

SUPPORTING INFORMATION

Chemical synthesis of the hexasaccharide related to the repeating unit of the capsular polysaccharide from carbapenem resistant *Klebsiella pneumoniae* 2796 and 3264

Vikramjit Sarkar and Balaram Mukhopadhyay

BM-VS-a76 in CDCl3

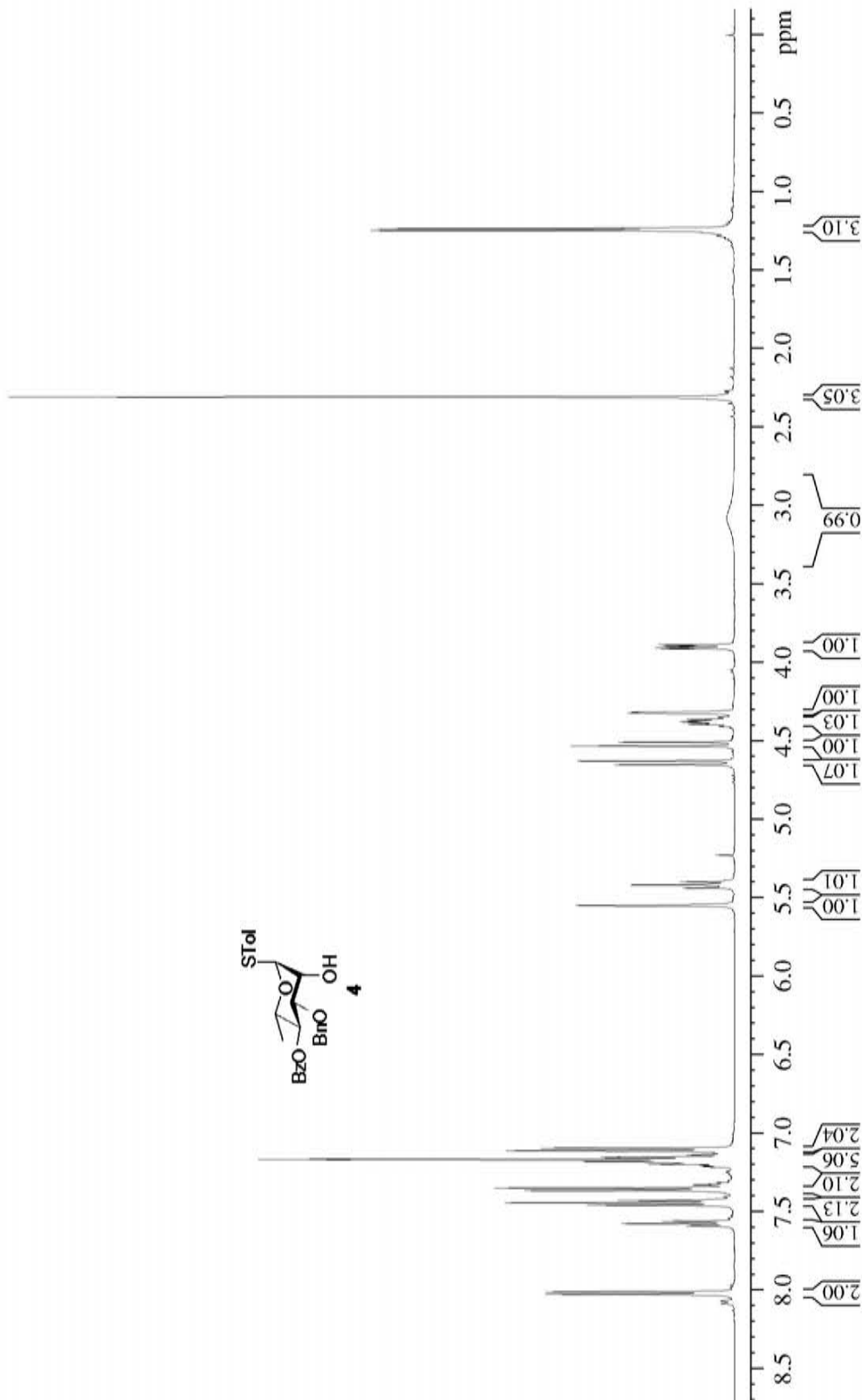


Current Data Parameters
NAME BM-VS-a76
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140415
Time 10:49
INSTRUM spect
PROBHD 5 mm PABBO B8
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14
DS 2
SWH 10930.570 Hz
FIDRES 0.157632 Hz
AQ 3.171943 sec
RG 221.6
CW 487.400 usec
DE 6.50 usec
TE 296.8 K
DI 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PL1 1.30 dB
PL1H 15.30635643 W
SFO1 500.2030889 MHz
F2 - Processing parameters
SI 32768
SF 500.2000384 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.027
8.013
8.010
7.591
7.576
7.562
7.459
7.444
7.428
7.366
7.350
7.329
7.215
7.210
7.205
7.197
7.191
7.183
7.181
7.170
7.166
7.159
7.155
7.152
7.138
7.112
7.096
5.548
5.437
5.418
5.399
4.651
4.627
4.532
4.508
4.394
4.387
4.381
4.375
4.369
4.362
4.322
4.317
3.912
3.906
3.893
3.887
2.306
1.246
1.233



BM-VS-a76 in CDC13

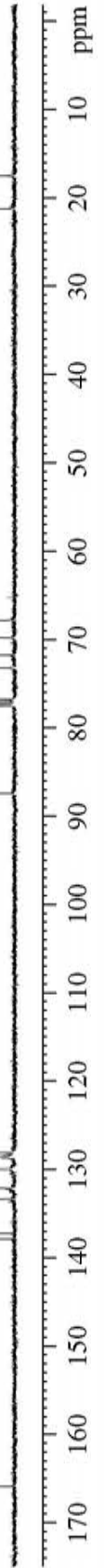
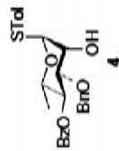


165.87
137.85
137.24
133.34
132.13
130.02
129.93
128.56
128.54
128.09
128.08

87.43
77.51
77.25
77.00
76.76
73.21
71.72
69.78
67.79

21.22
17.47

Current Data Parameters
 NAME BM-VS-a76
 EXPNO 21
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140415
 Time 10.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 ID 65336
 SOLVENT CDC13
 NS 59
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.456131 Hz
 AQ 1.1010048 sec
 RG 203
 DW 16.890 usec
 DE 29.58 usec
 TE 297.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 CHANNEL f1
 NUC1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 PL1W 90.1882531 W
 SF01 125.7879676 MHz
 CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 NUC2 80.00 usec
 PCPD2 1.30 dB
 PL2 16.00 dB
 PL12 20.00 dB
 PL13 15.30635643 W
 PL1W 0.51864596 W
 PL12W 0.20687706 W
 PL13W 500.2020008 MHz
 SF02
 F2 - Processing parameters
 SI 32768
 SF 125.7753660 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



BM-VS-a77 in CDCl3



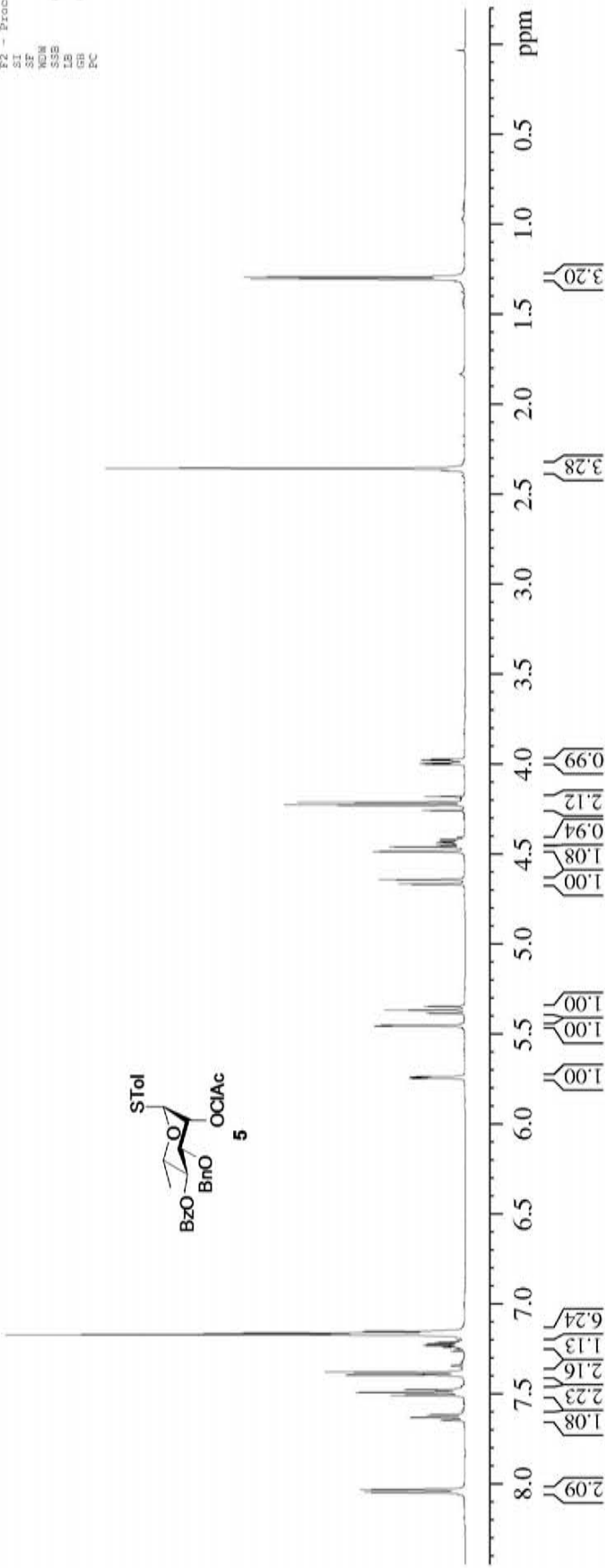
7.479
7.476
7.393
7.390
7.377
7.229
7.221
7.212
7.170
7.161
7.151
5.744
5.741
5.738
5.735
5.453
5.450
5.383
5.364
5.344
4.664
4.639
4.483
4.458
4.448
4.436
4.429
4.416
4.255
4.224
4.209
4.178
3.997
3.991
3.978
3.971
2.353
1.300
1.288

Current Data Parameters
Name BM-VS-a77
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 2010015
Time 10.25
INSTRUM spect
PROBHD 5 mm PABBO
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.878 Hz
FIDRES 0.157632 Hz
AQ 3.177842 sec
RG 322
DW 48.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
PU 14.25 usec
PL1 1.30 dB
PL1M 15.30635643 W
SFO1 500.2030889 MHz

F2 - Processing parameters
SI 32768
SF 500.2030889 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BM-VS-a77 in CDC13



166.73
165.51

138.31
136.87
133.21
132.41
129.96
129.78
129.52
129.17
128.33
128.28
128.03
127.81

86.10
77.25
77.00
76.75
74.20
72.66
71.81
71.31
67.92

40.81

21.04

17.30

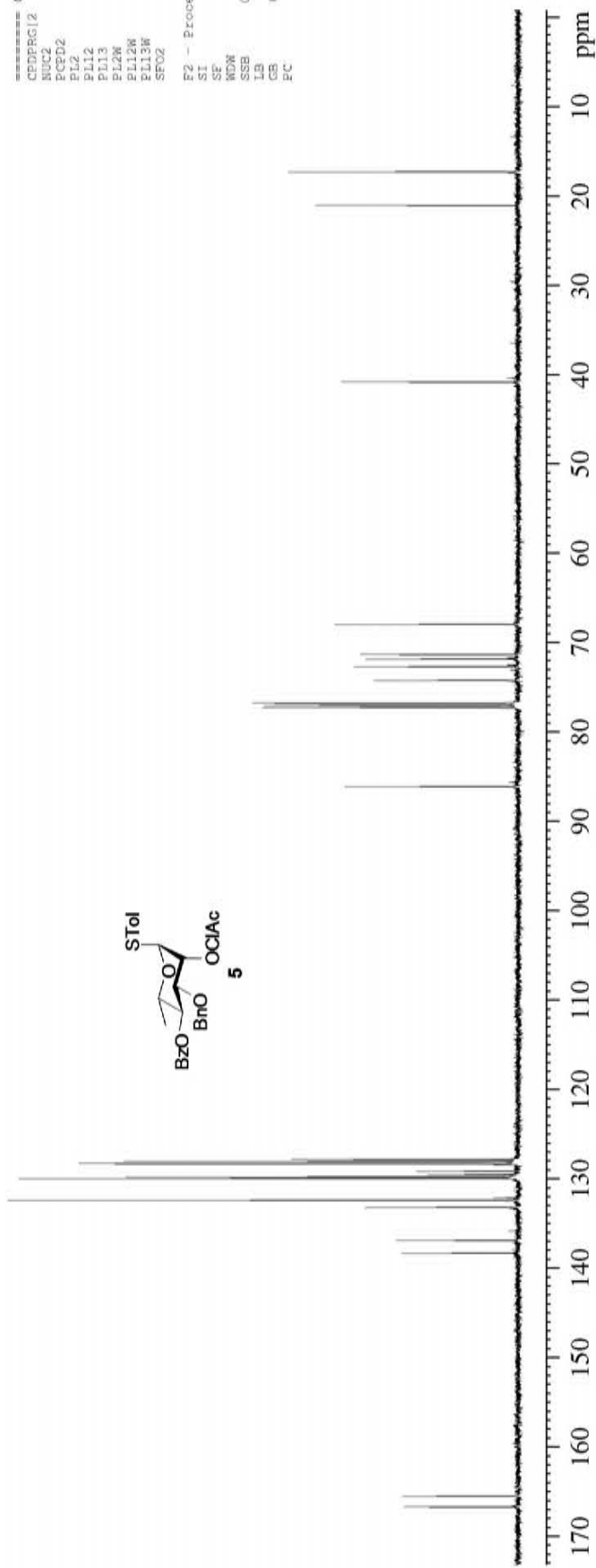
Current Data Parameters
 NAME BM-VS-a77
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140415
 Time 10.27
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 67
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 297.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 PL1W 90.18825331 W
 SFO1 125.7819676 MHz

===== CHANNEL f2 =====
 CPDPRG12 waitz16
 NUC2 1H
 P2 80.00 usec
 PL2 1.50 dB
 PL2W 16.00 dB
 PL13 16.00 dB
 PL14 15.30623643 W
 PL15W 0.31816166 W
 PL16W 0.20647706 W
 SFO2 500.2020008 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7754105 MHz
 SSB 0 EM
 LB 0
 GB 0
 EC 1.40



BM-VS-s14 in CDCl3

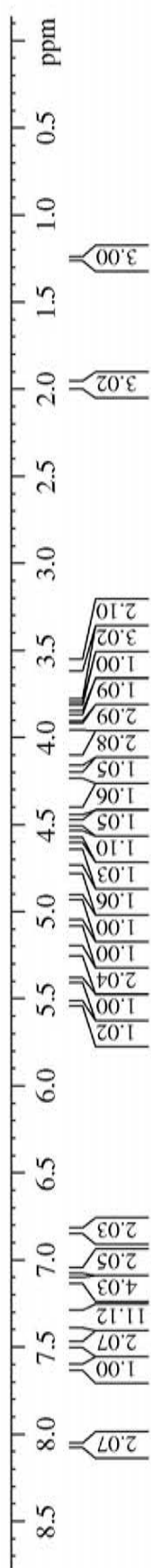
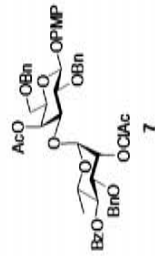


Current Data Parameters
NAME BM-VS-s14
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140611
Time 15:21
INSTRUM spect
PROBHD 5 mm PABBO BB-CP
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719423 sec
RG 45.2
DM 48.400 usec
DE 300.0 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.23 usec
PL1 1.30 dB
FLLW 15.30635643 W
SFO1 500.2030889 MHz

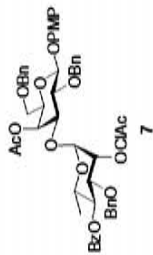
F2 - Processing parameters
SI 32768
SF 500.2000146 MHz
RG 4096
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





BM-VS-s14 in CDC13
HSQC

169.93
166.65
165.63
155.45
151.17
137.64
137.58
137.37
133.13
129.91
129.77
128.52
128.50
128.38
128.36
128.20
128.01
127.79
127.74
127.60
118.24
114.61
102.91
98.53
79.09
77.25
77.00
76.74
75.16
74.72
73.67
73.51
72.76
72.58
71.12
69.91
69.19
68.20
67.31
55.60
40.86
20.60
17.59



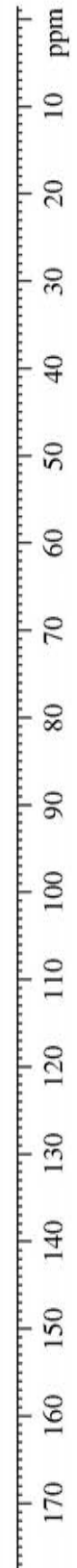
Current Data Parameters
NAME BM-VS-s14
EXPNO 53
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140811
Time 15:31
INSTRUM spect
PROBHD 5 mm PABBO-BS-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 682
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DM 16.800 usec
DE 6.50 usec
TE 302.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

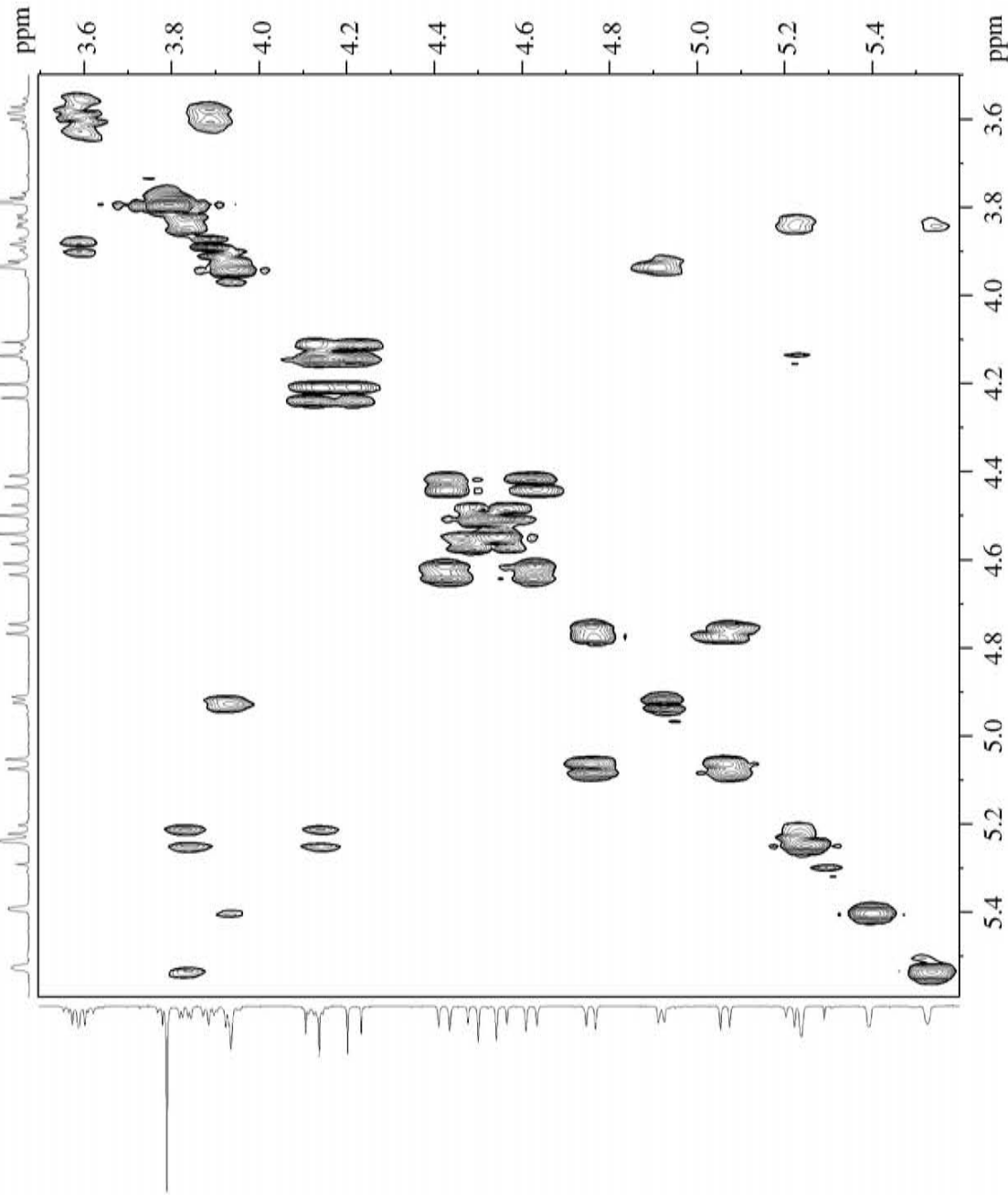
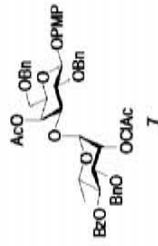
CHANNEL f1
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
PL1W 90.18825331 MHz
SFO1 125.7879876 MHz

CHANNEL f2
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.00 dB
PL13 20.00 dB
PL14 20.00 dB
PL15 15.30635643 W
PL12W 0.51864696 W
PL13W 0.20647706 W
SFO2 500.2020008 MHz

F2 - Processing parameters
SI 32768
SF 125.7753987 MHz
AQ 1.1010048 sec
RG 203
DM 16.800 usec
DE 6.50 usec
TE 302.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1



BM-VS-s14 in CDCl3



Current Data Parameters
NAME BM-VS-s14
EXNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140811
Time 13.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosyypqi
ID 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048000 sec
RG 45.2
DW 100.000 usec
DE 6.50 usec
TE 300.2 K
D0 0.00000300 sec
D1 1.4868198 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00019990 sec

CHANNEL f1
NUC1 1H
P0 14.25 usec
P1 14.25 usec
PL1 1.30 dB
PL1W 15.30635643 W
SFO1 500.2025010 MHz

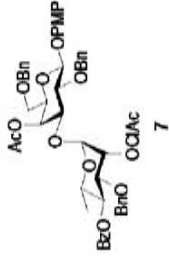
GRADIENT CHANNEL
GENM[1] SINE.100
GrZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 128
SFO1 500.2025 MHz
FIDRES 39.078320 Hz
SW 10.000 ppm
PRMODE QF

F2 - Processing parameters
SI 1024
SF 500.2000129 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2000157 MHz
SSB 0
SINE
IDB 0 Hz
CB 0

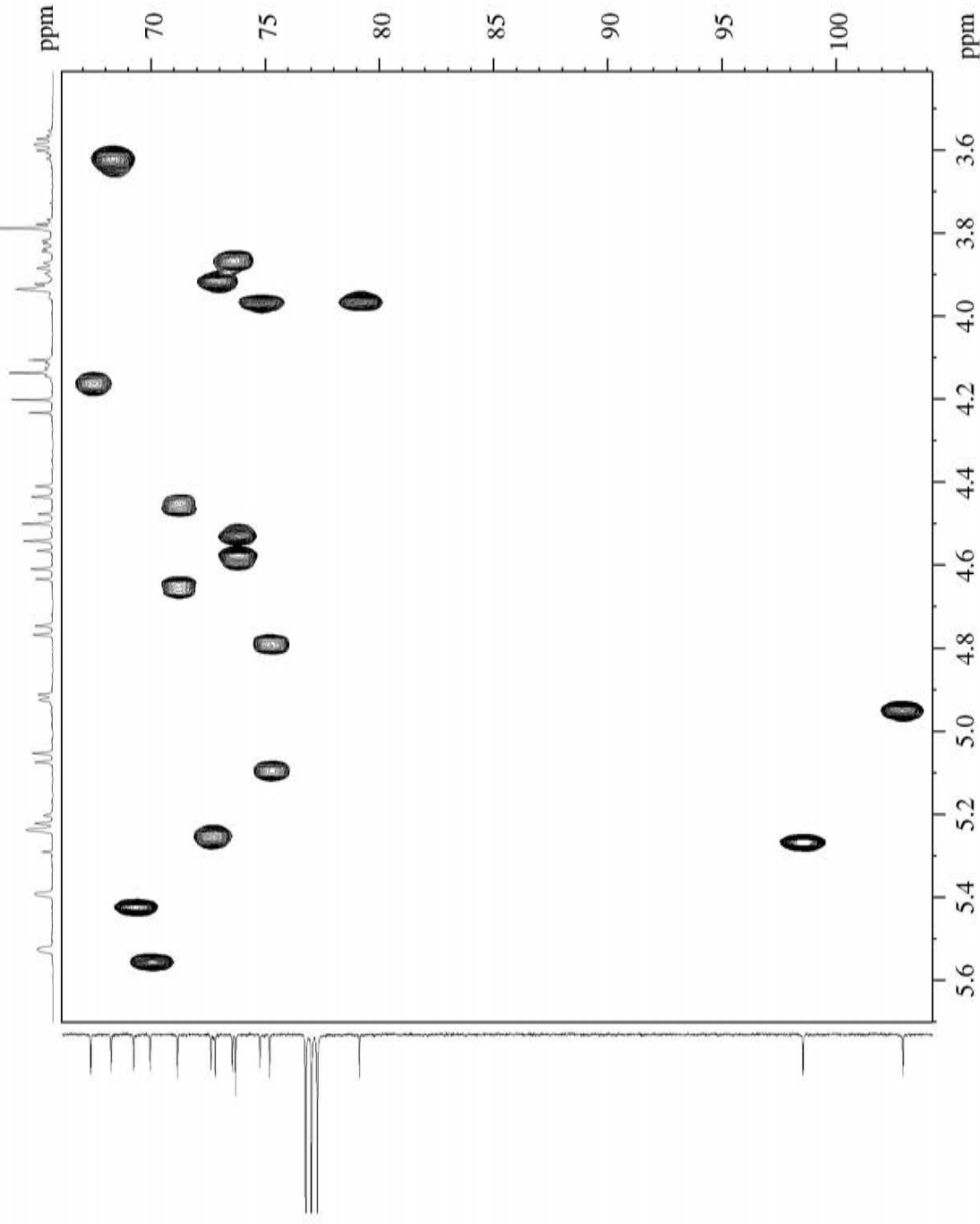
BM-VS-s14 in CDC13
HSQC



```

Current Data Parameters
NAME      BM-VS-s14
EXPNO    52
PROCNO   1
Date_    20140811
Time     15:27
INSTRUM  spect
PROBHD   5 mm PABBO-BE
PULPROG  zgpg30
TD       1024
SOLVENT  CDCl3
DS       16
SHE      5000.000 Hz
NUC1      13C
NUC2      13C
RG        0.1024000
AQ        85.2
RM        0.1024000
DS        16
SW        300.000 usac
TE        301.0 K
CH212    145.0000000
D0        0.0000000 sec
D1        0.0000000 sec
D2        0.0000000 sec
D3        0.0000000 sec
D4        0.0000000 sec
D5        0.0000000 sec
D6        0.0000000 sec
D7        0.0000000 sec
D8        0.0000000 sec
D9        0.0000000 sec
D10       0.0000000 sec
D11       0.0000000 sec
D12       0.0000000 sec
D13       0.0000000 sec
D14       0.0000000 sec
D15       0.0000000 sec
D16       0.0000000 sec
D17       0.0000000 sec
D18       0.0000000 sec
D19       0.0000000 sec
D20       0.0000000 sec
===== CHANNEL f1 =====
NUC1      13C
P1        14.25 usac
PC        25.00 usac
PR        1.10
P2        19.00 usac
PC        25.00 usac
PR        1.10
P3        19.00 usac
PC        25.00 usac
PR        1.10
P4        19.00 usac
PC        25.00 usac
PR        1.10
P5        19.00 usac
PC        25.00 usac
PR        1.10
P6        19.00 usac
PC        25.00 usac
PR        1.10
P7        19.00 usac
PC        25.00 usac
PR        1.10
P8        19.00 usac
PC        25.00 usac
PR        1.10
P9        19.00 usac
PC        25.00 usac
PR        1.10
P10       19.00 usac
PC        25.00 usac
PR        1.10
P11       19.00 usac
PC        25.00 usac
PR        1.10
P12       19.00 usac
PC        25.00 usac
PR        1.10
P13       19.00 usac
PC        25.00 usac
PR        1.10
P14       19.00 usac
PC        25.00 usac
PR        1.10
P15       19.00 usac
PC        25.00 usac
PR        1.10
P16       19.00 usac
PC        25.00 usac
PR        1.10
P17       19.00 usac
PC        25.00 usac
PR        1.10
P18       19.00 usac
PC        25.00 usac
PR        1.10
P19       19.00 usac
PC        25.00 usac
PR        1.10
P20       19.00 usac
PC        25.00 usac
PR        1.10
===== CHANNEL f2 =====
CPDPRG2  garp
NUC1      13C
P1        3.00 usac
PC        3.00 usac
PR        1.10
P2        3.00 usac
PC        3.00 usac
PR        1.10
P3        3.00 usac
PC        3.00 usac
PR        1.10
P4        3.00 usac
PC        3.00 usac
PR        1.10
P5        3.00 usac
PC        3.00 usac
PR        1.10
P6        3.00 usac
PC        3.00 usac
PR        1.10
P7        3.00 usac
PC        3.00 usac
PR        1.10
P8        3.00 usac
PC        3.00 usac
PR        1.10
P9        3.00 usac
PC        3.00 usac
PR        1.10
P10       3.00 usac
PC        3.00 usac
PR        1.10
P11       3.00 usac
PC        3.00 usac
PR        1.10
P12       3.00 usac
PC        3.00 usac
PR        1.10
P13       3.00 usac
PC        3.00 usac
PR        1.10
P14       3.00 usac
PC        3.00 usac
PR        1.10
P15       3.00 usac
PC        3.00 usac
PR        1.10
P16       3.00 usac
PC        3.00 usac
PR        1.10
P17       3.00 usac
PC        3.00 usac
PR        1.10
P18       3.00 usac
PC        3.00 usac
PR        1.10
P19       3.00 usac
PC        3.00 usac
PR        1.10
P20       3.00 usac
PC        3.00 usac
PR        1.10
===== GRABBLE CHANNEL =====
GPRGM11  SINE-100
GPRGM12  SINE-100
GPRGM13  SINE-100
GPRGM14  SINE-100
GPRGM15  SINE-100
GPRGM16  SINE-100
GPRGM17  SINE-100
GPRGM18  SINE-100
GPRGM19  SINE-100
GPRGM20  SINE-100
===== Acquisition parameters =====
SI       1024
SF       500.1364600 MHz
WDW      EM
SSB      0
GB        0
PC        1.00
===== Processing parameters =====
SI       1024
SF       500.1364600 MHz
WDW      EM
SSB      0
GB        0
PC        1.00

```

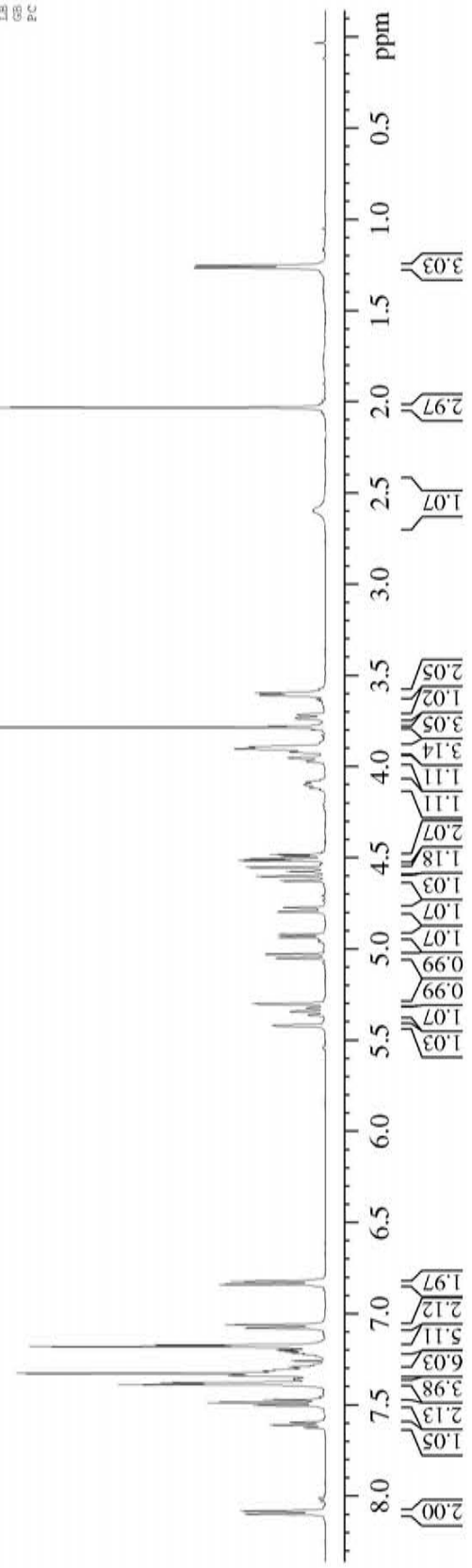
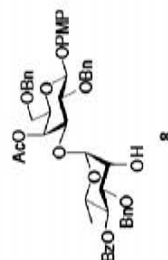


BM-VS-s15 in CDCl3



8.099
8.083
7.611
7.596
7.504
7.488
7.473
7.390
7.380
7.339
7.328
7.319
7.315
7.310
7.293
7.215
7.206
7.199
7.181
7.173
7.080
7.063
6.841
6.823
5.420
5.302
5.051
5.029
4.937
4.922
4.797
4.775
4.627
4.602
4.576
4.553
4.515
4.507
4.492
4.483
3.952
3.922
3.903
3.891
3.785
3.778
3.608
3.596
2.031
1.265
1.252

Current Data Parameters
 NAME BM-VS-s15
 EXPNO 50
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140814
 Time 13:48
 INSTRUM spect
 PROSHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157652 Hz
 AQ 3.1719425 sec
 RG 32
 DW 48.400 usec
 DE 6.50 usec
 FE 501.5 K
 FI 1.00000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 14.25 usec
 PL1 1.30 dB
 PL1W 15.30635643 W
 SP01 500.2030889 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.2000163 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BM-VS-s15 in CDCl3



169.88
165.71
155.37
151.26
137.85
137.69
137.43
133.02
129.93
129.80
128.44
128.32
128.29
128.27
127.84
127.74
127.71
127.70
127.63
118.29
114.53
102.94
100.57
79.02
77.25
77.00
76.75
75.80
75.44
75.01
73.58
72.88
72.80
71.26
69.57
68.35
68.17
66.88
55.55

```

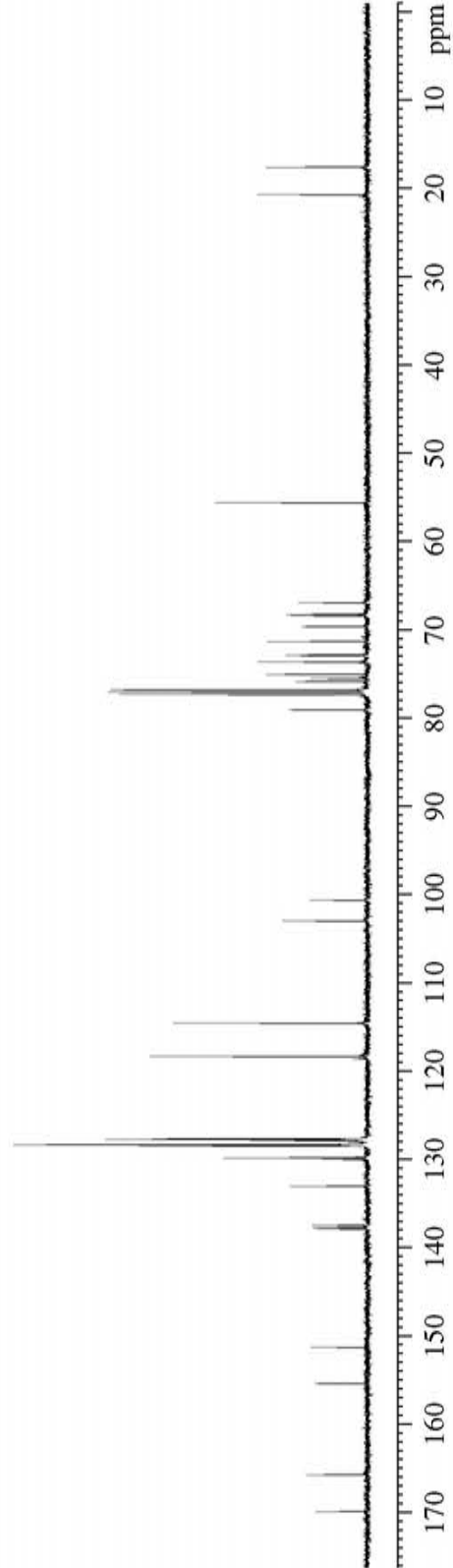
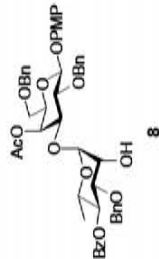
Current Data Parameters
NAME      EM-VS-s15
EXPNO    51
PROCNO   1

F2 - Acquisition Parameters
Date_    20140814
Time     13.50
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       65536
SOLVENT CDCl3
DS       104
SWH      29761.904 Hz
FIDRES   0.454131 Hz
AQ       1.1010048 sec
RG       203
DW       16.800 usec
DE       6.50 usec
TE       302.1 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

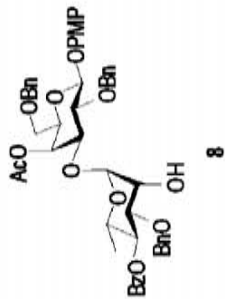
===== CHANNEL f1 =====
NUC1     13C
P1       9.50 usec
PL1      -0.50 dB
PL1W     90.18825531 W
SFO1     125.7879676 MHz

===== CHANNEL f2 =====
CPDPRG2  wait16
NUC2     13C
P2       80.00 usec
PL2      15.00 dB
PL12     15.00 dB
PL13     20.00 dB
PL14     20.00 dB
PL15     15.306355443 W
PL12W    0.51864696 W
PL13W    0.20647706 W
SFO2     500.2020008 MHz

P2 - Processing parameters
SI       32768
SF       125.7754059 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



BM-VS-s15 in CDC13



Current Data Parameters
NAME BM-VS-s15
EXPNO 52
PROCNO 1

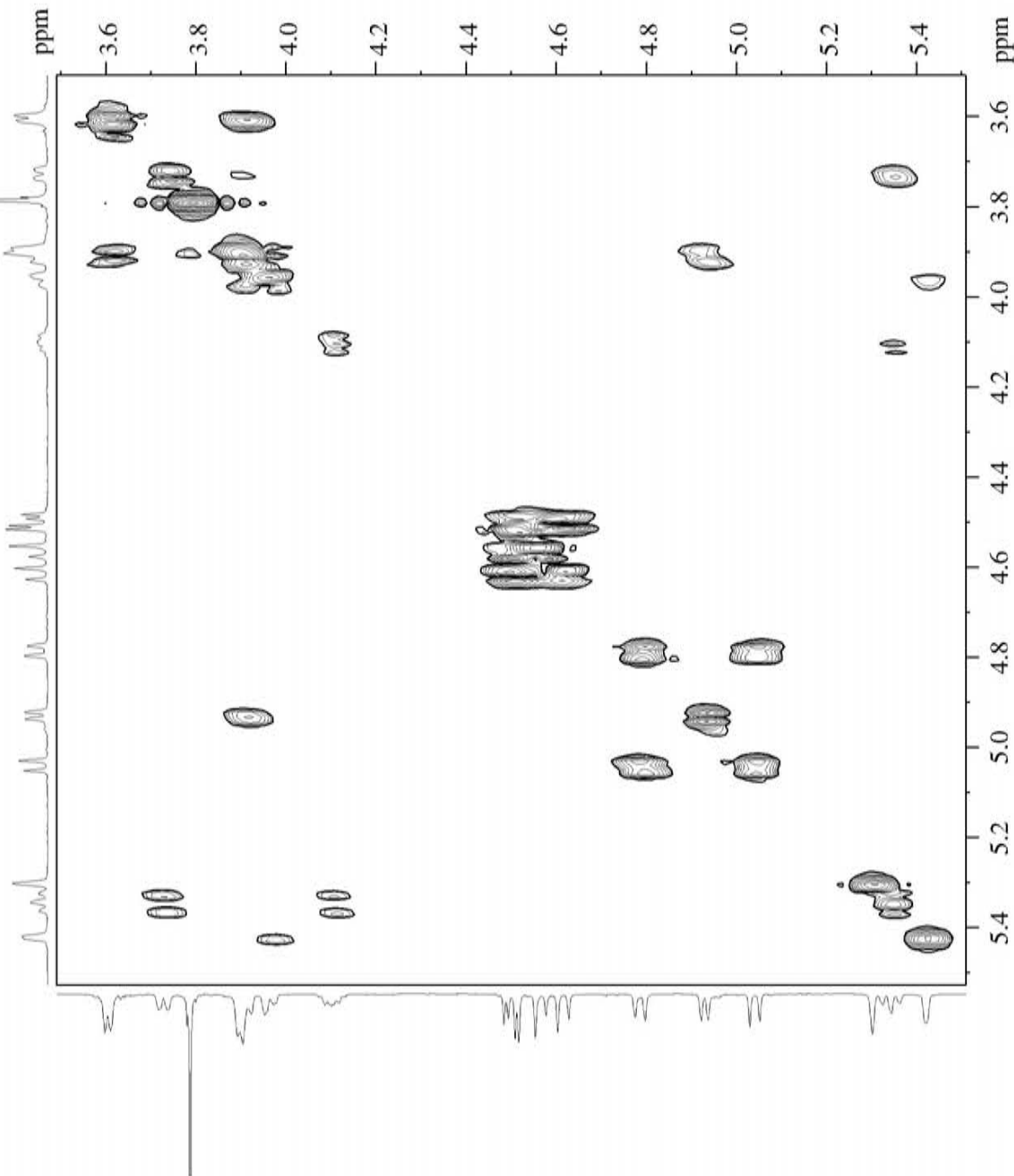
F2 - Acquisition Parameters
Date_ 20140814
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosy90qf
TD 2048
SOLVENT CDC13
NS 1
DS 8
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2048000 sec
RG 32
DW 100.000 usec
DE 6.50 usec
TE 302.1 K
DO 0.00000300 sec
D1 1.48689198 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019590 sec

==== CHANNEL f1 =====
NUC1 1H
P0 14.25 usec
P1 14.25 usec
PL1 1.30 dB
PL1W 15.30635643 W
SFO1 500.2025010 MHz
==== GRADIENT CHANNEL =====
CPNAM[1] SINE.100
GEZ1 10.00 &
P16 1000.00 usec

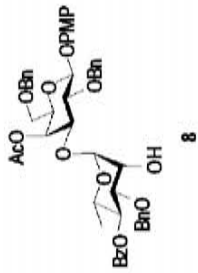
F1 - Acquisition parameters
ID 128
SFO1 500.2025 MHz
FIDRES 39.078320 Hz
SW 10.000 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 500.2000126 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
EC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2000143 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



BM-VS-s15 in CDC13
HSQCGP



Current Data Parameters
NAME BM-VS-s15
EXPNO 53
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140814
Time 14:01
INSTRUM spect
PROBHD 5 mm PABBO BB
TD 65536
SOLVENT CDCl3
NS 2
DS 1
SW 5000.000 Hz
FIDRES 4.882933 Hz
AQ 0.1024000 sec
RG 32
AQ 100.00 usec
SFO1 501.9 K
SFO2 145.0000000
SFO3 0.0000000 sec
SFO4 0.0000000 sec
SFO5 1.0000000 sec
SFO6 0.0300000 sec
SFO7 0.0000000 sec
SFO8 0.0000000 sec
SFO9 0.0000000 sec
SFO10 0.0000000 sec
SFO11 0.0000000 sec
SFO12 0.0000000 sec
SFO13 0.0000000 sec
SFO14 0.0000000 sec
SFO15 0.0000000 sec
SFO16 0.0000000 sec
SFO17 0.0000000 sec
SFO18 0.0000000 sec
SFO19 0.0000000 sec
SFO20 0.0000000 sec
SFO21 0.0000000 sec
SFO22 0.0000000 sec
SFO23 0.0000000 sec
SFO24 0.0000000 sec
SFO25 0.0000000 sec
SFO26 0.0000000 sec
SFO27 0.0000000 sec
SFO28 0.0000000 sec
SFO29 0.0000000 sec
SFO30 0.0000000 sec
SFO31 0.0000000 sec
SFO32 0.0000000 sec
SFO33 0.0000000 sec
SFO34 0.0000000 sec
SFO35 0.0000000 sec
SFO36 0.0000000 sec
SFO37 0.0000000 sec
SFO38 0.0000000 sec
SFO39 0.0000000 sec
SFO40 0.0000000 sec
SFO41 0.0000000 sec
SFO42 0.0000000 sec
SFO43 0.0000000 sec
SFO44 0.0000000 sec
SFO45 0.0000000 sec
SFO46 0.0000000 sec
SFO47 0.0000000 sec
SFO48 0.0000000 sec
SFO49 0.0000000 sec
SFO50 0.0000000 sec
SFO51 0.0000000 sec
SFO52 0.0000000 sec
SFO53 0.0000000 sec
SFO54 0.0000000 sec
SFO55 0.0000000 sec
SFO56 0.0000000 sec
SFO57 0.0000000 sec
SFO58 0.0000000 sec
SFO59 0.0000000 sec
SFO60 0.0000000 sec
SFO61 0.0000000 sec
SFO62 0.0000000 sec
SFO63 0.0000000 sec
SFO64 0.0000000 sec
SFO65 0.0000000 sec
SFO66 0.0000000 sec
SFO67 0.0000000 sec
SFO68 0.0000000 sec
SFO69 0.0000000 sec
SFO70 0.0000000 sec
SFO71 0.0000000 sec
SFO72 0.0000000 sec
SFO73 0.0000000 sec
SFO74 0.0000000 sec
SFO75 0.0000000 sec
SFO76 0.0000000 sec
SFO77 0.0000000 sec
SFO78 0.0000000 sec
SFO79 0.0000000 sec
SFO80 0.0000000 sec
SFO81 0.0000000 sec
SFO82 0.0000000 sec
SFO83 0.0000000 sec
SFO84 0.0000000 sec
SFO85 0.0000000 sec
SFO86 0.0000000 sec
SFO87 0.0000000 sec
SFO88 0.0000000 sec
SFO89 0.0000000 sec
SFO90 0.0000000 sec
SFO91 0.0000000 sec
SFO92 0.0000000 sec
SFO93 0.0000000 sec
SFO94 0.0000000 sec
SFO95 0.0000000 sec
SFO96 0.0000000 sec
SFO97 0.0000000 sec
SFO98 0.0000000 sec
SFO99 0.0000000 sec
SFO100 0.0000000 sec

===== CHANNEL F1 =====

NUC1 1H
P1 14.25 usec
F2 28.50 usec
F3 0.10 usec
SFO1 500.136300 MHz
SFO2 500.2025010 MHz

===== CHANNEL F2 =====

NUC2 13C
P2 9.50 usec
F4 19.00 usec
F5 70.00 usec
F6 17.00 usec
F7 17.00 usec
SFO3 90.18825431 MHz
SFO4 1.60779310 MHz
SFO5 125.7675675 MHz

===== GRADIENT CHANNEL =====

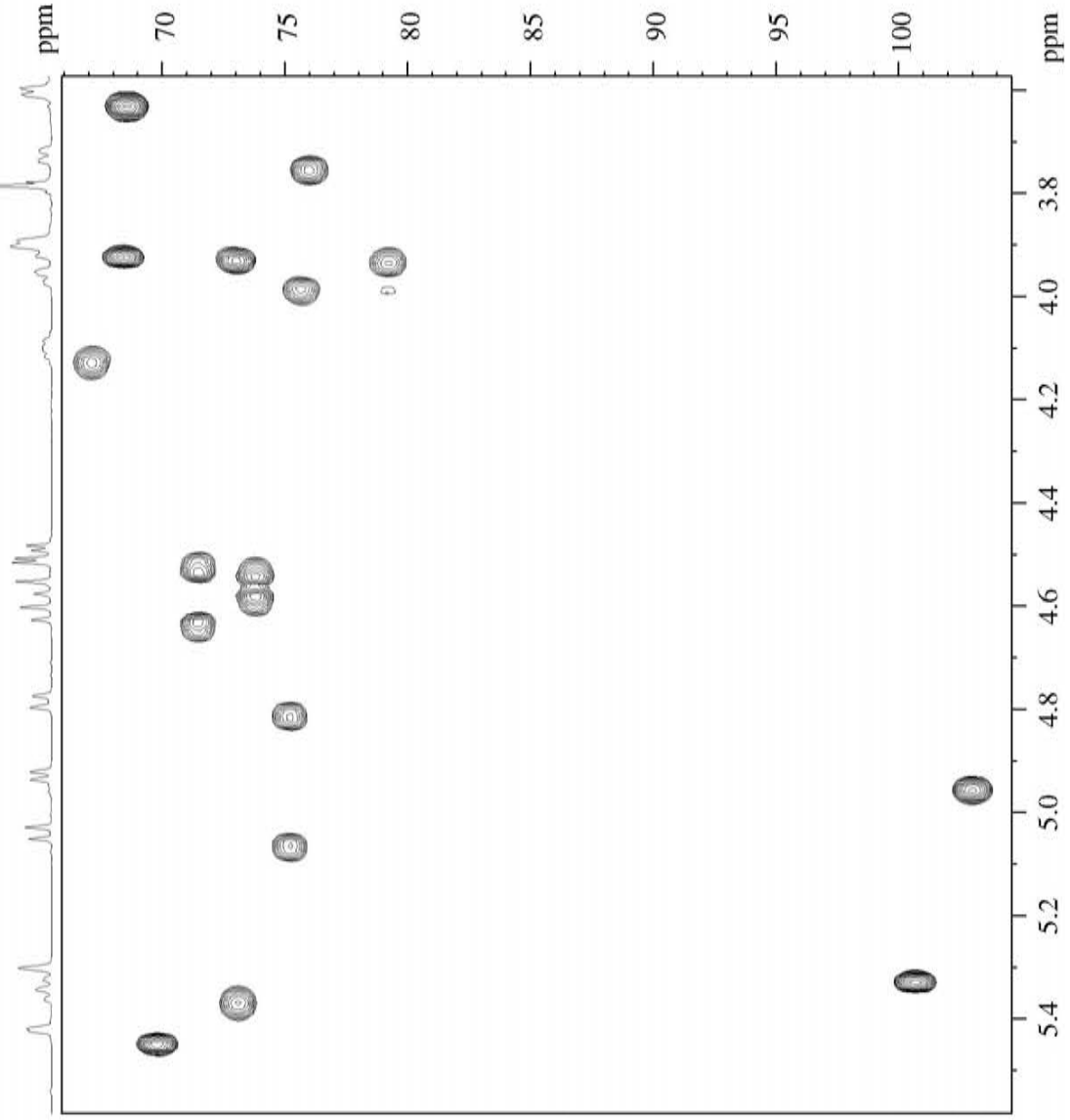
GRANM[1] SINE.100
GRANM[2] SINE.100
GRANM[3] SINE.100
GRANM[4] SINE.100
GRANM[5] SINE.100
GRANM[6] SINE.100
GRANM[7] SINE.100
GRANM[8] SINE.100
GRANM[9] SINE.100
GRANM[10] SINE.100
GRANM[11] SINE.100
GRANM[12] SINE.100
GRANM[13] SINE.100
GRANM[14] SINE.100
GRANM[15] SINE.100
GRANM[16] SINE.100
GRANM[17] SINE.100
GRANM[18] SINE.100
GRANM[19] SINE.100
GRANM[20] SINE.100
GRANM[21] SINE.100
GRANM[22] SINE.100
GRANM[23] SINE.100
GRANM[24] SINE.100
GRANM[25] SINE.100
GRANM[26] SINE.100
GRANM[27] SINE.100
GRANM[28] SINE.100
GRANM[29] SINE.100
GRANM[30] SINE.100
GRANM[31] SINE.100
GRANM[32] SINE.100
GRANM[33] SINE.100
GRANM[34] SINE.100
GRANM[35] SINE.100
GRANM[36] SINE.100
GRANM[37] SINE.100
GRANM[38] SINE.100
GRANM[39] SINE.100
GRANM[40] SINE.100
GRANM[41] SINE.100
GRANM[42] SINE.100
GRANM[43] SINE.100
GRANM[44] SINE.100
GRANM[45] SINE.100
GRANM[46] SINE.100
GRANM[47] SINE.100
GRANM[48] SINE.100
GRANM[49] SINE.100
GRANM[50] SINE.100
GRANM[51] SINE.100
GRANM[52] SINE.100
GRANM[53] SINE.100
GRANM[54] SINE.100
GRANM[55] SINE.100
GRANM[56] SINE.100
GRANM[57] SINE.100
GRANM[58] SINE.100
GRANM[59] SINE.100
GRANM[60] SINE.100
GRANM[61] SINE.100
GRANM[62] SINE.100
GRANM[63] SINE.100
GRANM[64] SINE.100
GRANM[65] SINE.100
GRANM[66] SINE.100
GRANM[67] SINE.100
GRANM[68] SINE.100
GRANM[69] SINE.100
GRANM[70] SINE.100
GRANM[71] SINE.100
GRANM[72] SINE.100
GRANM[73] SINE.100
GRANM[74] SINE.100
GRANM[75] SINE.100
GRANM[76] SINE.100
GRANM[77] SINE.100
GRANM[78] SINE.100
GRANM[79] SINE.100
GRANM[80] SINE.100
GRANM[81] SINE.100
GRANM[82] SINE.100
GRANM[83] SINE.100
GRANM[84] SINE.100
GRANM[85] SINE.100
GRANM[86] SINE.100
GRANM[87] SINE.100
GRANM[88] SINE.100
GRANM[89] SINE.100
GRANM[90] SINE.100
GRANM[91] SINE.100
GRANM[92] SINE.100
GRANM[93] SINE.100
GRANM[94] SINE.100
GRANM[95] SINE.100
GRANM[96] SINE.100
GRANM[97] SINE.100
GRANM[98] SINE.100
GRANM[99] SINE.100
GRANM[100] SINE.100

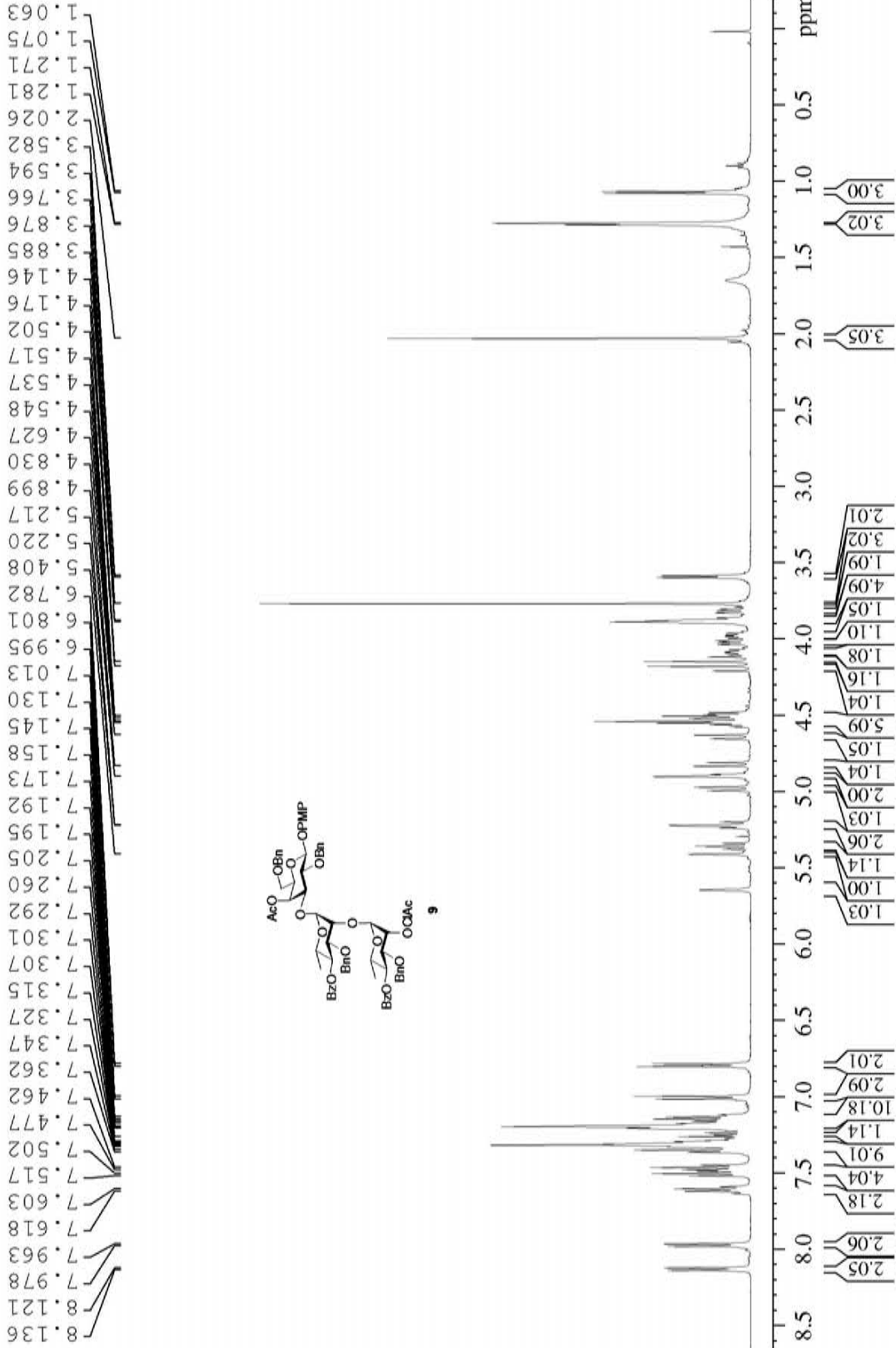
F1 - Acquisition Parameters

TD0 65536
SFO1 125.7675675 MHz
FIDRES 135.255975 Hz
SW 200.000 ppm
FREQ0 Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 500.2000000 MHz
WDW EM
SSB 0 Hz
GB 0 Hz
PC 1.40

F1 - Processing parameters

SI 1024
SF 125.7675675 MHz
WDW EM
SSB 0 Hz
GB 0 Hz
PC 1.40



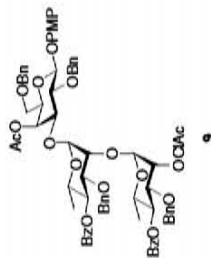
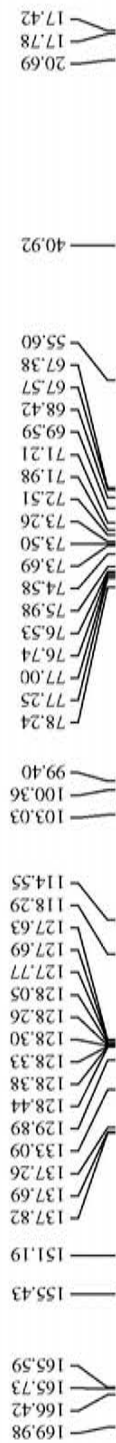


Current Data Parameters
 Name: BM-VS-s16
 ExpNO: 1
 F2 - Acquisition Parameters
 Date_: 20180806
 Time: 10:02
 INSTRUM: spect
 PROBHD: 5 mm PABBO BB-
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 2
 DS: 4
 SSB: 10350.578 Hz
 FIDRES: 0.157630 Hz
 AQ: 3.1719425 sec
 ZG: 0.0000000 sec
 ZM: 48.400 usec
 DE: 6.150 usec
 TE: 302.7 K
 DL: 1.00000000 sec
 TUG: 1

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 14.25 usec
 PL1: 0.00 dB
 FWHM: 15.3045730 Hz
 SFO1: 500.20130689 MHz

F2 - Processing parameters
 SI: 32768
 SF: 500.200156 MHz
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

BM-VS-s16 in CDC13



```

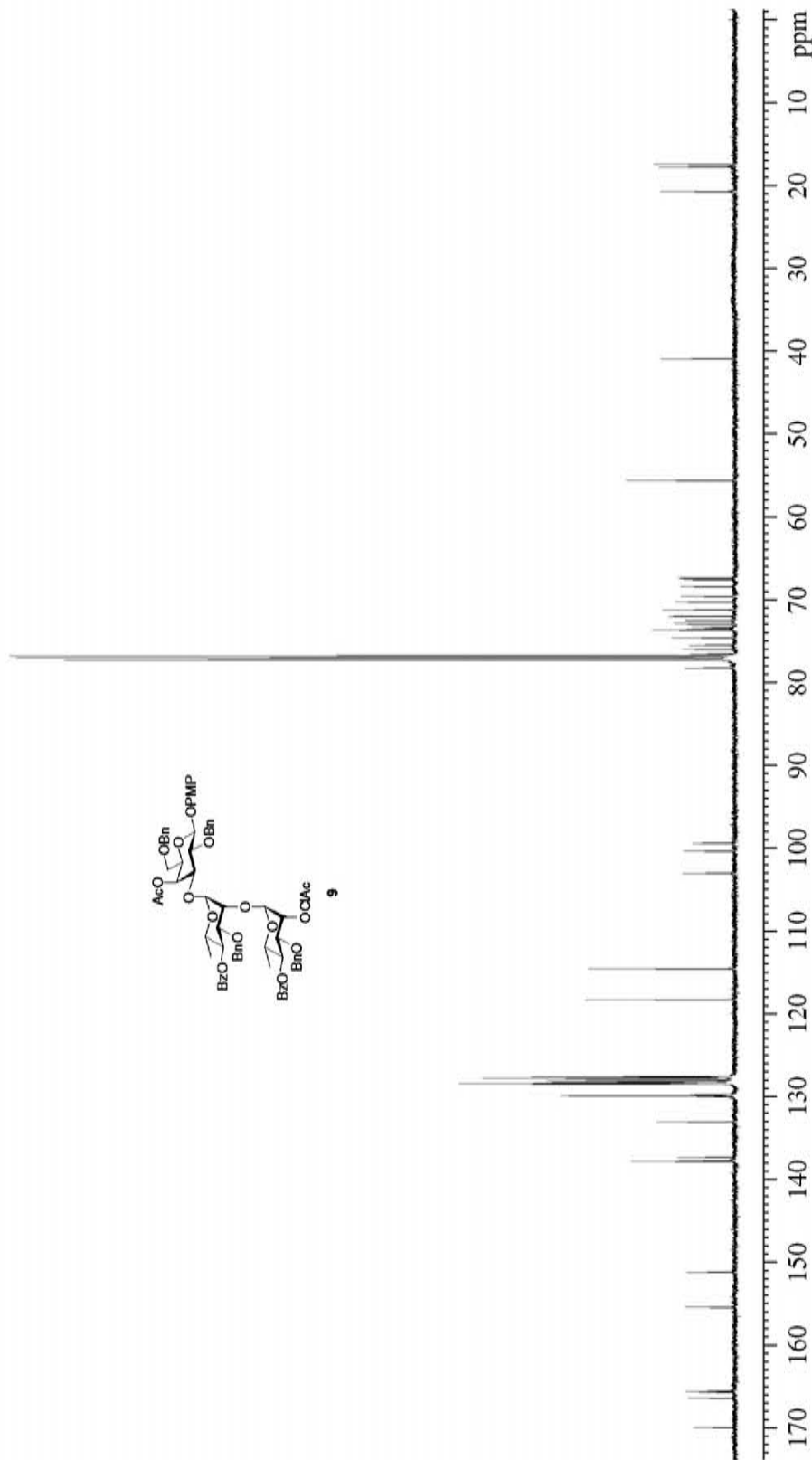
Current Data Parameters
NAME      BM-VS-s16
EXPNO    13
PROCNO   1

F2 - Acquisition Parameters
Date_    20140806
Time     11.05
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
ID       65536
SOLVENT  CDC13
NS       877
DS       4
SWH      23761.904 Hz
FIDRES   0.454131 Hz
AQ       1.1010048 sec
RG       203
DW       16.800 usec
DE       6.50 usec
TE       303.3 K
D1       2.00000000 sec
D11      0.05000000 sec
D10      1

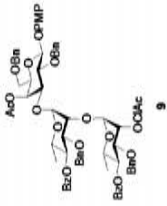
***** CHANNEL f1 *****
NUC1     13C
P1       9.15 usec
PL1      -0.50 dB
PL12     96.18825531 W
PL13     125.7879576 MHz
SFO1     500.2620008 MHz

***** CHANNEL f2 *****
CPDPRG12 waltz16
NUC2     1H
P2       80.00 usec
PCPD2    1.30 dB
PL2      16.00 dB
PL12     15.30635643 W
PL13     0.51864696 W
PL12W    0.20647706 W
PL13W    500.2620008 MHz
SFO2

F2 - Processing parameters
SI       32768
SF       125.7753967 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



BM-VS-s16 in CDC13



Current Data Parameters
NAME BM-VS-s16
EXPNO 11
PROCNO 1

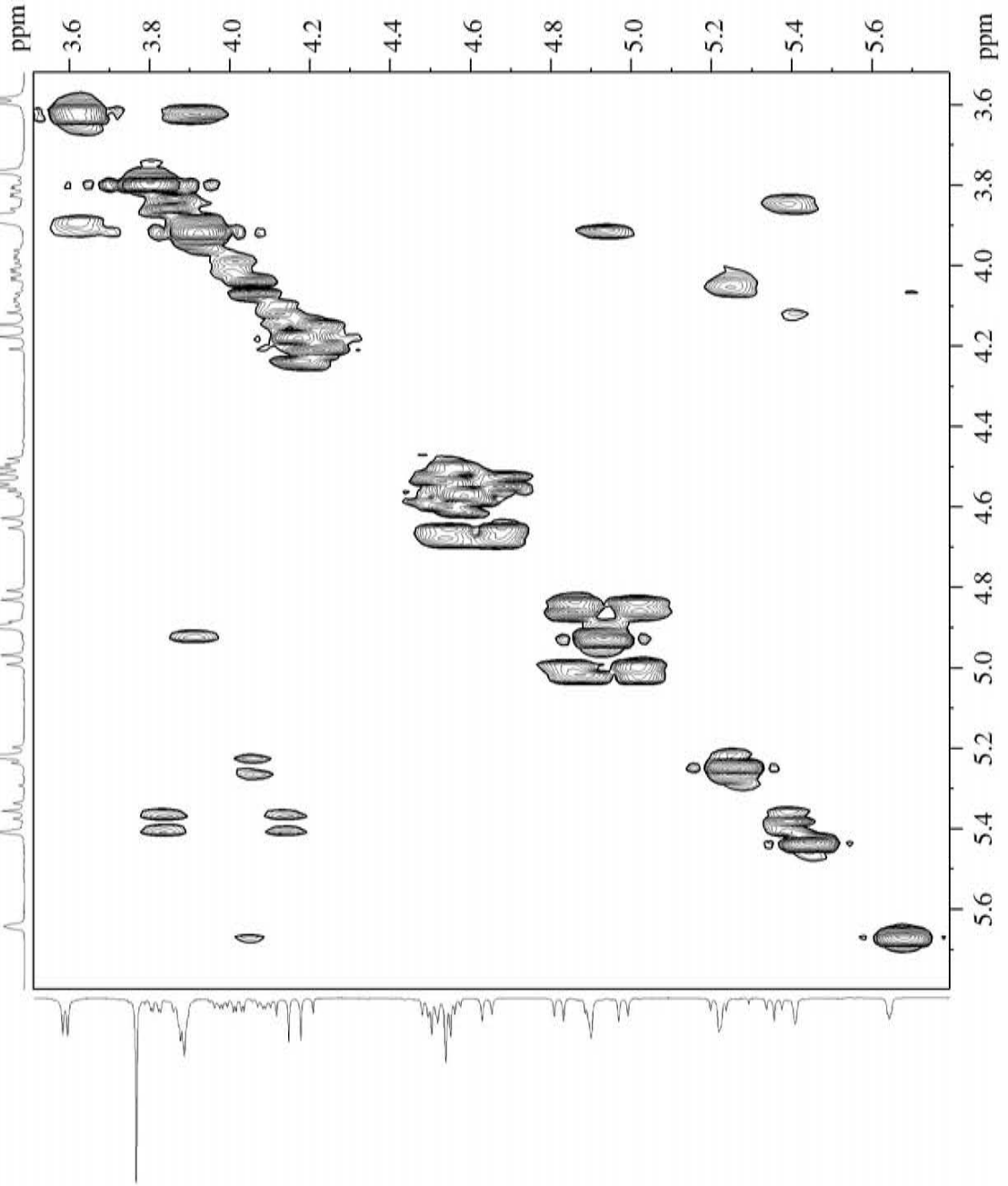
F2 - Acquisition Parameters
Date_ 20140806
Time 10.43
INSTRUM Spect
PROBHD 5 mm PABBO BB
PULPROG cosygqi
ID 2048
SOLVENT CDC13
NS 1
DS 8
SWH 6684.492 Hz
FIDRES 3.263912 Hz
AQ 0.1531904 sec
RG 50.8
DM 74.800 usec
DE 6.50 usec
TE 302.6 K
D0 0.00000300 sec
D1 1.48683198 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00014975 sec

CHANNEL f1
NUC1 1H
P0 14.25 usec
P1 14.25 usec
PL1 1.30 dB
PL1H 15.30635643 W
SF01 500.2030073 MHz
----- GRADIENT CHANNEL -----
GPNAM[f1] SINE.100
GPZ1 10.00 %
P16 1000.00 usec

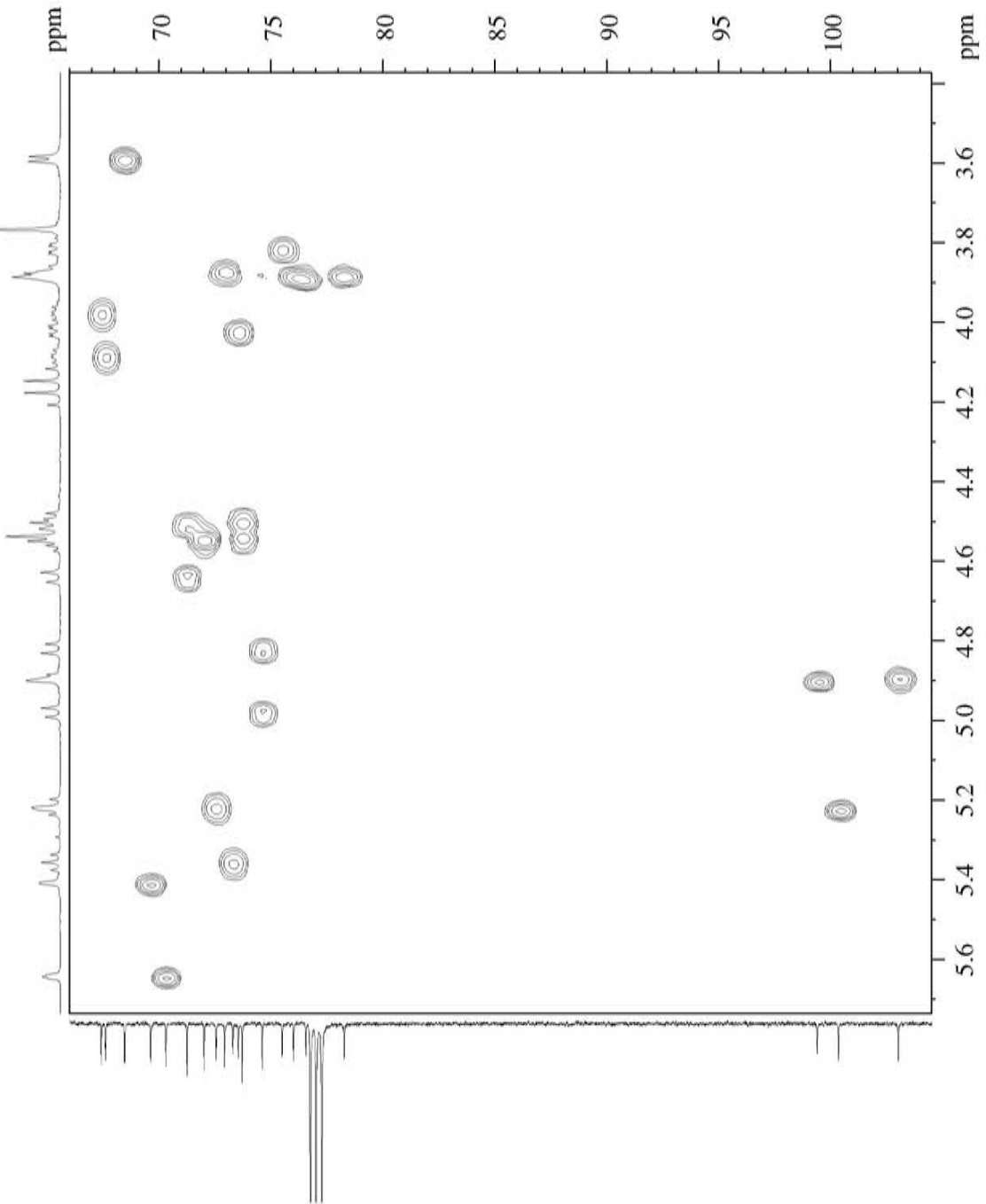
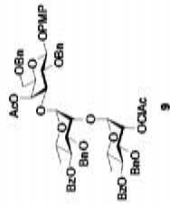
F1 - Acquisition parameters
ID 128
SF01 500.203 MHz
FIDRES 52.170712 Hz
SW 13.350 PPM
FMODE QF

F2 - Processing parameters
SI 1024
SF 500.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
SF 500.2000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



BM-VS-s16 in CDC13
HSQC



```

Current Data Parameters
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
=====
Date_ 2010.04.15
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
SOLVENT CDCl3
NS 2
DS 16
SS 4000.136 Hz
AQ 0.1024000 sec
RG 512
AQ 0.1024000 sec
RG 512
TE 303.2 K
CNS12 145.0000000
DO 0.00000300 sec
D1 0.00000000 sec
D11 0.00000000 sec
D13 0.00000400 sec
D16 0.00000000 sec
DE 0.00000000 sec
TM 0.00001365 sec
ZSQC7B5
=====
CHANNEL F1
NUC1 13
P1 14.25 usec
P2 28.50 usec
P3 0.10 usec
P4 15.30 usec
P5 15.30 usec
P6 15.30 usec
SFO1 500.2525010 MHz
=====
CHANNEL F2
NUC2 1H
P7 9.50 usec
P8 19.00 usec
P9 19.00 usec
P10 70.00 usec
P11 17.00 usec
P12 17.00 usec
P13 17.00 usec
P14 17.00 usec
P15 17.00 usec
P16 17.00 usec
P17 17.00 usec
P18 17.00 usec
P19 17.00 usec
SFO2 125.767875 MHz
=====
GRADIENT CHANNEL
=====
GPRAM[1] SINE,100
GPRAM[2] SINE,100
GPRAM[3] SINE,100
GPRAM[4] SINE,100
GPRAM[5] SINE,100
GPRAM[6] SINE,100
GPRAM[7] SINE,100
GPRAM[8] SINE,100
GPRAM[9] SINE,100
GPRAM[10] SINE,100
GPRAM[11] SINE,100
GPRAM[12] SINE,100
GPRAM[13] SINE,100
GPRAM[14] SINE,100
GPRAM[15] SINE,100
GPRAM[16] SINE,100
GPRAM[17] SINE,100
GPRAM[18] SINE,100
GPRAM[19] SINE,100
GPRAM[20] SINE,100
=====
E1 - Acquisition parameters
SFO1 125.768 MHz
SFO2 125.767875 MHz
FIDRES 98.371853 Hz
SFO 200.000000 MHz
FNAME Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 500.0000138 MHz
AQ 0.1024000 sec
RG 512
DE 0.00000000 sec
TE 303.2 K
GB 0
PC 1.00
=====
E1 - Processing parameters
SI 1024
SFO1 125.768 MHz
SFO2 125.767875 MHz
FIDRES 98.371853 Hz
SFO 200.000000 MHz
FNAME Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 500.0000138 MHz
AQ 0.1024000 sec
RG 512
DE 0.00000000 sec
TE 303.2 K
GB 0
PC 1.00
=====
E1 - Processing parameters
SI 1024
SFO1 125.768 MHz
SFO2 125.767875 MHz
FIDRES 98.371853 Hz
SFO 200.000000 MHz
FNAME Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 500.0000138 MHz
AQ 0.1024000 sec
RG 512
DE 0.00000000 sec
TE 303.2 K
GB 0
PC 1.00
=====

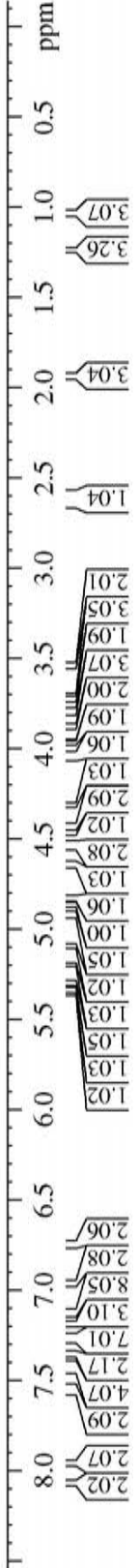
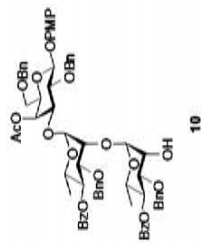
```



BM-VS-s17 CDCl3



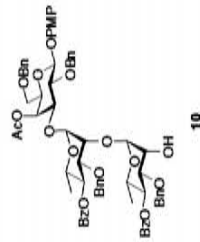
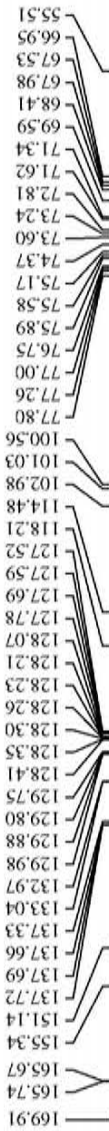
Chiront Data Parameters
 NAME BM-VS-s17
 EXPNO 30
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140821
 Time 14:32
 PROGM spect
 PULPROG zgpg30
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 PC 20.5 usec
 DR 48.44 usec
 DE 6.90 usec
 TE 302.6 K
 D1 1.00000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 14.25 usec
 PL 0.00 dB
 F1 500.136363 MHz
 SFO1 500.136363 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.136363 MHz
 SE 4
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BM-VS-s17 CDC13



169.91
165.74
165.67
155.34
151.14
137.72
137.69
137.66
137.33
133.04
132.97
129.98
129.88
129.80
129.75
128.41
128.35
128.30
128.26
128.23
128.21
128.07
127.78
127.69
127.59
127.52
118.21
114.48
102.98
101.03
100.56
77.80
77.26
77.00
76.75
75.89
75.58
75.17
74.37
73.60
73.24
72.81
71.62
71.34
69.59
68.41
67.98
67.53
66.95
55.51



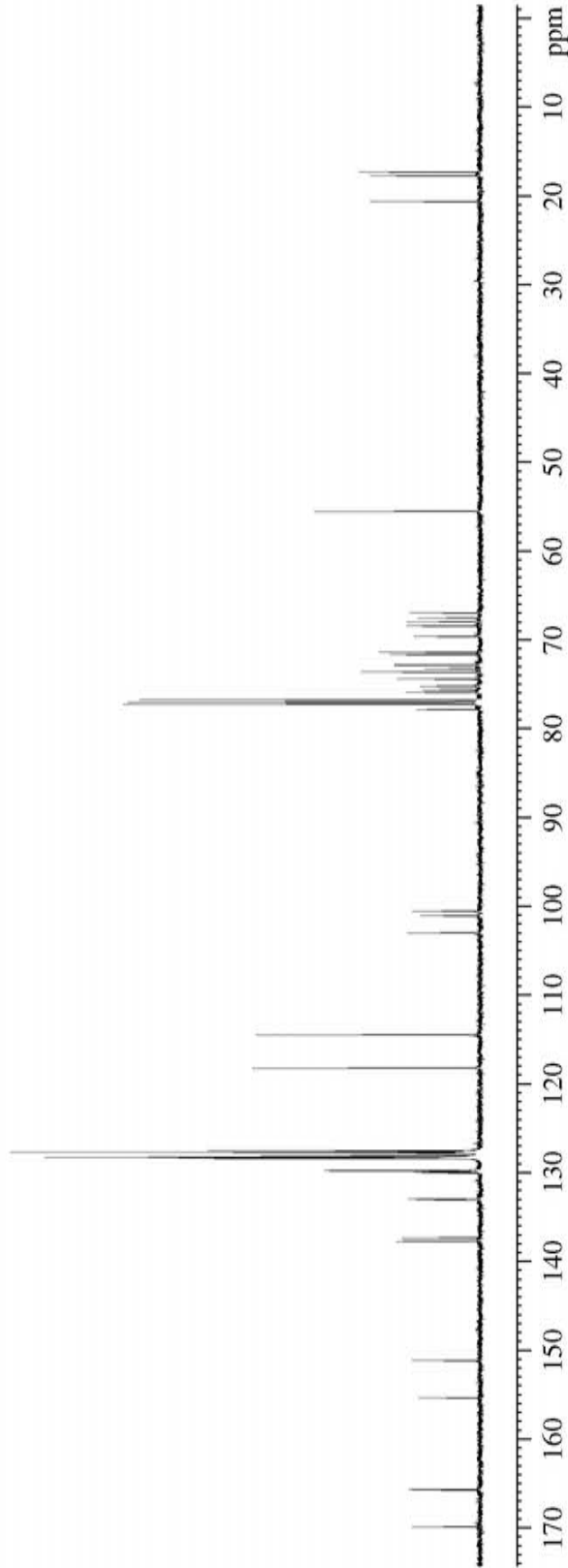
Current Data Parameters
 NAME BM-VS-s17
 EXPNO 31
 PROCNO 1

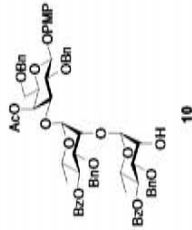
F2 - Acquisition Parameters
 Date_ 20140821
 Time 14.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 157
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 303.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 PL1W 90.1882531 W
 SF01 125.7879676 MHz

===== CHANNEL f2 =====
 CPDPRG[2] maltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.30 dB
 PL12 16.00 dB
 PL13 20.00 dB
 PL2W 15.30635643 W
 PL12W 0.51864696 W
 PL13W 0.20647706 W
 SF02 500.2020008 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7754095 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





```

Current Data Parameters
NAME      BM-VS-s17
EXPNO    32
PROCNO   1

F2 - Acquisition Parameters
Date_    20140921
Time     14.42
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  cosygpgfi
ID       2048
SOLVENT  CDCl3
NS       1
DS       8
SWH      5000.000 Hz
FIDRES   2.441406 Hz
AQ       0.2048000 sec
RG       28.5
DW       100.000 usec
DE       6.50 usec
TE       303.5 K
D0       0.00000300 sec
D1       1.4889198 sec
D13      0.00000400 sec
D16      0.00020000 sec
INO      0.00019990 sec

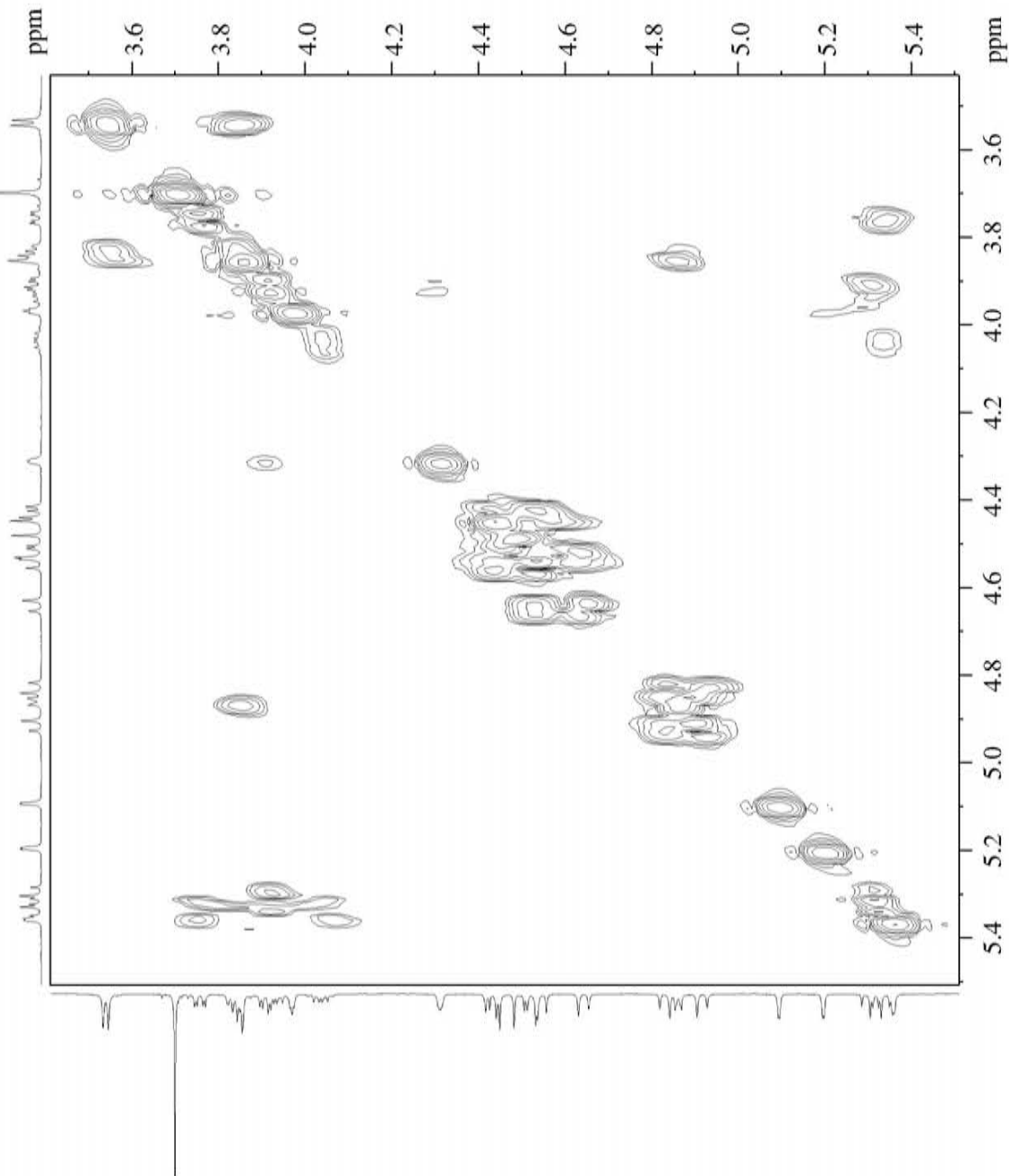
===== CHANNEL f1 =====
NUC1     1H
P0       14.25 usec
P1       14.25 usec
PL1      1.30 dB
PL1W     15.30635643 W
SF01     500.2025010 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GP21     10.00 %
P16      1000.00 usec

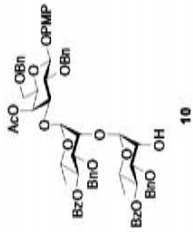
F1 - Acquisition Parameters
ID       128
SF01     500.2025 MHz
FIDRES   39.078320 Hz
SW       10.000 PPM
PRMODE   QF

F2 - Processing parameters
SI       1024
SF       500.2000505 MHz
WDW      SINE
SSB      0
LB       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       1024
MC2      QF
SF       500.2000540 MHz
WDW      SINE
SSB      0
LB       0 Hz
GB       0
  
```



BM-VS-s17 CDCl3
HSQC



Current Data Parameters
NAME: BM-VS-s17
EXPNO: 33
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20140821
Time: 14:48

AcqMeth: zgpg30
PROCNO: 33
PULPROG: zgpg30
TD: 1024

SOLVENT: CDCl3
DS: 4
DE: 14

SWH: 5000.000 Hz
FIDRES: 4.382813 Hz
AQ: 0.1024000 sec

RG: 655
DM: 100.000 umsc
DE: 6.50 umsc
TE: 303.0 K

CHGT2: 145.0000000 Hz
D1: 0.0000000 sec
D2: 1.5000000 sec

D4: 0.00172414 sec
D11: 0.03000000 sec
D13: 0.00000000 sec

D24: 0.00000000 sec
D24: 0.0008207 sec
IRB0: 0.00001955 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 14.25 umsc
PC: 88.50 umsc

P2: 1.0 umsc
P3: 1.0 umsc
P4: 1.0 umsc
P5: 1.0 umsc

PL1M: 15.30435643 M
RF01: 560.2025010 MHz
===== CHANNEL f2 =====

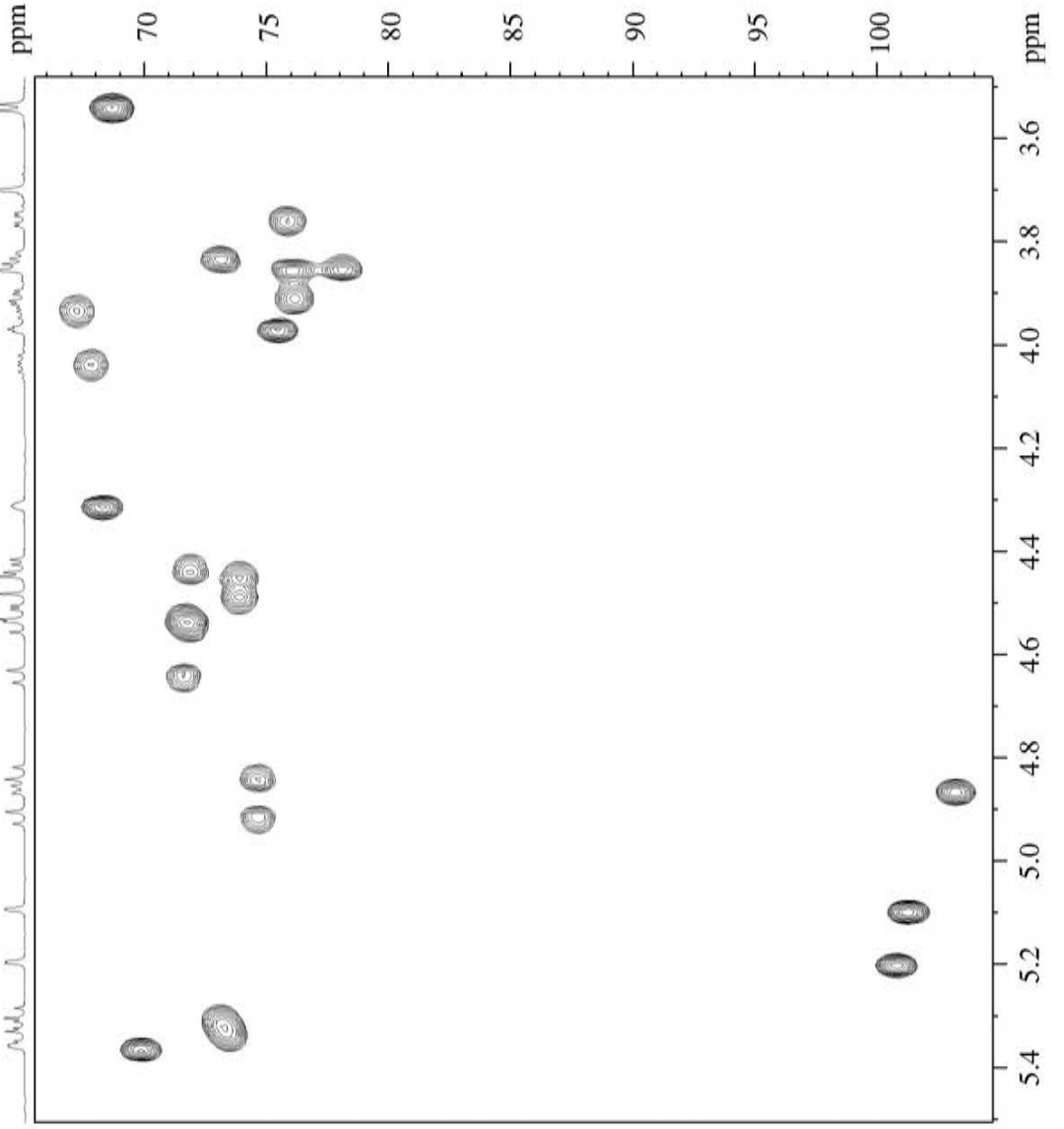
CPDPRG2: zgpg30
NUC2: 13C
P7: 9.50 umsc
P8: 19.00 umsc

P9: 9.50 umsc
P10: 19.00 umsc
P11: -0.50 umsc
P12: -0.50 umsc

P13: 17.00 umsc
P14: 17.00 umsc
P15: 90.18825531 M
P16: 1.60379910 M

P17: 125.7679615 MHz
===== GRADIENT CHANNEL =====
GPRM[1]: SINE-100
GPRM[2]: SINE-100
GPRM[3]: SINE-100

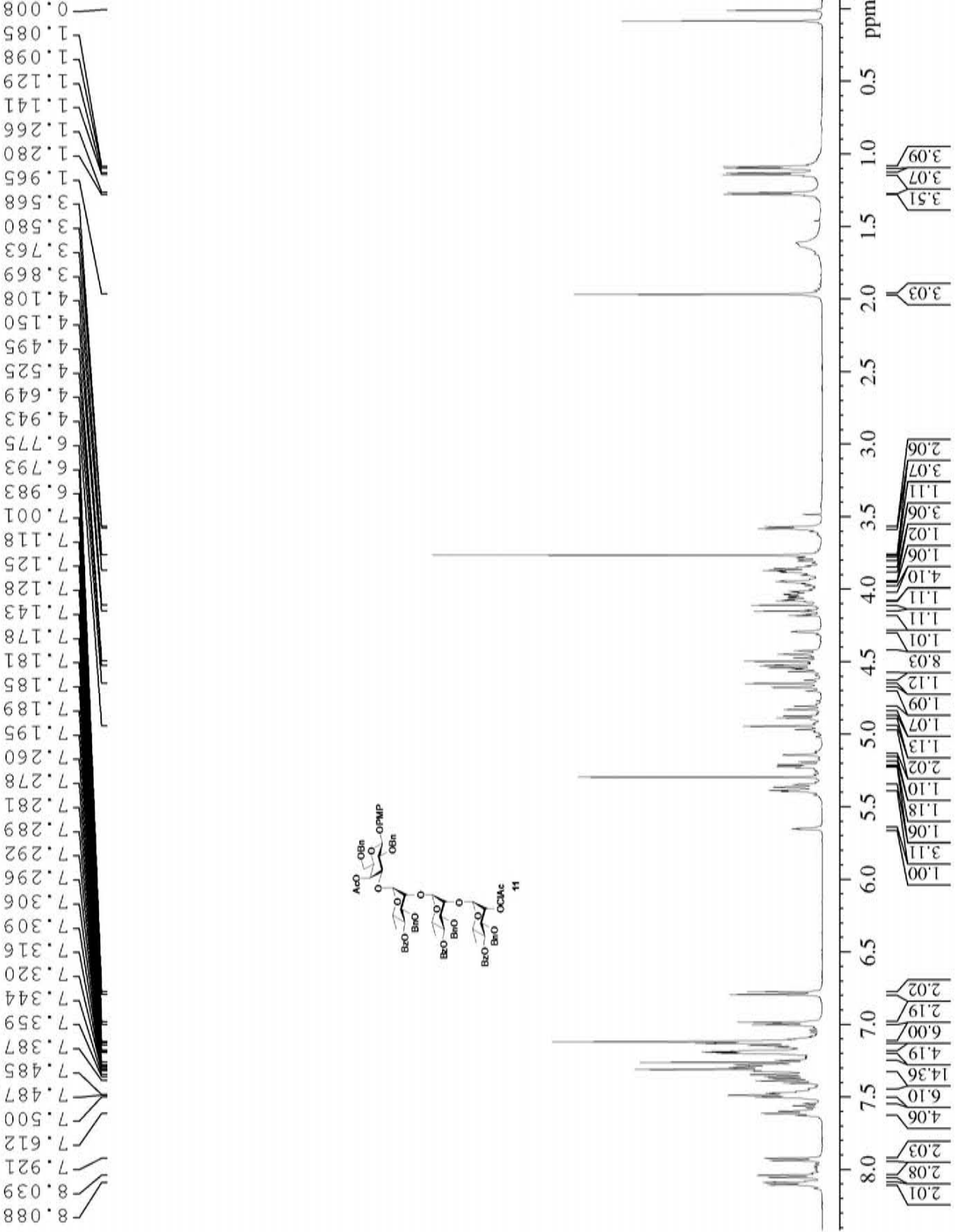
GPRM[4]: SINE-100
GPRM[5]: SINE-100
GPRM[6]: SINE-100
GPRM[7]: SINE-100



F2 - Processing parameters
SI: 1024
SF: 500.1360502 MHz
WDW: EM
SSB: 0 Hz
GB: 0
PC: 1.00

F1 - Processing parameters
SI: 1024
SF: 125.7679615 MHz
WDW: EM
SSB: 0 Hz
GB: 0
PC: 1.00

BM-VS-s18 in CDCl3



Current Data Parameters
 NMR BM-VS-s18
 PROCNO 50
 F2 - Acquisition Parameters
 Date 20140805
 Time 11.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 10330.576 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 101
 DW 48.400 usec
 DE 6.50 usec
 TE 302.0 K
 D1 1.00000000 sec
 TD0 1

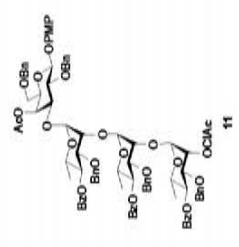
CHEMNAME: CHLOROFORM D
 CHANNEL f1 1H
 NUCL1 1H
 P1 14.21 usec
 PL1 1.30 dB
 PL1N 15.306356443 N
 SFO1 500.2030889 MHz

F2 - Processing Parameters
 SI 32768
 SF 500.2000165 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

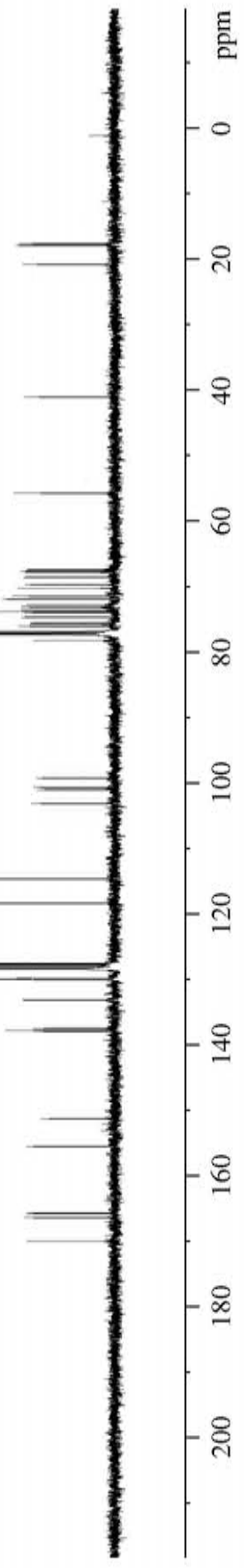
BM-VS-s18 in CDCl3



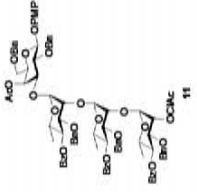
169.98
166.35
165.75
165.73
165.59
158.97
155.48
151.25
137.83
137.71
137.44
133.25
133.12
133.05
130.03
130.00
129.90
129.87
129.83
129.79
128.44
128.39
128.36
128.30
128.28
128.26
128.23
128.12
127.77
127.69
127.66
127.54
127.51
118.31
114.56
103.09
101.10
100.65
99.21
88.17
77.26
77.00
76.75
76.08
75.96
75.70
75.41
74.59
73.90
73.71
73.30
73.11
72.94
72.66
71.82
71.33
70.16
69.62
68.48
67.72
67.60
67.33
55.62
53.38
40.92
20.64
17.76
17.48



Current Data Parameters
 NAME BM-VS-s18
 EXPNO 33
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140805
 Time 11:48
 INSTRUM spect
 PROBRD 5 mm PARBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 295
 DS 4
 SFO1 29761.904 Hz
 FIDRES 0.454133 Hz
 AQ 1.1010046 sec
 RG 203
 DM 16.800 usec
 DE 6.50 usec
 TE 303.3 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1
 CHANNEL f1
 NUCL1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 PL1W 90.18625531 W
 SF01 125.7679676 MHz
 CHANNEL f2
 CPDPRG2 waltz16
 NUCL2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL2W 1.00 dB
 PL3 20.00 dB
 PL3W 15.306358643 W
 PL12W 0.51864696 W
 PL13W 0.20647706 W
 SF02 500.2020008 MHz
 F2 - Processing parameters
 SI 32768
 SF 125.7753941 MHz
 WHW 0
 SSB 0
 GB 0
 PC 1.40



BM-VS-s18 in CDC13



Current Data Parameters
 NAME BM-VS-s18
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140805
 Time 11.18
 INSTRUM spect
 PROBD 5 mm FAPBO BB-
 PULPROG cosygpfH
 TD 2048
 SOLVENT CDC13
 NS 1
 DS 8
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048000 sec
 RG 101
 RC 1
 DW 100.000 usec
 DE 6.50 usec
 TE 302.0 K
 D0 0.00000300 sec
 D1 1.48689198 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019990 sec

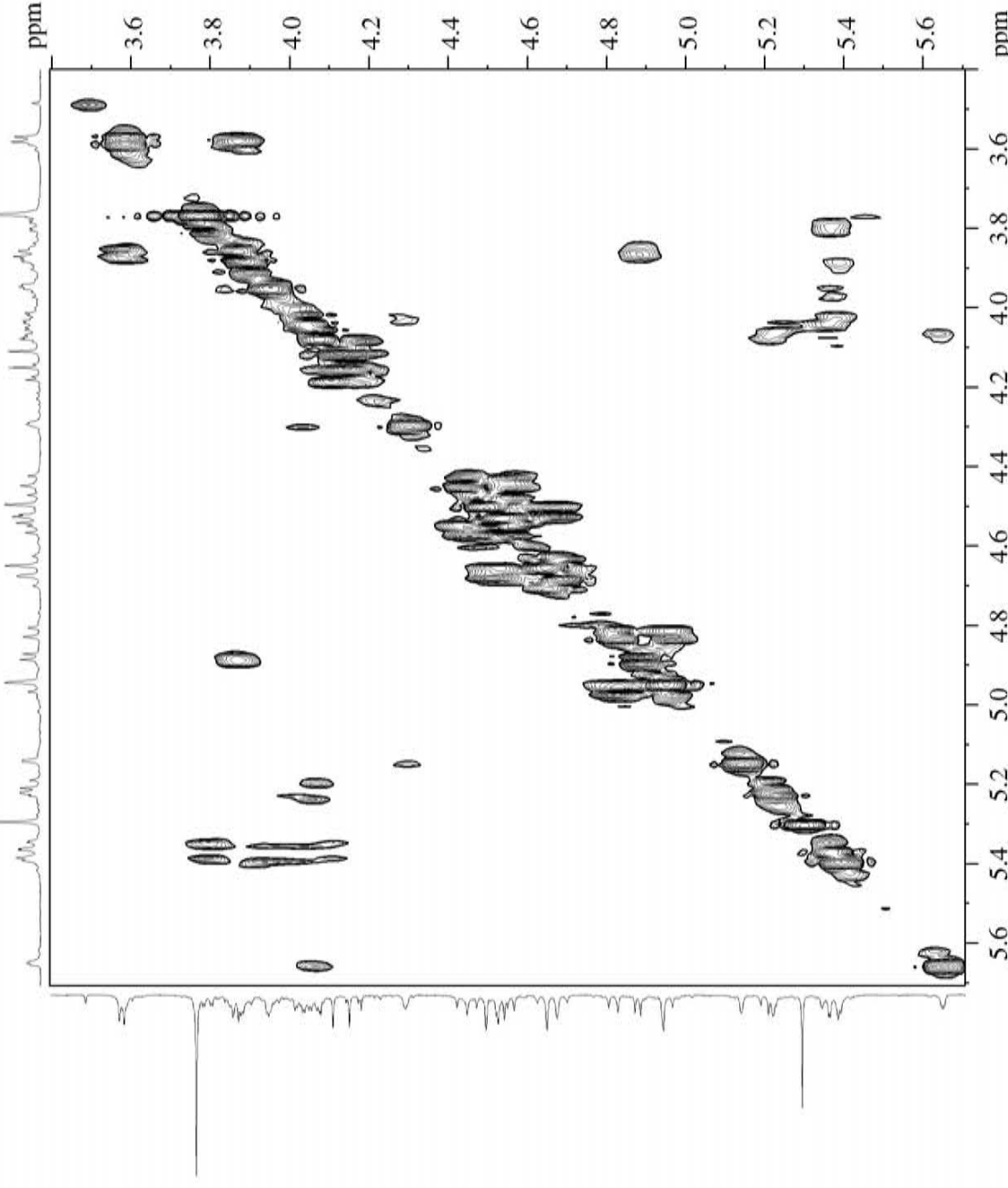
===== CHANNEL f1 =====
 NUC1 1H
 P0 14.25 usec
 P1 14.25 usec
 PL1 1.30 dB
 PL1W 15.30635643 W
 SF01 500.2025010 MHz

===== GRADIENT CHANNEL =====
 GENAM[1] SINE.100
 GP21 10.00 %
 P16 1000.00 usec

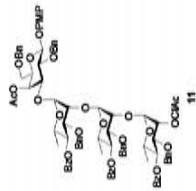
F1 - Acquisition parameters
 ID 128
 SF01 500.2025 MHz
 FIDRES 39.078320 Hz
 SW 10.000 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 500.2000143 MHz
 WDM 0
 SSB 0 Hz
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MCT QF
 SF 500.2000135 MHz
 WDM 0
 SSB 0 Hz
 LB 0 Hz
 CB 0



BM-VS-s18 in CDC13
HSQCGP



Current Data Parameters:
NAME BM-VS-s18
EXPNO 32
PROCNO 1

F1 - Acquisition Parameters
Date_ 20140903
Time 11:25
INSTRUM spect
PROBHD 5 mm PABBO ED
PULPROG zgpg30
TD 1024
SOLVENT CDC13
NS 2
DS 8
SWH 5000.000 Hz
FIDRES 4.882013 Hz
AQ 0.1024000 sec
RG 320
AQ 0.1024000 sec
RG 320
TE 302.1 K
CNS12 145.0000000
DO 0.0000000 sec
D1 0.0000000 sec
D2 0.0000000 sec
D3 0.0017244 sec
D4 0.003000000 sec
D11 0.030000000 sec
D13 0.000004000 sec
D16 0.000200000 sec
D18 0.000000000 sec
L8 0.000000000 sec
L9 0.000000000 sec
SFOFTS 0.0000185 sec

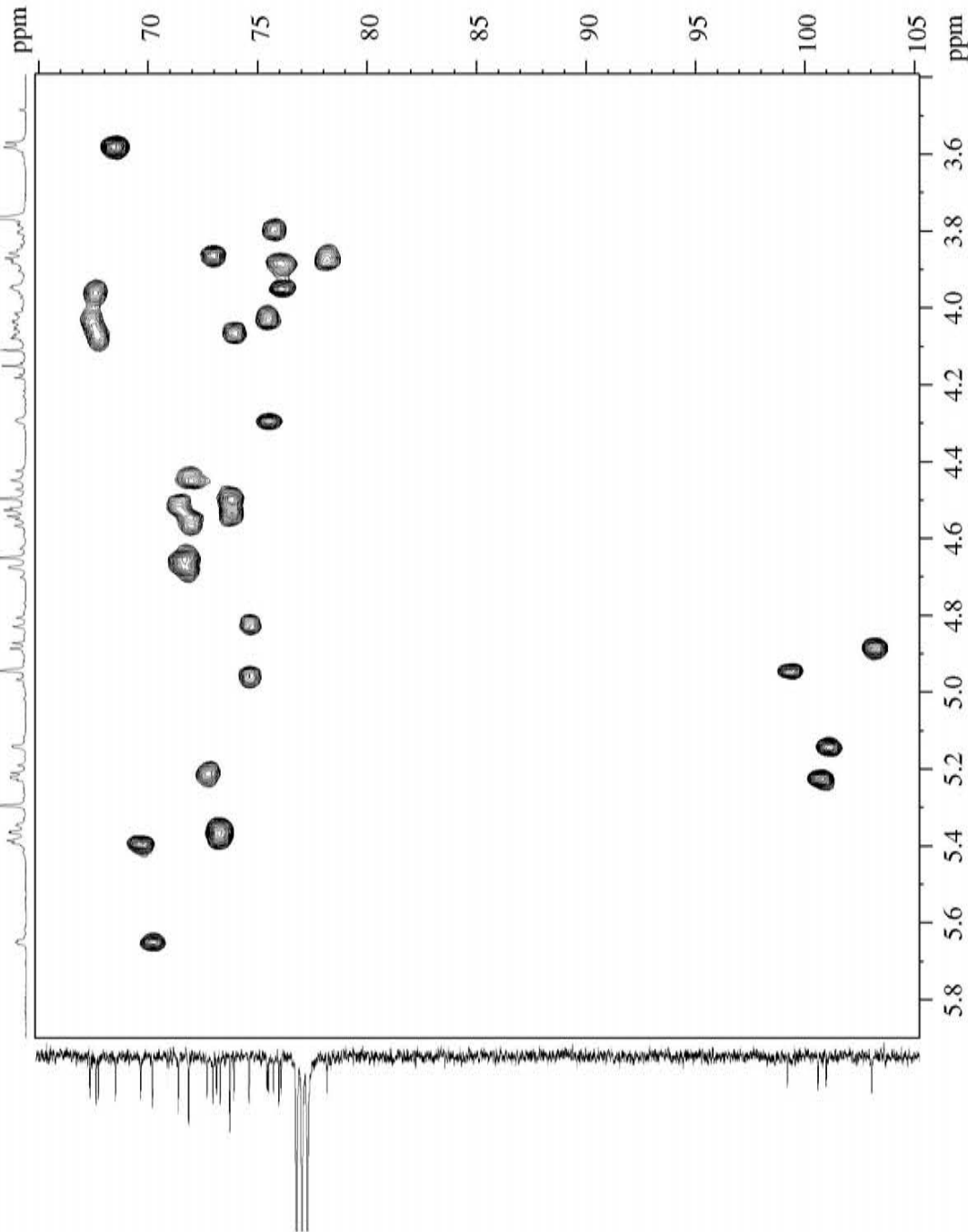
===== CHANNEL f1 =====
NUC1 14.25 usec
P1 14.25 usec
P2 28.50 usec
P2R 0.10 usec
P11 15.30 usec
P11R 15.30 usec
SFO1 500.20245010 MHz

===== CHANNEL f2 =====
CPDPRG2 gpc
NUC2 9.55 usec
P3 9.55 usec
P4 19.00 usec
PCPD2 70.00 usec
P1 17.00 usec
P12 17.00 usec
P12R 17.00 usec
P12M 90.18825531 M
P11M 1.86379410 M
SFO2 125.7878473 MHz

===== GRADIENT CHANNEL =====
GPMAG[1] SINE-100
GPMAG[2] SINE-100
GPMAG[3] SINE-100
GPMAG[4] SINE-100
GP21 50.00 %
GP22 20.10 %
GP23 13.00 %
GP24 5.00 %
P13 500.00 usec

F1 - Acquisition parameters
ID 001 125.788 MHz
FIDRES 98.271851 Hz
SW 200.000 ppm
FWDRES Echo-Antiecho
F2 - Processing parameters
SI 1024
SF 500.2000130 MHz
GB 0 Hz
PC 1.00

F1 - Processing parameters
SI 1024
M22 echo-antiecho
SF 125.7733827 MHz
GB 0 Hz

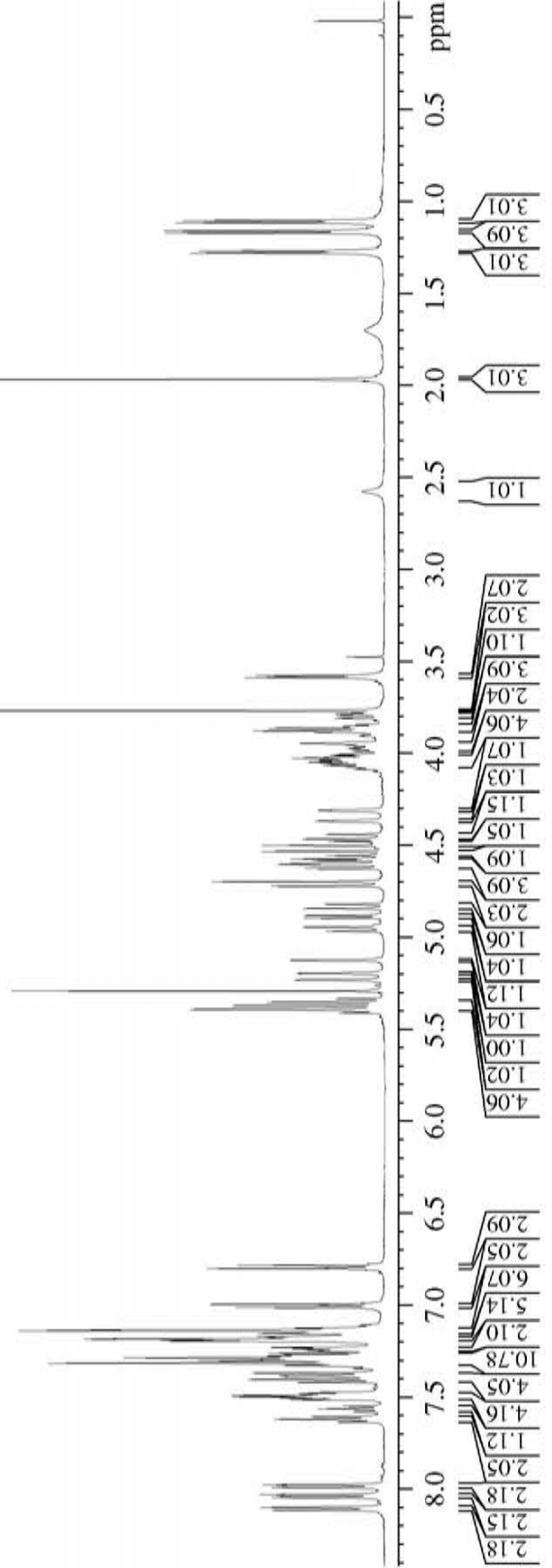
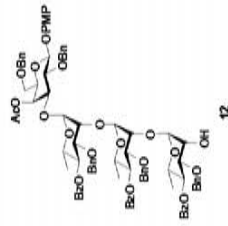




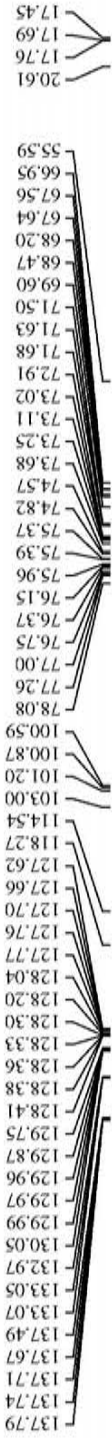
BM-VS-s22 in CDC13

8.112
8.098
8.043
8.029
7.990
7.975
7.496
7.489
7.402
7.367
7.314
7.299
7.295
7.284
7.275
7.260
7.228
7.194
7.189
7.184
7.181
7.174
7.170
7.152
7.137
7.133
7.011
6.993
6.800
6.782
5.389
5.370
5.352
5.290
4.720
4.696
4.531
4.500
3.876
3.862
3.766
3.586
3.574
1.964
1.281
1.269
1.168
1.156
1.113
1.101

Current Data Parameters
 NAME BM-VS-s22
 EXPNO 40
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140805
 Time 12.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 45.2
 DW 48.400 usec
 DE 6.50 usec
 TE 302.1 K
 D1 1.00000000 sec
 TD0 1
 CHANNEL f1
 NUC1 1H
 P1 14.25 usec
 PL1 1.30 dB
 FLLW 15.30635643 W
 SFO1 500.2030889 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.2000166 MHz
 EM
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BM-VS-s22 in CDC13



```

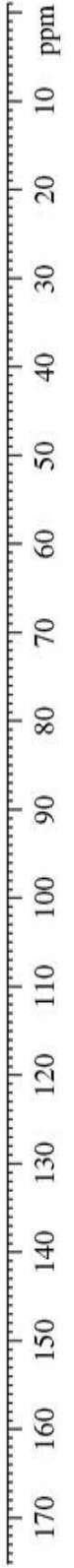
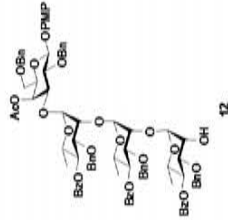
Current Data Parameters
NAME      BM-VS-s22
EXPNO     41
PROCNO    1

F2 - Acquisition Parameters
Date_     20140605
Time      12.15
INSTRUM   spect
PROBHD    5 mm FAPBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         359
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ          1.1010048 sec
RG          203
DW          16.800 usec
DE          6.50 usec
TE          302.7 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

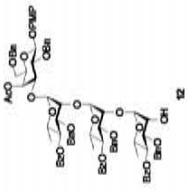
===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        0.150 dB
PL1W       90.18625531 W
SFO1       125.7879676 MHz

===== CHANNEL f2 =====
CDEPRG[2] waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.30 dB
PL12       16.00 dB
PL13       20.00 dB
PL2W       15.30635643 W
PL12W      0.51864696 W
PL13W      0.20647706 W
SFO2       500.2020008 MHz

F2 - Processing parameters
SI         32768
SF         125.7753978 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



BM-VS-s22 in CDCl3



Current Data Parameters
NAME BM-VS-s22
EXPNO 42
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140805
Time 12.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpqr
ID 2048
SOLVENT CDCl3
NS 1
DS 8
SMH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.20498000 sec
RG 45.2
DM 100.000 usec
DE 6.50 usec
TE 302.15 K
D0 0.00000000 sec
D1 1.48683198 sec
D12 0.00000000 sec
D16 0.00000000 sec
INV 0.00019990 sec

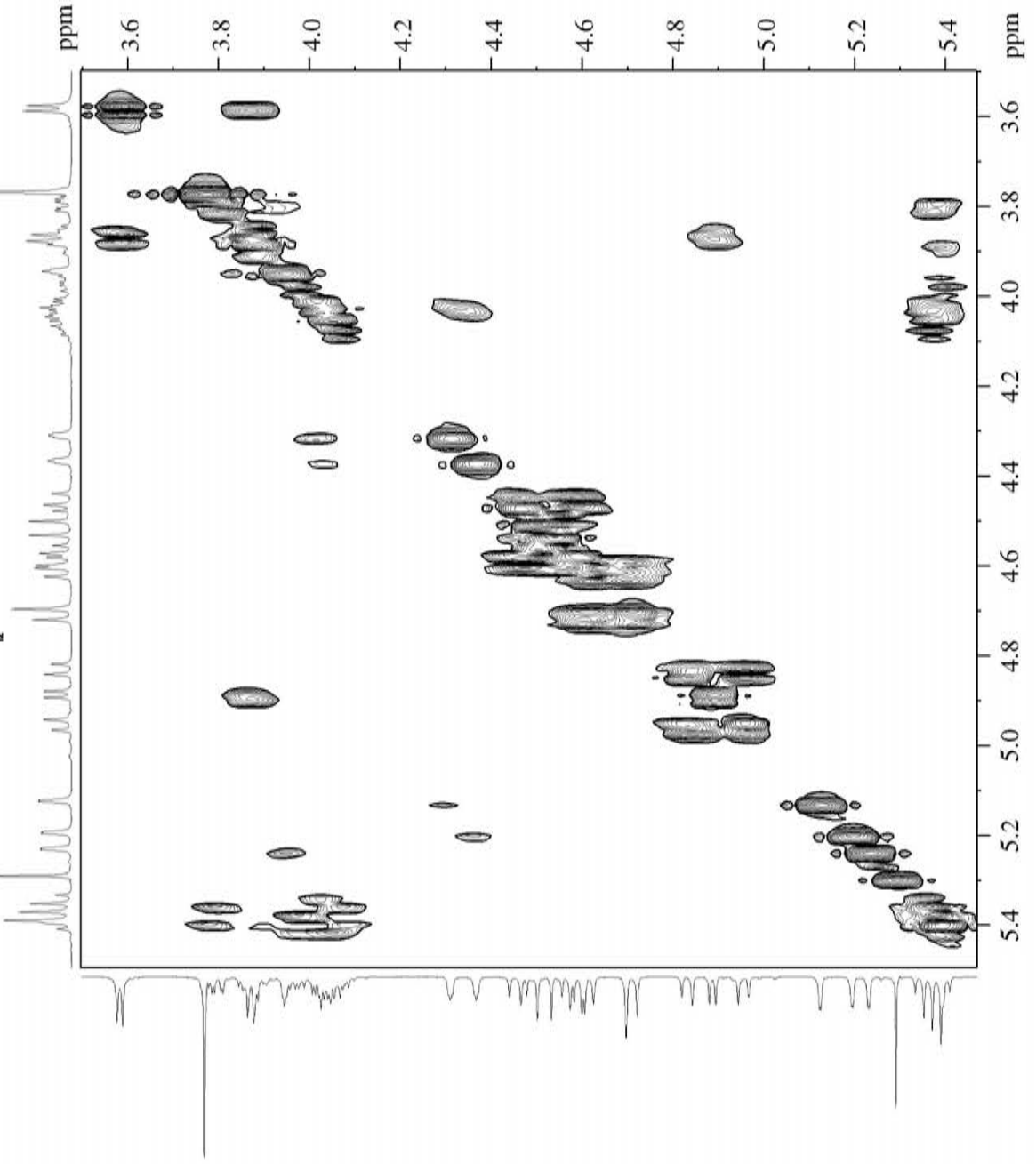
CHANNEL f1
NUC1 1H
P0 14.25 usec
P1 14.25 usec
PL1 1.30 dB
PL1M 15.30635643 W
SFO1 500.2023010 MHz

GRADIENT CHANNEL
GPNAM(1) SINE.100
GP21 10.00 *
p16 1000.00 usec

F1 - Acquisition Parameters
TD 128
SFO1 500.2025 MHz
FIDRES 39.078320 Hz
SH 10.000 ppm
FmMODE CF

F2 - Processing Parameters
SI 1024
SF 500.2000134 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 CF
SF 500.2000136 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



BM-VS-s22 in CDC13
HSQC



Current Data Parameters
NAME: BM-VS-s22
EXPNO: 43
PROCNO: 1

F2 - Acquisition Parameters

Date_ 20140805
Time 12.39
INSTRUM spect
PROBHD 5 mm zgr301
PULPROG zgpg30
TD 1024
SOLVENT CDCl3
DS 4
DE 16
FIDRES 5000.000 Hz
AQ 4.852813 Hz
RG 0.1024000 sec
WDW EM
SSB 0
LB 100.000 usec
GB 6.50 usec
TR 302.0 K
CRST2 145.000000 sec
D0 1.50000000 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D12 0.00004000 sec
D13 0.03000000 sec
D14 0.00066207 sec
D15 0.00001985 sec
ZDELTA 0

***** CHANNEL f1 *****

NUC1 1H
P1 14.25 usec
F2 28.50 usec
P3 1.50 usec
F4 1.50 usec
P5 1.50 usec
F5 15.30435643 W
SF01 500.2025010 MHz
***** CHANNEL f2 *****
CPDPRG2 zgpg
NUC2 13C
P3 9.50 usec
F4 19.00 usec
P5 19.00 usec
F5 -20.50 usec
P6 17.00 usec
F6 17.00 usec
P7 90.18825531 W
F8 11.60379910 W
SF02 125.7679715 MHz
***** GRADIENT CHANNEL *****
GPM11 SINE.100
GPM12 SINE.100
GPM13 SINE.100
GPM14 SINE.100
GPM15 SINE.100
GPR1 80.00 %
GPR2 50.10 %
GPR3 15.00 %
GPR4 15.00 %
P18 1000.00 usec
P19 600.00 usec

F1 - Acquisition Parameters

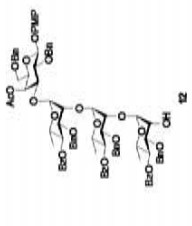
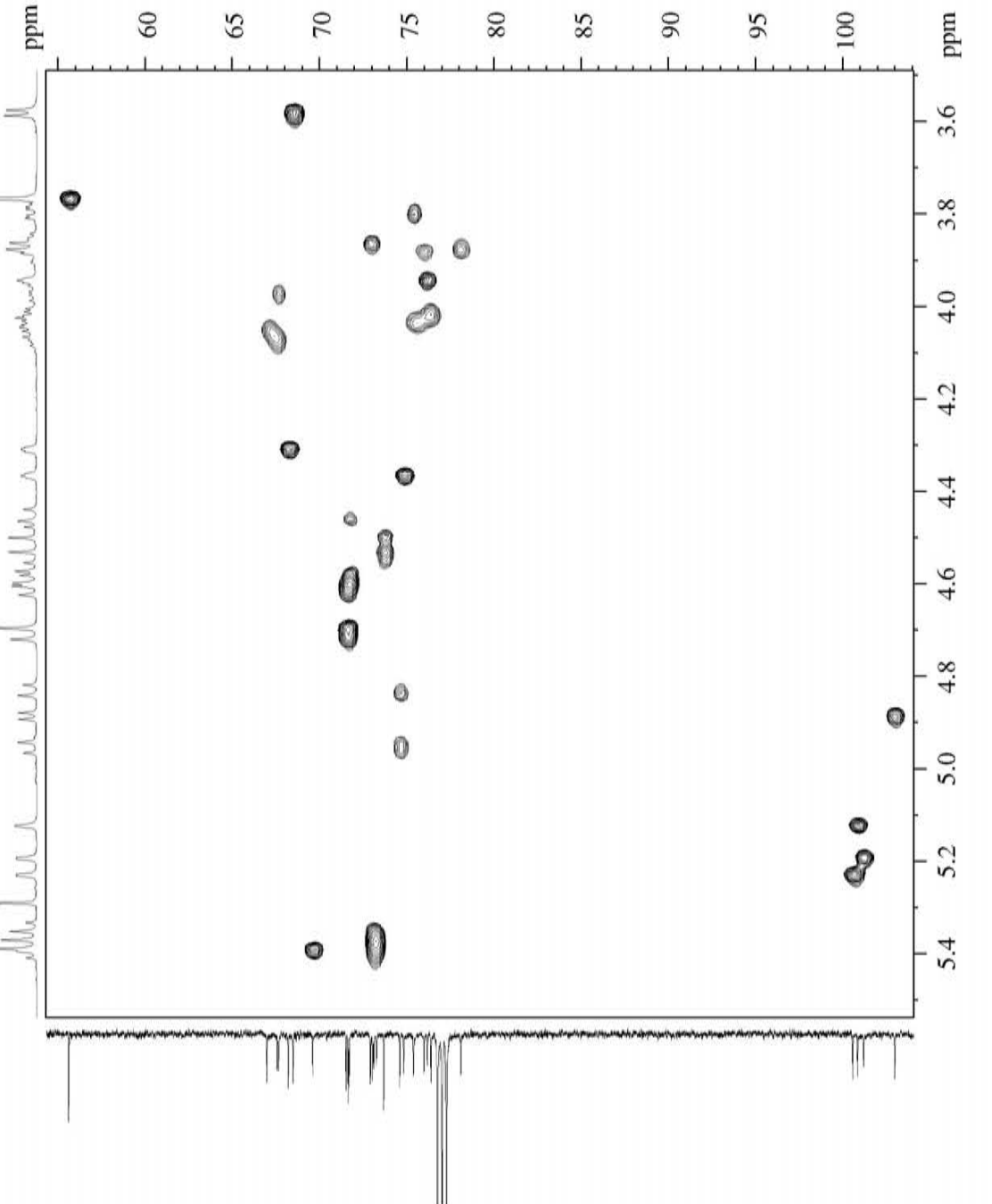
TD 256
SF01 125.768 MHz
FIDRES 98.271851 Hz
WDW EM
SSB 0
LB 0 Hz
GB 0

F2 - Processing parameters

SI 1024
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
WDW EM
SSB 0
LB 0 Hz
GB 0

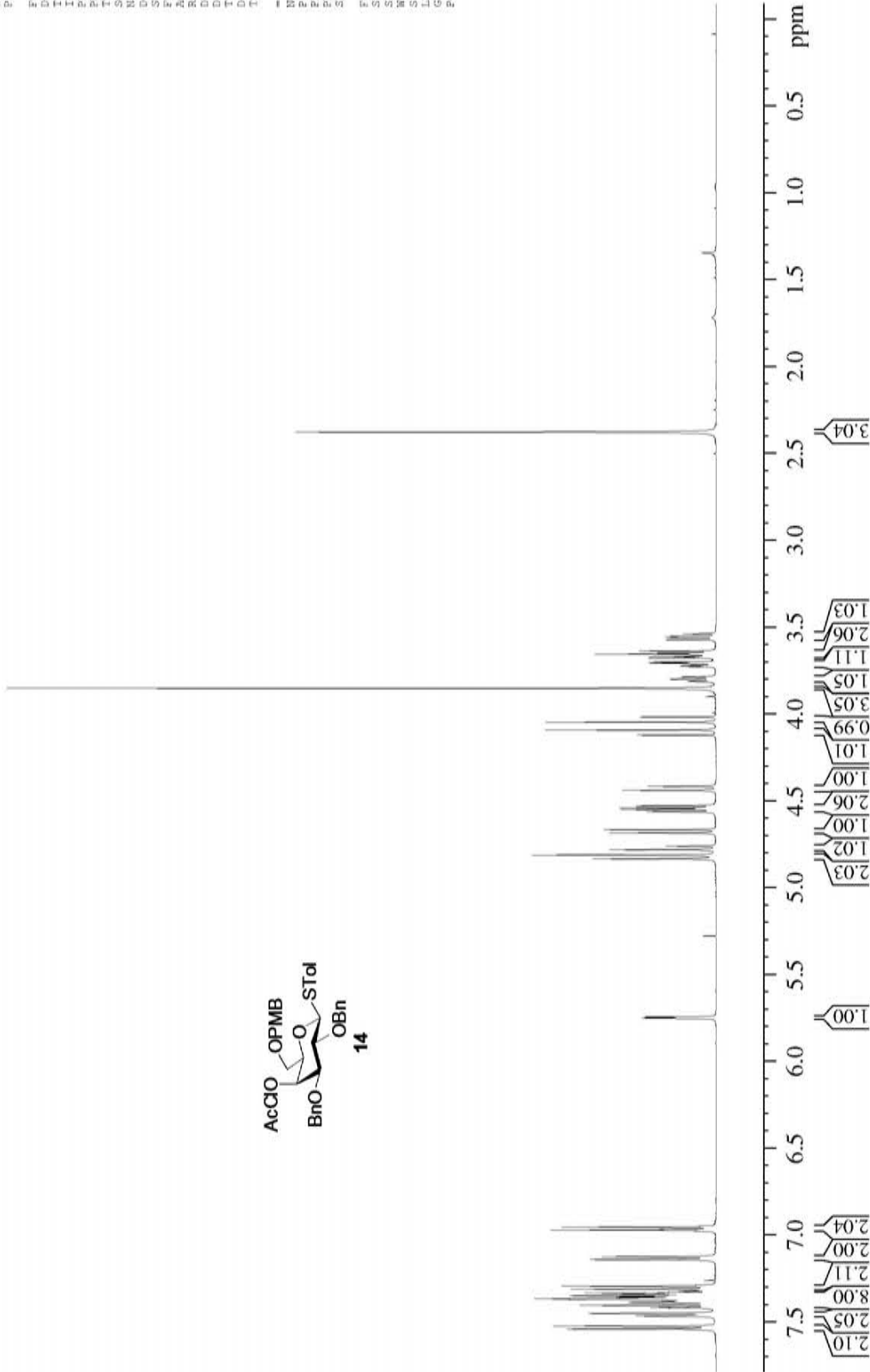
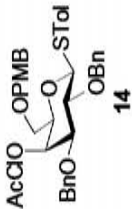


BM-VS-s24 in CDCl3

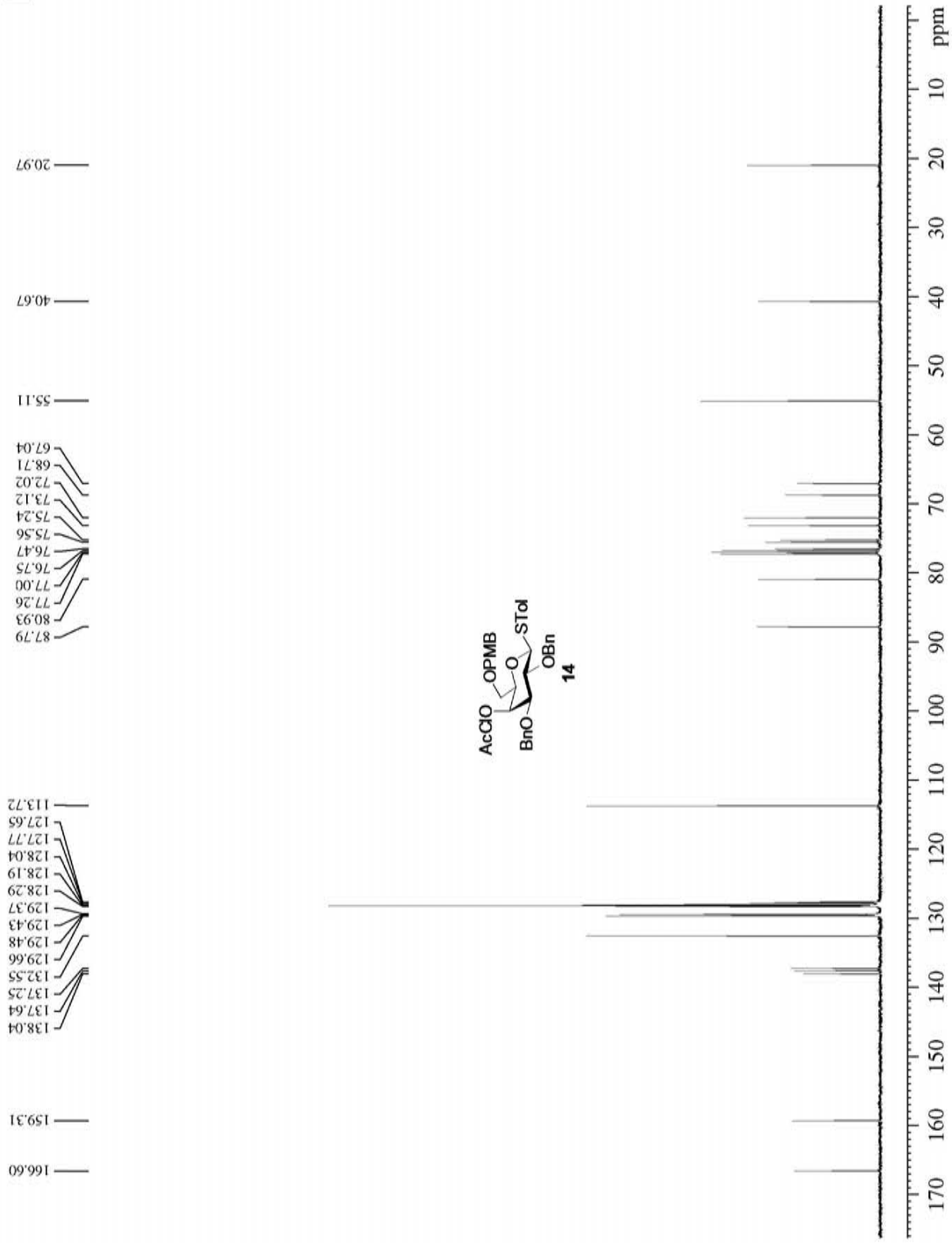


7.540
7.524
7.466
7.464
7.450
7.416
7.402
7.399
7.387
7.380
7.371
7.368
7.365
7.360
7.354
7.348
7.344
7.338
7.333
7.329
7.310
7.293
7.140
7.124
6.970
6.953
5.749
5.743
4.832
4.810
4.779
4.683
4.664
4.561
4.547
4.538
4.526
4.437
4.414
4.120
4.090
4.045
4.015
3.849
3.706
3.700
3.673
3.654
3.647
3.636
2.374

Current Data Parameters
 NAME BM-VS-s24
 ACQNO 40
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140902
 Time 14.00
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 EQ 10330.572
 FIDRES 0.137832 Hz
 AQ 3.1719425 sec
 RG 22.6
 DW 48.400 usec
 DE 6.50 usec
 TE 301.3 K
 D1 1.00000000 sec
 TD0 1
 ----- CHANNEL f1 -----
 NUC1 1H
 P1 14.25 usec
 PL1 0.00
 FLN 15.30635440 MHz
 SFO1 500.2030689 MHz
 F2 - Processing Parameters
 SI 32768
 SF 500.2000163 MHz
 NLW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BM-VS-s24 in CDC13



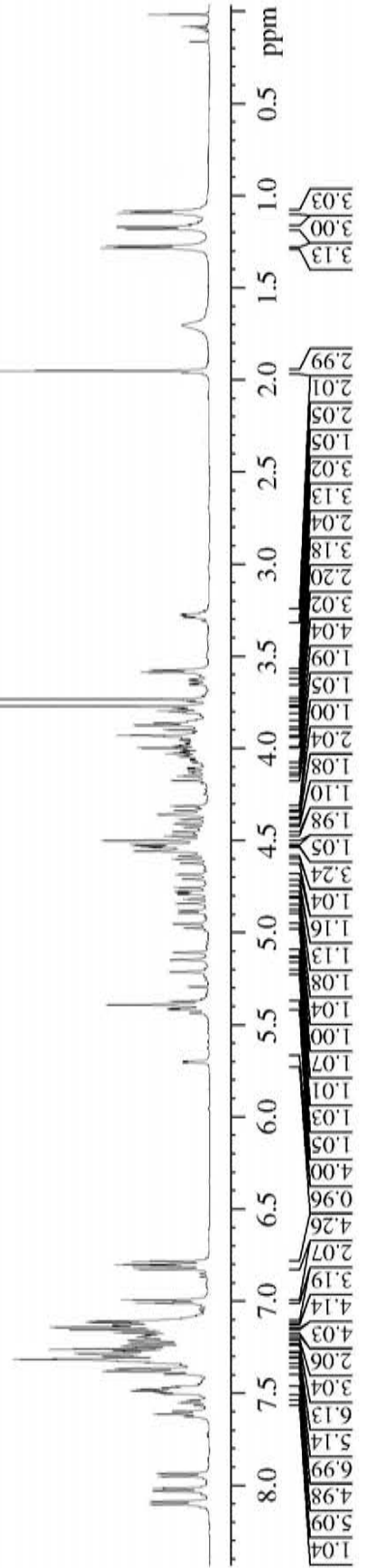
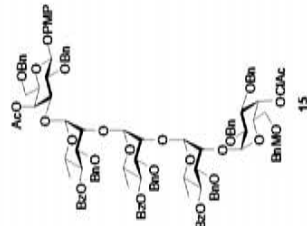
Current Data Parameters
NAME BM-VS-s24
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160902
Time 14:03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 71
DS 4
SWE 25761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DM 16.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL F1
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
PL1W 90.18625531 W
SF01 125.7679676 MHz
CHANNEL F2
CPCPRG12 waltz16
NUC2 1H
P2 80.00 usec
PL2 1.00 dB
PL2W 0.00000000 W
PL3 20.00 dB
PL3W 15.30635643 W
PL12N 0.51864696 M
PL13N 0.20647706 M
SF02 500.2620008 MHz
F2 - Processing parameters
SI 32768
SF 125.7754214 MHz
WDW EM
SSS 0
LB 0
GB 0
PC 1.40

BM-VS-s25r in CDCl3

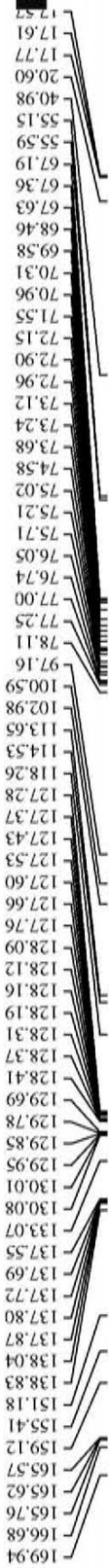


7.486
7.478
7.380
7.365
7.325
7.315
7.312
7.301
7.299
7.295
7.287
7.284
7.272
7.268
7.260
7.253
7.244
7.229
7.214
7.211
7.194
7.172
7.155
7.141
7.133
7.129
7.116
7.108
7.011
6.783
6.801
6.808
6.826
6.826
6.993
6.993
3.928
3.873
3.770
3.731
1.949
1.285
1.273
1.180
1.167
1.093
1.081

Current Data Parameters
 NAME BM-VS-s25
 EXPNO 20
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140904
 Time 10:36
 INSTRUM Spect
 PROBED 5 mm PABBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 10330.578 Hz
 SFO 0.157632 Hz
 FIDRES 3.1719425 sec
 AQ 45.2
 DW 48.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 D10
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 14.25 usec
 PL1 1.30 dB
 PL1W 15.30635643 W
 SF01 500.2030889 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.200159 MHz
 WGM 5M
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BM-VS-s25r in CDCl3



```

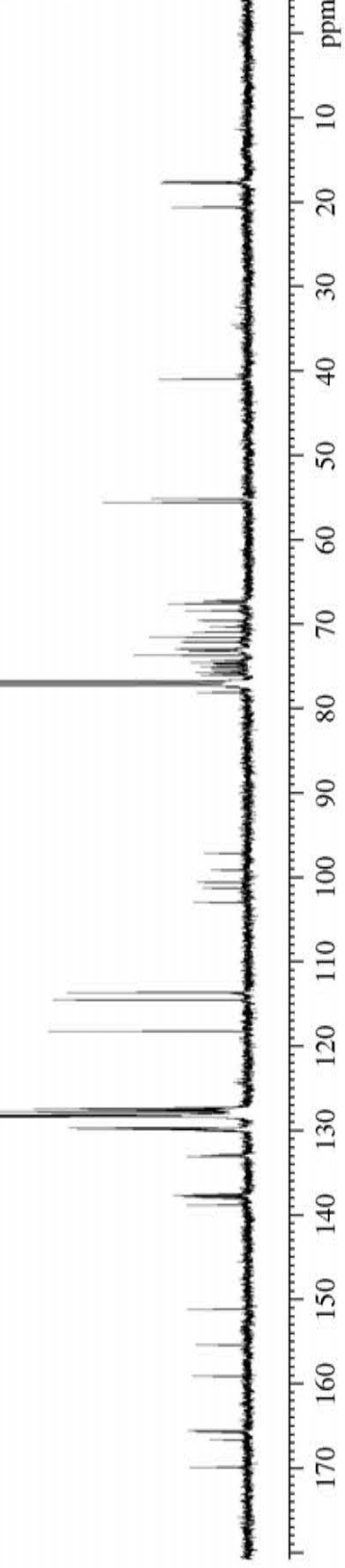
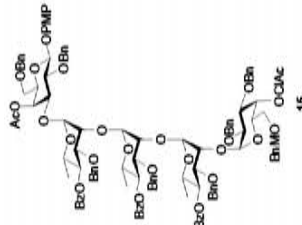
Current Data Parameters
NAME      BM-VS-s25
EXPNO    23
PROCNO   1

F2 - Acquisition Parameters
Date_    20140904
Time     10.58
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       65536
SOLVENT CDCl3
NS       1024
DS       4
SWH      29761.904 Hz
FIDRES   0.454131 Hz
AQ       1.1010048 sec
RG       203
DM       16.000 usec
DE       6.50 usec
HE       300.42 K
H1       2.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1      -0.50 dB
PL12     90.18825531 W
PL13     125.7879676 MHz
SF01

===== CHANNEL f2 =====
CPDPRG2  wait16
NUC2      1H
PCPD2    80.00 usec
PL2      1.30 dB
PL12     16.00 dB
PL13     20.00 dB
PL14     15.30635643 W
PL15     0.51864696 W
PL16     0.20647706 W
SF02     500.2020008 MHz

F2 - Processing parameters
SI        32768
SF        125.7753975 MHz
MORF      EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```



BM-VS-s25r in CDCl3



Current Data Parameters
 NAME BM-VS-s25
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140904
 Time_ 10.37
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG cosygpgf
 TD 2048
 SOLVENT CDCl3
 NS 1
 DS 8
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048000 sec
 RG 45.2
 DW 100.000 usec
 DE 6.50 usec
 TE 298.3 K
 D0 0.00000300 sec
 D1 1.4868198 sec
 D13 0.00000400 sec
 D16 0.0002000 sec
 INO 0.00019990 sec

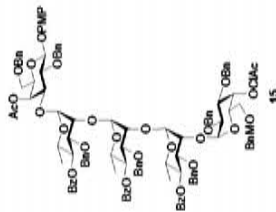
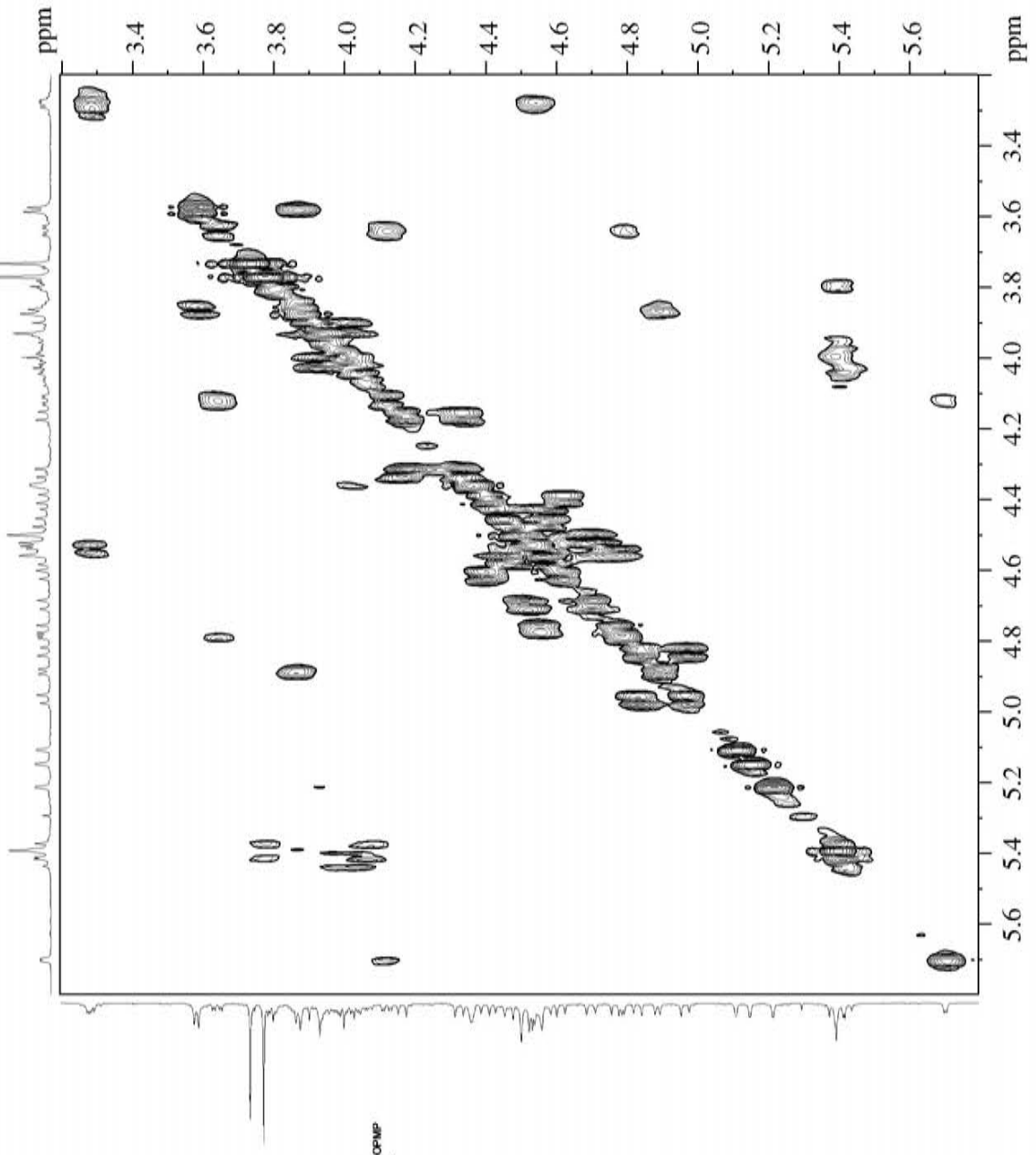
CHANNEL f1
 NUC1 1H
 P0 14.25 usec
 P1 14.25 usec
 P11 14.25 usec
 P12 1.30 dB
 P13 15.30635643 W
 SFO1 500.2025010 MHz

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

F1 - Acquisition parameters
 TD 128
 SF01 500.2025 MHz
 FIDRES 39.078320 Hz
 SW 10.000 ppm
 ENMODE QF

F2 - Processing parameters
 SI 1024
 SF 500.2000150 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.2000144 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0



BM-VS-s25r in CDCl3
HSQCGP



Current Data Parameters
 NAME BM-VS-s25
 EXPRNO 22
 PROCNO 1

F1 - Acquisition Parameters
 Date_ 20140904
 Time 10:43
 INSTRUM spect
 PROBHD 5 mm F4001 BBO
 PULPROG zgpg30
 TD 1024
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 5000.000 Hz
 FIDRES 4.862813 Hz
 AQ 0.1024000 sec
 RG 451.2
 DW 100.000 usec
 DE 1.500 usec
 TE 293.2 K
 CHST2 145.0000000
 D0 0.0000300 sec
 D1 1.0000000 sec
 D4 0.0017244 sec
 D11 0.0300000 sec
 D13 0.0000400 sec
 D16 0.0002000 sec
 D18 0.0000000 sec
 D19 0.0001585 sec
 D20 0.0001585 sec
 SCANS 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.25 usec
 P2 28.50 usec
 P3 0.10 usec
 PL1 0.00 dB
 PL2 15.7063530 dB
 PL3 0.00 dB
 SFO1 500.2625010 MHz

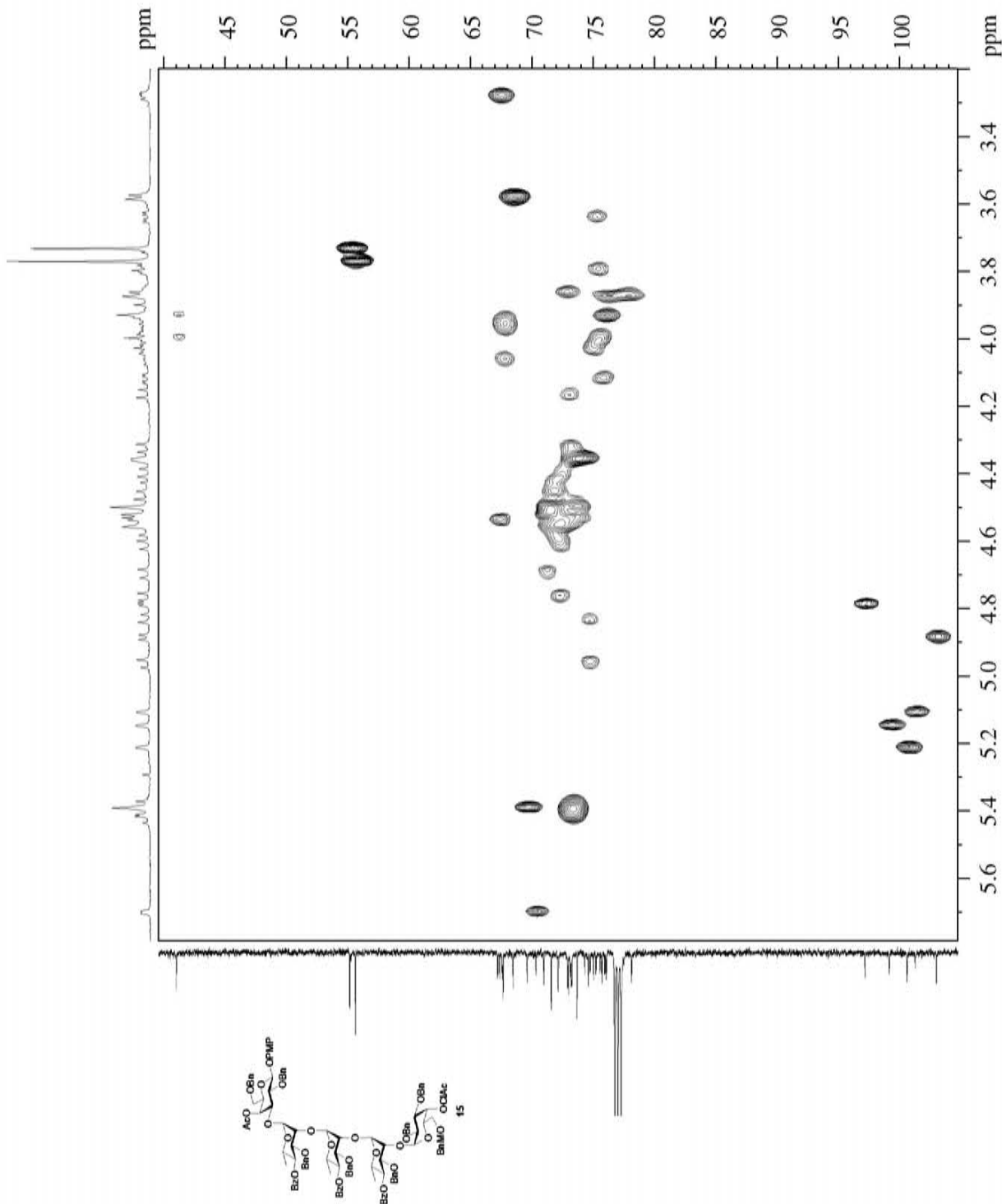
===== CHANNEL f2 =====
 NUC2 13C
 P3 9.50 usec
 P4 19.00 usec
 PCPD2 70.00 usec
 PL1 0.00 dB
 PL2 17.00 dB
 PL3 0.00 dB
 PL4 90.1824531 W
 PL12W 1.6037310 W
 SFO2 125.7673475 MHz

===== GRADIENT CHANNEL =====
 GPRAM(1) SINE.100
 GPRAM(2) SINE.100
 GPRAM(3) SINE.100
 GPRAM(4) SINE.100
 GRD1 80.00 %
 GRD2 20.10 %
 GRD3 11.00 %
 GRD4 5.00 %
 GRD5 100.00 usec
 GRD6 500.00 usec

F1 - Acquisition parameters
 SI 1024
 SF 500.1362795 MHz
 FIDRES 222.633575 Hz
 SFO 500.1362795 MHz
 PULPROG zgpg30
 ECHO antiecho

F2 - Processing parameters
 SI 1024
 SF 125.7673475 MHz
 WDW EM
 SSB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 echo-antiecho
 SF 125.7673475 MHz
 WDW EM
 SSB 0 Hz
 GB 0

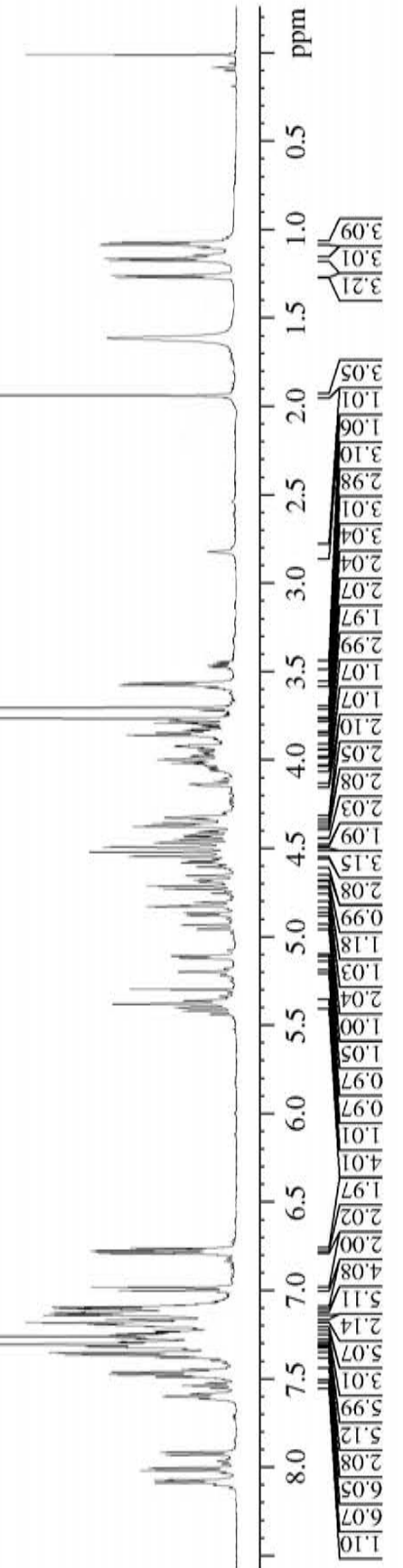
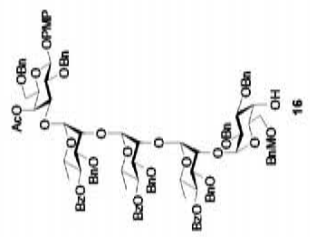


BM-VS-s26 in CDCl3

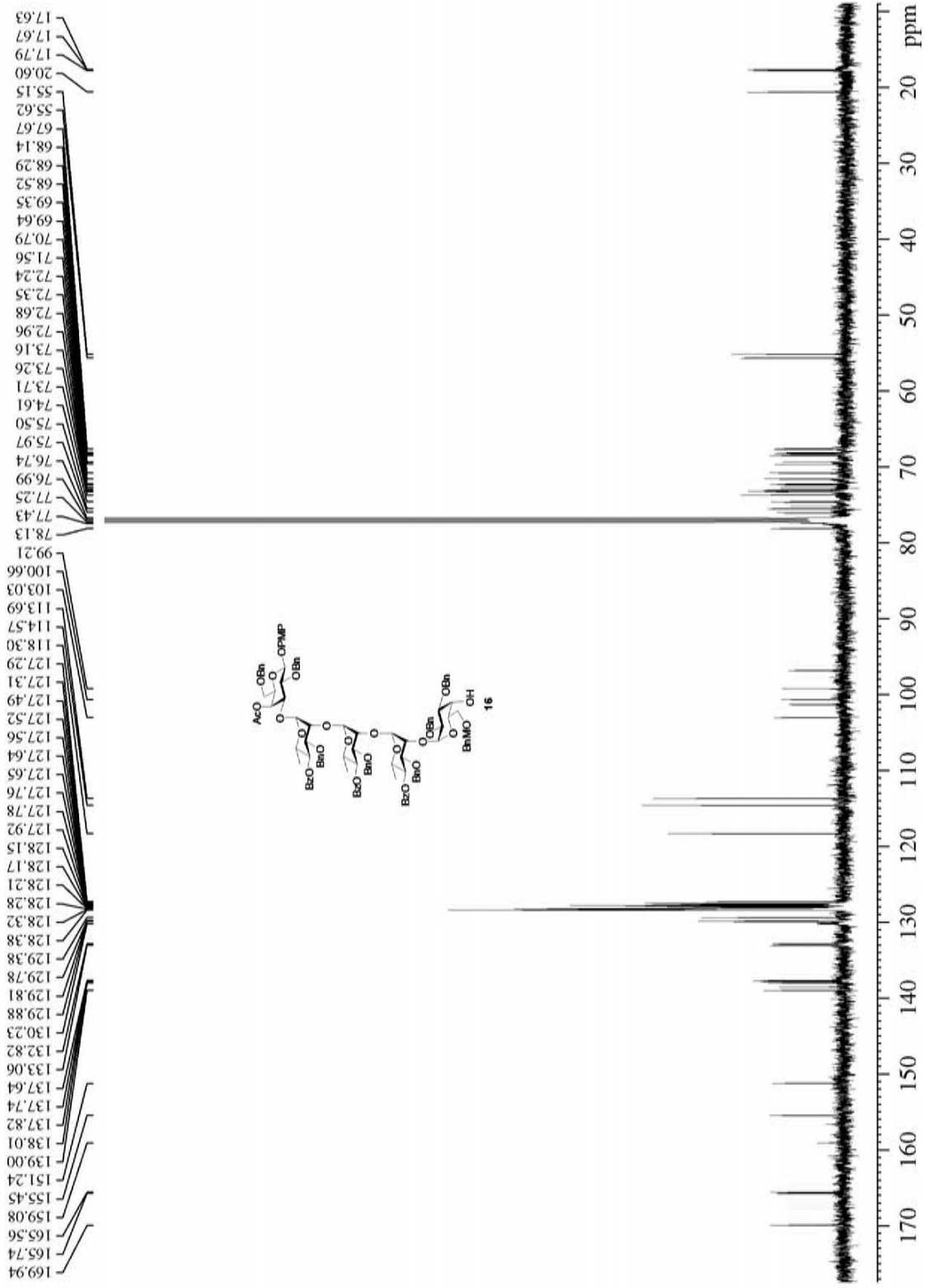


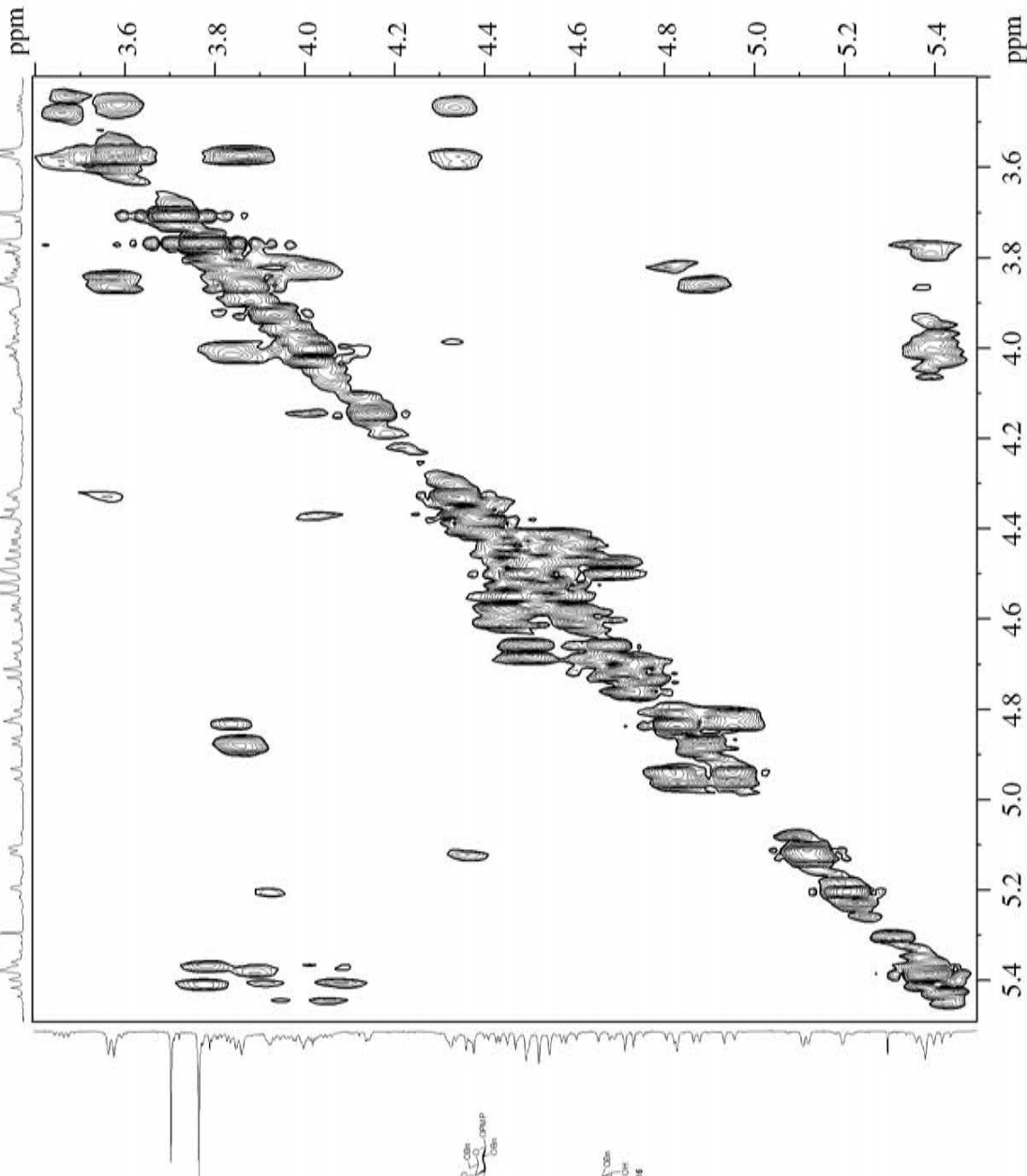
Current Data Parameters
 NAME BM-VS-s26
 EXPNO 60
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140908
 Time 16:34
 INSTRUM spect
 PROBED 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.171945 sec
 RQ 0.0444
 DN 48.400 usec
 DE 6.50 usec
 TE 303.1 K
 D1 1.0000000 sec
 IDU 1
 CHANNEL f1
 NUC1 1H
 P1 14.25 usec
 PL1 1.30 dB
 PLL 15.30635643 W
 SFO1 500.2030689 MHz
 F2 - Processing parameters
 SI 32768
 SF 506.2000169 MHz
 NCMF EM
 SSB 0
 LB 0
 GB 0
 PC 1.00

7.474
7.461
7.364
7.351
7.317
7.304
7.301
7.291
7.288
7.266
7.260
7.251
7.244
7.191
7.182
7.164
7.140
7.135
7.126
7.121
7.107
7.104
7.100
7.094
7.091
6.999
6.981
6.790
6.777
6.772
6.760
5.379
5.295
4.543
4.519
4.490
4.374
3.857
3.763
3.700
3.573
3.561
1.935
1.274
1.266
1.265
1.173
1.160
1.081
1.069



BM-VS-s26 in CDCl3





```

Current Data Parameters
NAME      BM-VS-s26
EXPNO    61
PROCNO   1

F2 - Acquisition Parameters
Date_    20140908
Time     15.35
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  cosygpgr
TD        2048
SOLVENT  CDC13
NS        1
DS        8
SMH       5000.000 Hz
FIDRES   2.441406 Hz
AQ        0.2048000 sec
RG        144
FW        100.000 usec
DE        6.50 usec
TE        303.1 K
D0        0.00000300 sec
D1        1.48689199 sec
D13       0.00000400 sec
D16       0.00020000 sec
INO       0.00019990 sec

===== CHANNEL f1 =====
NUC1      1H
P0        14.25 usec
P1        14.25 usec
P2        14.25 usec
PL1       1.30 dB
PL2       1.30 dB
PL12      15.30635643 W
SF01      500.2025010 MHz

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

F1 - Acquisition parameters
TD        128
SF01      500.2025 MHz
FIDRES   39.076320 Hz
SW        10.000 ppm
ENHMODE   QF

F2 - Processing parameters
SI        1024
SF        500.2000126 MHz
WDW       SINE
SSB       0
LB        0 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
MC2       QF
SF        500.2000131 MHz
WDW       SINE
SSB       0
LB        0 Hz
GB        0
    
```

BM-VS-s26 in CDC13
HSQCGP

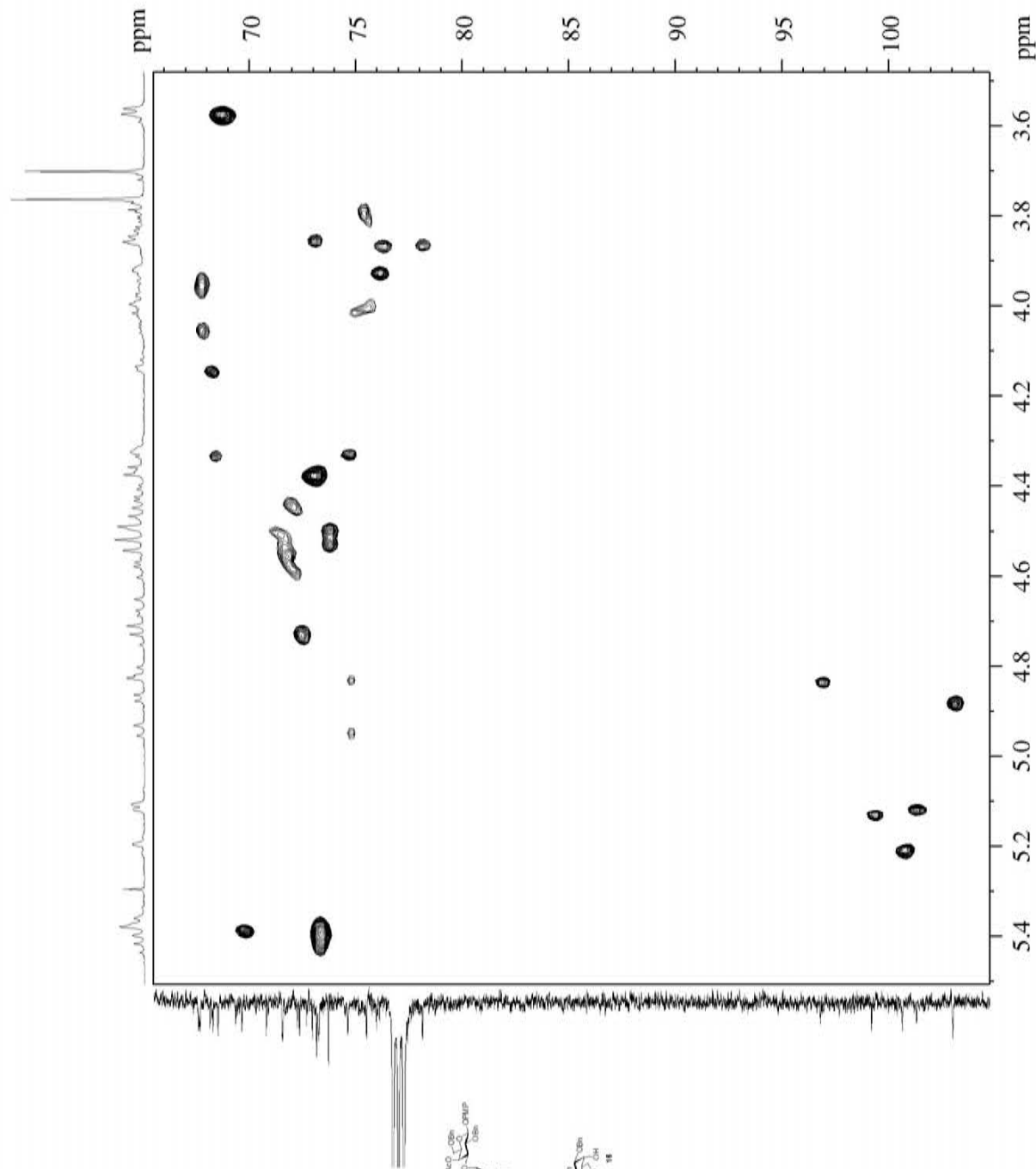


Current Data Parameters
NAME BM-VS-s26
EXPNO 62
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140906
Time 16:40
INSTRUM spect
PULPROG zgpg30
PROCNO 1
TD 1024
SOLVENT CDC13
DS 4
DS2 1
DS3 1
SFO1 500.0000 MHz
F1RES 4.882813 Hz
AQ 0.1024000 sec
RG 327.5
WM 100.000 usec
WB 6.50 usec
TE 303.2 K
CRST2 145.000000 sec
DE 1.00000000
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000000 sec
D15 0.00000000 sec
D24 0.0006207 sec
INVO 0.00001583 sec
EXORF2S

===== CHANNEL f1 =====
NUC1 1H
P1 14.23 usec
P2 28.50 usec
P3 1.0 usec
P4 1.0 usec
P11M 15.365543 M
SFO1 500.0025010 MHz
===== CHANNEL f2 =====
CPDPRG2 gpcp
NUC2 13C
P3 9.50 usec
P4 19.00 usec
P5 9.50 usec
P6 20.50 usec
P11 1.00 usec
P112 17.00 usec
P12W 90.18825531 M
P13W 1.0319910 M
SFO2 125.7697675 MHz

===== GRADIENT CHANNEL =====
GPMN[1] SINE-100
GPMN[2] SINE-100
GPMN[3] SINE-100
GPMN[4] SINE-100
GR21 80.00 %
GR22 20.10 %
GR23 14.90 %
GR24 4.00 %
P15 1000.00 usec
P16 600.00 usec
P17 600.00 usec
F1 - Acquisition parameters
TD 256
SFO1 125.768 MHz
F1RES 98.271853 Hz
AQ 200.000 ppm
PULPROG Echo-AnticHo
F2 - Processing parameters
SI 1024
SF 500.0000112 MHz
WDW EM
SSB 0 Hz
L8 0 Hz
L9 1.00
F1 - Processing parameters
SI 1024
SF 125.7700000 MHz
WDW EM
SSB 0 Hz
L8 0 Hz
L9 0





BM-VS-s28 in CDCl3

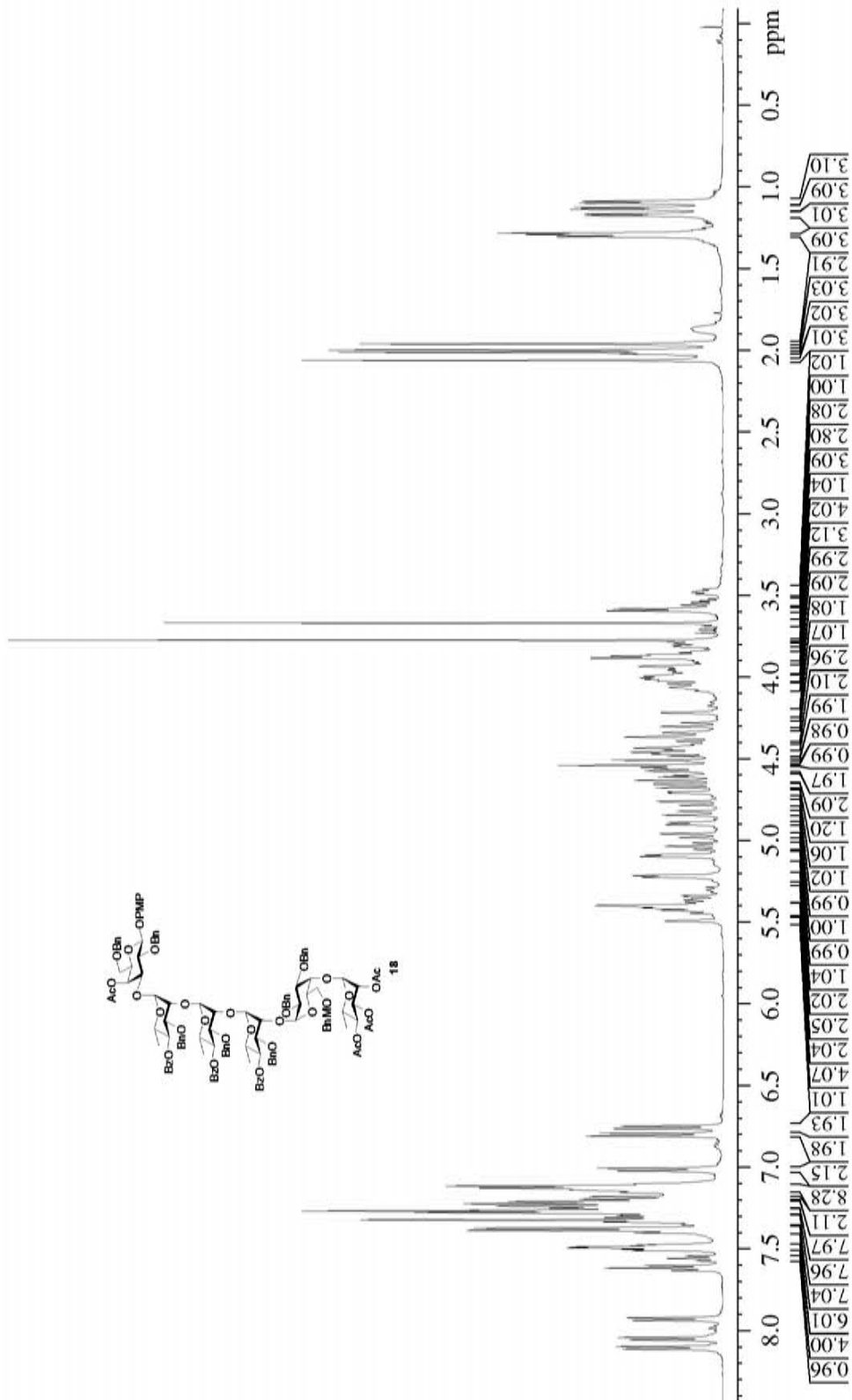
8.097
8.041
7.616
7.493
7.487
7.385
7.371
7.333
7.322
7.308
7.296
7.277
7.267
7.260
7.249
7.237
7.222
7.209
7.195
7.179
7.136
7.126
7.115
7.023
7.005
6.809
6.791
6.763
5.396
4.538
4.506
3.882
3.870
3.773
3.667
3.594
3.582
2.060
2.011
1.997
1.959
1.302
1.290
1.174
1.162
1.135
1.123
1.097
1.085

Current Data Parameters
 NAME BM-VS-s28
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180915
 Time 10:38
 INSTRUM spect
 PROBRD 5 mm PABBO-SE
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 36
 DW 48.400 usec
 DE 6.50 usec
 TE 296.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.25 usec
 PL1 1.30 dB
 PL1W 15.30635643 W
 SF01 500.2330891 MHz

F2 - Processing parameters
 SI 32768
 SF 500.2300153 MHz
 SW 0
 SE 0
 LB 0.30 Hz
 GB 0
 PC 1.00



0.96
4.00
6.01
7.04
7.96
7.97
8.28
2.15
1.98
1.93
1.01
4.07
2.04
2.05
2.02
1.04
0.99
1.00
0.99
1.02
1.06
1.20
2.09
1.97
0.99
0.98
1.99
2.10
2.96
1.07
1.08
2.09
2.99
3.12
4.02
1.04
3.09
2.80
2.08
1.00
1.02
3.01
3.02
3.03
2.91
3.09
3.01
3.01
3.09
3.10

BM-VS-s28 in CDCl3



170.00
169.91
169.72
169.54
165.53
158.91
155.35
151.15
138.96
138.47
137.94
137.74
137.65
137.47
133.04
129.97
129.83
129.79
129.21
128.44
128.37
128.34
128.27
128.19
128.15
128.12
128.10
128.06
127.78
127.74
127.72
127.70
127.62
127.51
127.23
127.09
118.21
114.48
113.54
102.93
98.61
87.08
78.08
77.25
76.99
76.74
76.04
74.58
73.64
73.06
72.87
72.74
72.55
71.64
71.47
70.36
69.72
69.55
69.38
68.43
67.53
55.55
55.02
20.81
20.78
20.73
20.57
17.75
17.61
17.57
17.40

```

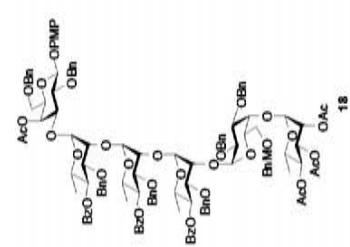
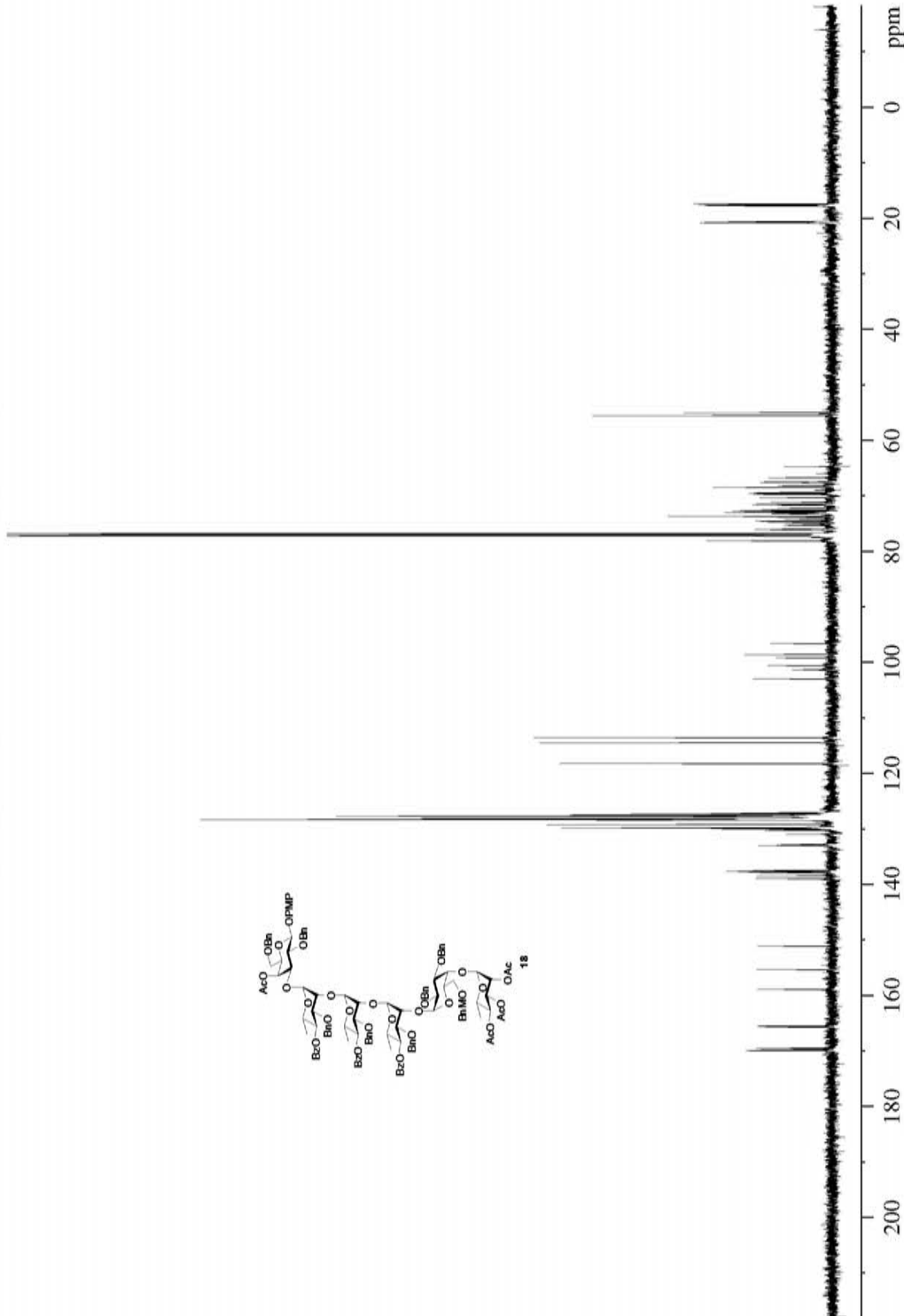
Current Data Parameters
Name      BM-VS-s28
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20140915
Time     10.41
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        651
DS        4
SWH       25761.904 Hz
FIDRES    0.454131 Hz
AQ         1.1010048 sec
RG         203
DW         16.800 usec
DE         6.50 usec
TE        300.2 K
D1         2.0000000 sec
d11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
PL12      90.1825531 W
SFO1      125.7625000 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
P2        80.00 usec
PL2       1.30 dB
PL12      16.00 dB
PL13      20.00 dB
PL14      15.30635643 W
PL15      0.51064596 W
PL16      0.27570000 W
SFO2      500.2320009 MHz

F2 - Processing parameters
SI        32768
SF        125.7625000 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



18

BM-VS-s28 in CDC13



Current Data Parameters
 NAME BM-VS-s28
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140315
 Time 11.16
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG cosygpozf
 TD 2048
 SOLVENT CDC13
 NS 1
 DS 8
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048000 sec
 RG 36
 LW 100.000 usec
 DE 6.50 usec
 TE 298.2 K
 DO 0.00000300 sec
 D1 1.48889198 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INU 0.00019990 sec

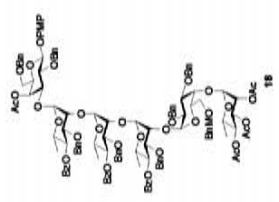
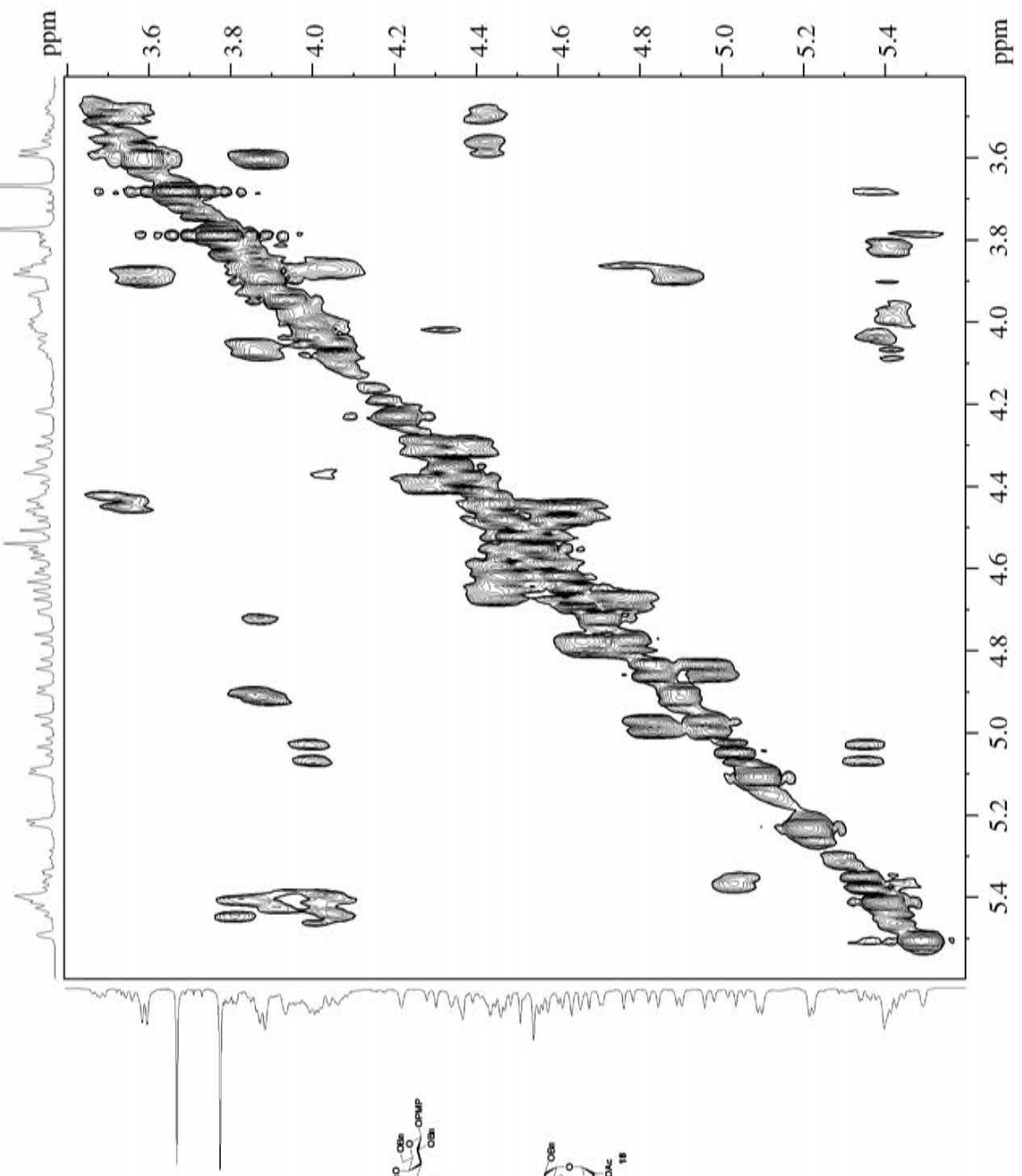
===== CHANNEL f1 =====
 NUC1 1H
 P0 14.25 usec
 PL 14.25 usec
 PL1 1.30 dB
 PL1W 15.30635643 W
 SF01 500.2325012 MHz

===== GRADIENT CHANNEL =====
 GENAM[L] SINE.100
 GPZ1 10.00 %
 PL6 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SF01 500.2325 MHz
 FIDRES 39.080666 Hz
 SW 10.000 ppm
 FWHODE QF

F2 - Processing parameters
 SI 1024
 SF 500.2300098 MHz
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 OF
 SF 500.2300144 MHz
 SSB 0
 LB 0 Hz
 GB 0



BM-VS-s28 in CDC13
HSQC



Current Data Parameters
NAME: BM-VS-s28
EXPNO: 13
PROCNO: 1

F2 - Acquisition Parameters
Date_ 20140915
Time: 11.21

PROBHD 5 mm pspc-1
PULPROG waqzgpg12
TD 1024
SOLVENT CDC13
DS 16
SWH 5000.0000 Hz
FIDRES 4.882813 Hz
AQ 0.1024000 sec
RG 655
IN 180.000 usec
DE 6.50 usec
TE 297.8 K
CHST2 145.000000 sec
D3 1.50000000 sec
D4 0.0017244 sec
D11 0.03000000 sec
D13 0.00000000 sec
D14 0.00000000 sec
D24 0.00084207 sec
IND 0.00001395 sec
SCOPYING

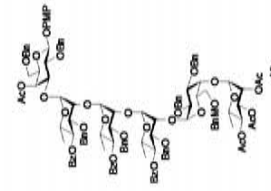
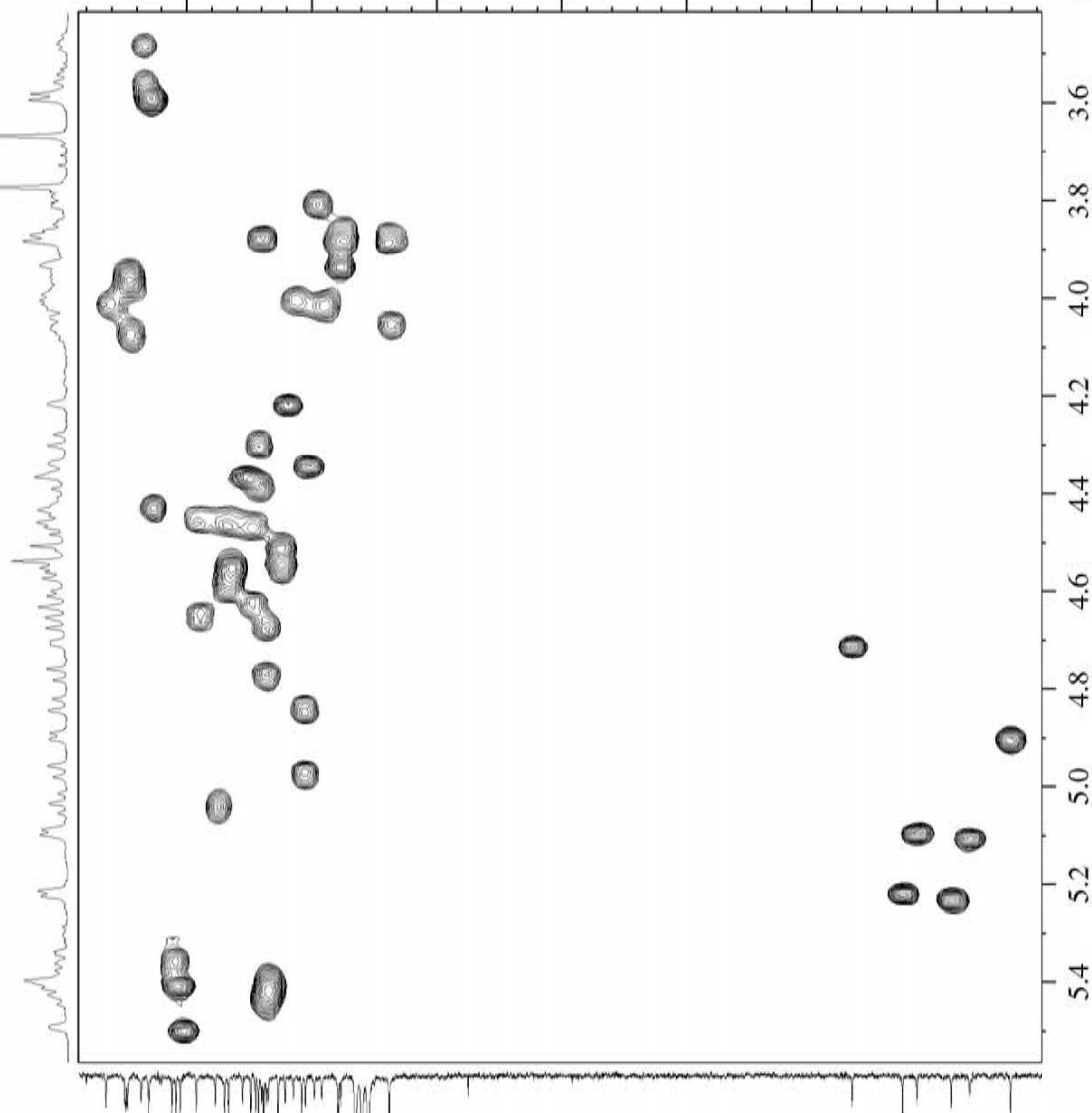
===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PC 28.20 usec
PL1 0.00 dB
PL2 0.00 dB
PL3 1.10 dB
PL4 1.10 dB
PL1W 15.30435443 W
SFO1 500.2325012 MHz

===== CHANNEL f2 =====
CPDPRG2 gcp
NUC2 13C
P2 5.50 usec
PC 19.00 usec
PL2 0.00 dB
PL3 -0.20 dB
PL4 -0.20 dB
PL12 17.00 dB
PL2W 90.1882531 W
PL3W 1.60379910 W
SFO2 125.7625012 MHz

===== GRADIENT CHANNEL =====
GPRM[1] SINE.100
GPRM[2] SINE.100
GPRM[3] SINE.100
GPRM[4] SINE.100
GPRM[5] SINE.100
GPRM[6] SINE.100
GPRM[7] SINE.100
GPRM[8] SINE.100
GPRM[9] SINE.100
GPRM[10] SINE.100
GPRM[11] SINE.100
GPRM[12] SINE.100
GPRM[13] SINE.100
GPRM[14] SINE.100
GPRM[15] SINE.100
GPRM[16] SINE.100
GPRM[17] SINE.100
GPRM[18] SINE.100
GPRM[19] SINE.100
GPRM[20] SINE.100

F1 - Acquisition parameters
TD 256
SFO1 125.7355 MHz
SFO2 500.2325012 MHz
FIDRES 98.277740 Hz
SW 200.0000 PPM
F2 - Processing parameters
SI 1024
SF 500.2500118 MHz
WDW 60112
SSB 0 Hz
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
SF 125.7625012 MHz
WDW 60112
SSB 0 Hz
LB 0 Hz
GB 0
PC 1.40



BM-VS-s29 in CDC13



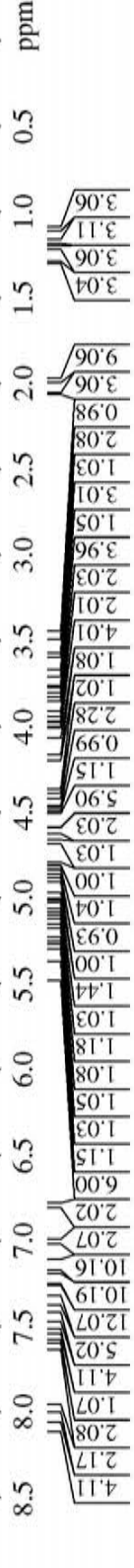
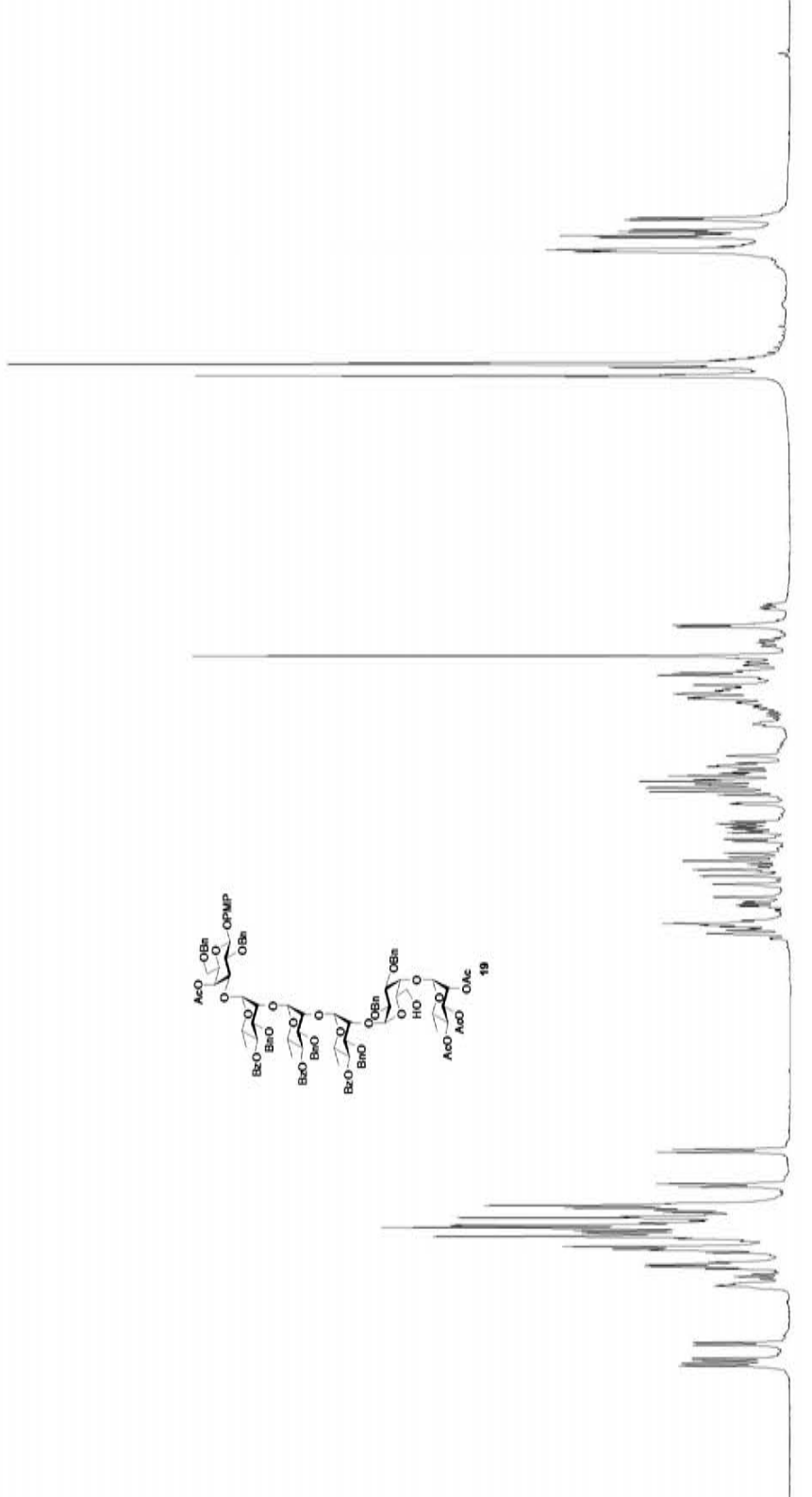
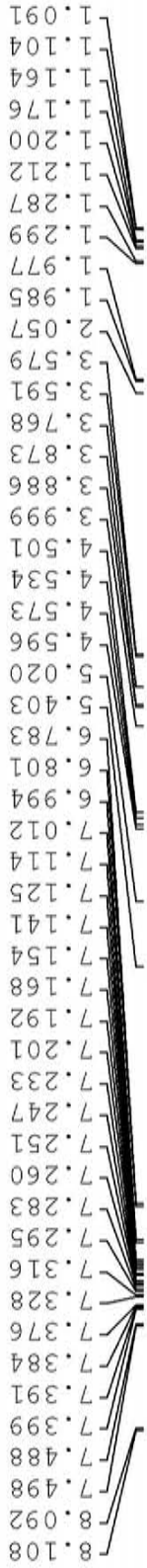
```

Current Data Parameters
NAME: BM-VS-s29
EXPNO: 70
PROCNO: 1

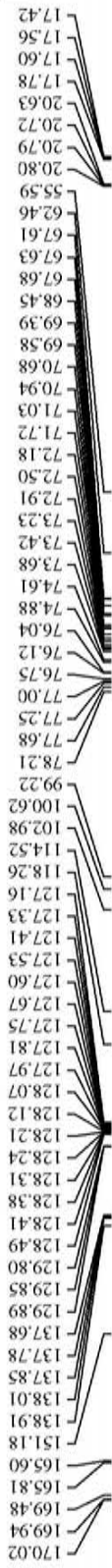
F2 - Acquisition Parameters
Date_: 20140917
Time: 11.13
INSTRUM: spect
PROBHD: 5 mm PABBO BR-
PULPROG: zg30
TD: 65536
SOLVENT: CDC13
NS: 16
DS: 2
SWH: 10330.578 Hz
FIDRES: 0.157622 Hz
AQ: 3.1719425 sec
RG: 45.2
LW: 48.400 usec
DE: 8.50 usec
TE: 297.6 K
D1: 1.00000000 sec
TD0: 1

===== CHANNEL f1 =====
NUC1: 1H
P1: 14.25 usec
PL1: 1.30 dB
PL12: 15.30635643 M
SFO1: 500.2330891 MHz

F2 - Processing parameters
SI: 32768
SF: 500.2300152 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
    
```



BM-VS-s29 in CDC13



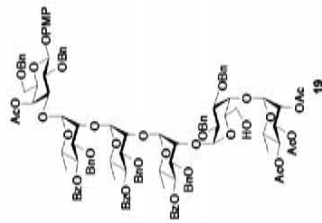
Current Data Parameters
 NAME BM-VS-s29
 EXENO 90
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140917
 Time 12.26
 INSTRUM spect
 PROBH 5 mm PARBO BB-
 PULPROG zgpg
 ID 65536
 SOLVENT CDC13
 NS 1147
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 PL1W 90.18825531 W
 SF01 125.7955118 MHz

===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 PCED2 80.00 usec
 PL2 1.30 dB
 PL2W 15.30635643 W
 PL2W 0.51866696 W
 SF02 500.2320009 MHz

F2 - Processing Parameters
 SI 32768
 SF 125.7829417 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

BM-VS-s29 in CDC13



Current Data Parameters
 NAME BM-VS-s29
 EXENO 71
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140917
 Time 11.15
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG cosy3Df
 ID 2048
 SOLVENT CDC13
 NS 1
 DS 8
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048000 sec
 RG 45.2
 DW 100.000 usec
 DE 6.50 usec
 TE 297.6 K
 D0 0.00000300 sec
 D1 1.48683198 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019990 sec

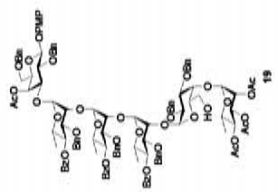
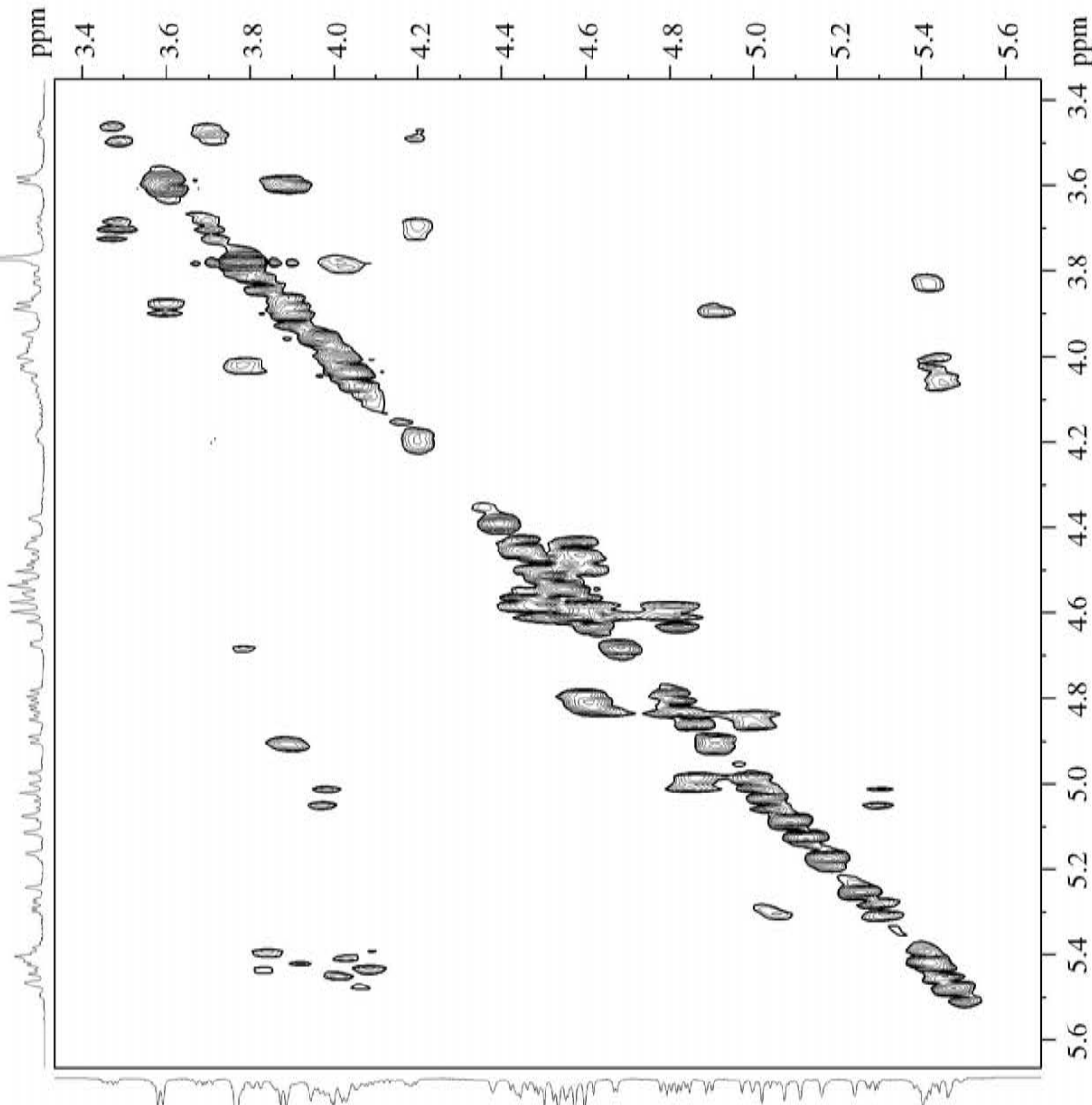
===== CHANNEL f1 =====
 NUC1 1H
 P0 14.25 usec
 P1 14.25 usec
 PL1 1.30 dB
 PL1W 15.30635643 W
 SF01 500.2325012 MHz

===== GRADIENT CHANNEL =====
 GPRAM[1] SINE.100
 GPZ1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SF01 500.2325 MHz
 FIDRES 39.080666 Hz
 SW 10.000 PPM
 FTMODE QF

F2 - Processing parameters
 SI 1024
 SF 500.2300108 MHz
 SINE
 WDW 0
 SSB 0 Hz
 LB 0
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.2300104 MHz
 WDW SINE
 SSB 0 Hz
 LB 0
 GB 0



BM-VS-s29 in CDC13
 HSQCGP



NAME BM-VS-s29
 EXPNO 110
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140917
 Time 14.24
 INSTRUM spect
 PULPROG zgpg30
 F2PROG zgpg30
 TO 1024
 SOLVENT CDC13
 NS 2
 DS 2
 SWH 5000.000 Hz
 FIDRES 4.882813 Hz
 AQ 0.1024000 sec
 RG 45.2
 DE 100.000 umsec
 TE 300.1 K
 CNST2 145.0000000
 DD 0.0000300 sec
 D1 0.0017284 sec
 D4 0.0300000 sec
 D11 0.0300000 sec
 D13 0.0000400 sec
 D18 0.0002000 sec
 D19 0.0002000 sec
 INO 0.0001985 sec

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

NUC1 13
 P1 14.25 umsec
 P2 28.50 umsec
 P3 0.10 umsec
 PL1 0.00 dB
 PL2 15.3043542 dB
 PL3 500.2325012 MHz

===== CHANNEL f2 =====

CPDPRG2 zgpg30
 NUC2 13C
 P1 9.50 umsec
 P2 17.00 umsec
 P3 70.00 umsec
 PL1 0.00 dB
 PL2 17.00 dB
 PL3 90.18825531 dB
 PL4 1.69373910 dB
 PL5 125.7955123 MHz

===== GRADIENT CHANNEL =====

GPMAX[1] 5.00
 GPMAX[2] 5.00
 GPMAX[3] 5.00
 GPMAX[4] 5.00
 GRP1 80.00 %
 GR2 20.10 %
 GR3 11.00 %
 GR4 5.00 %
 P13 1000.00 umsec
 P14 600.00 umsec

F1 - Acquisition Parameters

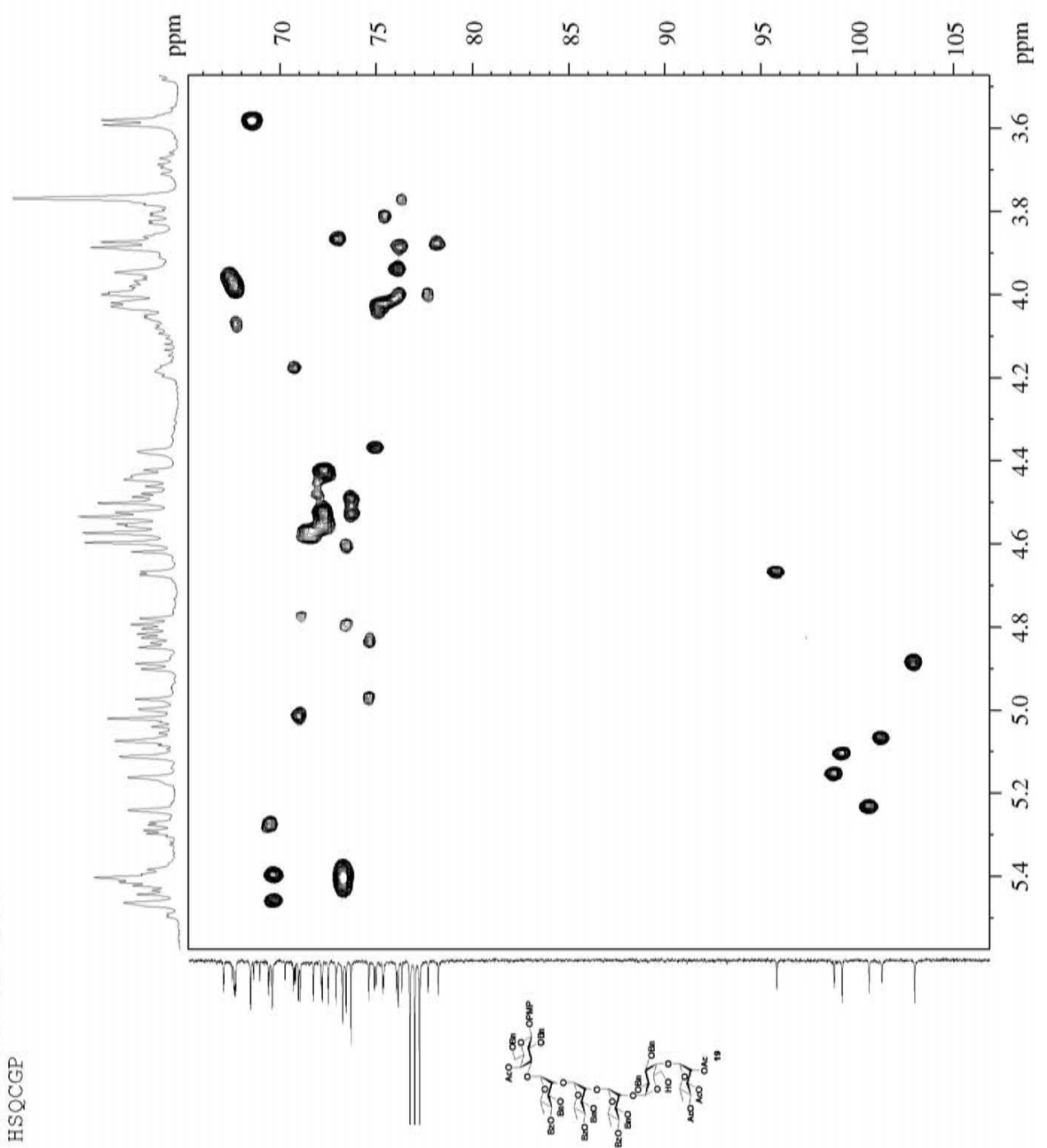
PROBHD 5mm QNP1H
 X301 125.7845 MHz
 F1FRES 98.277740 Hz
 SW 200.0000000 ppm
 FWD08 Echo-Anticcho

F2 - Processing parameters

SI 1024
 SF 500.2300173 MHz
 GB 0 Hz
 AS 0 Hz
 Z 1
 PC 1.00

F1 - Processing parameters

SI 1024
 MK2 echo-antico
 SF 125.7829403 MHz
 GB 0 Hz
 AS 0 Hz
 Z 0



BM-VS-hf in MeOD

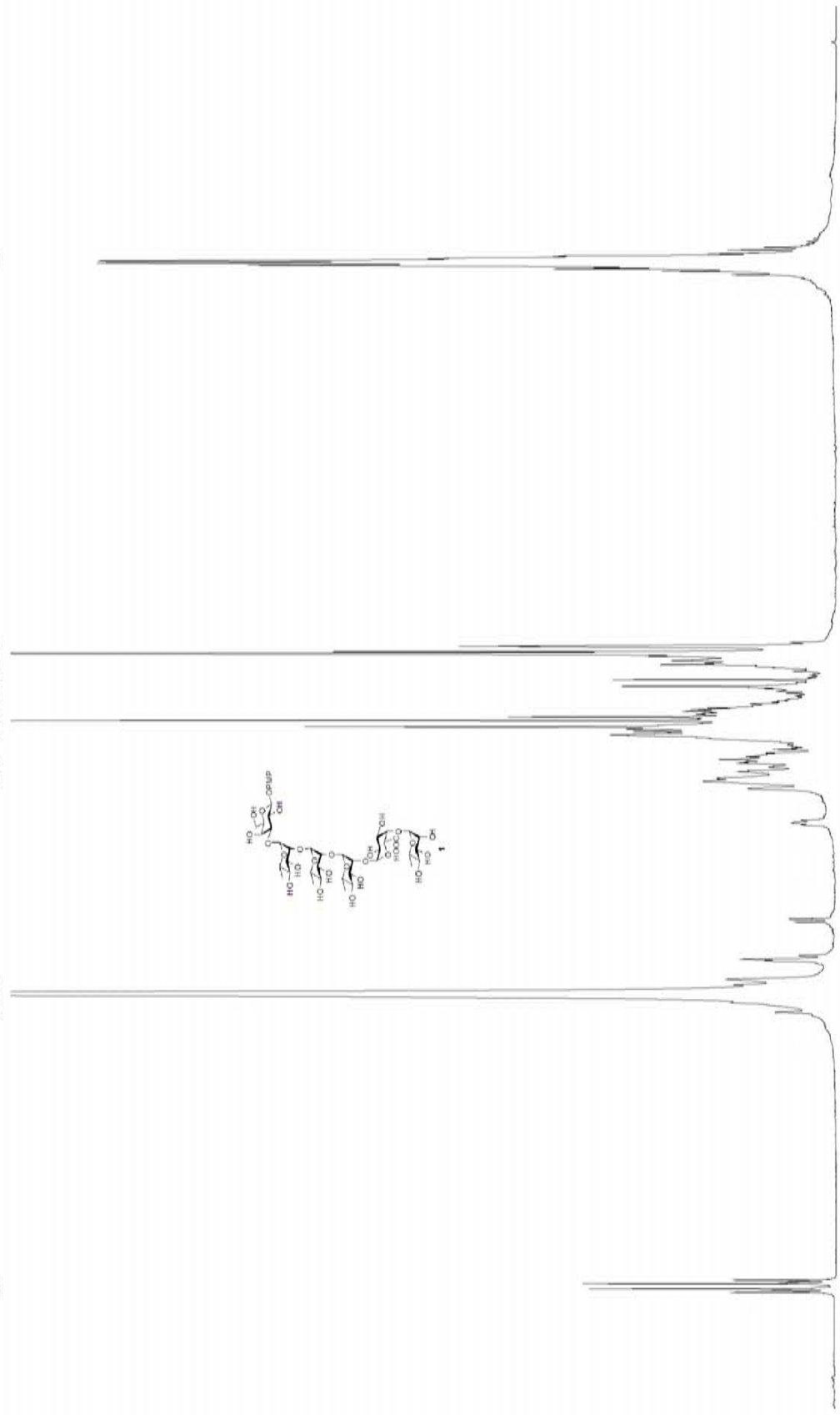


6.751
6.732
6.704
6.686
5.260
5.208
5.159
5.114
5.085
4.029
4.016
4.011
3.913
3.801
3.795
3.786
3.782
3.776
3.768
3.763
3.750
3.738
3.731
3.720
3.706
3.697
3.686
3.673
3.668
3.662
3.657
3.647
3.644
3.638
3.638
3.613
3.310
3.307
1.280
1.270
1.268
1.257
1.256
1.247
1.243

Current Data Parameters
 NAME BM-VS-Hf
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20141117
 Time 13:05:13
 INSTRUM spect
 PROBRD 5 mm PABBO ZB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 49
 DS 4
 SWH 10330.578 Hz
 FIDRES 0.1576332 Hz
 AQ 3.1719425 sec
 SFO1 500.1360610 MHz
 DW 49.400 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.00000000 sec
 TDO 1

***** CHANNEL f1 *****
 NUC1 1H
 P1 14.25 usec
 PL1 0 dB
 FWH 15.3661150 dB
 SFO1 500.1360610 MHz

F2 - Processing Parameters
 SI 32768
 SF 500.1360610 MHz
 WDW EM
 SSF 0
 LB 0.30 Hz
 GB 0
 PC 1.00



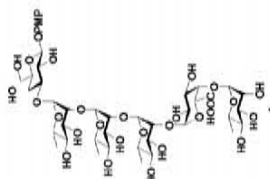
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

BM-VS-hf in MeOD

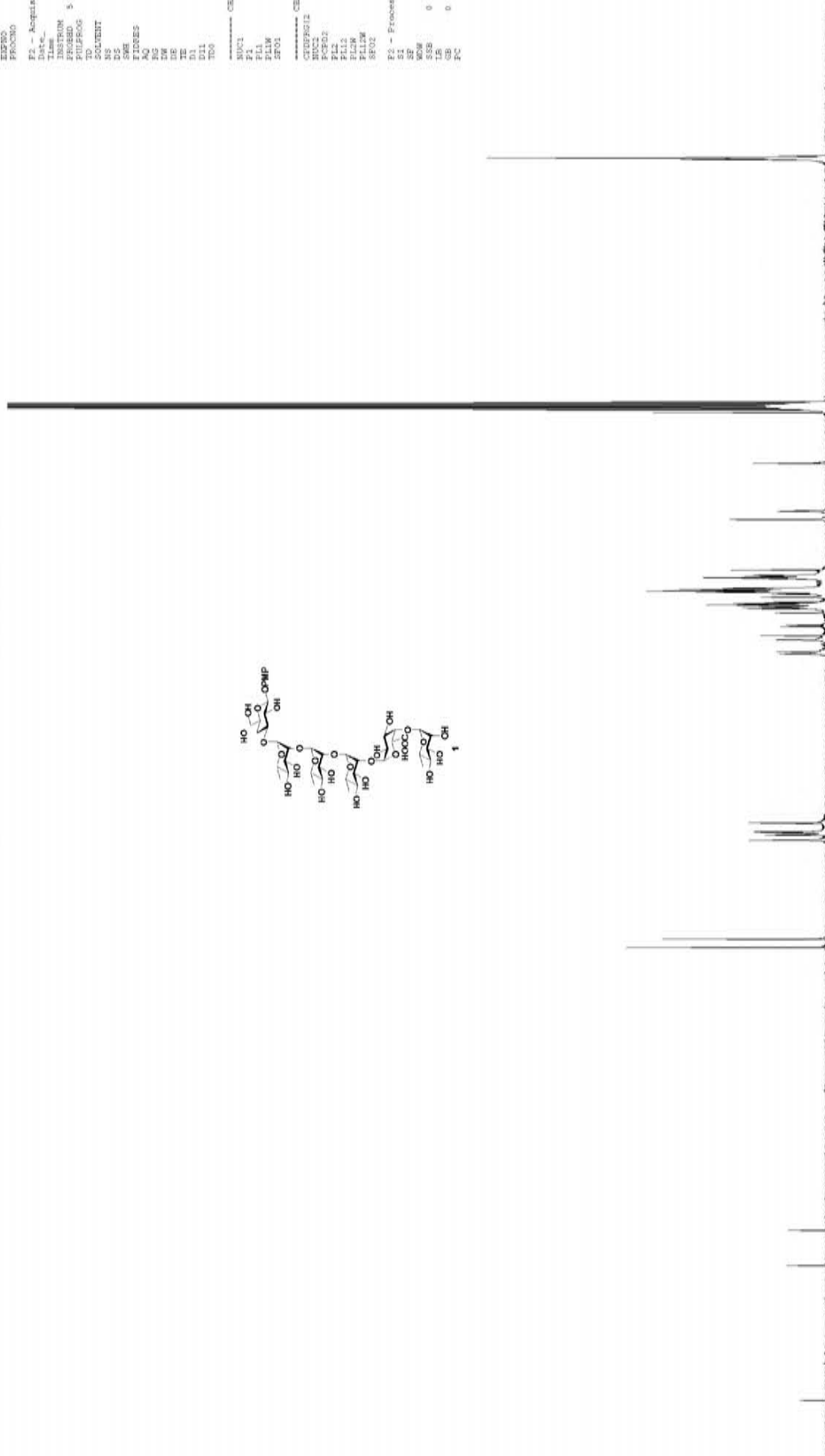


173.39
156.54
152.14

116.75
115.69
103.34
102.70
102.62
102.38
102.27
101.17
80.04
79.75
78.25
77.73
76.61
76.41
74.88
74.38
74.25
73.90
73.72
73.55
72.34
72.23
72.14
72.09
71.93
71.78
70.50
70.48
70.28
70.15
69.53
63.90
63.21
56.16
49.85
49.51
49.46
49.34
49.17
49.00
48.83
48.66
48.49
18.14
18.01
17.96
17.92



Current Data Parameters
NAME BM-VS-hf
PROCNO 211
F2 - Acquisition Parameters
Date_ 201111
Time_ 10.00
INSTRUM spect
PROBHD 5 mm F4001 BE-
TD1PROB 65356
SOLVENT MeOD
NS 18779
DS 2
SWH 20761.004 Hz
FIDRES 0.454131 Hz
AQ 1.1010018 sec
RG 327.5
WDW EM
SS 16.300 uSAC
SB 6.50 uSAC
BE 2.0000000 K
D11 0.05000000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 9.50 uSAC
PL1 0.00 dB
FLW 30.1832553 W
SF01 125.7625118 MHz
----- CHANNEL f2 -----
C13CPROG2 waltz16
NUC2 13C
P2 1.00 uSAC
PL2 0.00 dB
FL2 16.00 W
FLN 15-30635643 W
FLM 15-31181609 W
SF02 500.135099 MHz
F2 - Processing parameters
SI 327.5
SF 125.7625118 MHz
WDW EM
SSB 0
GB 0
PC 1.40



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm