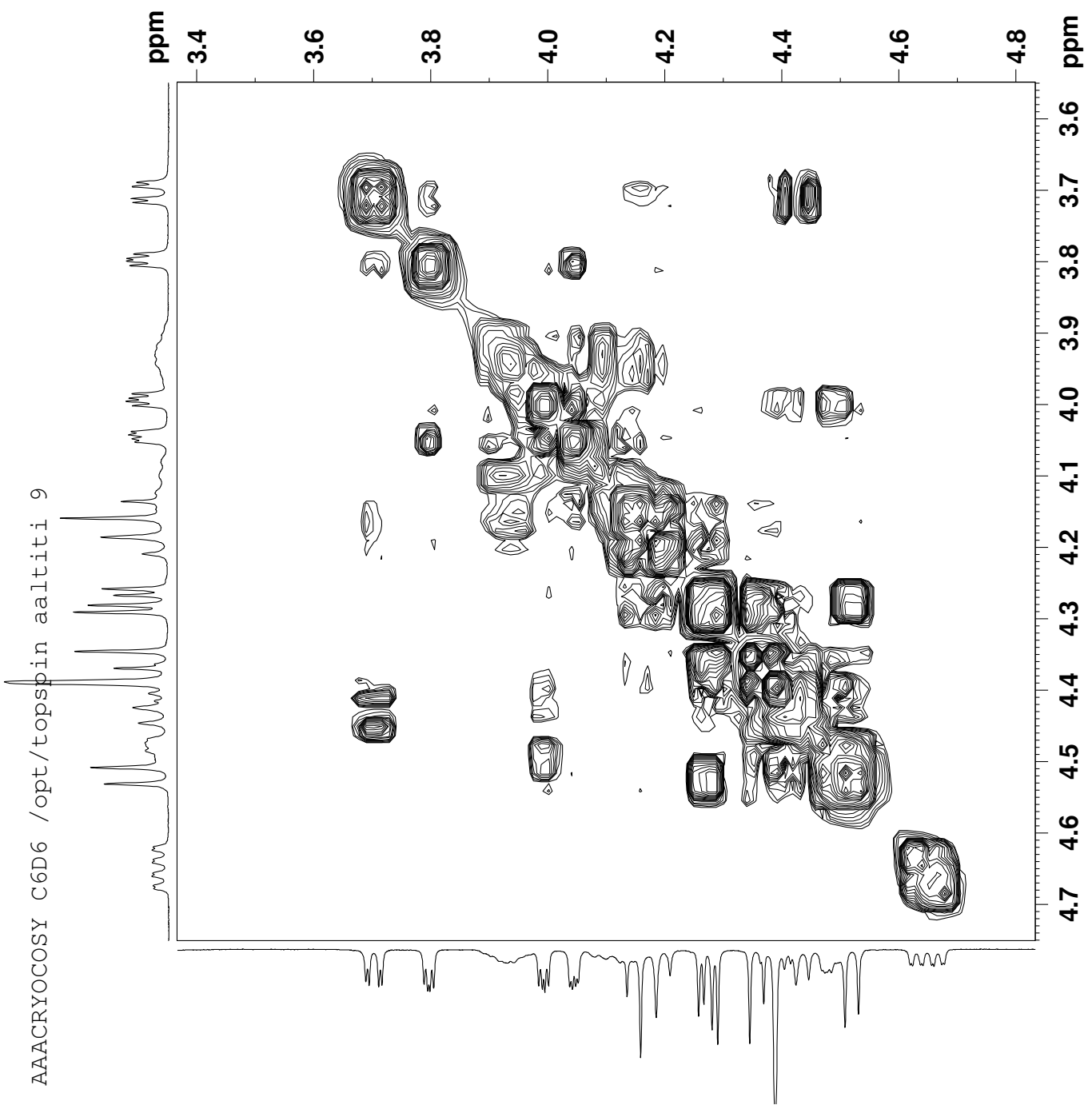
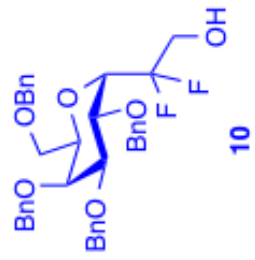


AAACRYOCARBON C6D6 /opt/topspin aaltiti 9



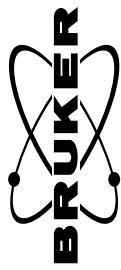
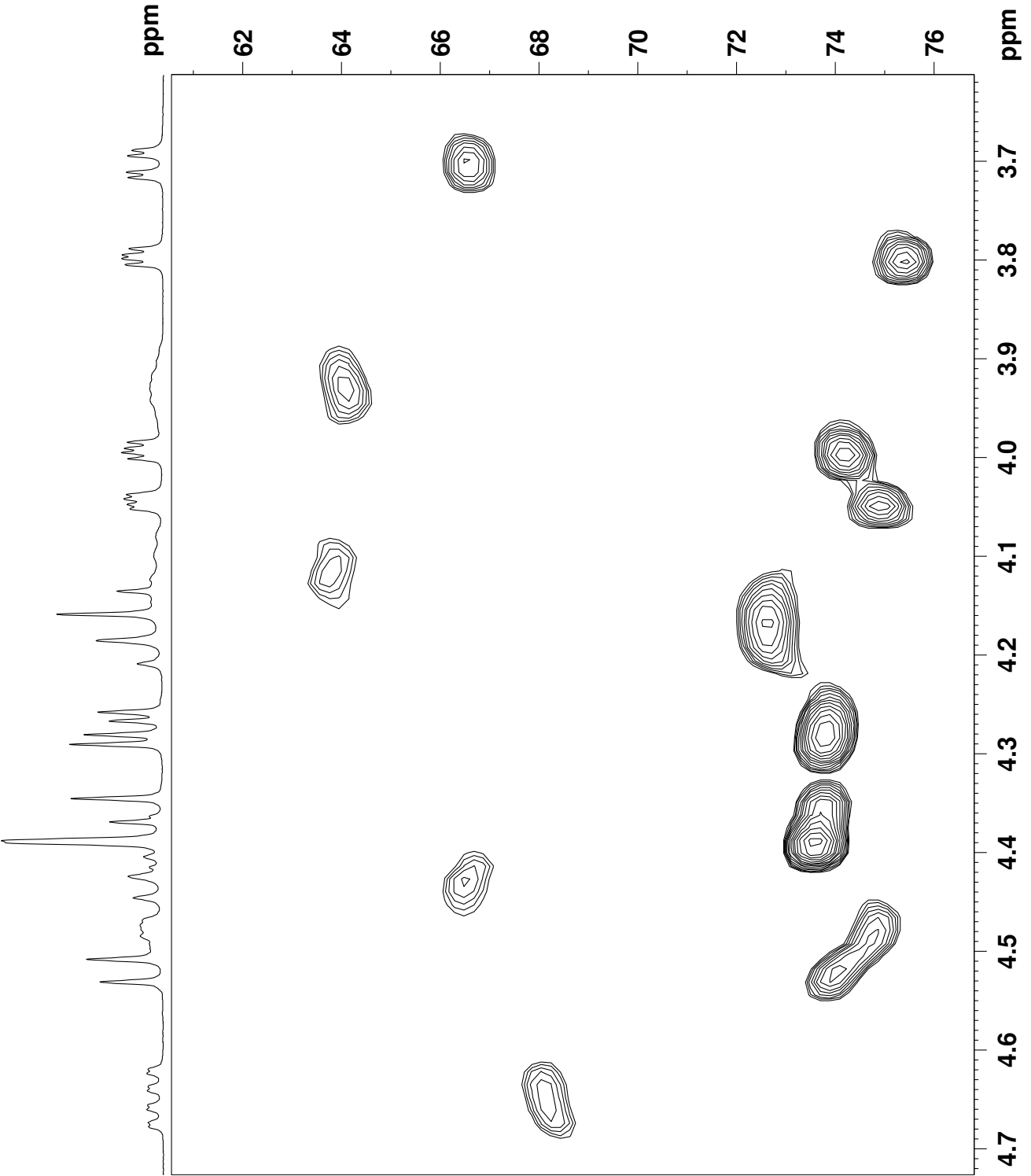


NAME 20150616-difluorocatalcohol-C6D6-Moct-09
 EXPNO 5
 PROCNO 5
 F2ACQNO 20150617
 Time 10.43
 F2PROC 1
 PULPROG 5 mm cpdchf13c
 BULPROG cosy90sf
 SOLVENT C6D6
 NS 1
 SWH 6666.667 Hz
 FIDRES 3.255208 Hz
 RG 0.1352256 sec
 DW 75.000 usec
 DE 0.00000000 usec
 TE 298.2 K
 UO 0.00000000 sec
 U1 0.00000000 sec
 d13 0.00000000 sec
 d16 0.00000000 sec
 d18 0.00000000 sec
 d30 0.00000000 sec
 NUC1 1H
 P0 10.25 usec
 PL1 -0.50 dB
 PL2 -0.50 dB
 SFO1 500.1320069 MHz
 GRADIENT CHANNEL
 GPMAX1 SINE.100
 P1.6 1000.00 usec
 TD 128
 SFO2 500.133 MHz
 F2FREQ 52.13730 ppm
 SW 4.00 Hz
 F2MODE 1D OF
 SF 500.1300491 MHz
 SFO 500.1300491 MHz
 LB 0.00 Hz
 GB 0
 S1 1.45
 S2 1024
 SFO2 500.1300509 MHz
 SFO 500.1300509 MHz
 LB 0.00 Hz
 GB 0



AAACRYOCOSY C6D6 /opt/topspin aaltiti 9

AAACRYOHSQC C6D6 /opt/topspin aaltiti 9

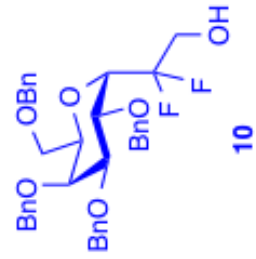


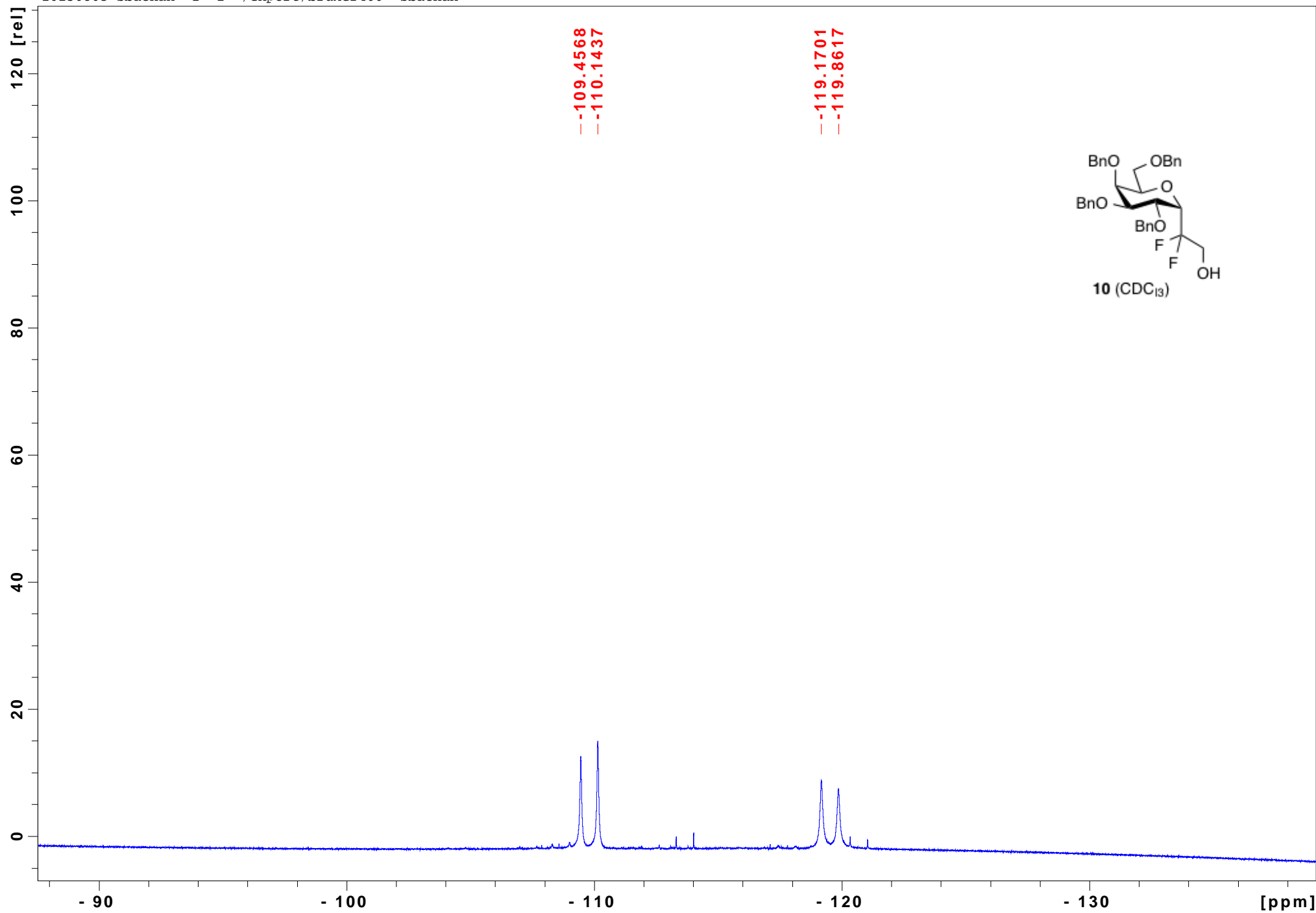
20130616-difluoroinol-C6D6-Most.oo
 NAME: 1
 PROCNO: 1
 Date_: 20150617
 TIME: 12:59:59
 INSTRUM: spect
 PRBHD: 5 mm CHXCH 13C
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: C6D6
 DS: 4
 SFO1: 125.7678496 MHz
 SFO2: 500.1300699 MHz
 SWH: 6666.667 Hz
 FIDRES: 0.07769250 Hz
 AQ: 0.07769250 Hz
 RG: 329.93
 DE: 6.00 usec
 TE: 300.2 K
 CH22: 145.0029812 K
 G0: 0.00003000 Hz
 D1: 1.20000005 sec
 d11: 0.00000000 sec
 d12: 0.00000000 sec
 DELTA: 0.00122650 sec
 DELTA1: 0.00071614 sec
 STCNT: 0
 ZGPGTNS: 0

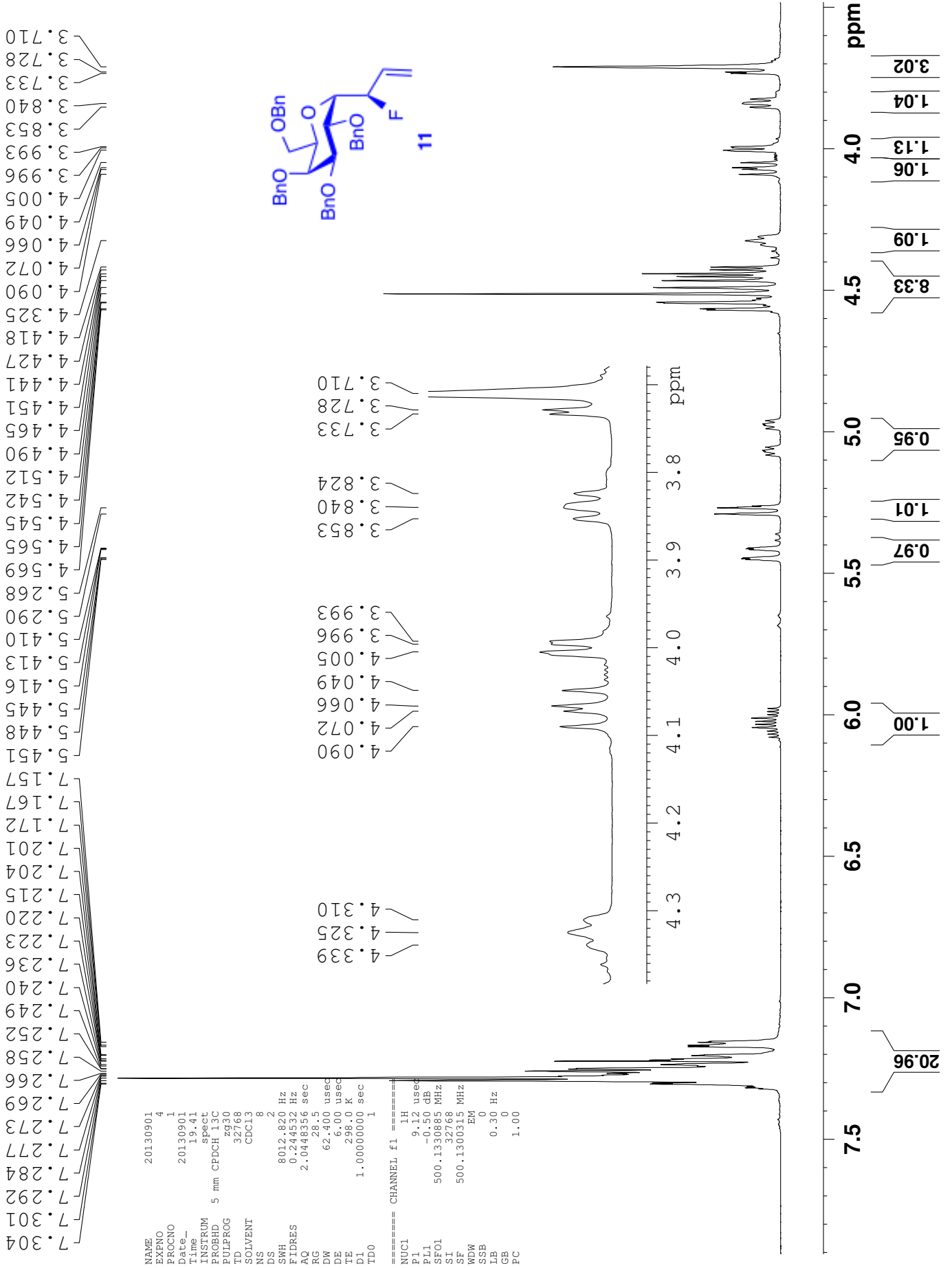
===== CHANNEL f1 =====
 NUC1: 13C
 P1: 12.00 usec
 F2: 20.50 usec
 F28: 2000.00 usec
 SFO1: 500.1300699 MHz

===== CHANNEL f2 =====
 CDPRG2: gfpf
 NUC2: 13C
 P4: 12.00 usec
 F4: 28.00 usec
 FCPD2: 70.00 usec
 F11: 17.48 dB
 F12: 17.48 dB
 SFO2: 125.7678496 MHz

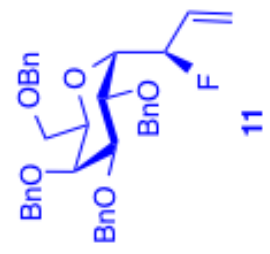
===== GRADIENT CHANNEL =====
 GRNM1: SINE, 1.00
 GRP1: 80.00 %
 GRP2: 20.10 %
 GRP3: 100.00 %
 ND0: 1000.00 usec
 ND1: 125.7678496 MHz
 FIDRES: 196.2895716 Hz
 SW: 199.778 Ppm
 F2MODE: Echo-ant-1024
 S1: 500.1300699 MHz
 S2: 125.7678496 MHz
 LB: 0.00 Hz
 FC: 1.40
 MC2: 1024
 SF: 125.7577132 MHz
 SSW: 65192
 L1B: 0.00 Hz
 CB: 0







138.46
138.80
138.04
134.86
134.72
128.63
128.60
128.58
128.54
128.51
128.39
128.16
127.93
127.90
127.85
127.80
127.74
127.70
127.67
118.01
117.91
90.97
89.63
77.48
77.22
76.97
75.27
74.72
74.05
73.60
73.55
73.35
73.24
71.82
69.68
69.45
65.84



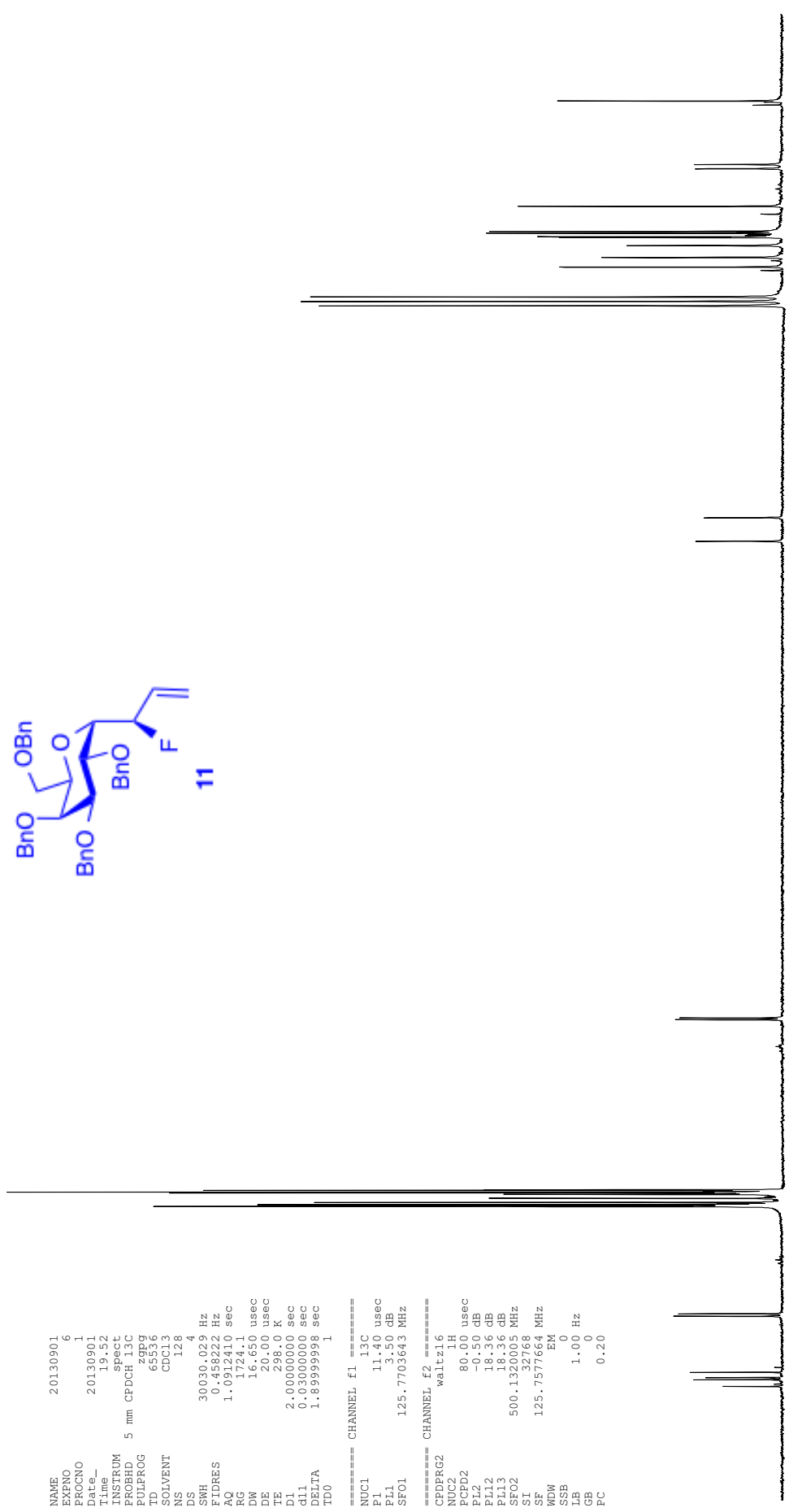
```

NAME                20130901
EXPNO                6
PROCNO               1
F2 -                  20130901
F1 -                  19.52
INSTRUM              spect
PROBHD               5 mm CPDCH13C
PULPROG              zgpg2
TD                   65536
SOLVENT              CDCl3
NS                   128
DS                   4
SWH                  30030.029 Hz
FIDRES              0.458222 Hz
AQ                   1.0912410 sec
RG                   1724.1
DW                   16.650 usec
DE                   20.00 usec
TE                   298.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA               1.89999998 sec
TD0                 1

===== CHANNEL f1 =====
NUC1                 13C
P1                   11.40 usec
PL1                  3.50 dB
SFO1                 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2             waltz16
NUC2                 1H
PCPD2               80.00 usec
PL2                 -0.50 dB
PL12                18.36 dB
PL13                18.36 dB
SFO2                 500.1320005 MHz
SI                  32768
SF                   125.7577664 MHz
WDW                  EM
SSB                  0
LB                   1.00 Hz
GB                   0
PC                   0.20

```



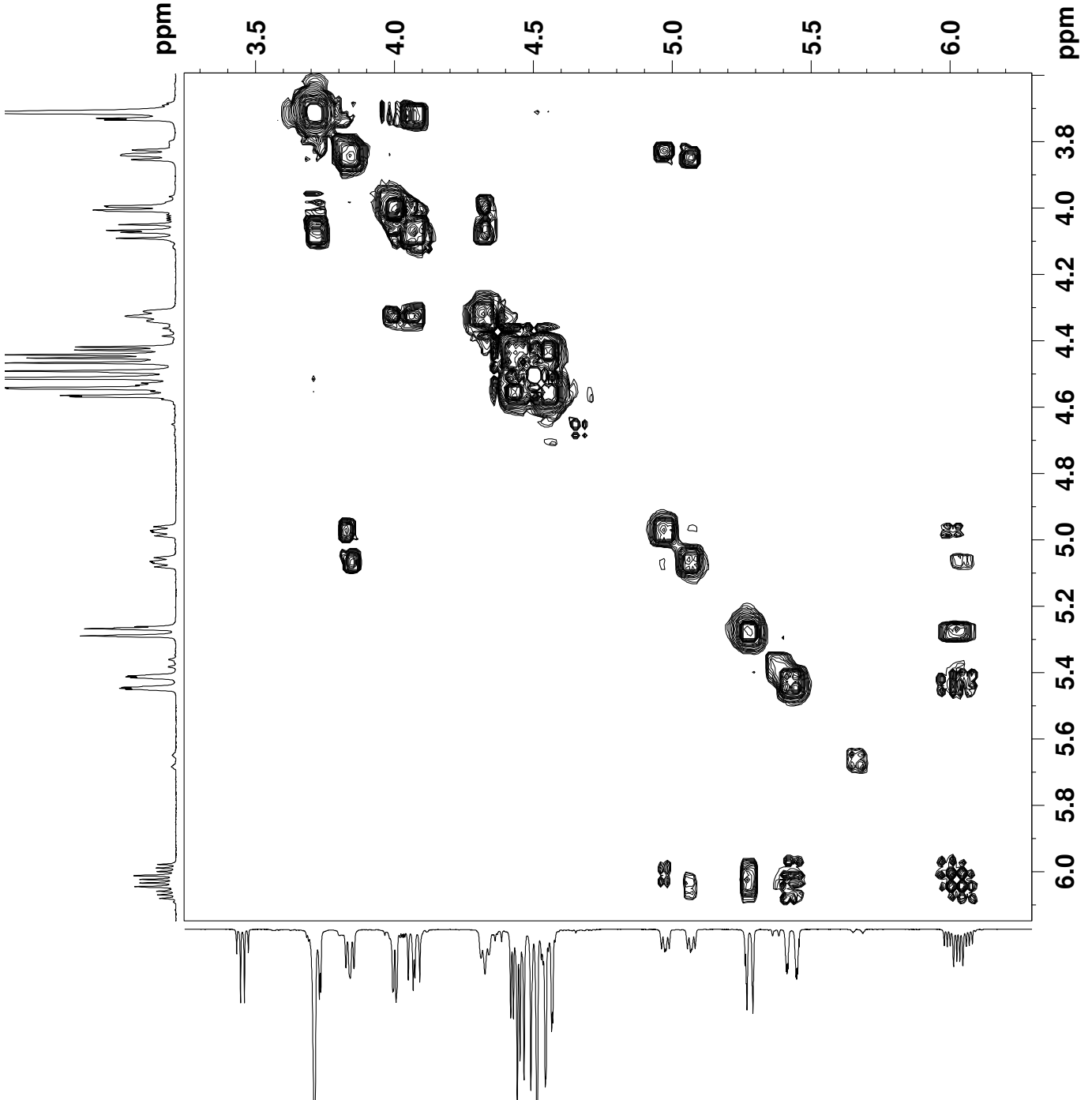
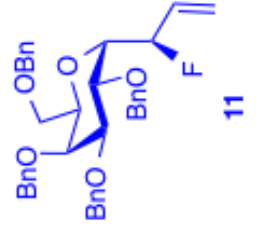
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 ppm



20130901
NAME
EXPNO 5
PROCNO 1
Date_ 20130901
Time 19.41
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG cosygpsf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 6666.667 Hz
FIDRES 3.254208 Hz
AQ 0.1537250 sec
RG 22.6
DW 75.000 usec
DE 6.00 usec
TE 298.0 K
d0 0.0000300 sec
d1 1.48689198 sec
d13 0.0000400 sec
d16 0.0002000 sec
IN0 0.00015000 sec

==== CHANNEL f1 =====
NUC1 1H
P0 9.12 usec
PL 9.12 usec
SFO1 500.1330069 MHz

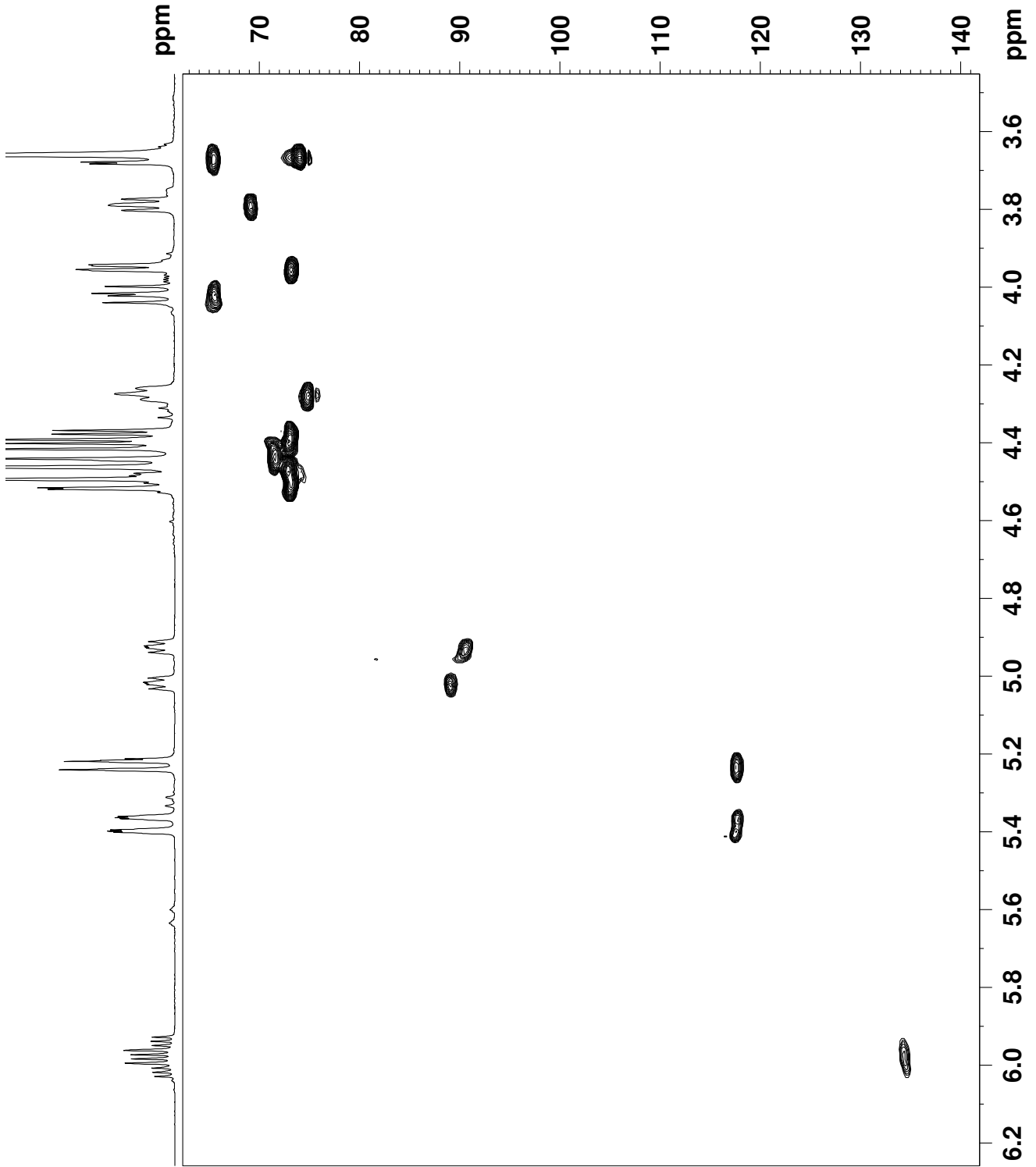
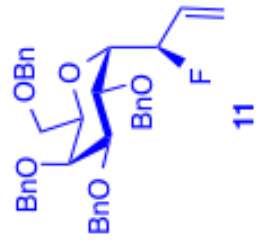
==== GRADIENT CHANNEL =====
GENM1 SINE.100
P16 10.00 %
ND0 1
SFO1 500.133 MHz
FIDRES 52.083332 Hz
SW 13.330 ppm
FMODE QF
SI 1024
SF 500.1300308 MHz
WDW
SSB 0
LB 0.00 Hz
GB 0
EC 1.0
SC 1024
MG2 OF
SF 500.1300301 MHz
WDW
SSB 0
LB 0.00 Hz
GB 0





```

NAME      20130902
EXPNO     1
PROCNO    1
Time      20130911
Time      0.25
INSTRUM   spect
PROBHD    5 mm cryo-
PULPROG   zgpg30
RG         655
AQ         0.0752950 sec
FIDRES    0.0001390 Hz
AQRES     0.0001390 Hz
SFO1      500.1350693 MHz
SFO2      125.7678496 MHz
===== CHANNEL f1 =====
NUC1      1H
P1        18.72 usec
PC        1.30 usec
PR        22.80 usec
RF1       500.1350693 MHz
===== CHANNEL f2 gnd =====
NUC2      13C
P2        19.00 usec
PC        1.40 usec
PR        22.80 usec
RF2       125.7678496 MHz
===== GRADIENT CHANNEL =====
GPRAMP1   SINE 100
GR21      80.00 %
GR22      80.00 %
GR23      100.00 usec
MD0       1.2
SFO1      125.7678496 MHz
P1DRBS    196.283976 Hz
ECHO-ANTI ECHO PPM
P1WDW     500.1350693 MHz
SFB       0.5
GB         0
PC         1.40
MC2       echo-anti echo
SFO1      125.7678496 MHz
SFB       0.5
GB         0.00 Hz
  
```



ppm

70

80

90

100

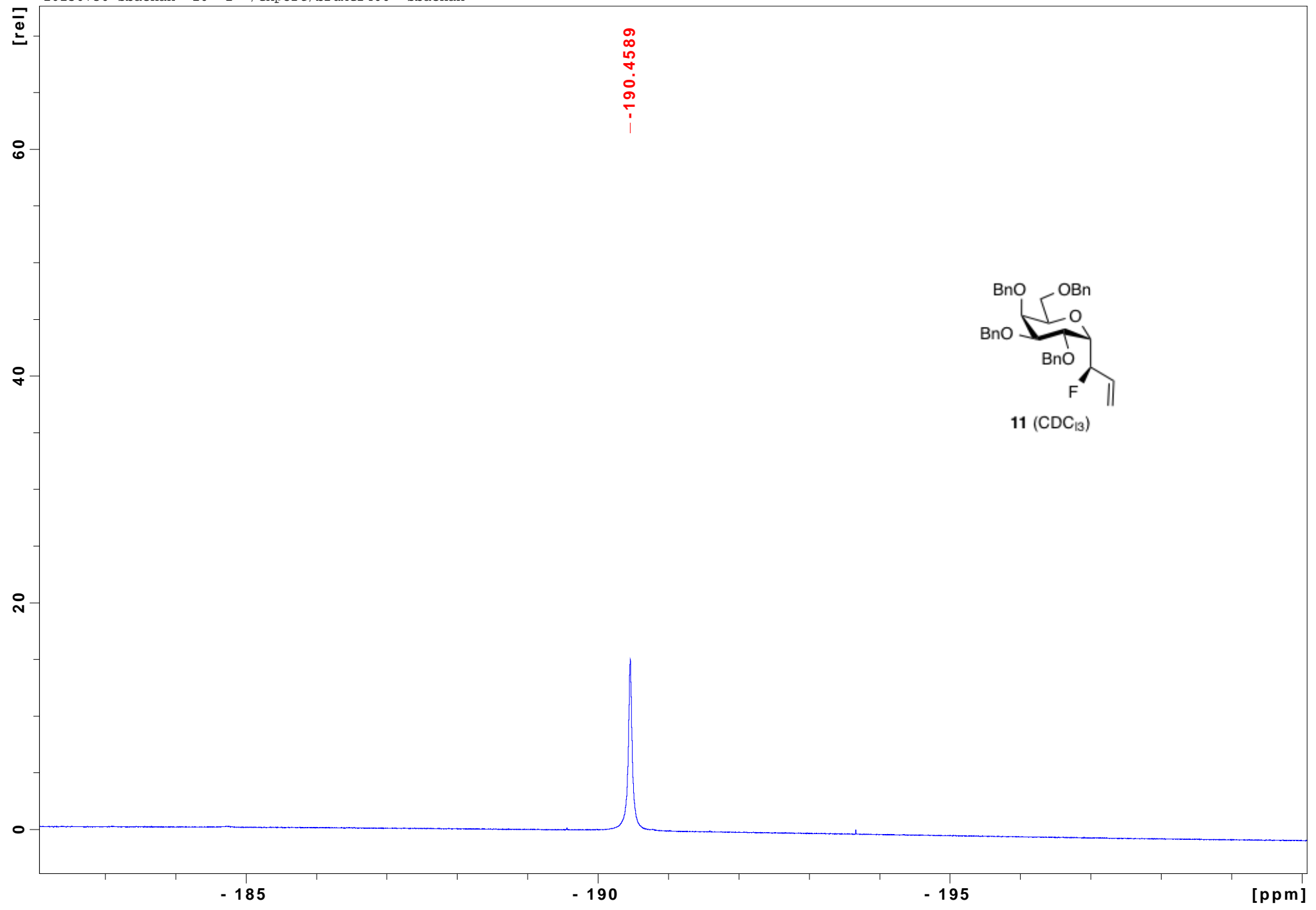
110

120

130

140

ppm

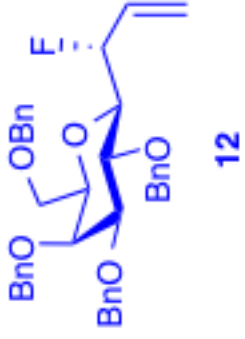


7.300
7.284
7.271
7.268
7.255
7.246
7.242
7.233
7.229
7.225
7.222
7.210
7.206
7.200
7.196
7.194
7.183
5.998
5.343
5.340
5.335
5.308
5.301
5.229
5.208
4.925
4.860
4.860
4.698
4.674
4.640
4.629
4.618
4.605
4.592
4.568
4.410
4.386
4.359
4.336
4.097
4.078
4.059
3.911
3.907
3.562
3.558
3.543
3.535
3.522
3.462
3.450

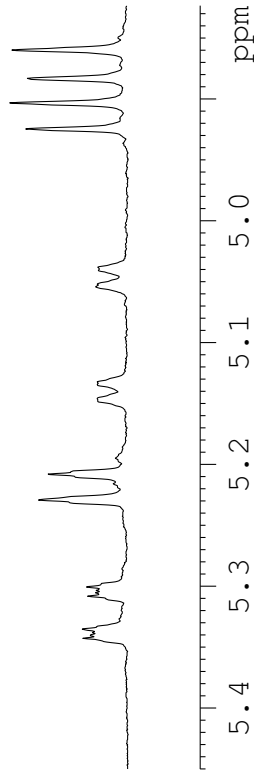
```

NAME      20141231
EXPNO     1
PROCNO    1
Date_     20141231
Time      17.43
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         18
DS         2
SWH        8012.820 Hz
FIDRES     0.244832 Hz
AQ         2.0448856 sec
RG         31.9
DE         62.400 usec
TE         298.20 K
D1         1.00000000 sec
TD0        1

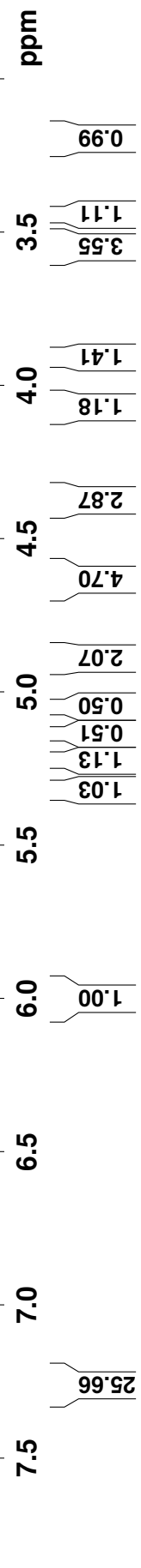
===== CHANNEL f1 =====
NUC1       1H
P1         9.50 usec
PL1        -0.50 dB
SFO1       500.1330085 MHz
SI         32768
SF         500.1300085 MHz
WDW        EM
SSB        0
LB         0.00 Hz
GB         0
PC         1
  
```



5.43
5.42
5.40
5.38
5.35
5.308
5.306
5.303
5.301
5.229
5.208
5.146
5.132
5.038
4.925
4.860
4.860
4.698
4.674
4.640
4.629
4.618
4.605
4.592
4.568
4.410
4.386
4.359
4.336
4.097
4.078
4.059
3.911
3.907
3.562
3.558
3.543
3.535
3.522
3.462
3.450



5.4 5.3 5.2 5.1 5.0 ppm



1.18 4.9
1.18 8.21
1.18 6.7
1.18 5.1
1.18 6.3
1.18 6.0
1.18 5.4
1.18 5.0
1.18 4.0
1.18 3.7
1.18 2.9
1.18 1.6
1.18 1.3
1.18 0.8
1.18 0.5
1.18 0.3
1.18 0.0
1.18 9.8
1.18 9.5
1.18 9.1
1.18 8.8
1.18 8.3
1.18 8.1
1.18 7.7
1.18 7.3
1.18 7.1
1.18 6.99
1.18 6.90

```

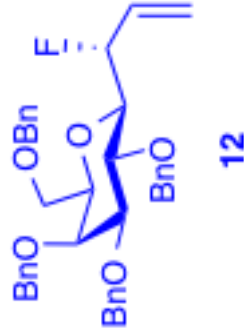
NAME          20141231
EXPNO         3
PROCNO        1
Date_         20141231
Time_         17.55
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       zgpg
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            26008
DW            16.650 usec
DE            40.00 usec
TE            298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TDO           1
    
```

```

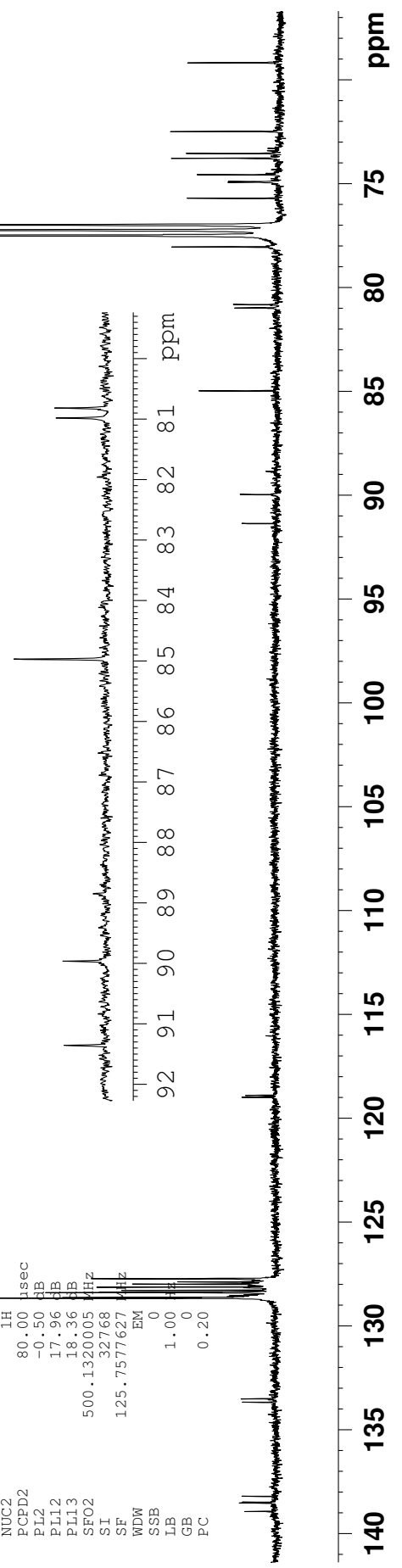
===== CHANNEL f1 =====
NUC1          13C
P1            10.50 usec
PL1           3.50 dB
SFO1          125.7703643 MHz

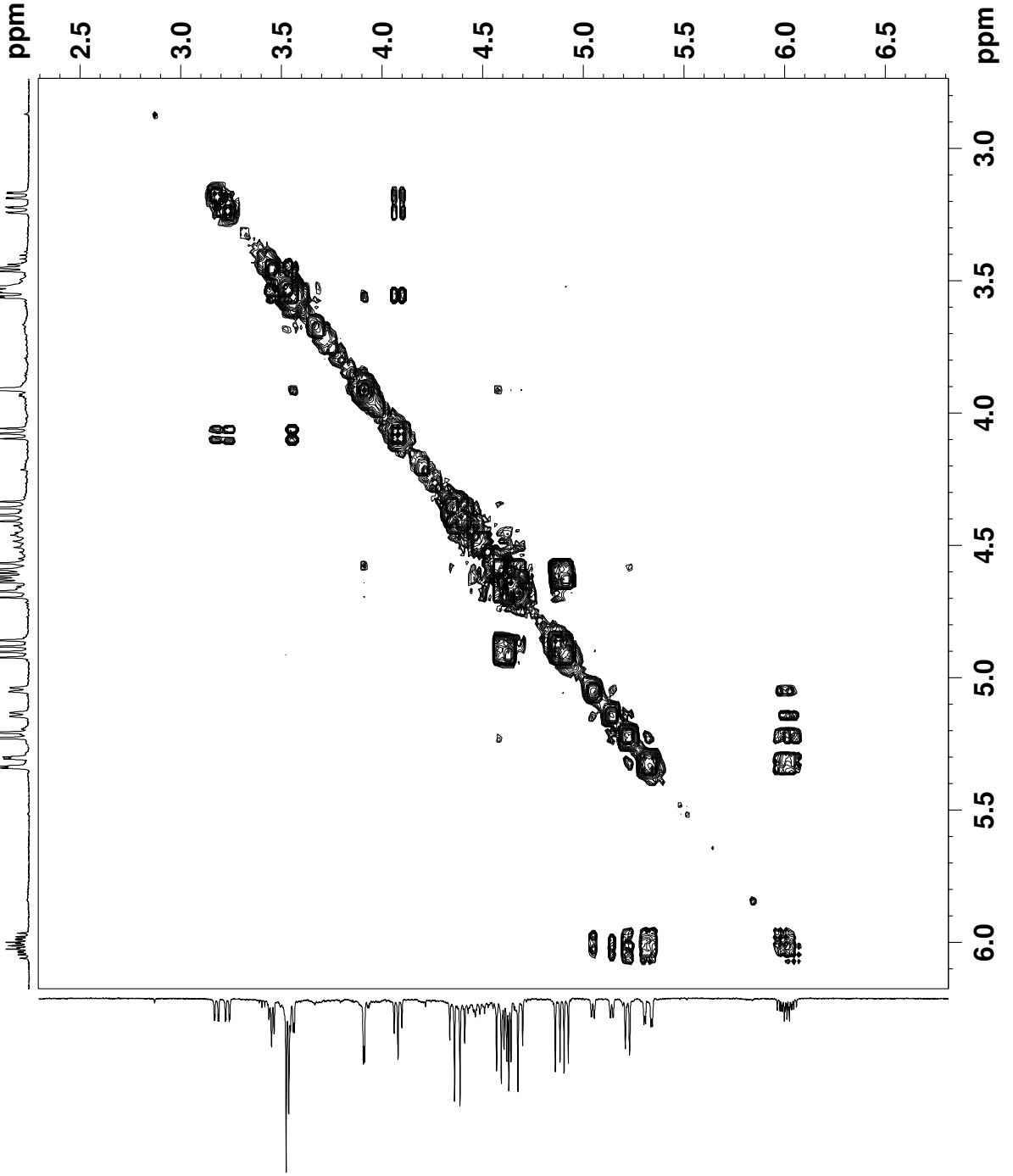
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -0.50 dB
PL12          17.96 dB
PL13          18.36 dB
SFO2          500.1320005 MHz
SI            32768
SE            125.7577627 MHz
WDM           EM
SSB           0
LB            1.00
GB            0
PC            0.20
    
```

91.36
89.96
84.97
80.98
80.82
78.04
77.37
75.69
74.92
74.89
74.56
73.77
73.54
72.48
69.17



91.357
89.964
84.967



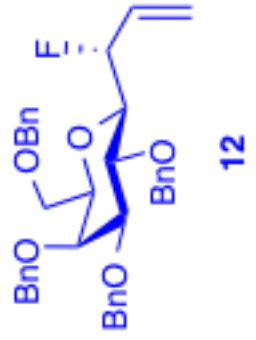


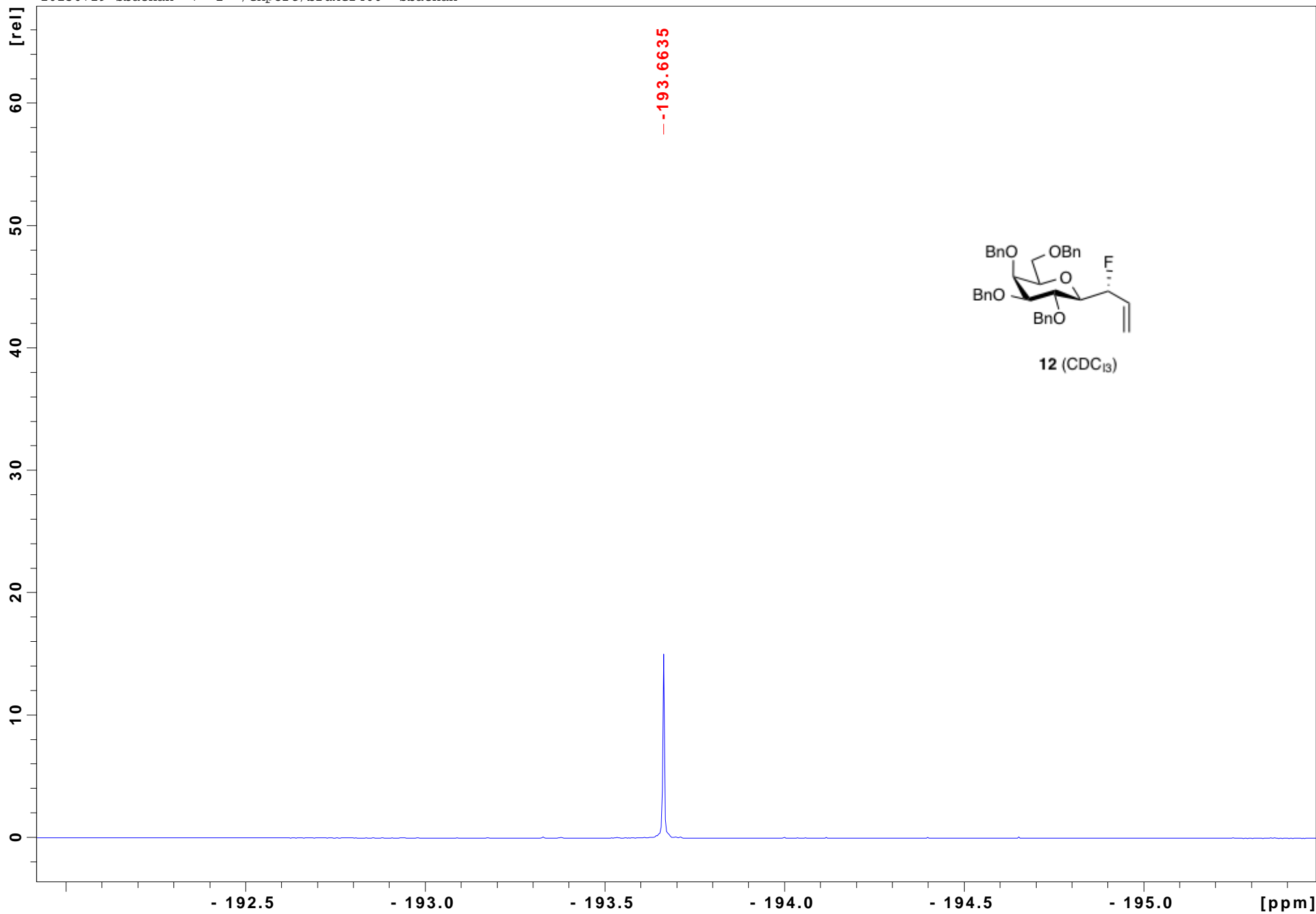
```

NAME      20141231
PROCNO    1
Date_     20141231
Time      17.44
INSTRUM   spect
PROBHD    5 mm CPDCH-13C
PULPROG   zgpg30
TD        2048
SOLVENT   CDCl3
NS        1
DS        8
AQ        6666.666 Hz
FIDRES    3.255208 Hz
RG        0.1537250 sec
DW        75.000 usec
TE        298.00 usec
DE        998.00 usec
DO        0.00000300 sec
D1        1.48689198 sec
d13       0.00000400 sec
D16       0.00020000 sec
IN0       0.00015000 sec

===== CHANNEL f1 =====
NUC1      1H
PC        9.50 usec
PL1       0.50 usec
PL2       0.50 usec
PL3       0.50 usec
SFO1      500.1330069 MHz

===== GRADIENT CHANNEL =====
GENAM1    SINE.100
PC1       0.00 usec
PL1       0.00 usec
PL2       0.00 usec
PL3       0.00 usec
PL6       1000.00 usec
NDO       1
TD        128
SFO1      500.133 MHz
SF        52.083332 MHz
SWH        13.333 Ppm
FMODE     OF
SI        1024
SF        500.1300463 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40
SI        1024
SC2       0
SFO2      500.1300463 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
    
```

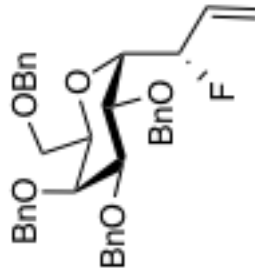




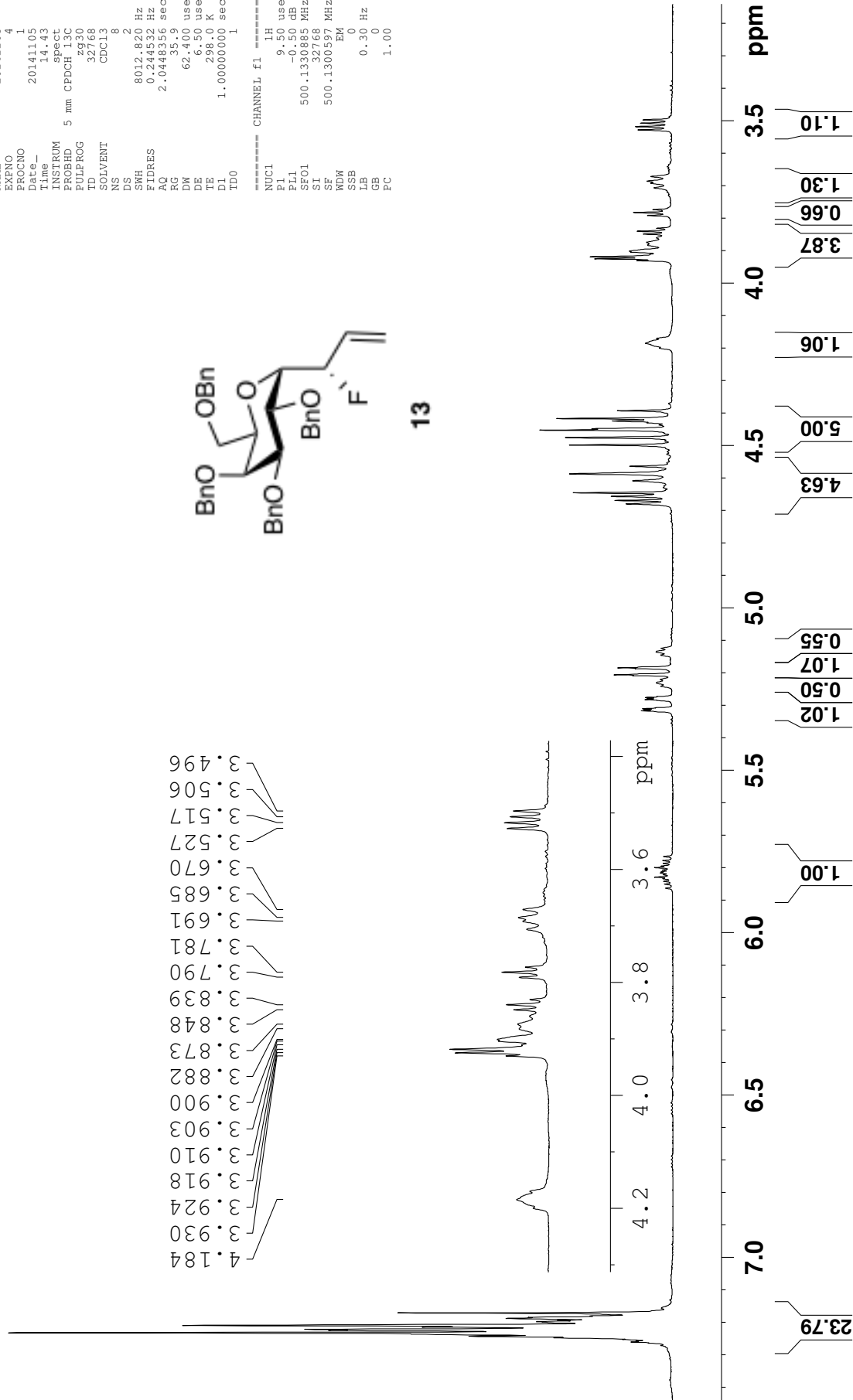
7.260
7.258
7.253
7.247
7.242
7.232
7.224
7.221
7.214
7.209
7.197
7.194
7.188
7.184
7.180
7.171
5.316
5.313
5.309
5.282
5.275
5.207
5.205
5.203
5.186
5.184
4.679
4.668
4.656
4.645
4.608
4.586
4.563
4.497
4.474
4.452
4.448
4.423
4.416
4.392
4.184
3.930
3.924
3.918
3.903
3.900
3.848
3.839
3.81
3.527
3.517
3.506
3.496

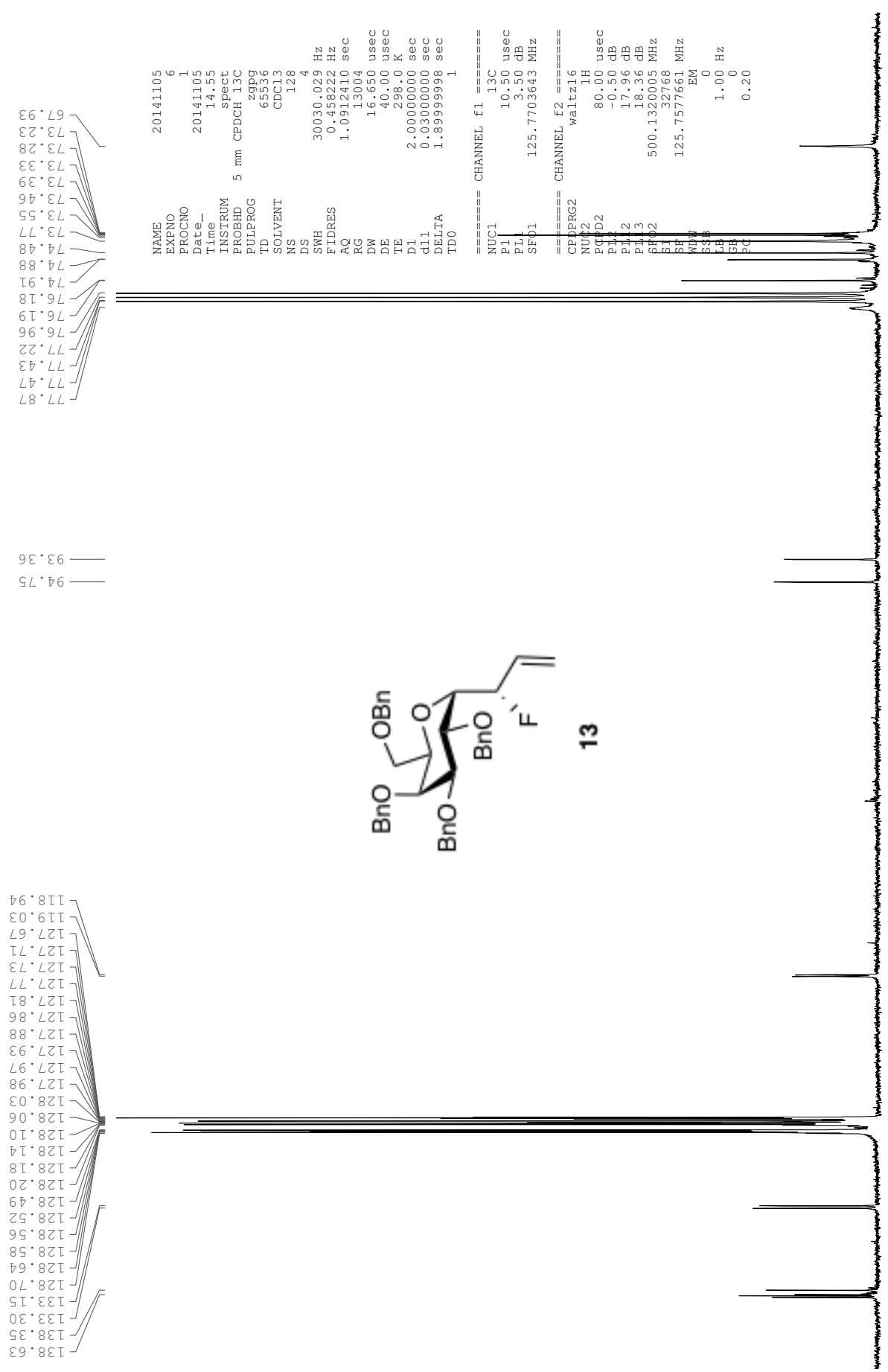
```

NAME      20141105
EXPNO     4
PROCNO    1
Date_     20141105
Time      14.43
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
RG         327.0
SOLVENT   CDCl3
NS         2
DS         2
SRH        8012.820 Hz
FIDRES    0.244532 Hz
AQ         2.0448356 sec
RG         35.9
DW         62.400 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
TD0        1
===== CHANNEL f1 =====
NUC1       1H
P1         9.50 usec
PL1        -0.50 dB
SFO1       500.1330885 MHz
SI         327.68
SE         500.1300597 MHz
WDW        EM
SSB        0
GB         0.30 Hz
PC         1.00
    
```

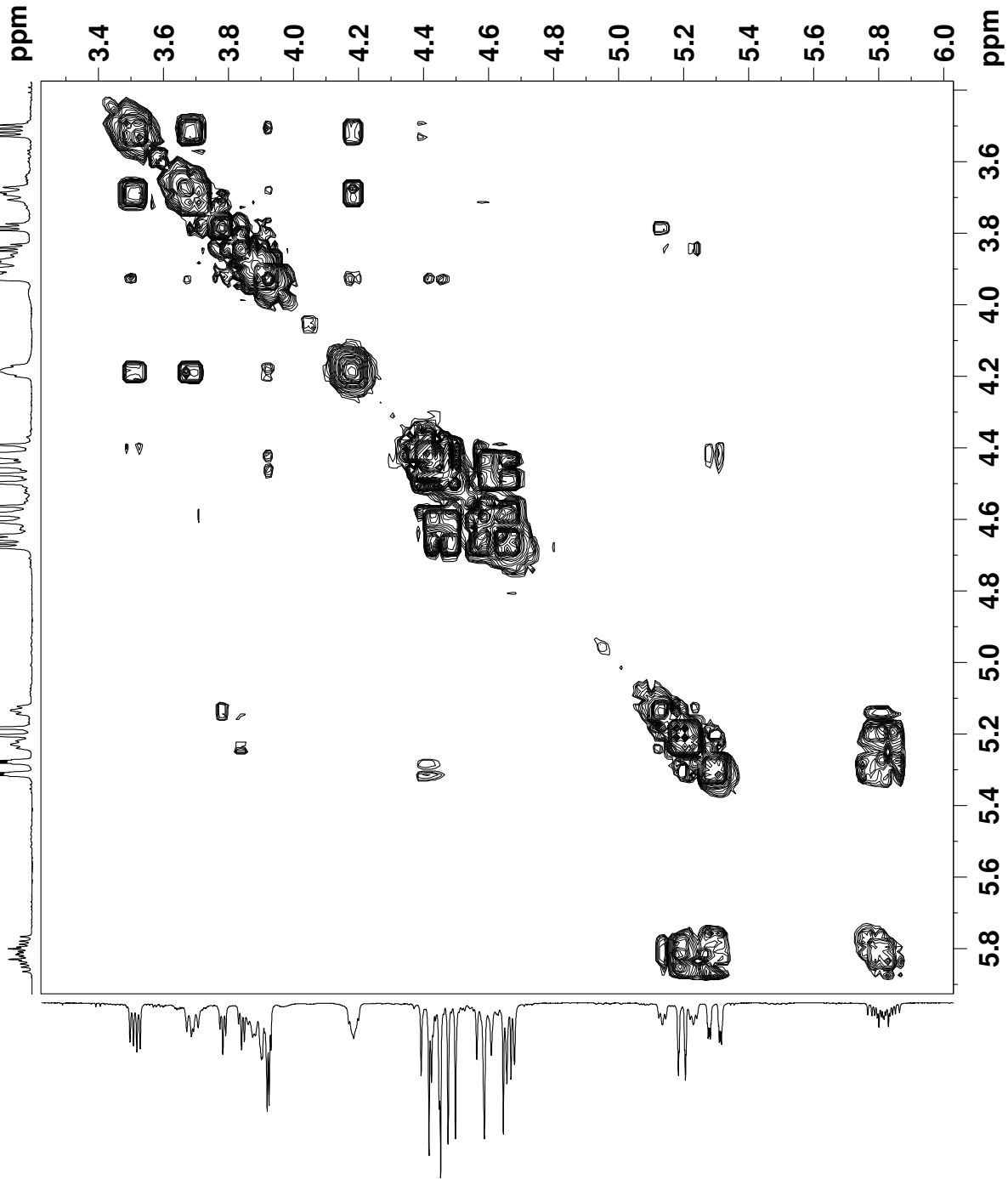


4.184
4.184
3.930
3.924
3.918
3.910
3.903
3.900
3.882
3.873
3.848
3.839
3.790
3.781
3.691
3.685
3.670
3.527
3.517
3.506
3.496



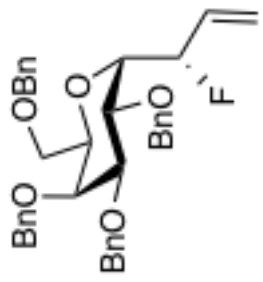


AAACRYOCOSY CDC13 /opt/topspin aaltiti 9



```

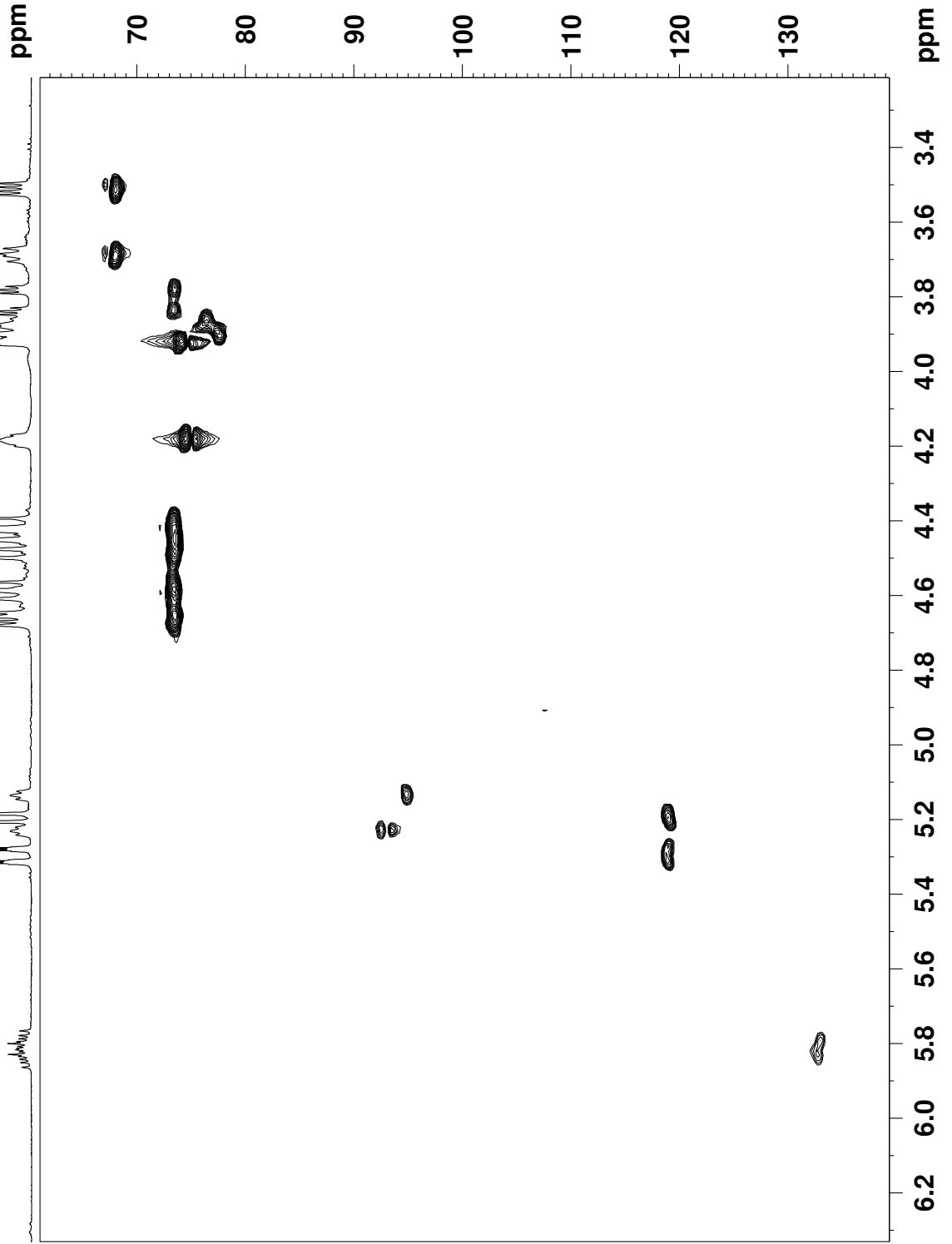
NAME          20141105
EXPNO         5
PROCNO        1
F2F1          20141101
Time          14:44
INSTRUM       spect
PROBHD        5 mm CPDCH 13C
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1
DS            4
AQ            6666.666 Hz
FIDRES        3.255208 Hz
RG            0.1537250 sec
RG            28.5
DW            75.000 usec
DE            298.0 K
TE            298.0 K
d0            0.00000300 sec
d1            1.4889198 sec
d2            0.00000000 sec
d3            0.00000000 sec
d4            0.00020000 sec
d5            0.00000000 sec
d6            0.00015000 sec
d7            0.00015000 sec
d8            0.00015000 sec
d9            0.00015000 sec
d10           0.00015000 sec
d11           0.00015000 sec
d12           0.00015000 sec
d13           0.00015000 sec
d14           0.00015000 sec
d15           0.00015000 sec
d16           0.00015000 sec
d17           0.00015000 sec
d18           0.00015000 sec
d19           0.00015000 sec
d20           0.00015000 sec
d21           0.00015000 sec
d22           0.00015000 sec
d23           0.00015000 sec
d24           0.00015000 sec
d25           0.00015000 sec
d26           0.00015000 sec
d27           0.00015000 sec
d28           0.00015000 sec
d29           0.00015000 sec
d30           0.00015000 sec
d31           0.00015000 sec
d32           0.00015000 sec
d33           0.00015000 sec
d34           0.00015000 sec
d35           0.00015000 sec
d36           0.00015000 sec
d37           0.00015000 sec
d38           0.00015000 sec
d39           0.00015000 sec
d40           0.00015000 sec
d41           0.00015000 sec
d42           0.00015000 sec
d43           0.00015000 sec
d44           0.00015000 sec
d45           0.00015000 sec
d46           0.00015000 sec
d47           0.00015000 sec
d48           0.00015000 sec
d49           0.00015000 sec
d50           0.00015000 sec
d51           0.00015000 sec
d52           0.00015000 sec
d53           0.00015000 sec
d54           0.00015000 sec
d55           0.00015000 sec
d56           0.00015000 sec
d57           0.00015000 sec
d58           0.00015000 sec
d59           0.00015000 sec
d60           0.00015000 sec
d61           0.00015000 sec
d62           0.00015000 sec
d63           0.00015000 sec
d64           0.00015000 sec
d65           0.00015000 sec
d66           0.00015000 sec
d67           0.00015000 sec
d68           0.00015000 sec
d69           0.00015000 sec
d70           0.00015000 sec
d71           0.00015000 sec
d72           0.00015000 sec
d73           0.00015000 sec
d74           0.00015000 sec
d75           0.00015000 sec
d76           0.00015000 sec
d77           0.00015000 sec
d78           0.00015000 sec
d79           0.00015000 sec
d80           0.00015000 sec
d81           0.00015000 sec
d82           0.00015000 sec
d83           0.00015000 sec
d84           0.00015000 sec
d85           0.00015000 sec
d86           0.00015000 sec
d87           0.00015000 sec
d88           0.00015000 sec
d89           0.00015000 sec
d90           0.00015000 sec
d91           0.00015000 sec
d92           0.00015000 sec
d93           0.00015000 sec
d94           0.00015000 sec
d95           0.00015000 sec
d96           0.00015000 sec
d97           0.00015000 sec
d98           0.00015000 sec
d99           0.00015000 sec
d100          0.00015000 sec
  
```



13

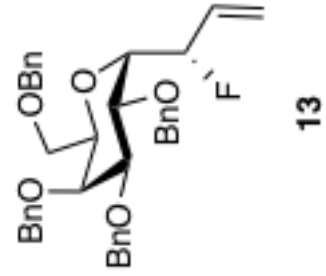


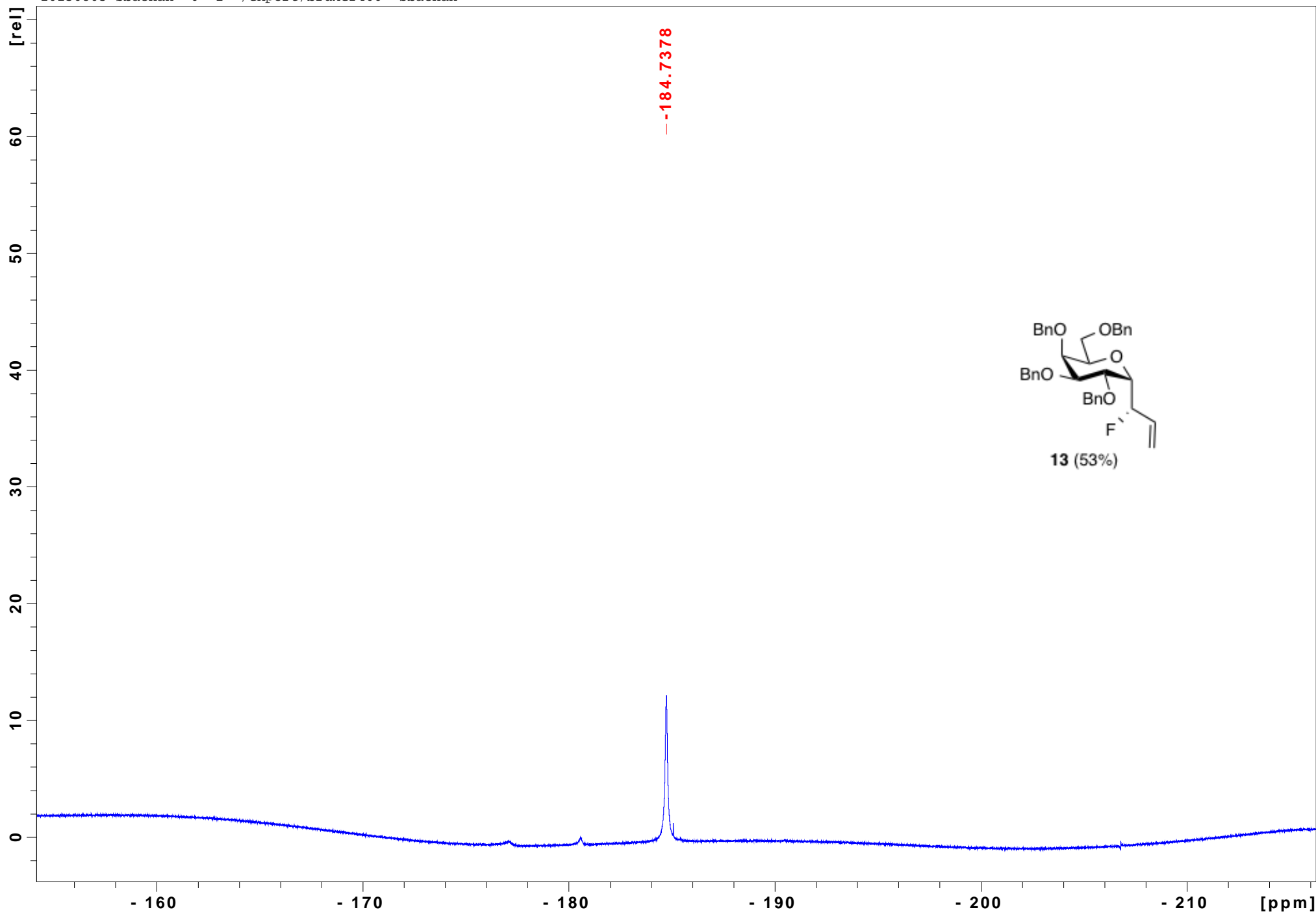
AAACRYOHSQC CDC13 /opt/topspin aaltiti 9

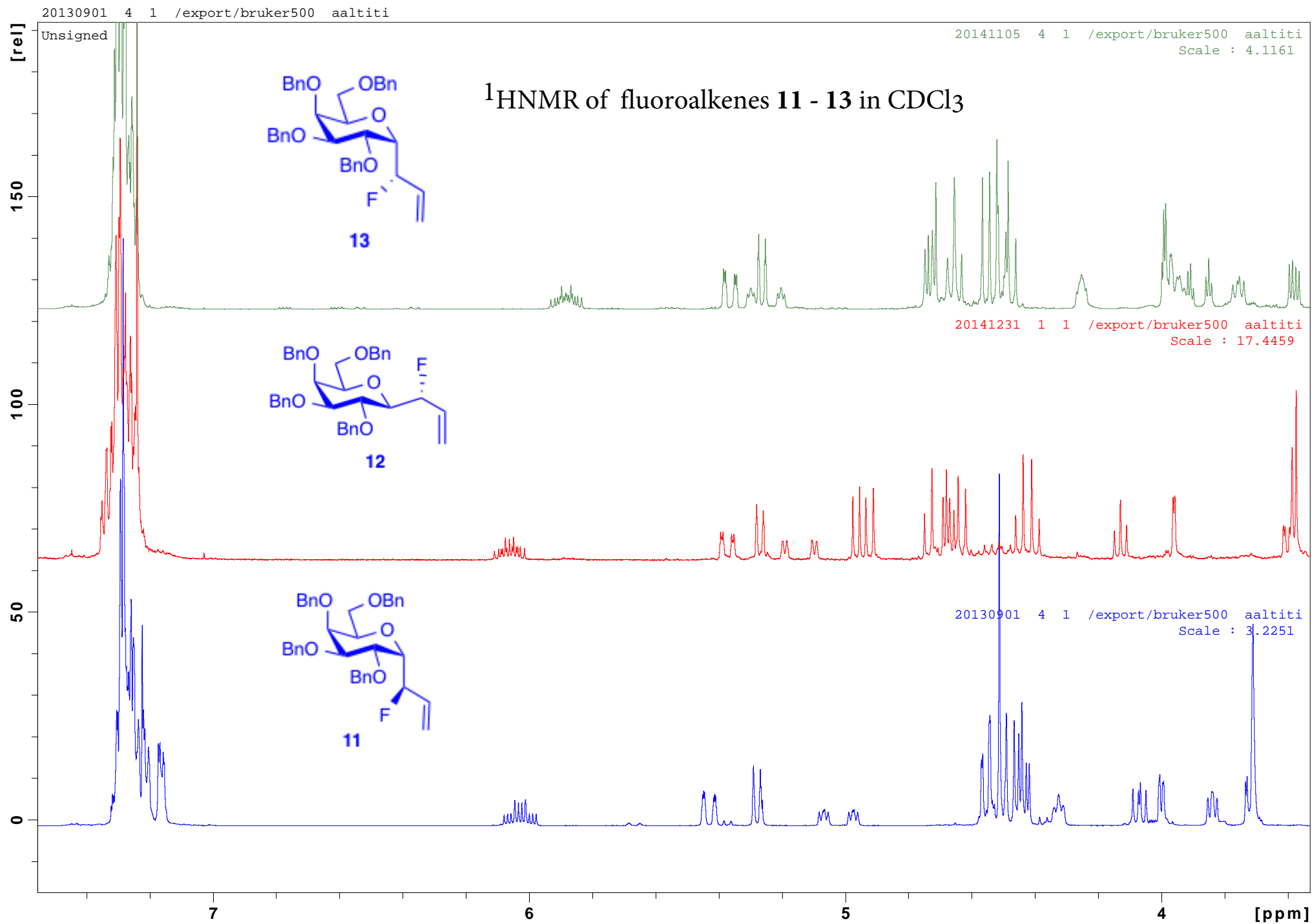


```

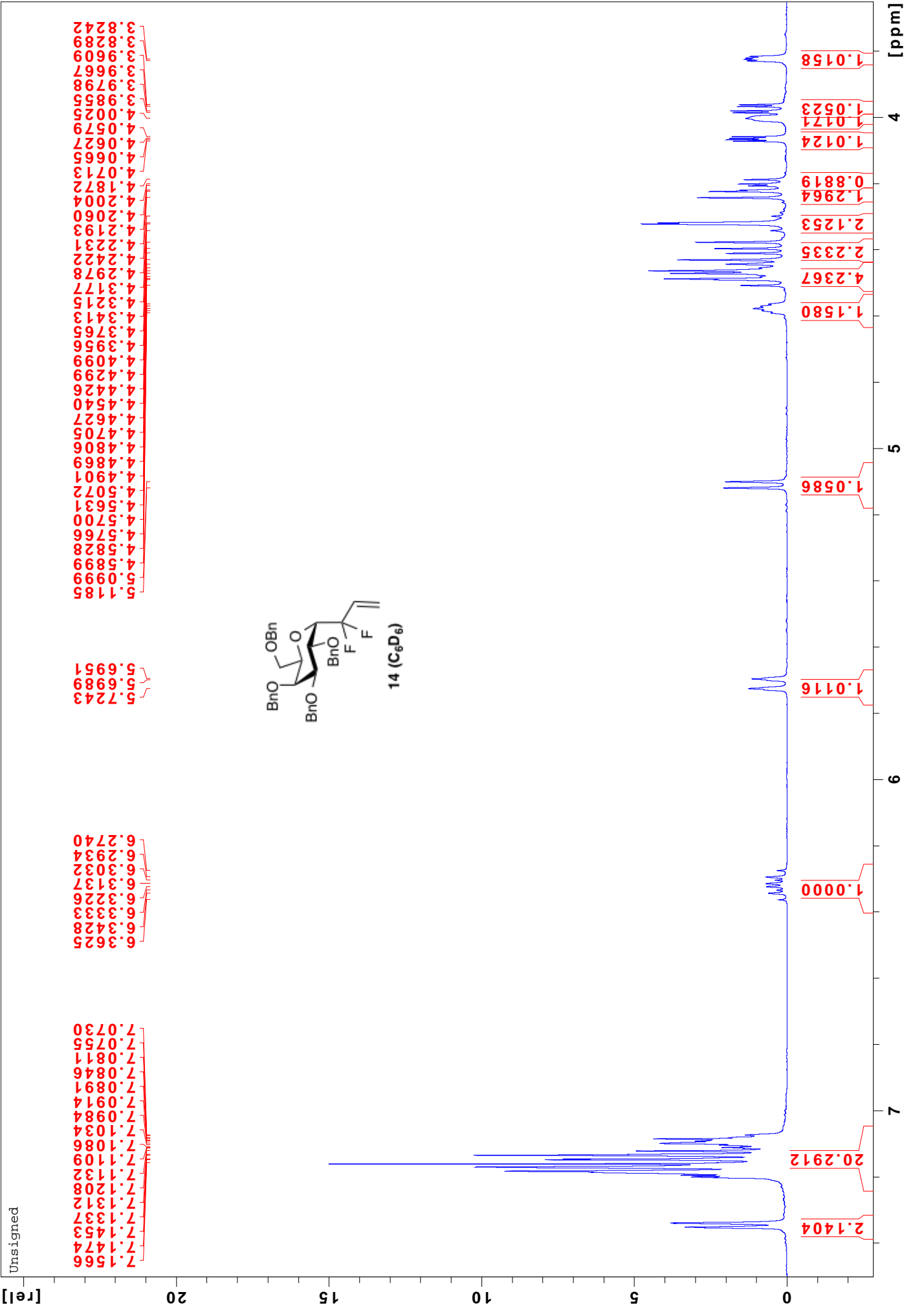
NAME 20141105
EXPER 7
Date_ 20141105
Time 14.156
INSTRUM spect
PROBHD 5 mm CTPCH 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
DS 4
AQ 6.666667 Hz
RG 655.360000
AQRES 0.07692250 sec
RG 655.360000
DM 75.000 UHRG
DE -6.00 UHRG
CHST2 145.0000000 K
NUC1 13C
P2 9.1H UHRG
P3 19.00 UHRG
P4 19.00 UHRG
P7 19.00 UHRG
SFO1 500.1330069 MHz
===== CHANNEL f2 =====
CPDPRG2 gfpf
P3 10.50 UHRG
P4 21.00 UHRG
P7 21.00 UHRG
P8 21.00 UHRG
P9 3.50 dB
P12 3.50 dB
P13 3.50 dB
SFO2 125.7678496 MHz
===== GRADIENT CHANNEL =====
GPMAM1 SINE:100
GPMAM2 SINE:100
GPR22 20.10 %
GPR23 1000.00 %
ND0 1000.00 %
TD 65536
FIDRES 207.649826 Hz
SW 199.778 ppm
  
```



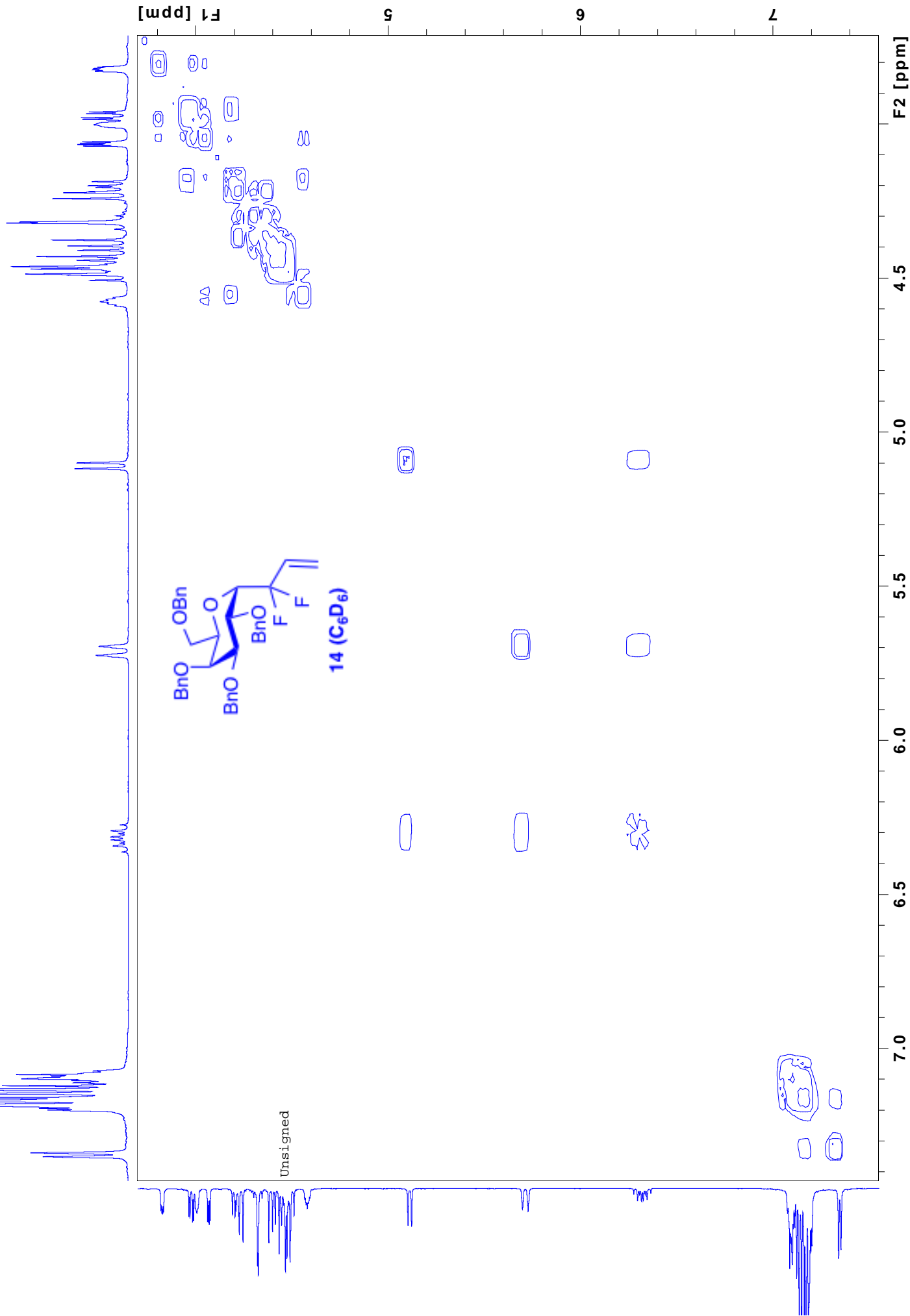




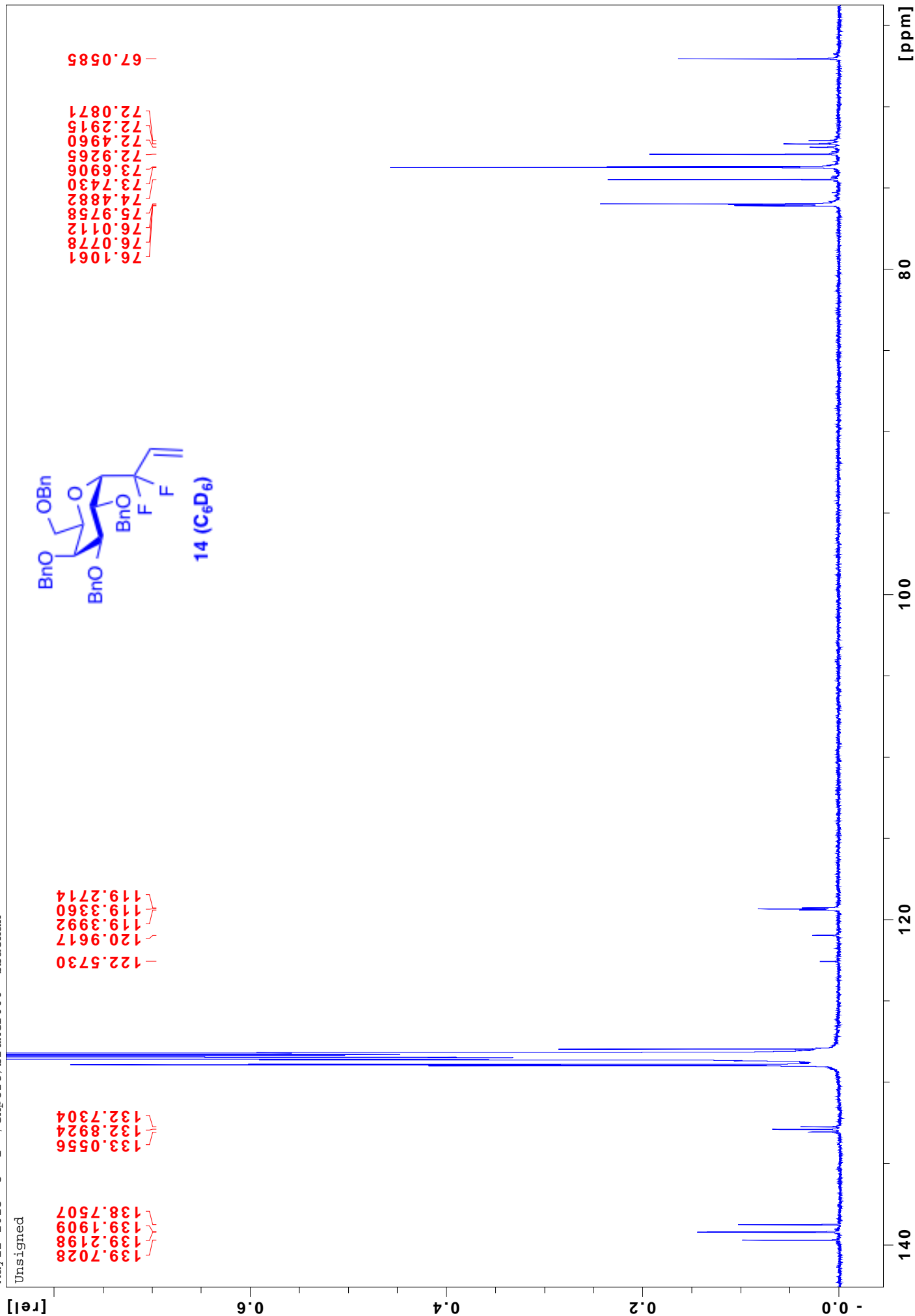
May12-2015 1 1 /export/bruker600 sbachan



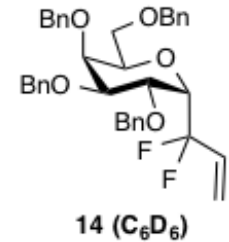
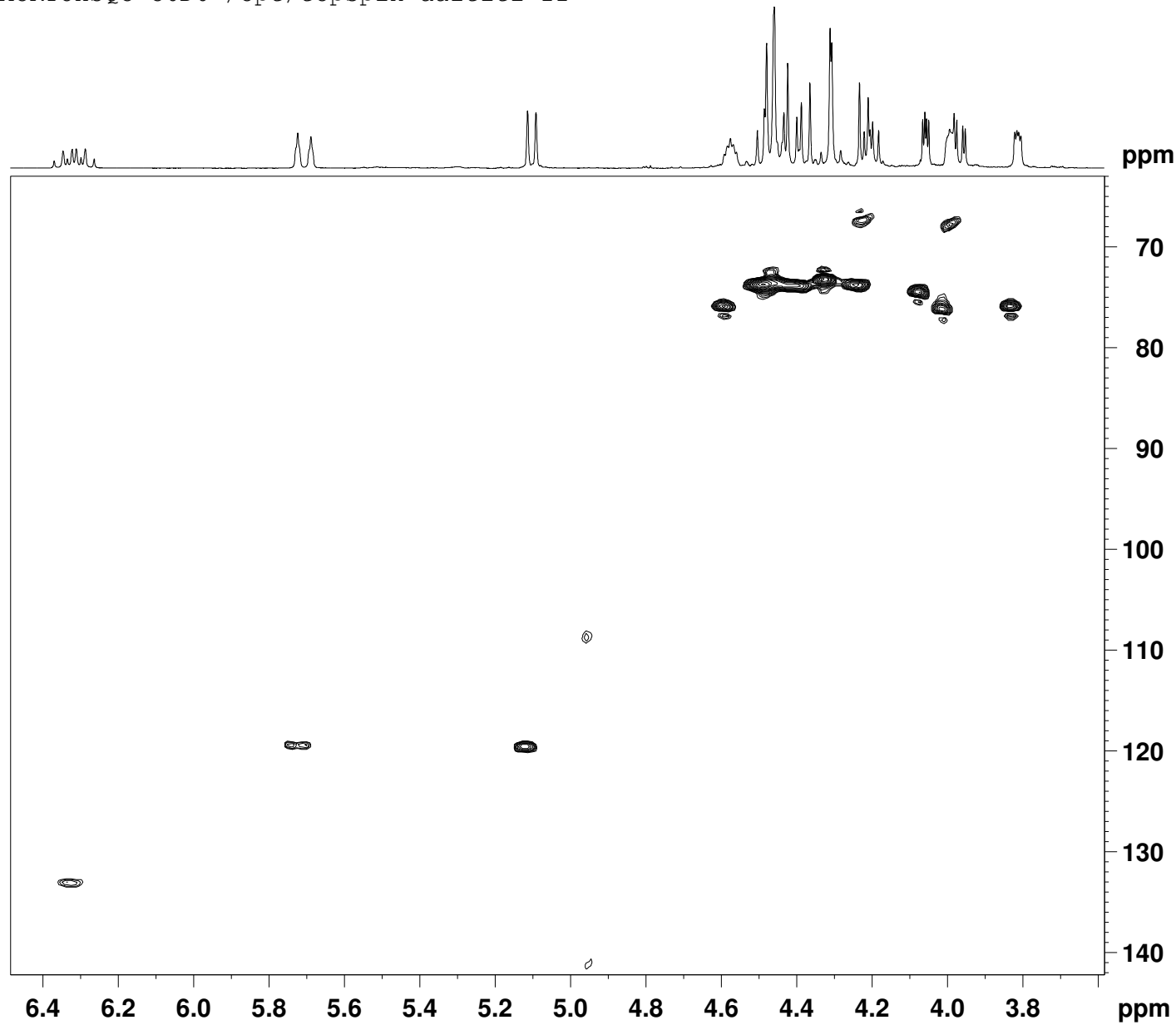
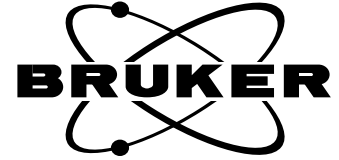
May12-2015 6 1 /export/bruker600 sbachan

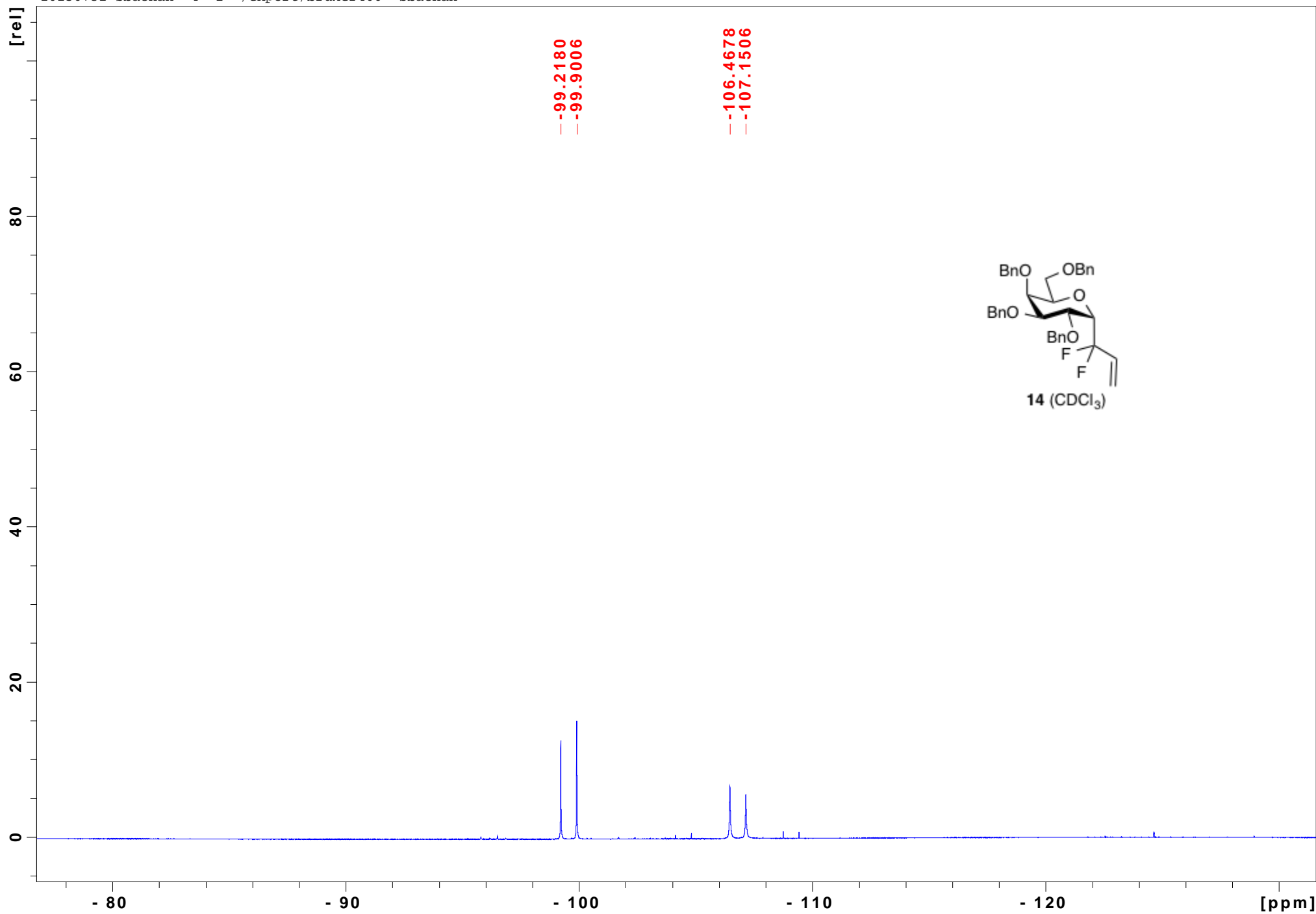


May12-2015 5 1 /export/bruker600 sbachan

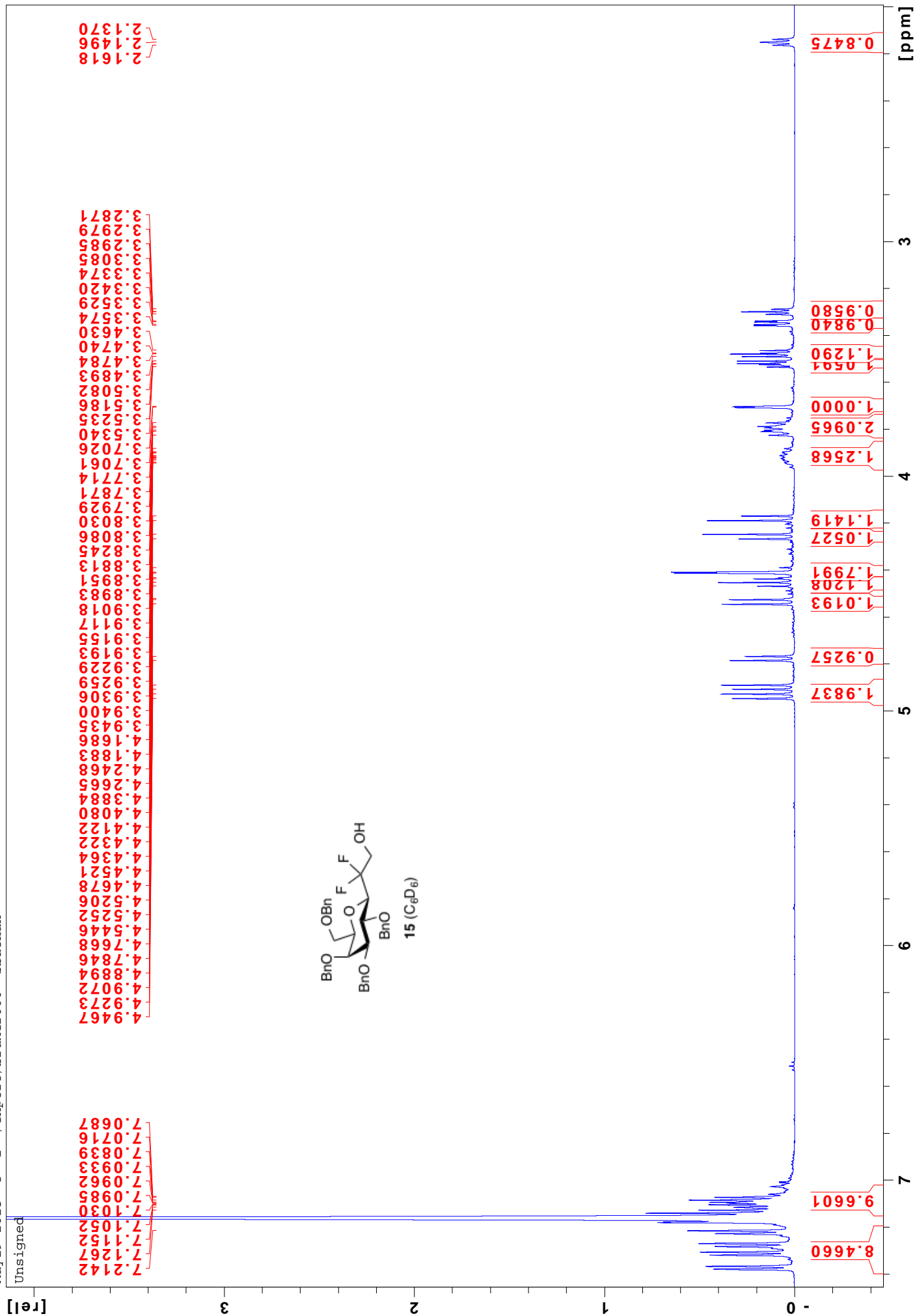


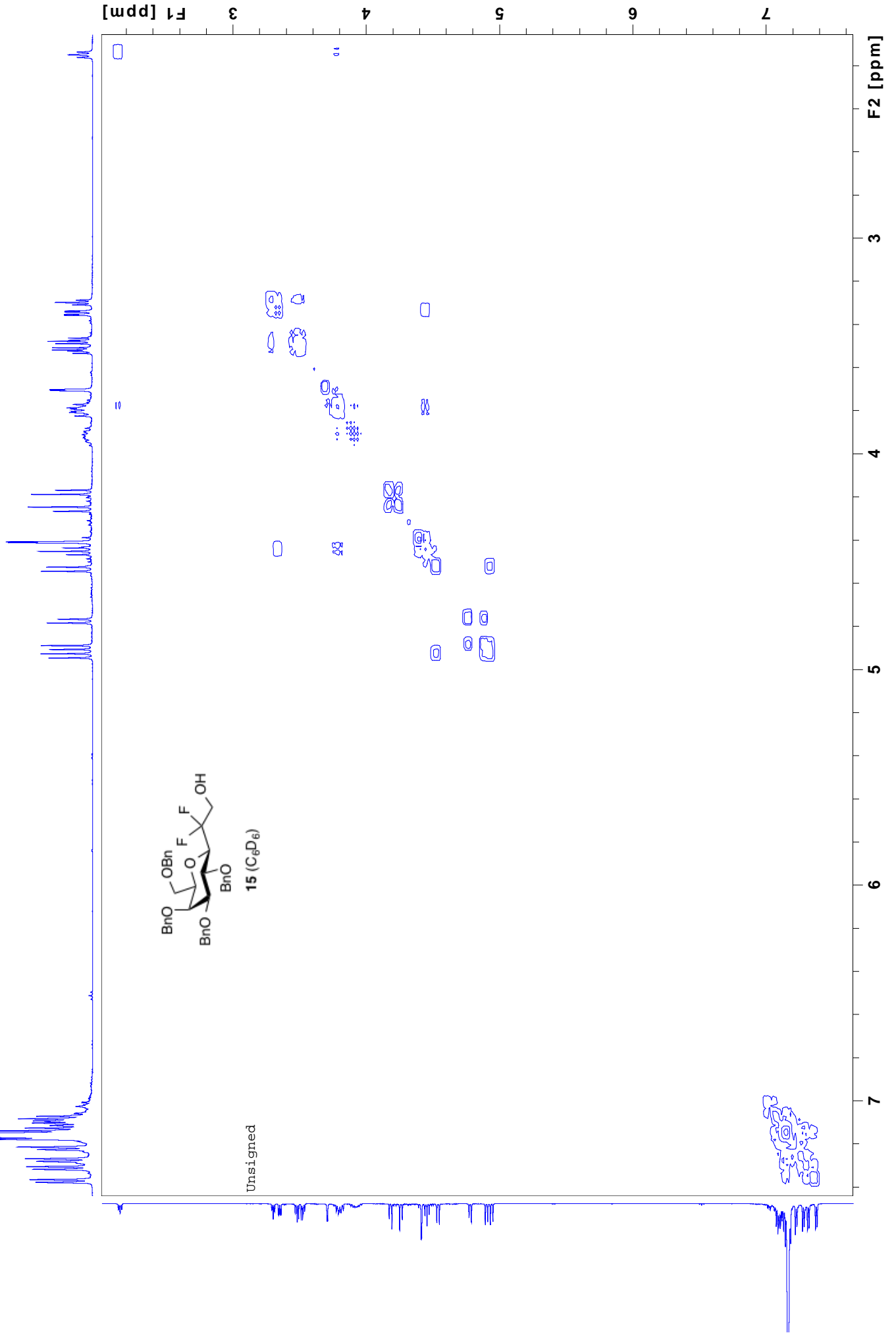
AAACRYOHSQC C6D6 /opt/topspin aaltiti 11



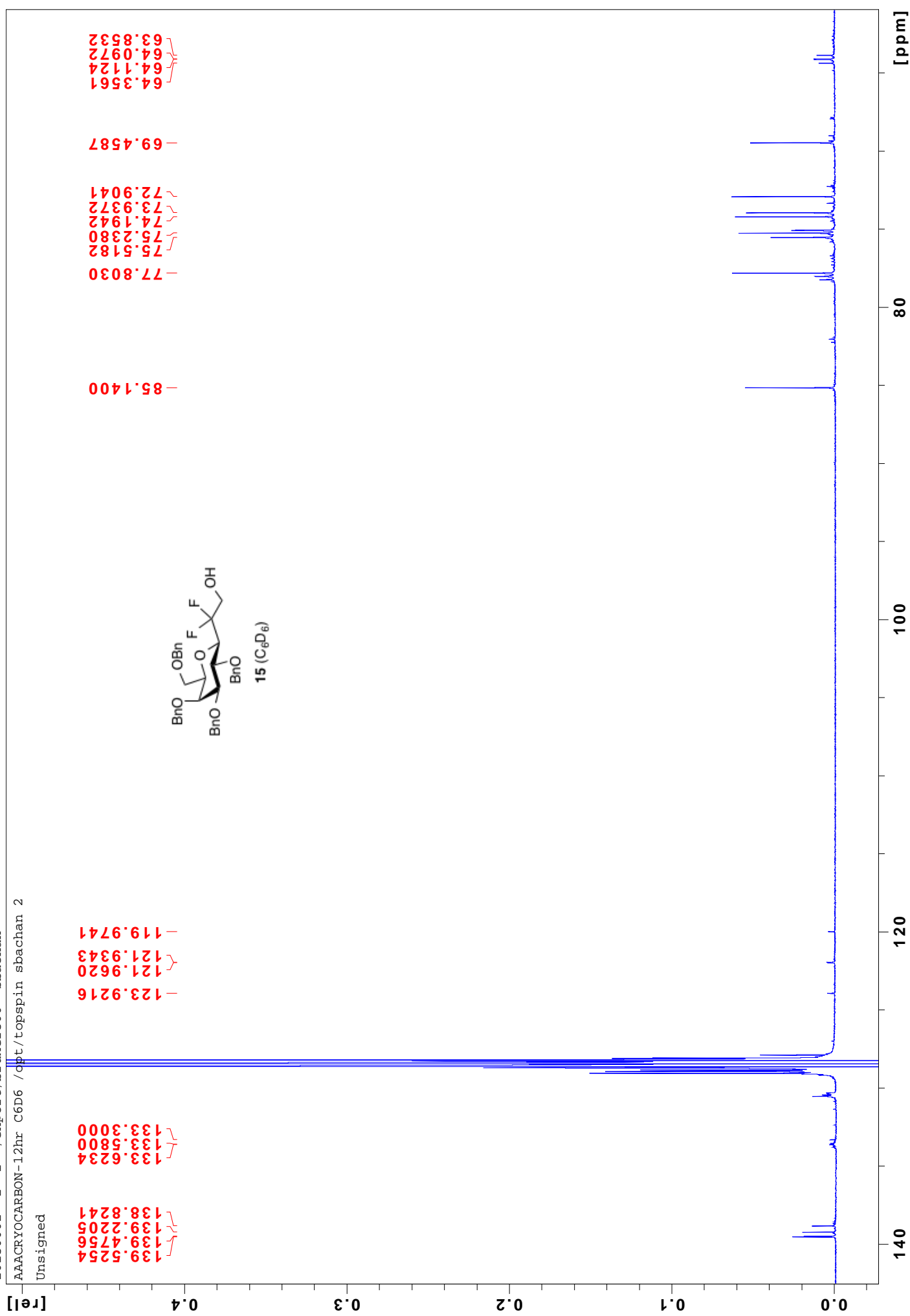


May29-2015 3 1 /export/bruker600 sbachan

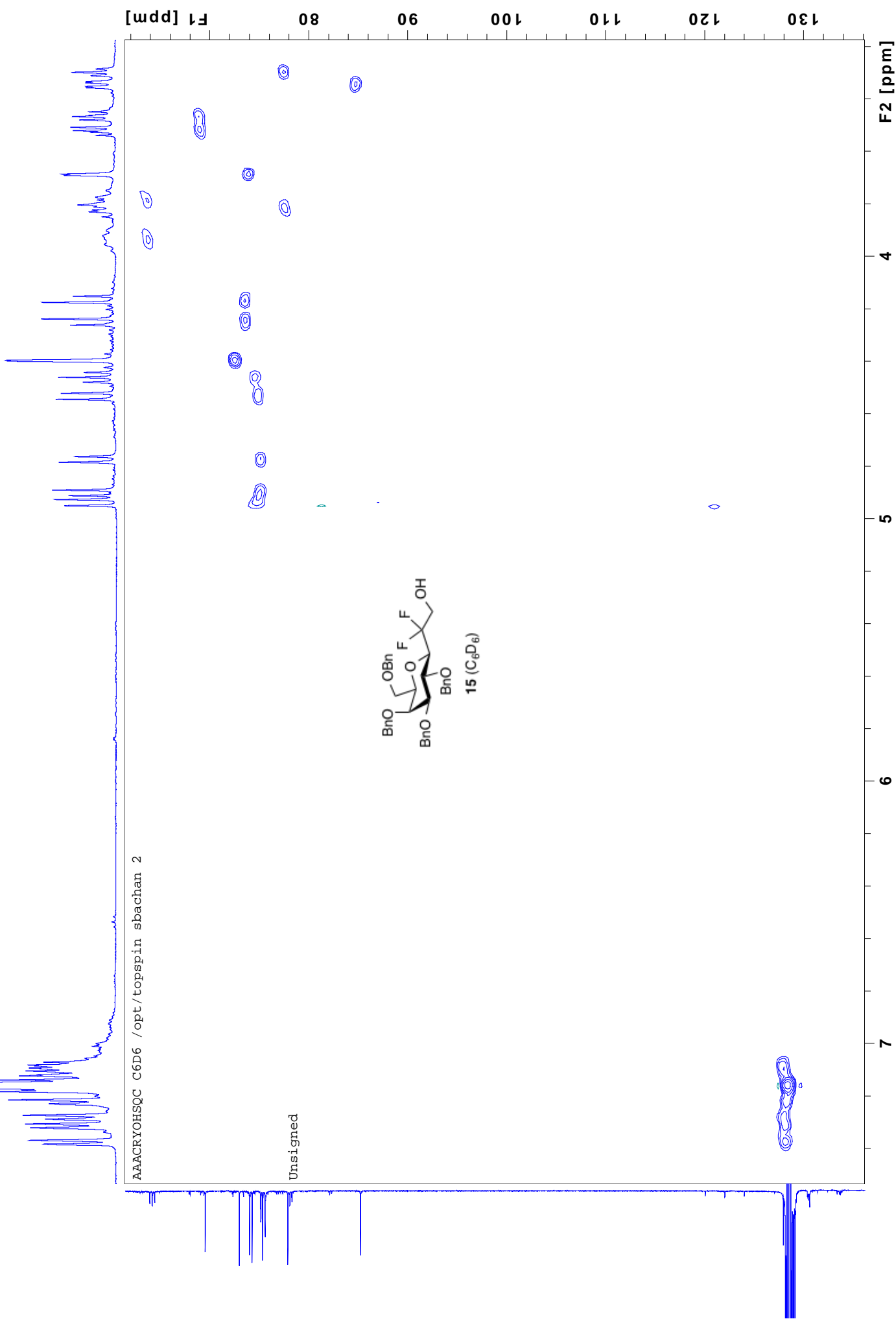




20150602 2 1 /export/bruker500 sbachan
AAACRYCARBON-12hr C6D6 /opt/topsp.in sbachan 2



Unsigned



AACRYOHSQC C6D6 /opt/topspin sbachan 2



