Supporting Information

Deactivating Influence of 3-*O*-Glycosyl Substituent on Anomeric Reactivity of Thiomannoside Observed in Oligomannoside Synthesis

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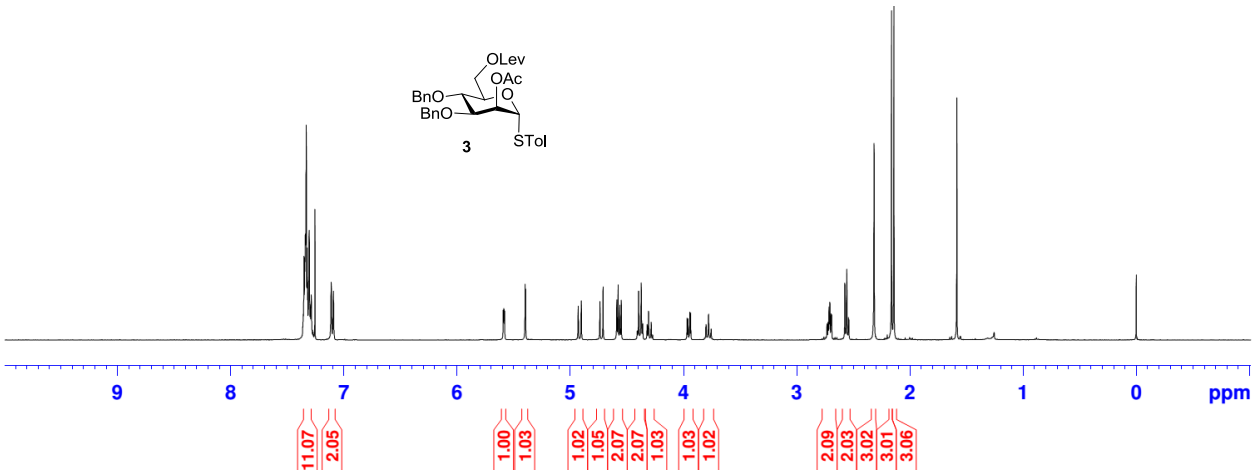
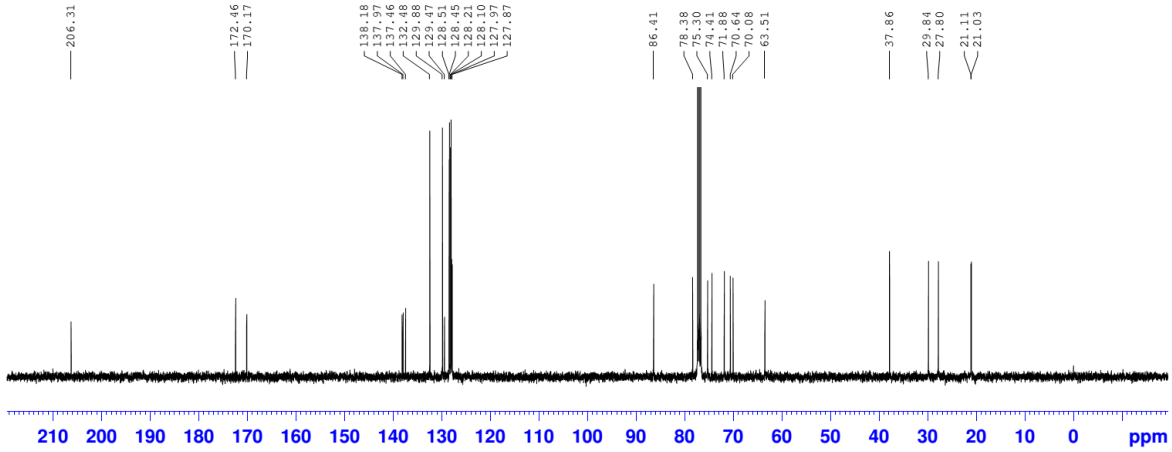
Table of Contents

1. 1D and 2D NMR Spectra for all new compounds (and selected HRMS)

Compound	Page	Copies of Spectra	Compound	Page	Copies of Spectra
3	S3	^{1}H NMR, ^{13}C NMR	**42**	S24	^{1}H NMR, ^{13}C-APT, HSQC
4	S3	^{1}H NMR, ^{13}C NMR	**43**	S25	^{1}H NMR, ^{13}C NMR, HSQC
5	S4	^{1}H NMR, ^{13}C NMR	**44**	S26	^{1}H NMR, ^{13}C-APT, HSQC
6	S4	^{1}H NMR, ^{13}C-APT NMR	**45**	S27	^{1}H NMR, ^{13}C-APT, HSQC
7	S5	^{1}H NMR, ^{13}C-APT NMR	**46**	S28	^{1}H NMR, ^{13}C NMR, HSQC,
8	S5	^{1}H NMR, ^{13}C NMR	**48**	S29	^{1}H NMR, ^{13}C NMR, HSQC, COSY, HMBC
10	S6	^{1}H NMR, ^{13}C NMR	**49**	S31	^{1}H NMR, ^{13}C NMR, HSQC
11	S6	^{1}H NMR, ^{13}C NMR	**50**	S32	^{1}H NMR, ^{13}C NMR, HSQC
12	S7	^{1}H NMR, ^{13}C NMR	**51**	S33	^{1}H NMR, ^{13}C NMR, HSQC
13	S7	^{1}H NMR, ^{13}C NMR	**55**	S34	^{1}H NMR, ^{13}C-APT, HSQC
14	S8	^{1}H NMR, ^{13}C-APT NMR	**56**	S35	^{1}H NMR, ^{13}C-APT, HSQC
15	S8	^{1}H NMR, ^{13}C NMR	**57**	S36	^{1}H NMR, ^{13}C NMR, HSQC
16	S9	^{1}H NMR, ^{13}C NMR	**58**	S37	^{1}H NMR, ^{13}C-APT, HSQC
18	S9	^{1}H NMR, ^{13}C NMR	**59**	S38	^{1}H NMR, ^{13}C-APT, HSQC
19	S10	^{1}H NMR, ^{13}C NMR	**60**	S39	^{1}H NMR, ^{13}C-APT, HSQC
20	S10	^{1}H NMR, ^{13}C-APT NMR	**61**	S40	^{1}H NMR, ^{13}C NMR, HSQC
22	S11	^{1}H NMR, ^{13}C NMR	**62**	S41	^{1}H NMR, ^{13}C-APT, HSQC
23	S11	^{1}H NMR, ^{13}C NMR	**63**	S42	^{1}H NMR, ^{13}C-APT, HSQC
24	S12	^{1}H NMR, ^{13}C NMR	**64**	S43	^{1}H NMR, ^{13}C-APT, COSY, HSQC
26	S12	^{1}H NMR, ^{13}C NMR	**65**	S45	^{1}H NMR, ^{13}C-APT, COSY, HSQC
27	S13	^{1}H NMR, ^{13}C NMR	**66**	S47	^{1}H NMR, ^{13}C-APT, HSQC
29	S13	^{1}H NMR, ^{13}C-APT NMR	**67**	S48	^{1}H NMR, ^{13}C-APT, COSY, HSQC
31	S14	^{1}H NMR, ^{13}C NMR	**68**	S50	^{1}H NMR, ^{13}C-APT, COSY, HSQC
32	S14	^{1}H NMR, ^{13}C-APT NMR	**69**	S52	^{1}H NMR, ^{13}C-APT, COSY, HSQC
33	S15	^{1}H NMR, ^{13}C NMR, HSQC	**70**	S54	^{1}H NMR, ^{13}C-APT, COSY, HSQC
34	S16	^{1}H NMR, ^{13}C NMR, HSQC	**71**	S56	^{1}H NMR, ^{13}C-APT, COSY, HSQC
35	S17	^{1}H NMR, ^{13}C NMR, HSQC	**72**	S58	^{1}H NMR, ^{13}C-APT, COSY, HSQC
36	S18	^{1}H NMR, ^{13}C NMR, HSQC	**73**	S60	^{1}H NMR, ^{13}C-APT, COSY, HSQC
37	S19	^{1}H NMR, ^{13}C NMR, HSQC	**74**	S62	^{1}H NMR, ^{13}C-APT, COSY, HSQC
38	S20	^{1}H NMR, ^{13}C NMR, HSQC	**75**	S64	^{1}H NMR, ^{13}C-APT, COSY, HSQC
39	S21	^{1}H NMR, ^{13}C-APT, HSQC	**76**	S66	^{1}H NMR, ^{13}C-APT, COSY, HSQC, HSQC-TOCSY, HMBC, ^{31}P-NMR, HRESIMS
40	S22	^{1}H NMR, ^{13}C-APT, HSQC	**77**	S70	^{1}H NMR, ^{13}C-APT, COSY, HSQC, ^{31}P-NMR
41	S23	^{1}H NMR, ^{13}C-APT, HSQC	**78**	S72	^{1}H NMR, ^{13}C-APT, COSY, HSQC, HSQC-TOCSY, HMBC
1	S75	^{1}H NMR, ^{13}C-APT, HSQC, coupled-HSQC, COSY, HSQC-TOCSY, HMBC,ROESY, ^{31}P-NMR, HRESIMS			

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **3**





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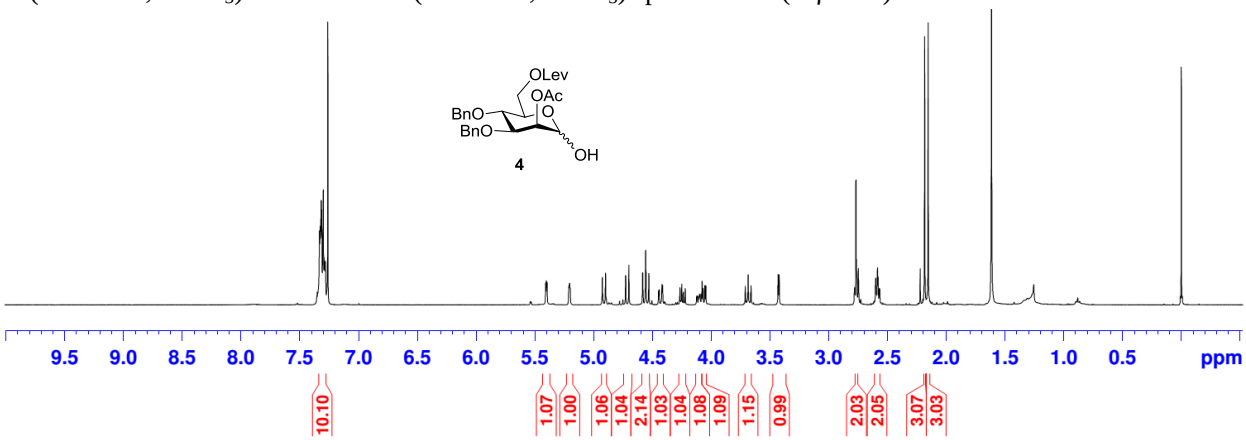
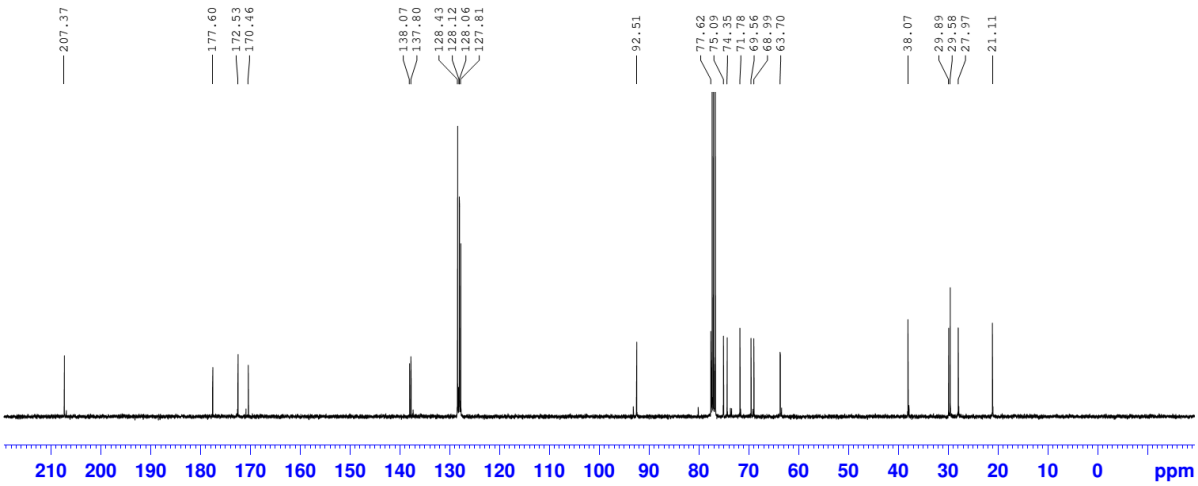
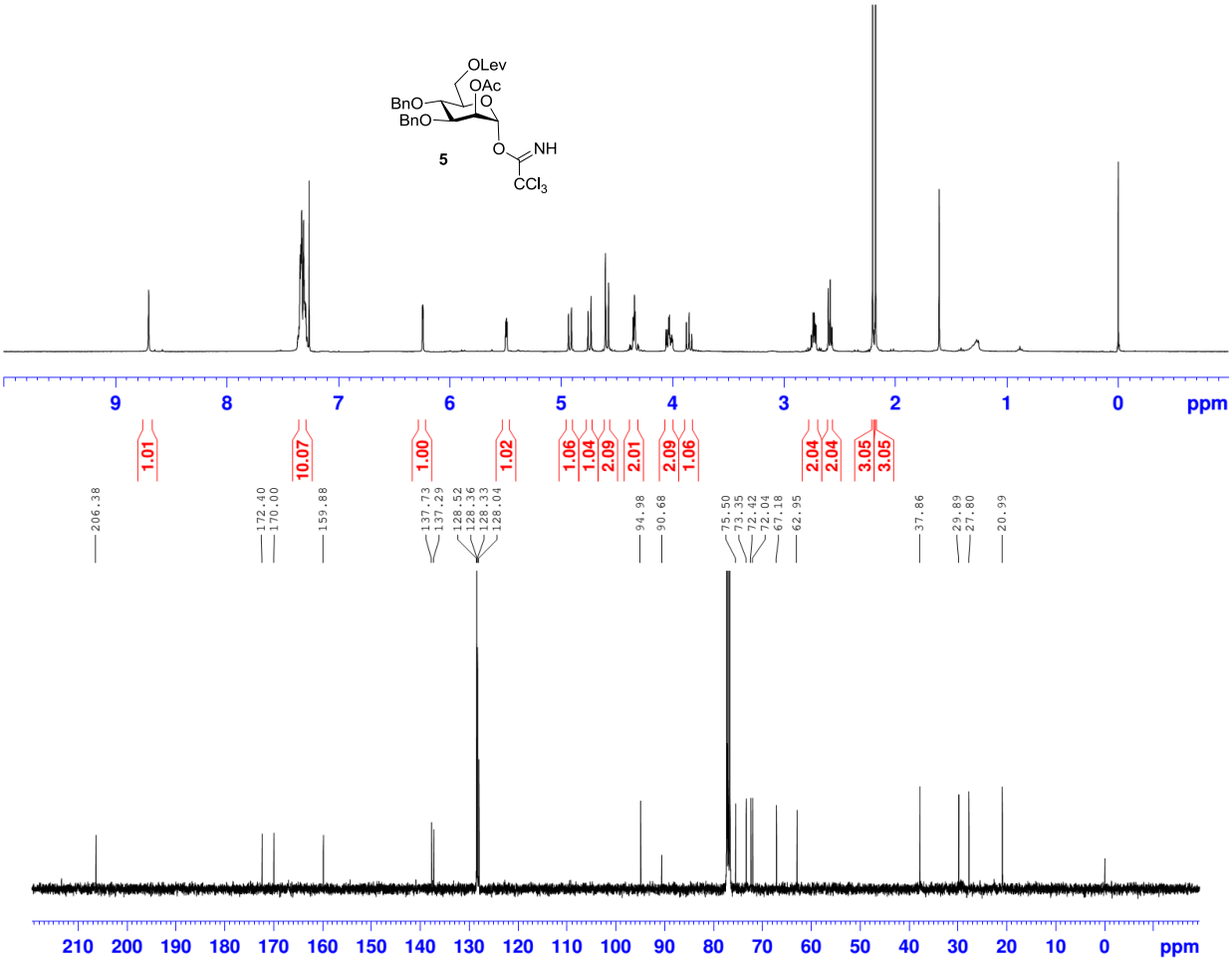




^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **5**



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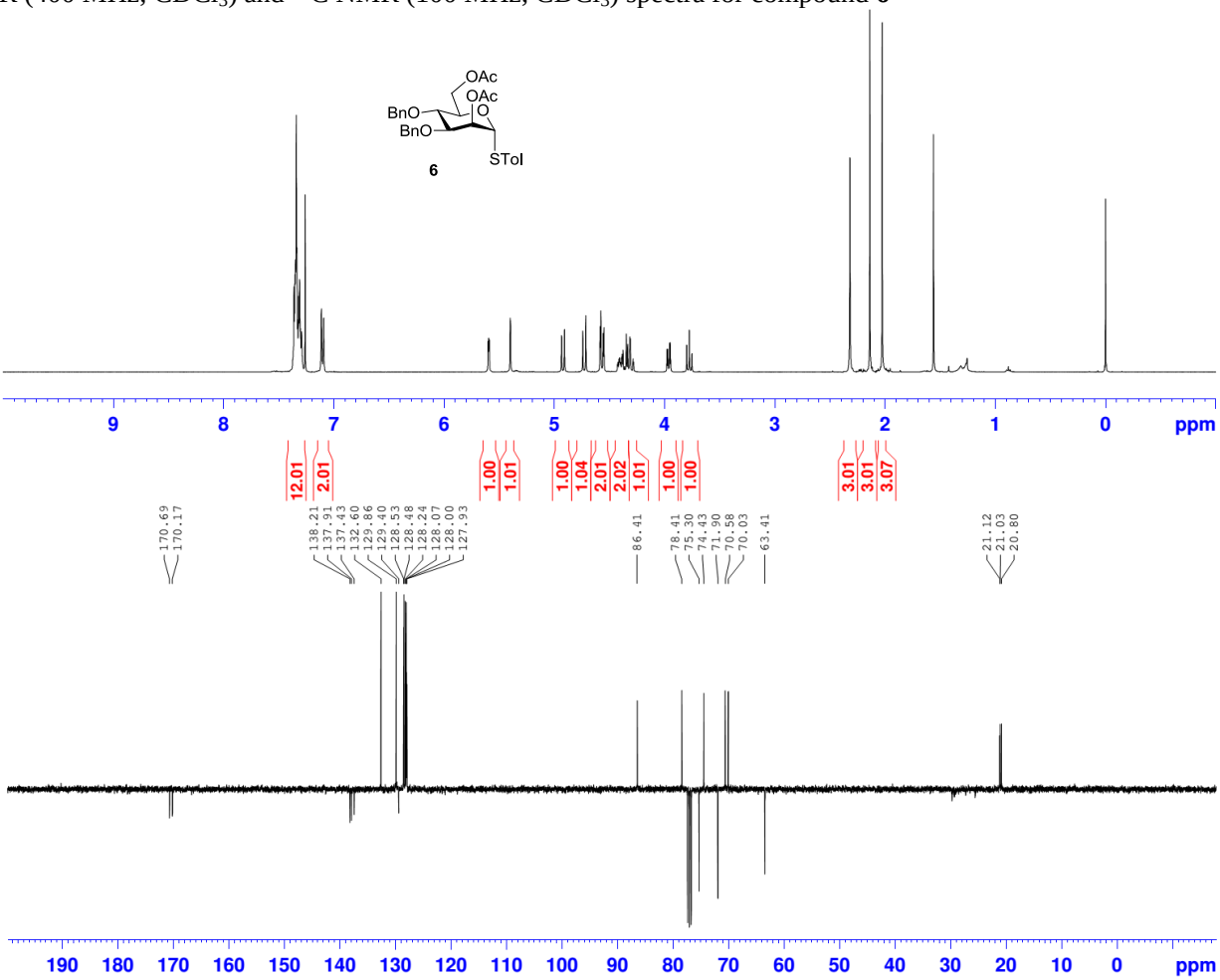

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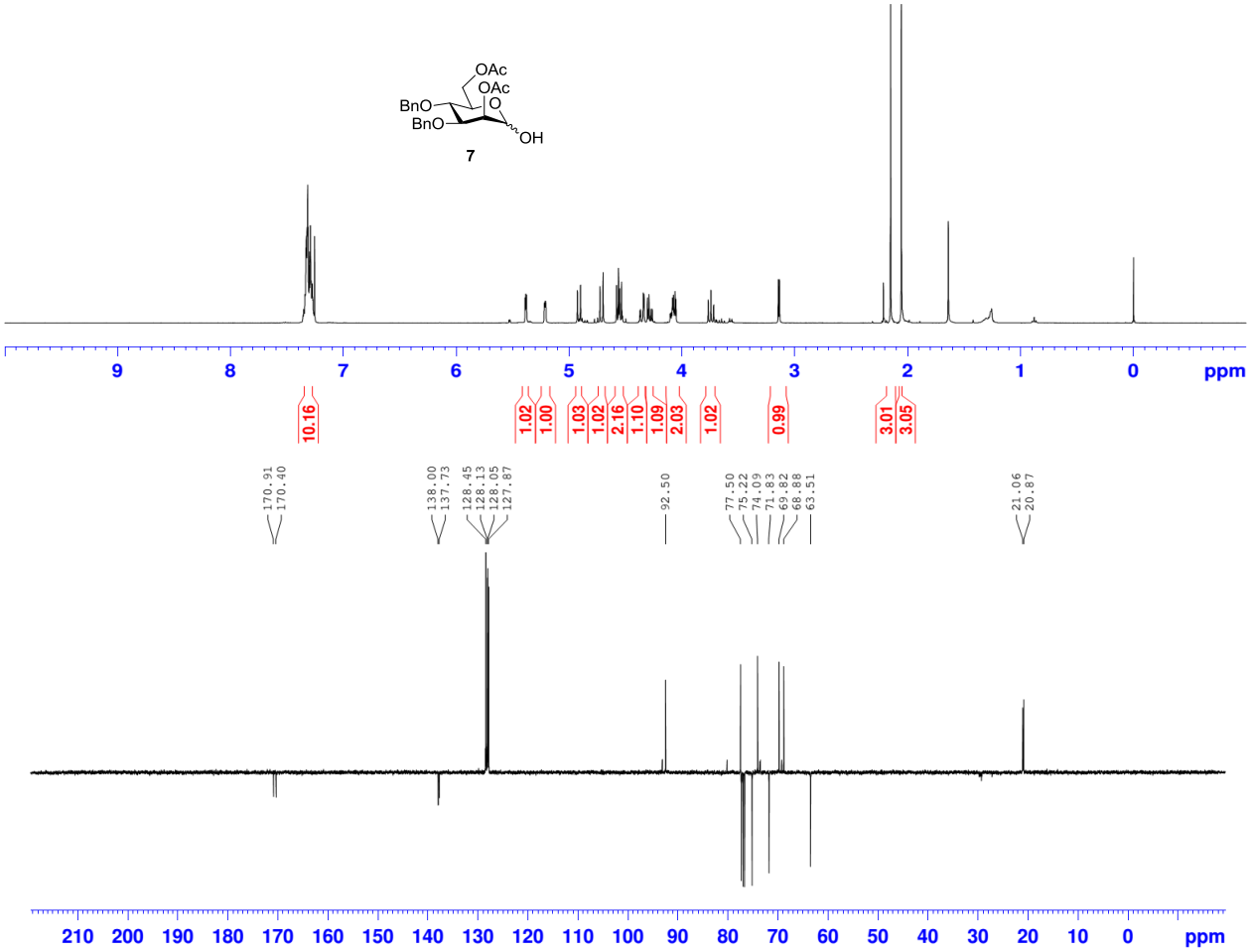

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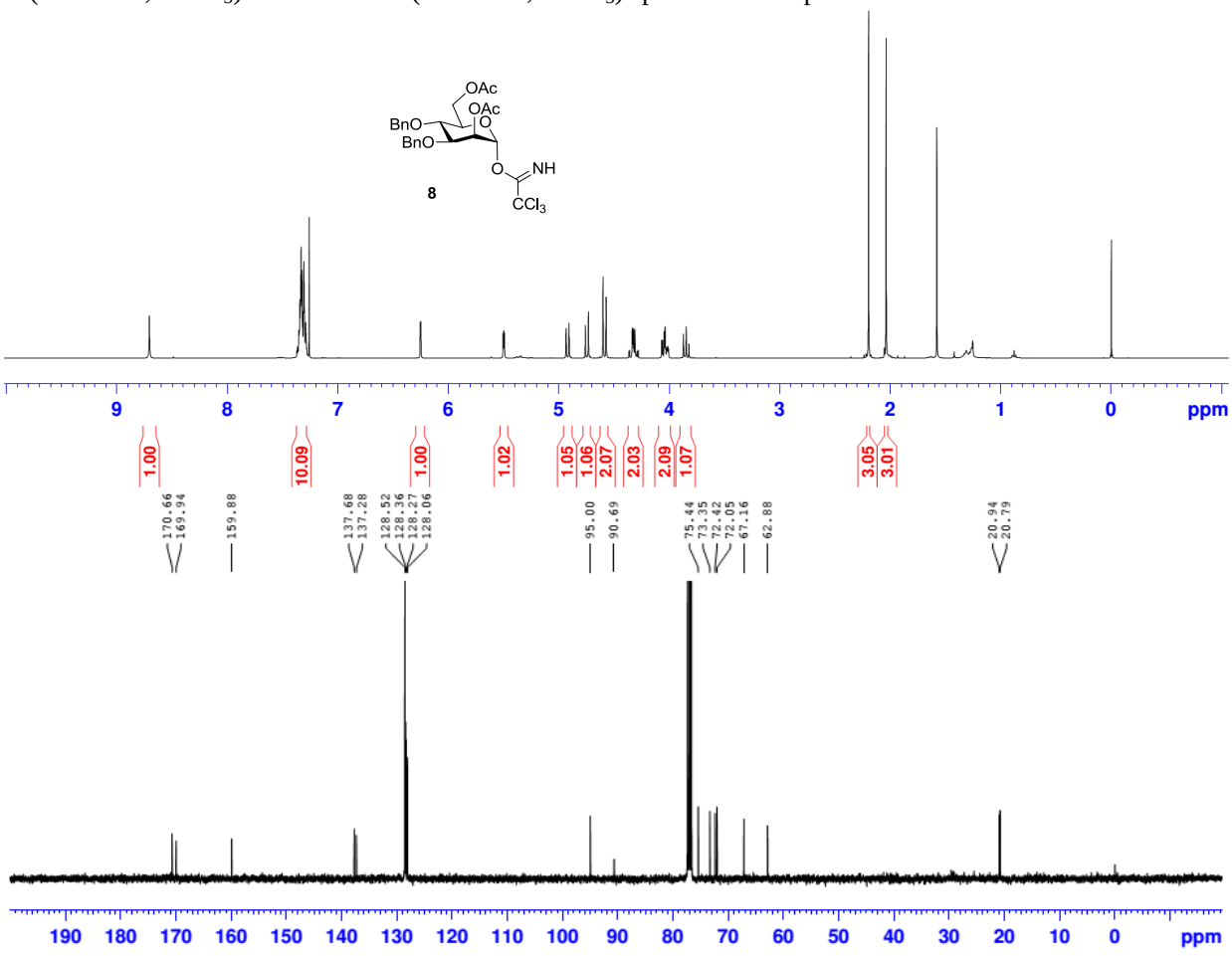
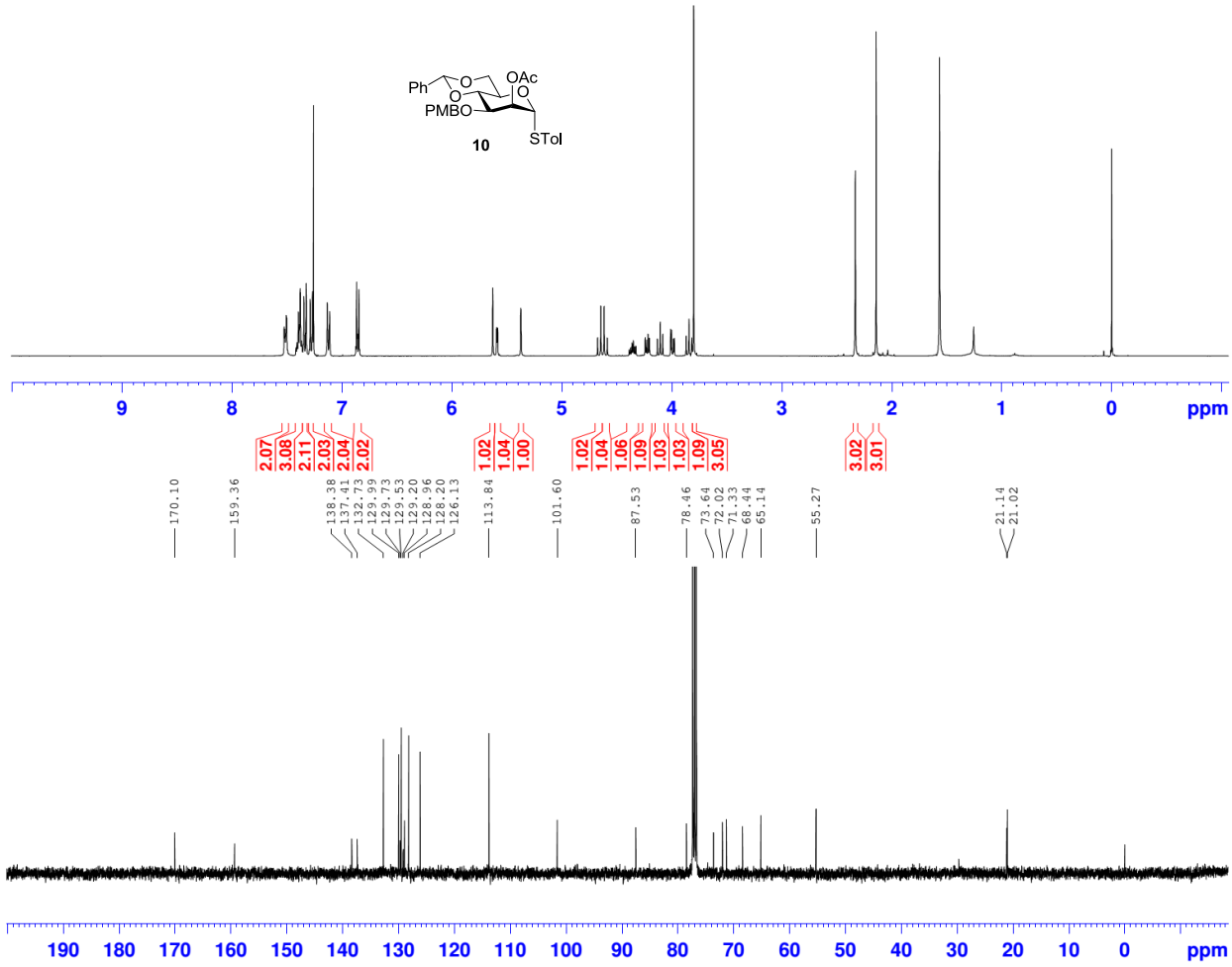
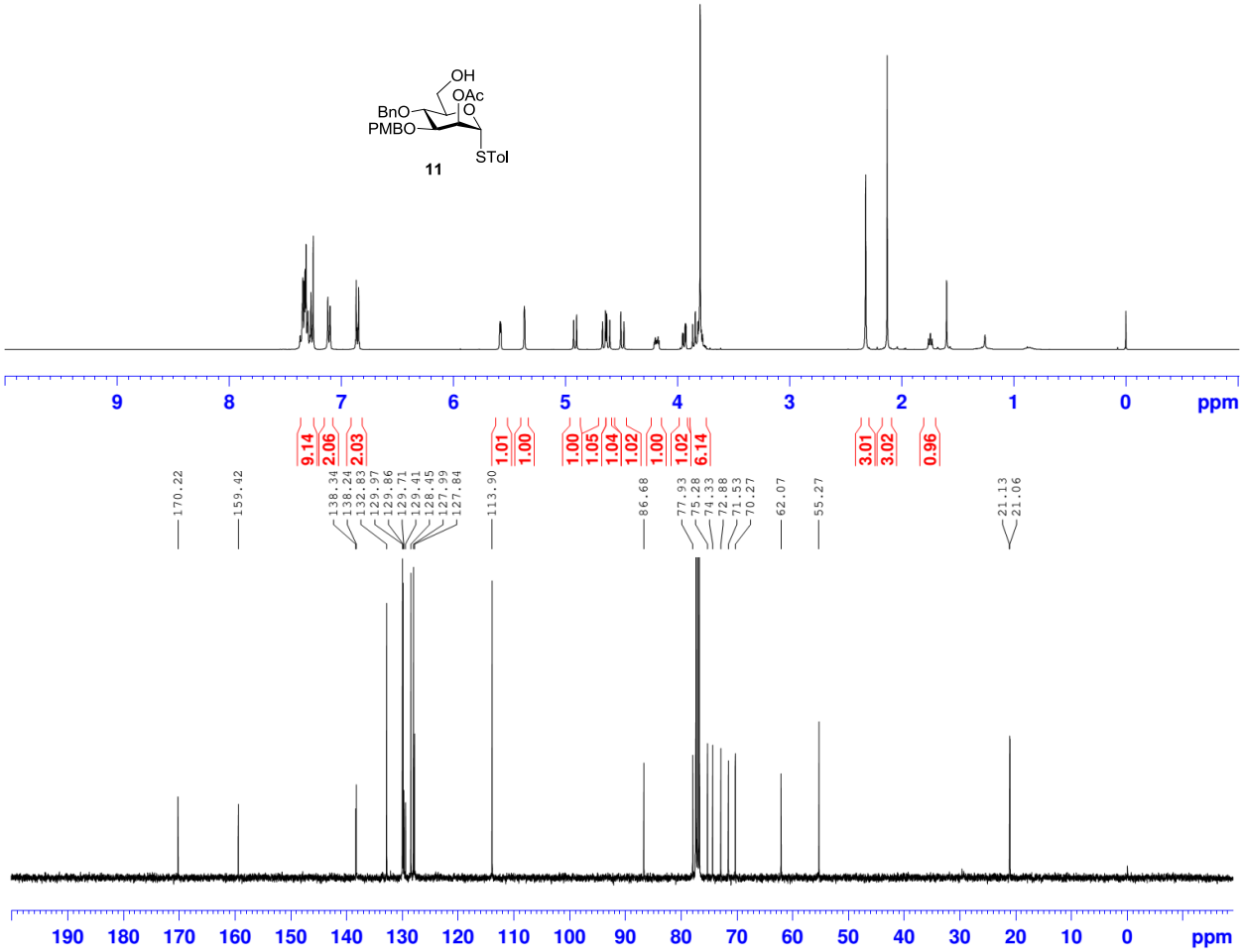


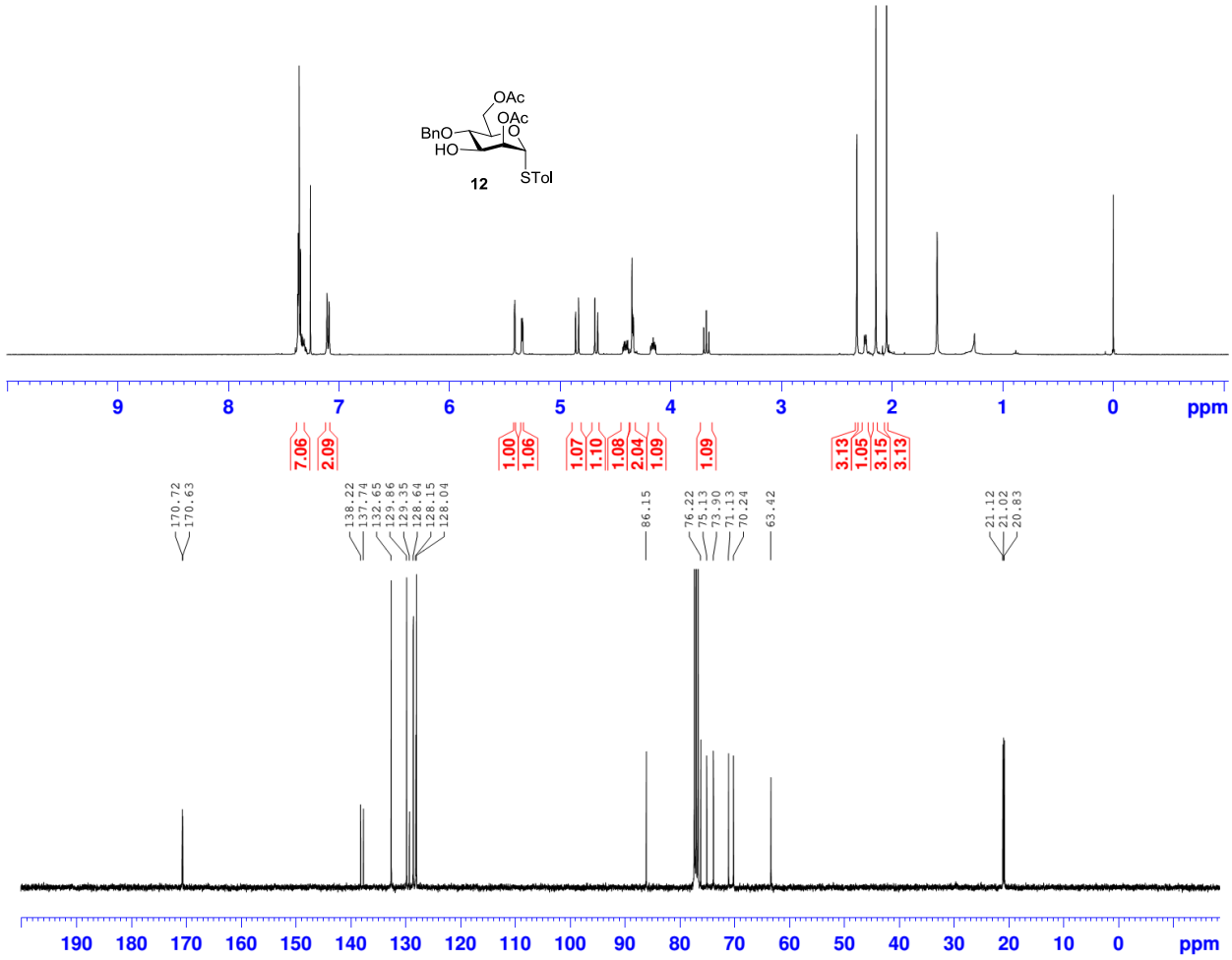
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **10**



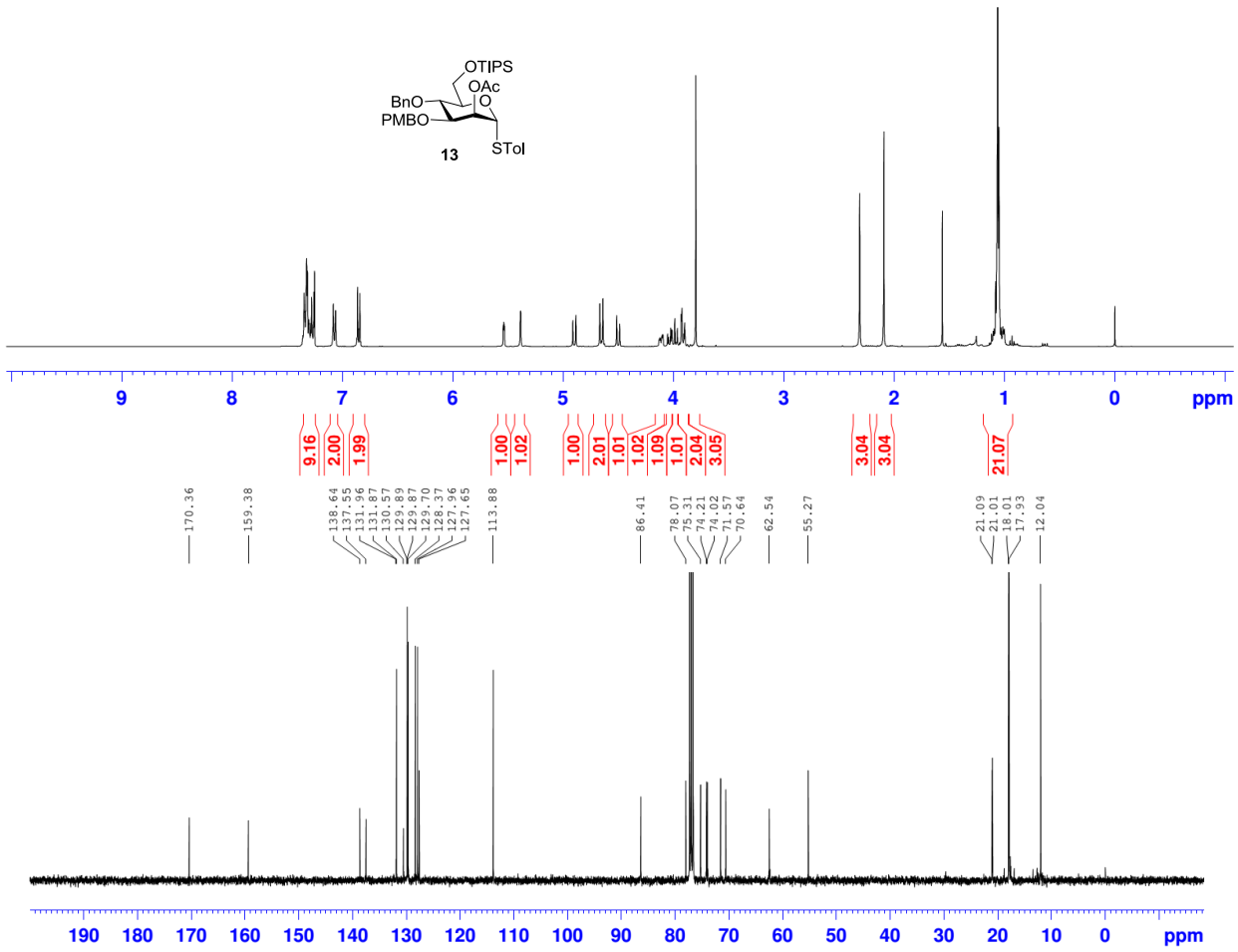
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **11**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **12**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **13**



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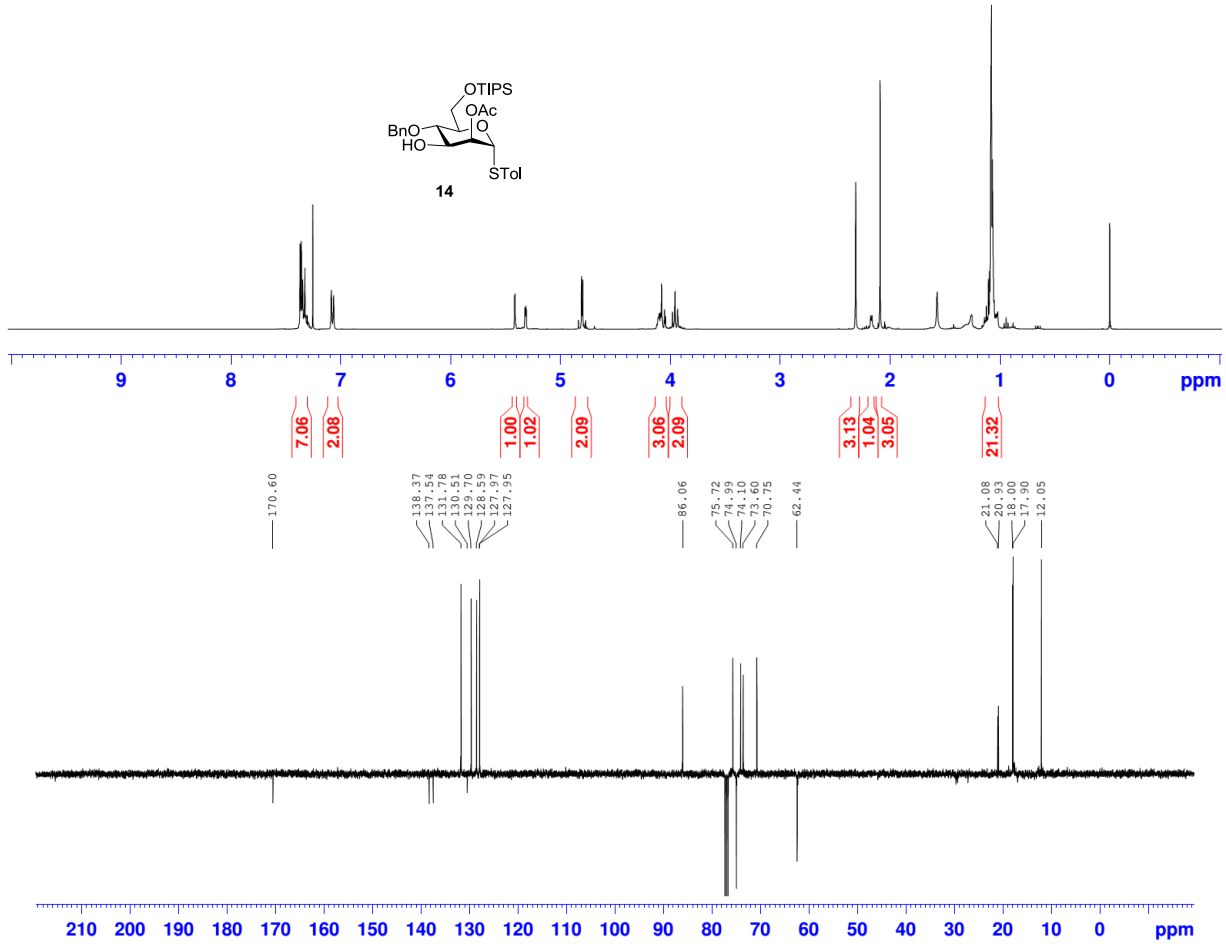
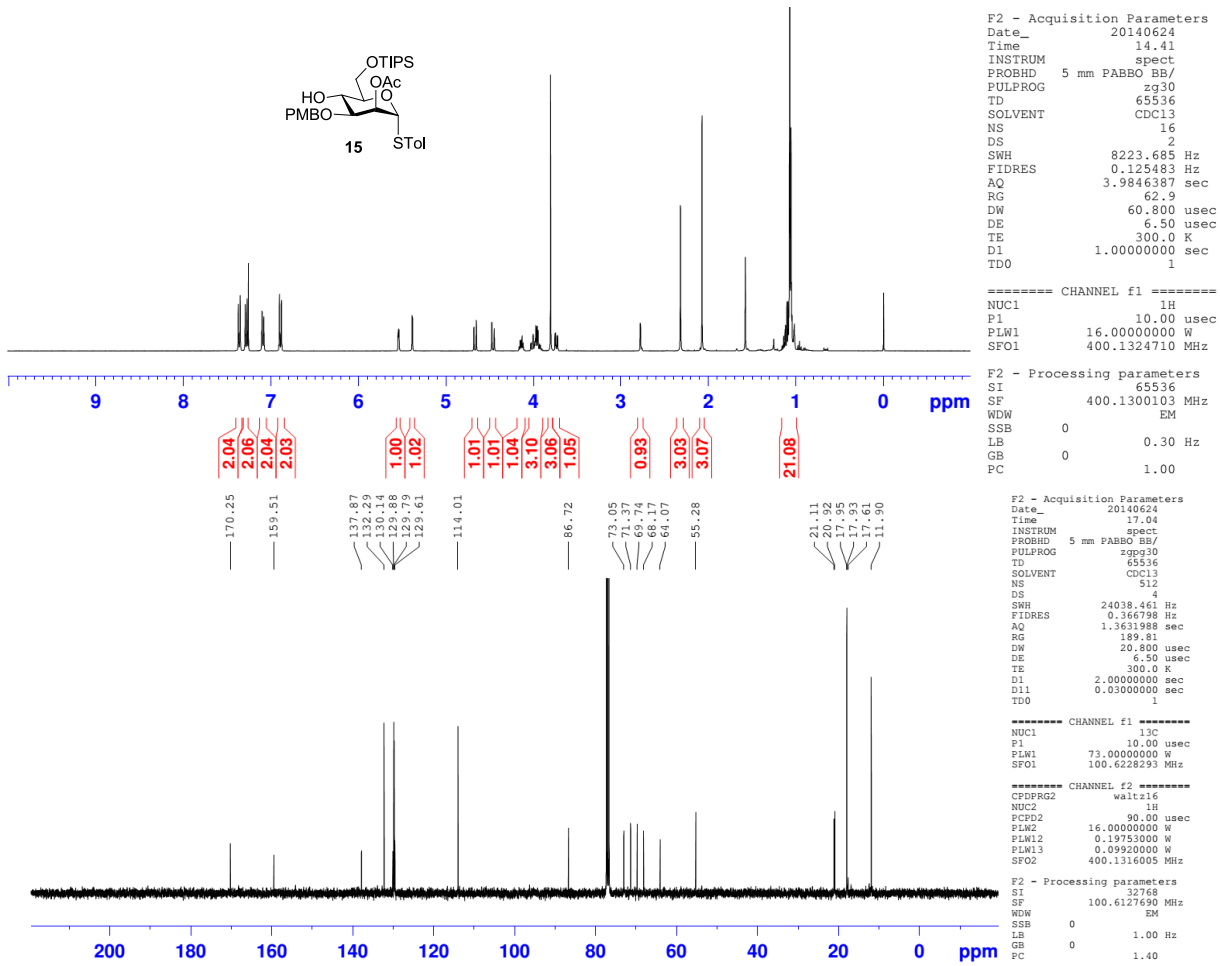
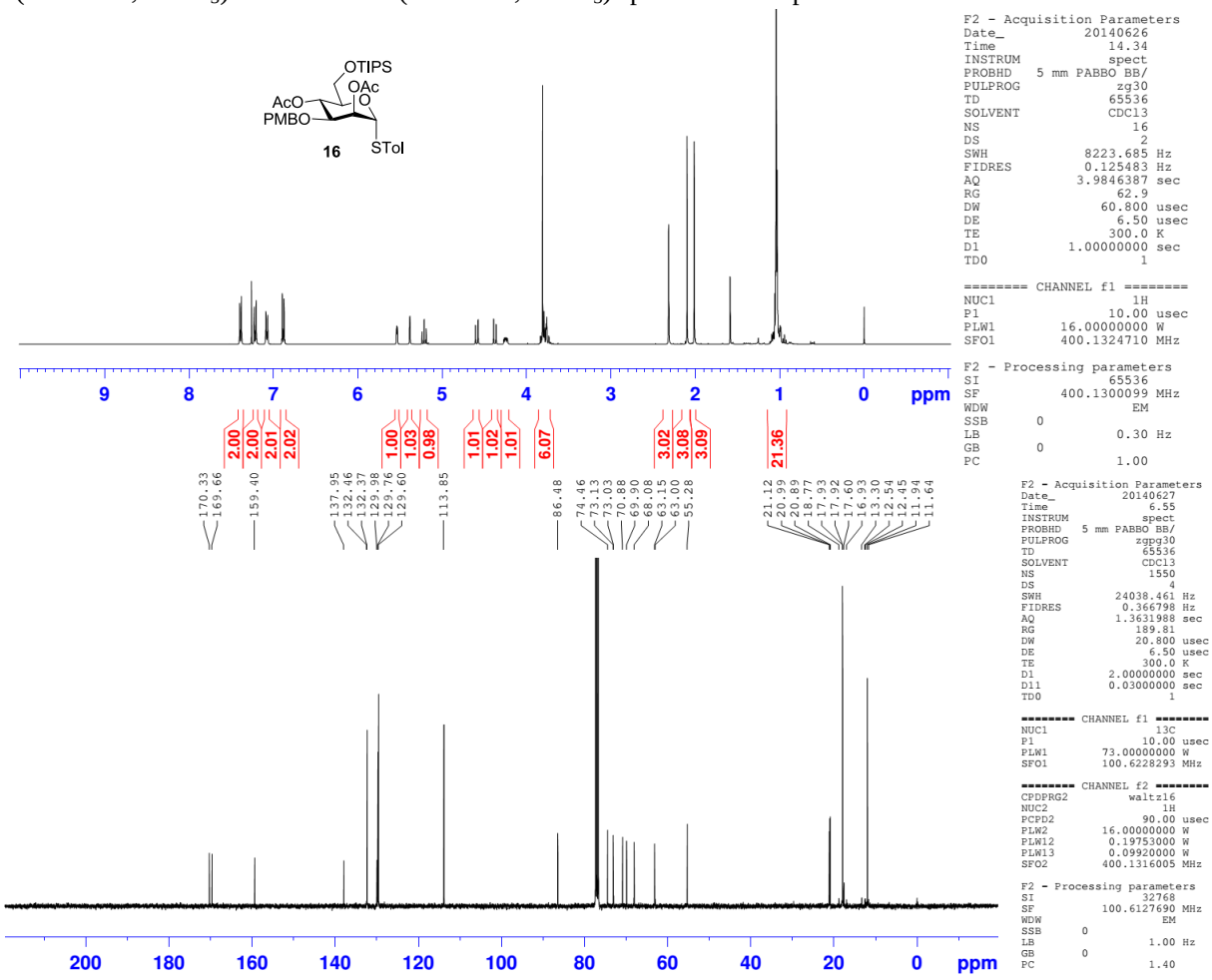


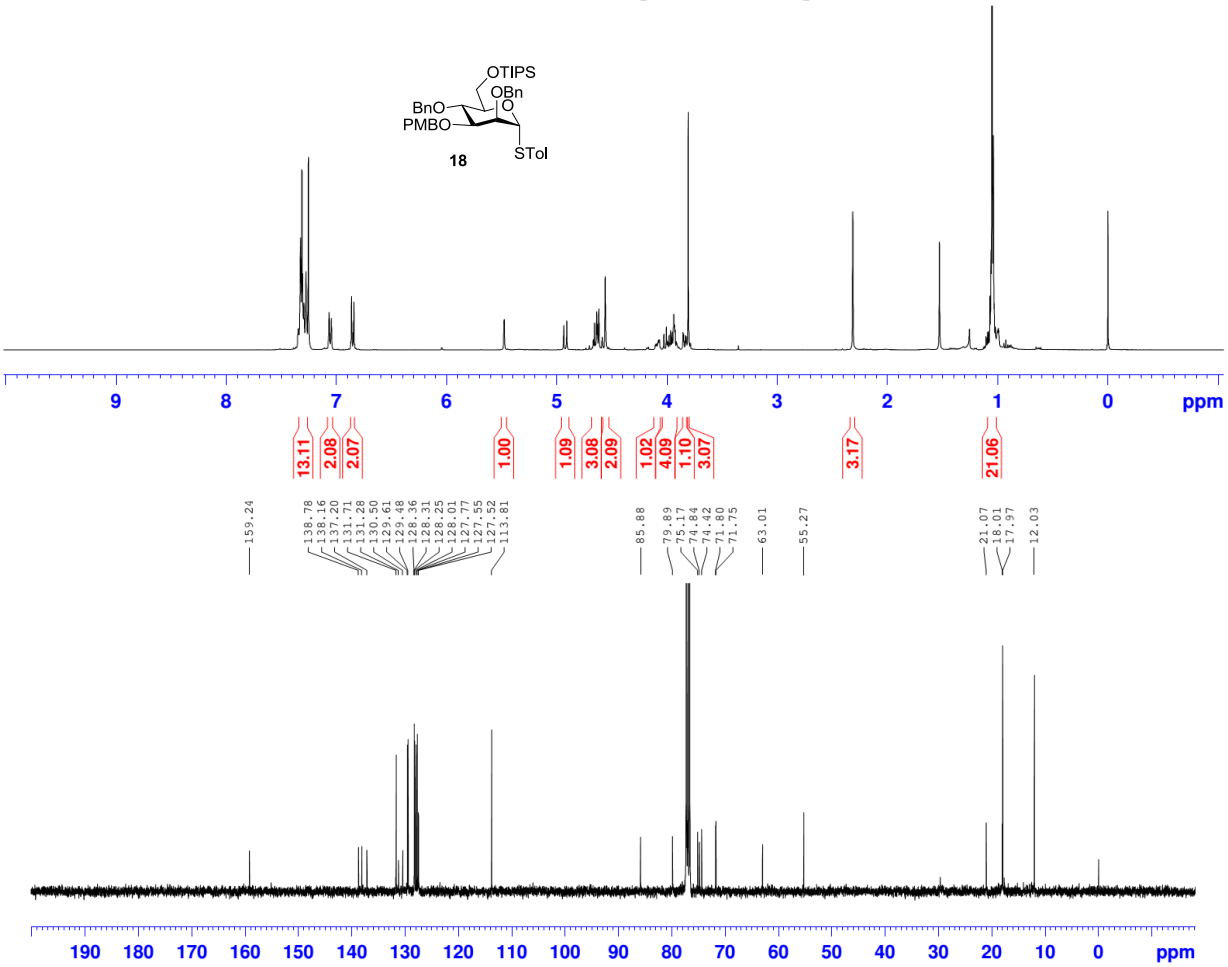
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **15**



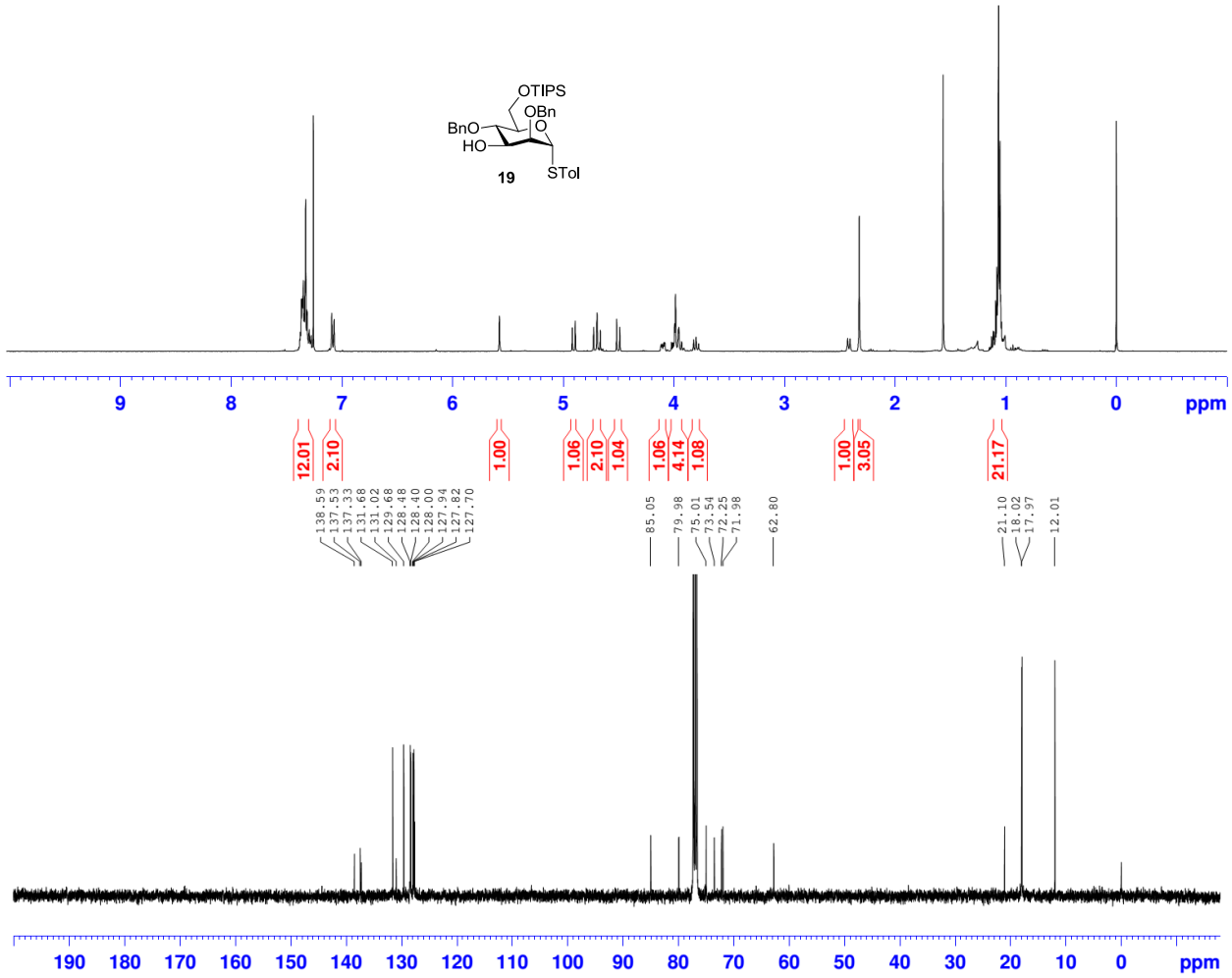
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **16**



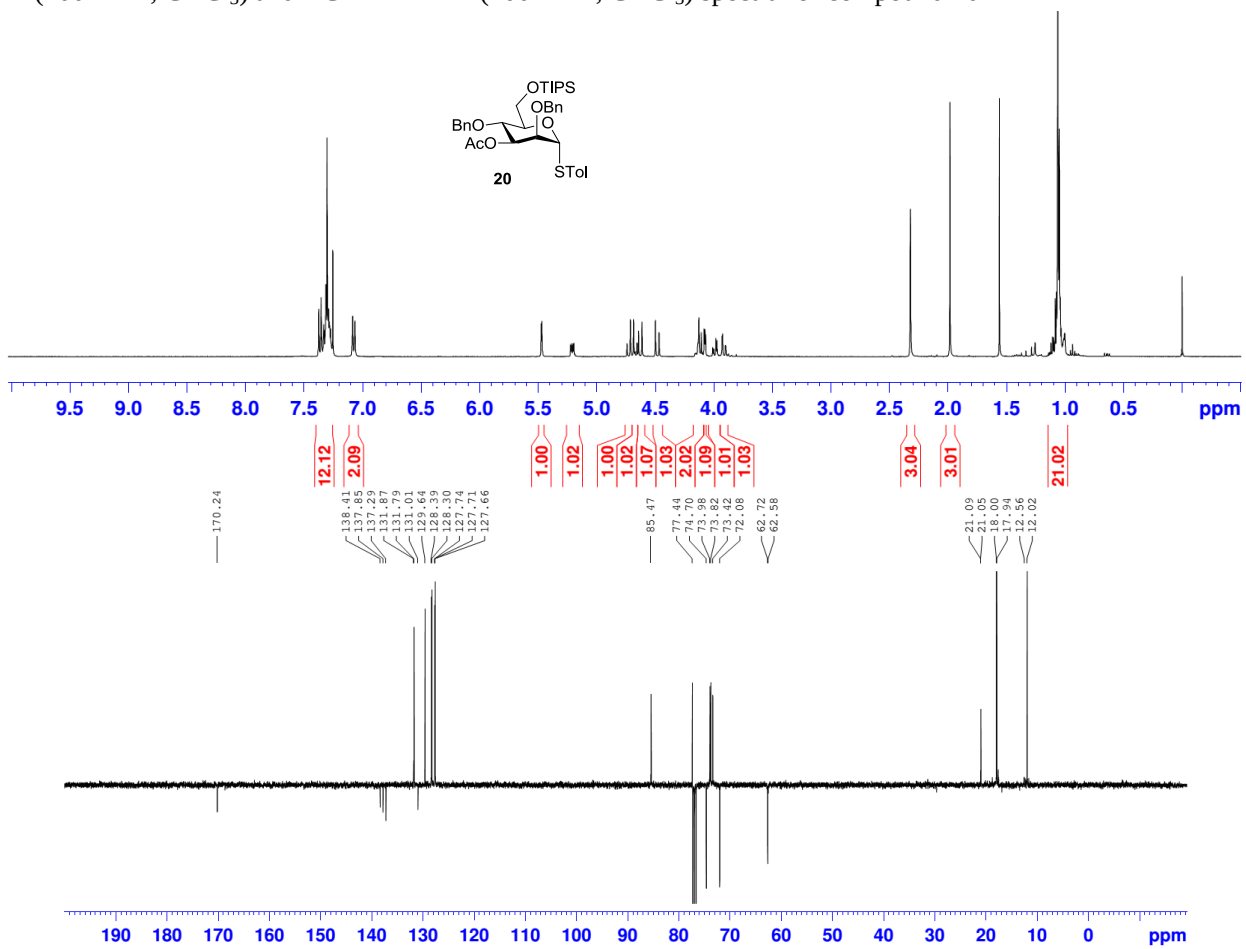
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **18**



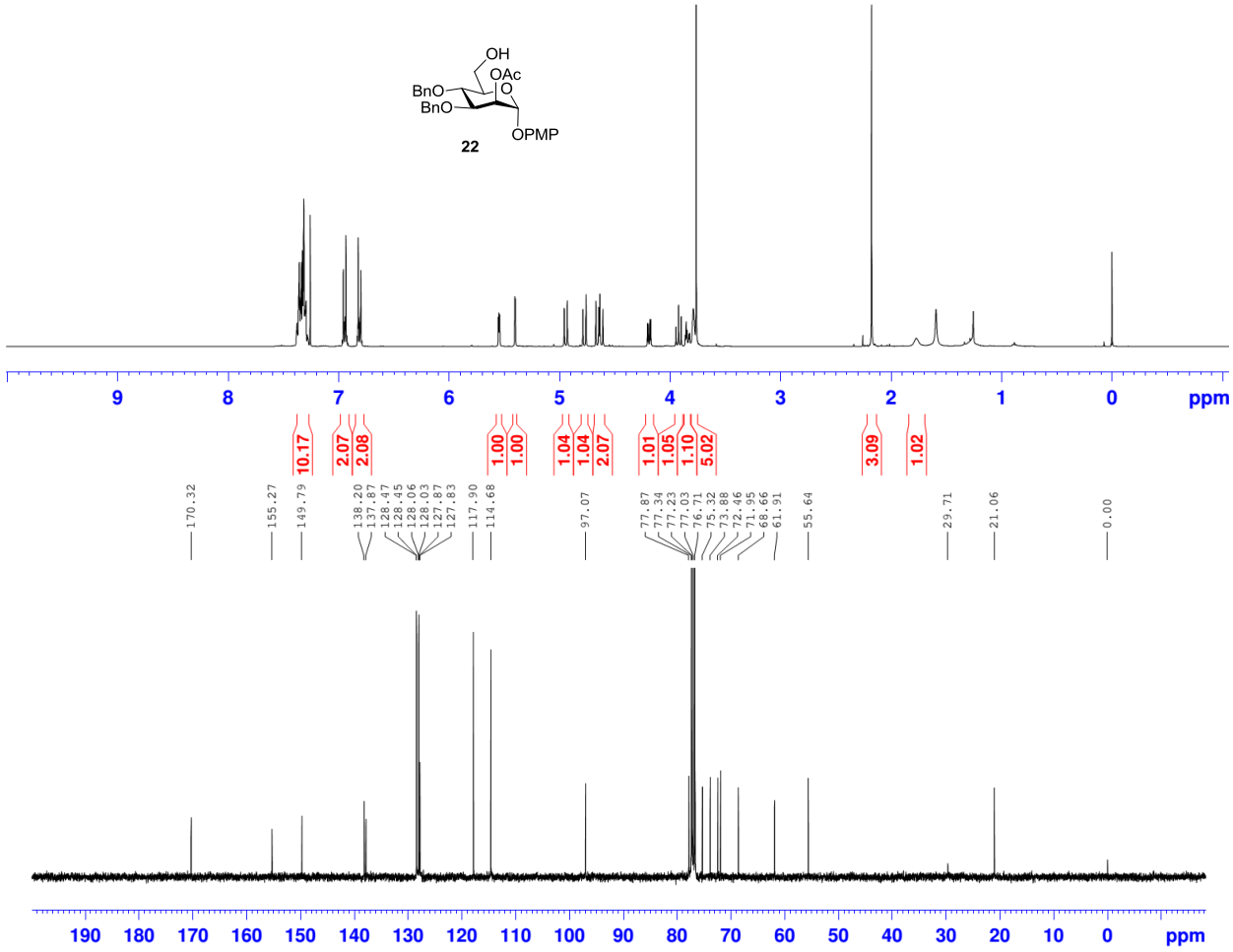
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **19**



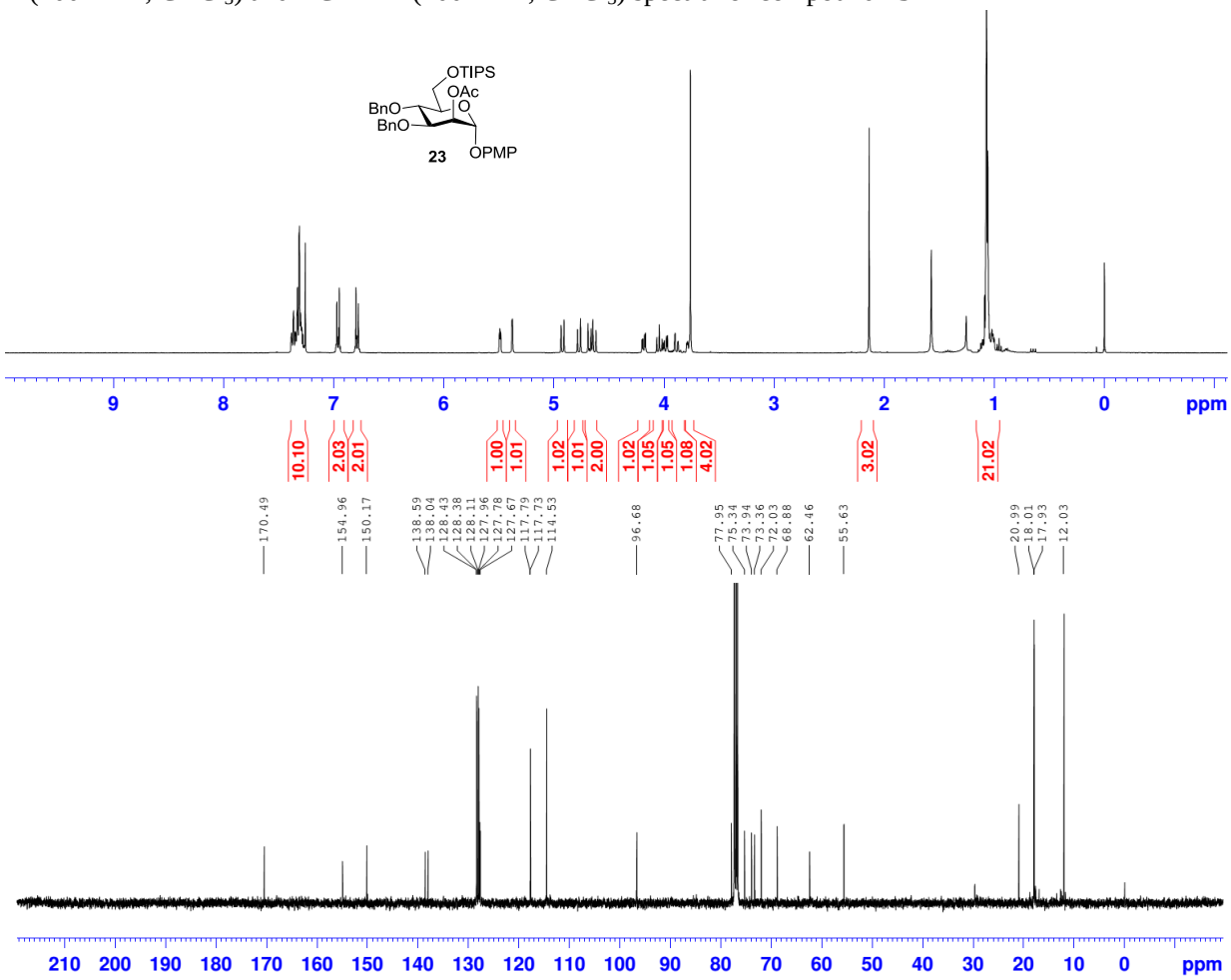
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **20**



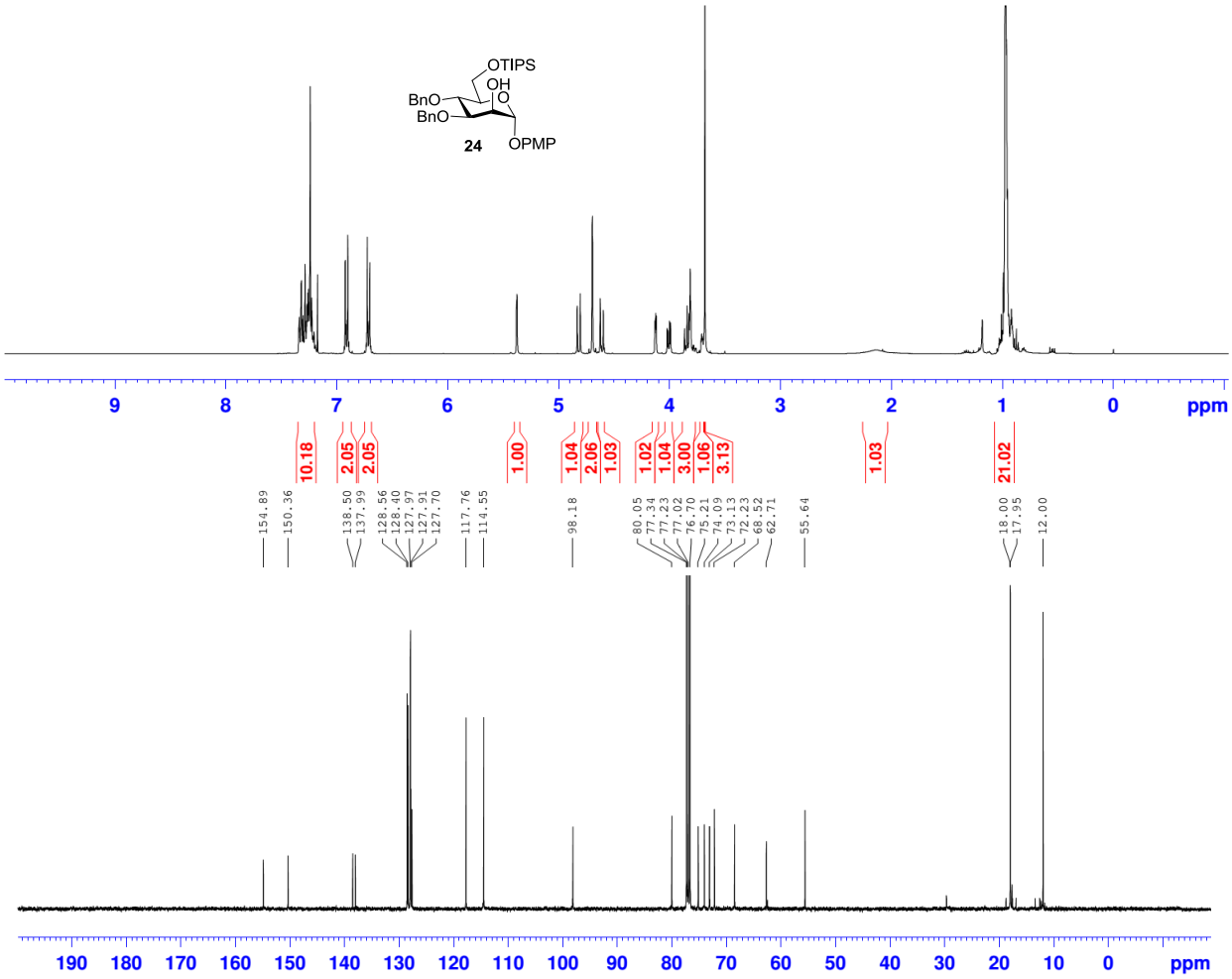
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **22**



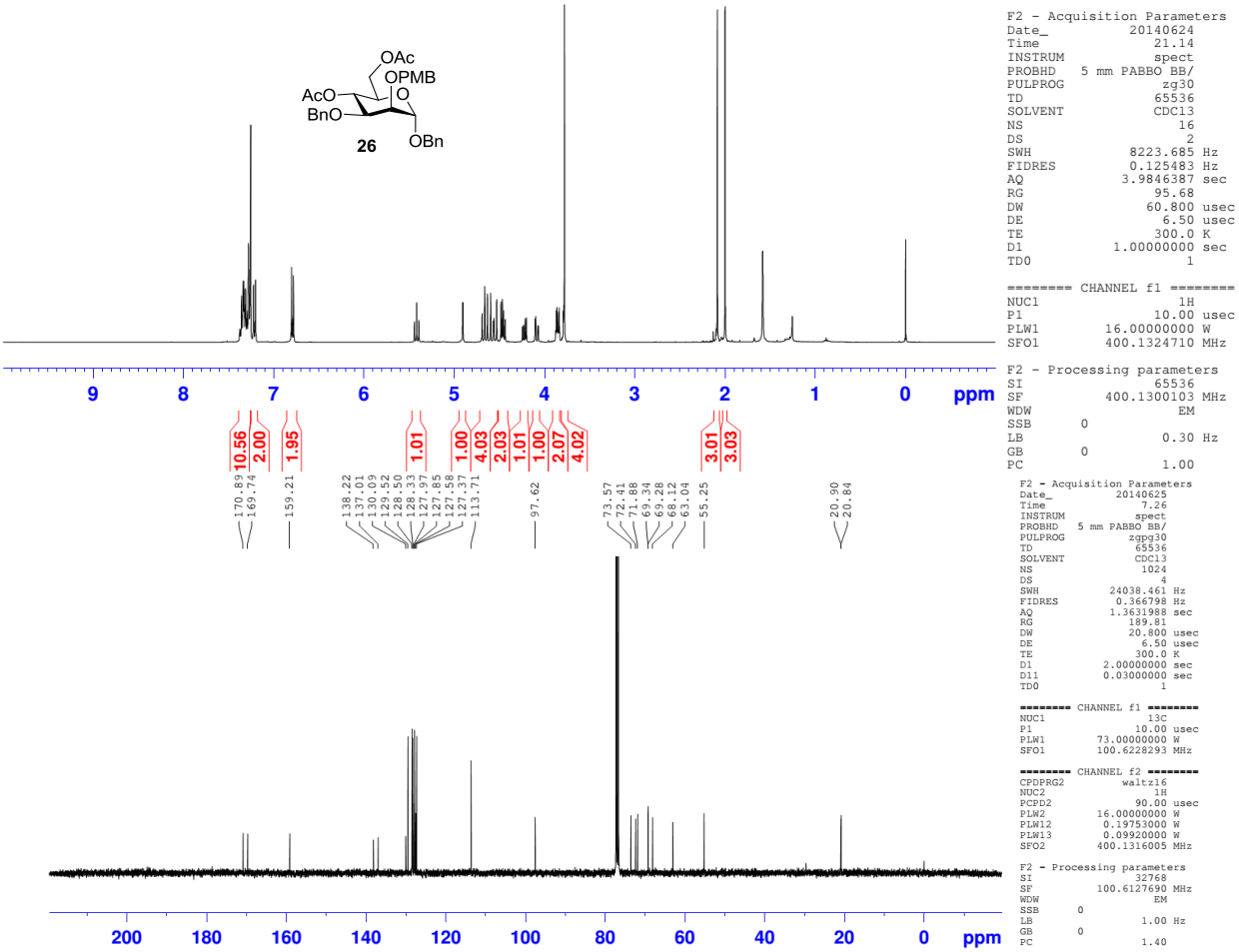
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **23**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **24**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **26**

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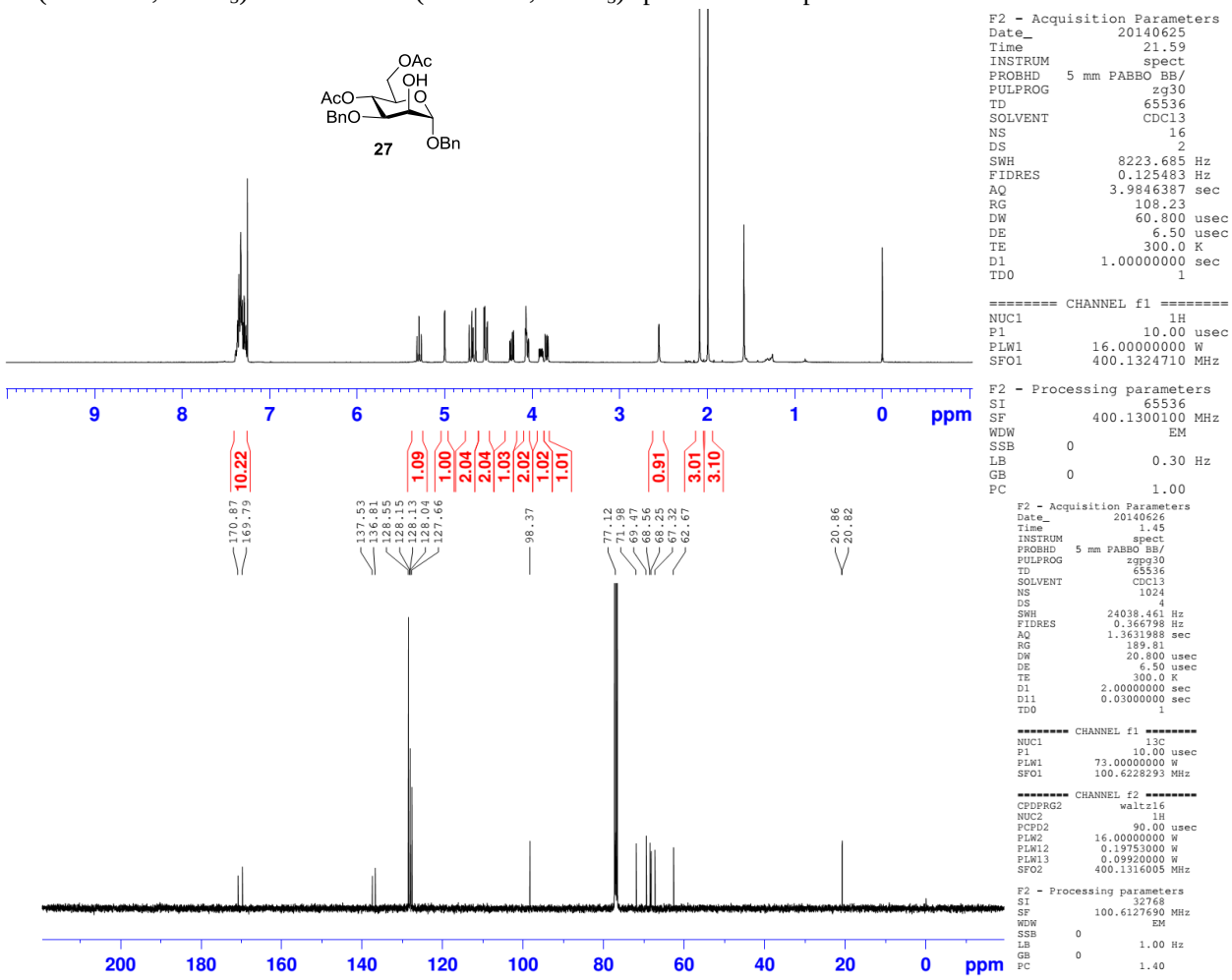
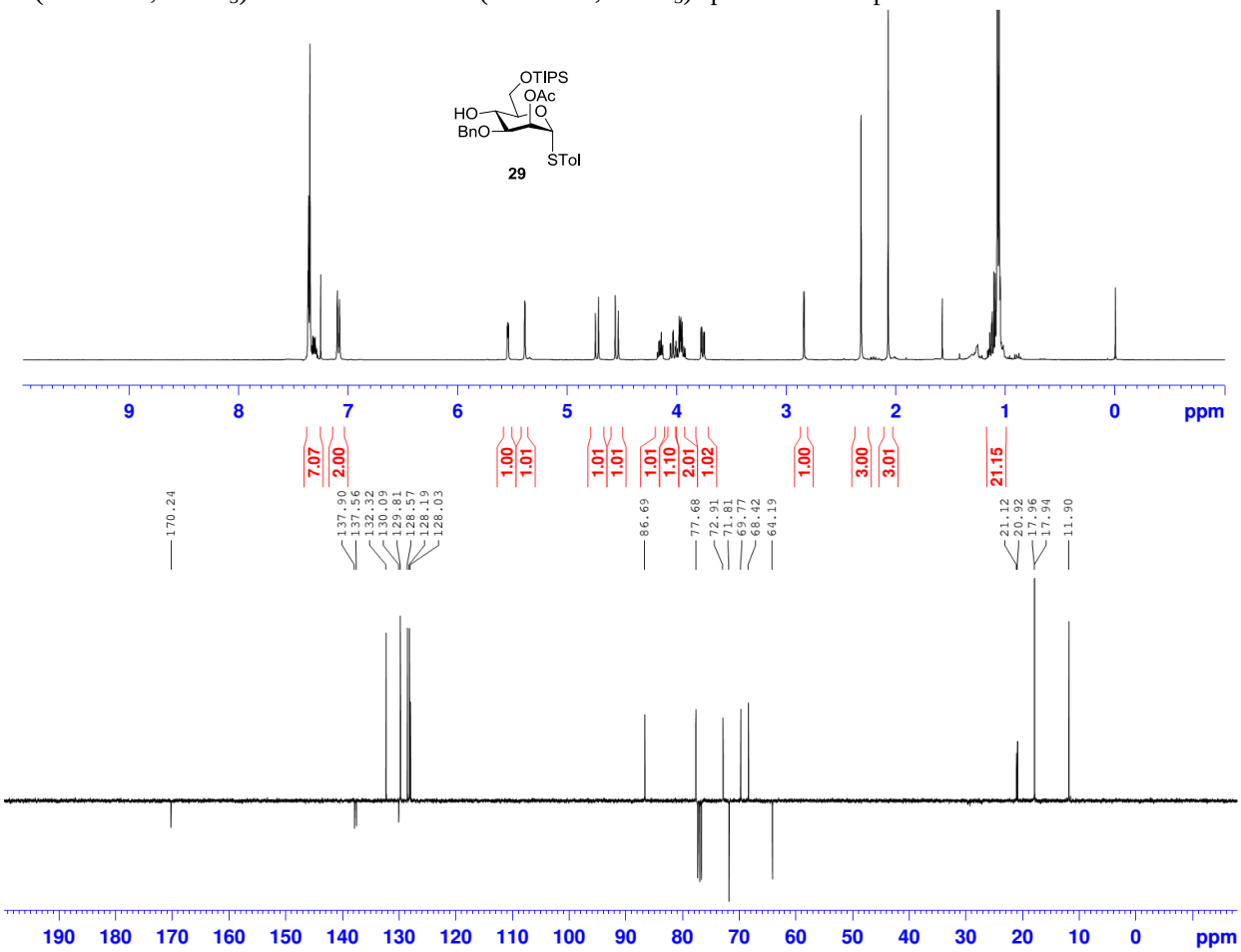
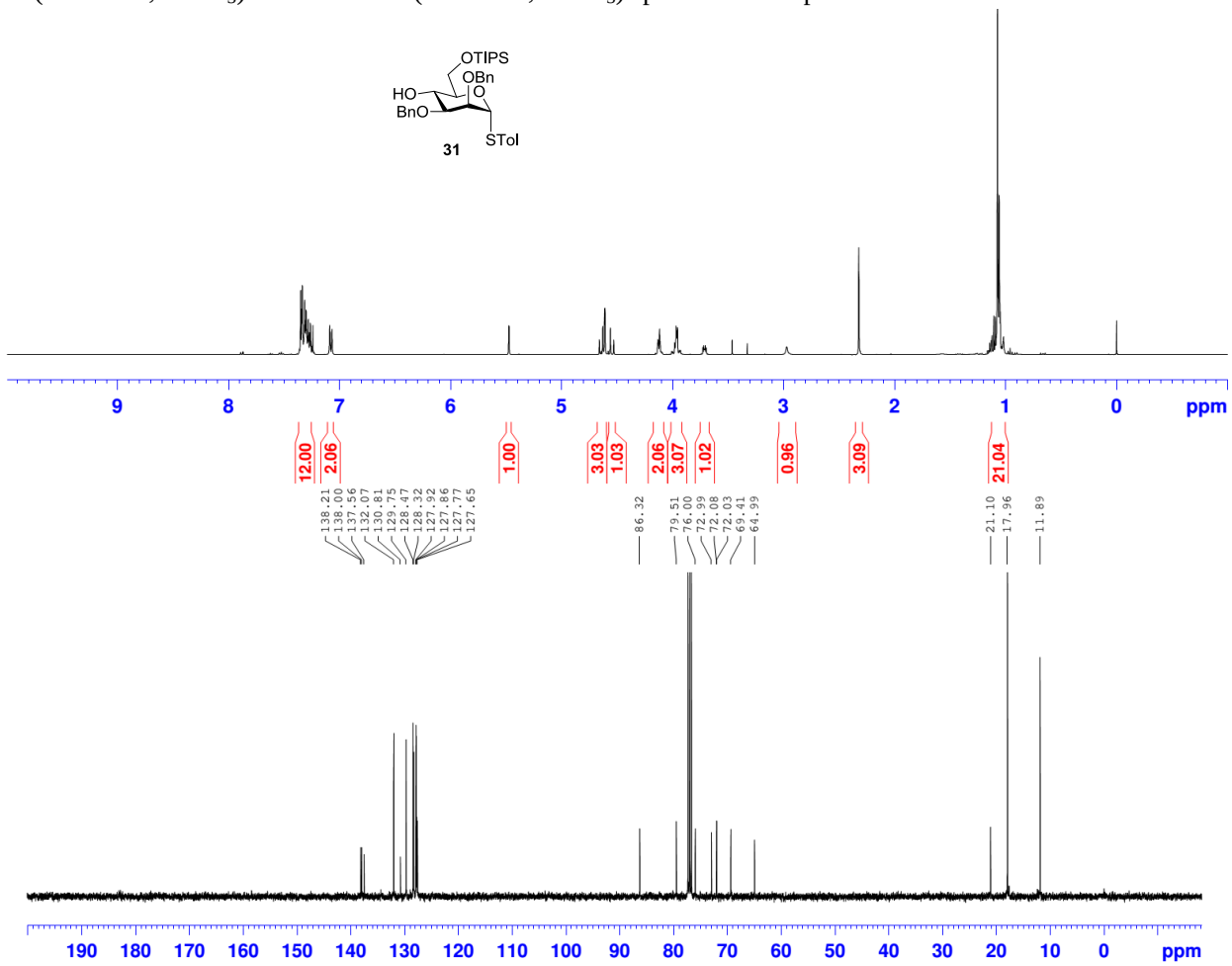
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **27**



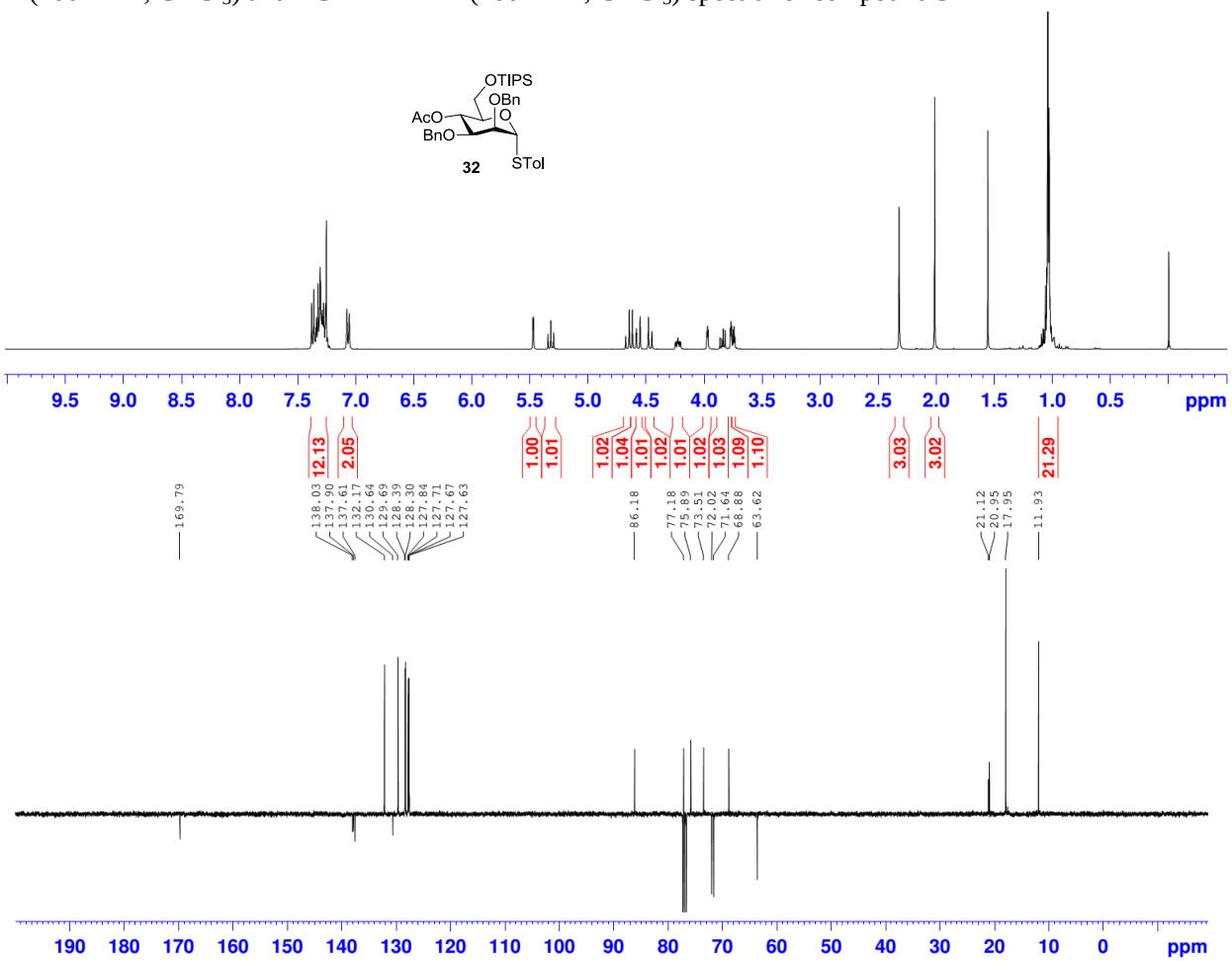
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **29**



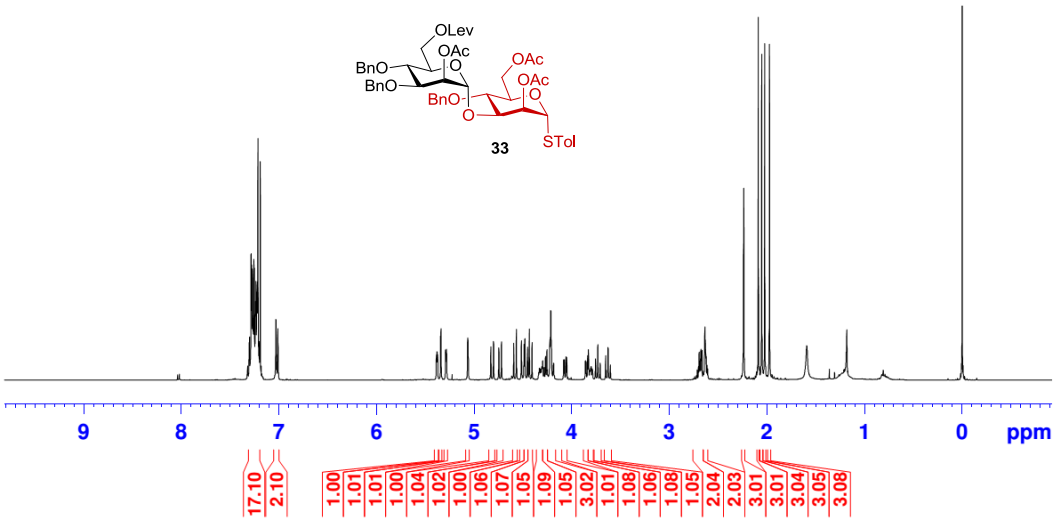
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **31**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **32**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **33**

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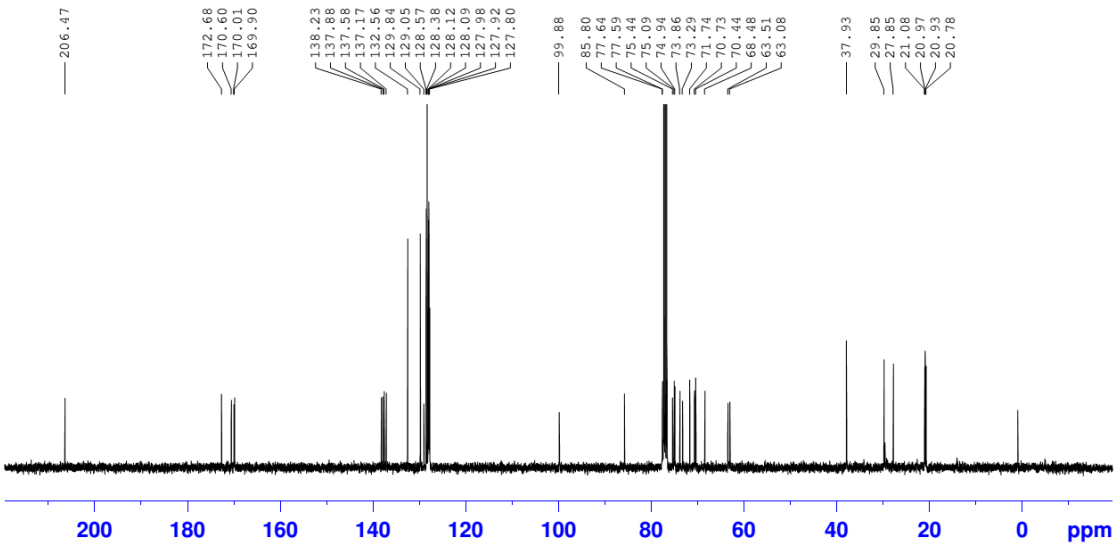


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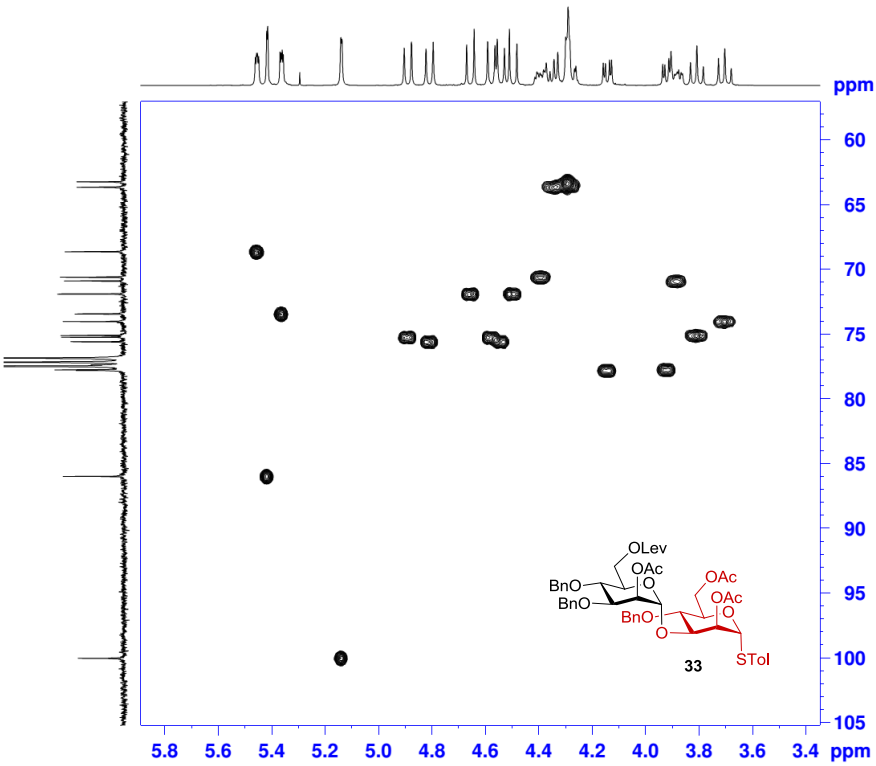
HSQC spectra (400 MHz, $CDCl_3$) for compound **33**

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IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
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======== CHANNEL f2 ========
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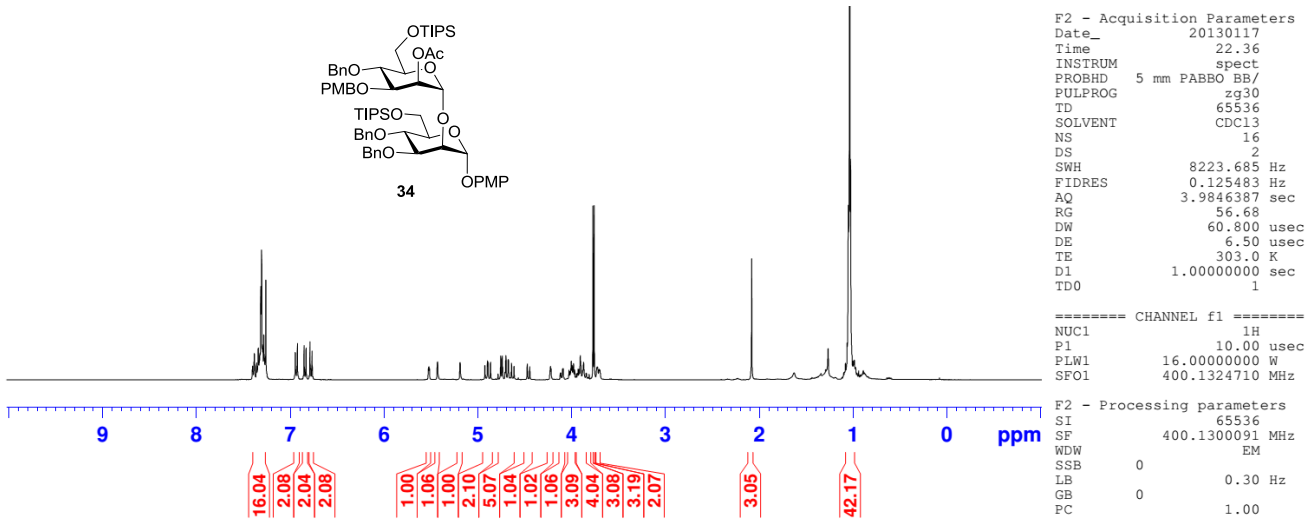
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPNAM3        SMSQ10.100
GPNAM4        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

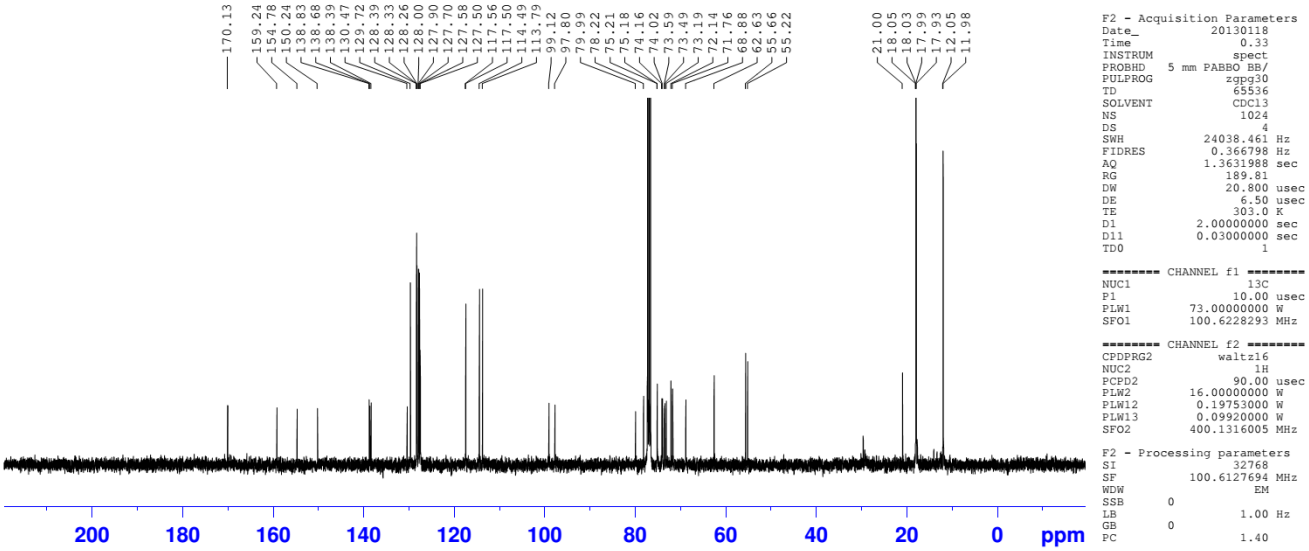
F1 - Acquisition parameters
TD                    256
SFO1            100.6203 MHz
FIDRES          65.108414 Hz
SW                165.650 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF            400.1300059 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                   1.40

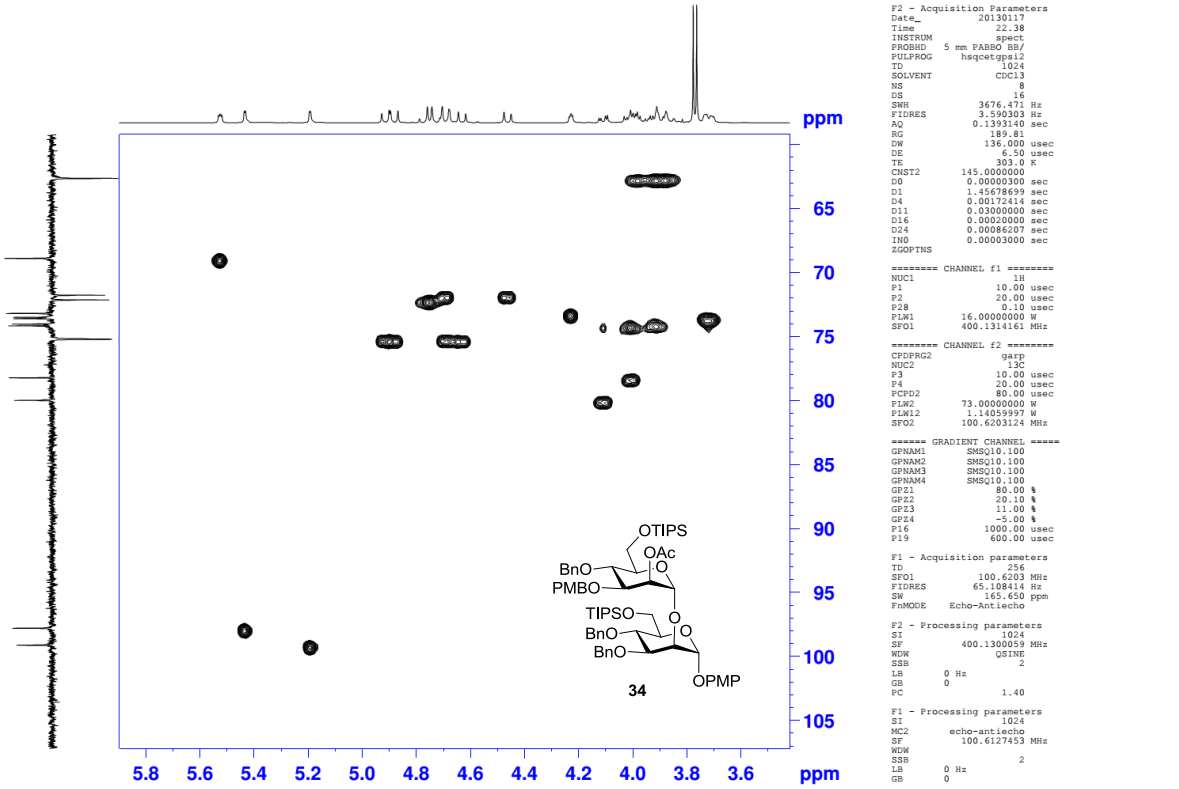
F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF             100.6127497 MHz
WDW
SSB                      2
LB         0 Hz
GB         0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **34**

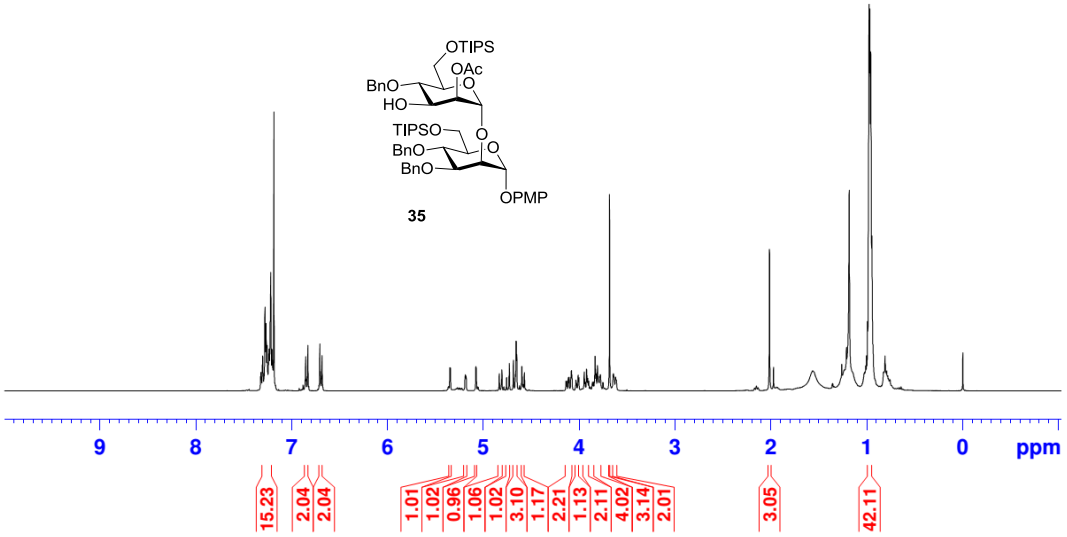




HSQC spectra (400 MHz, $CDCl_3$) for compound **34**



^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **35**

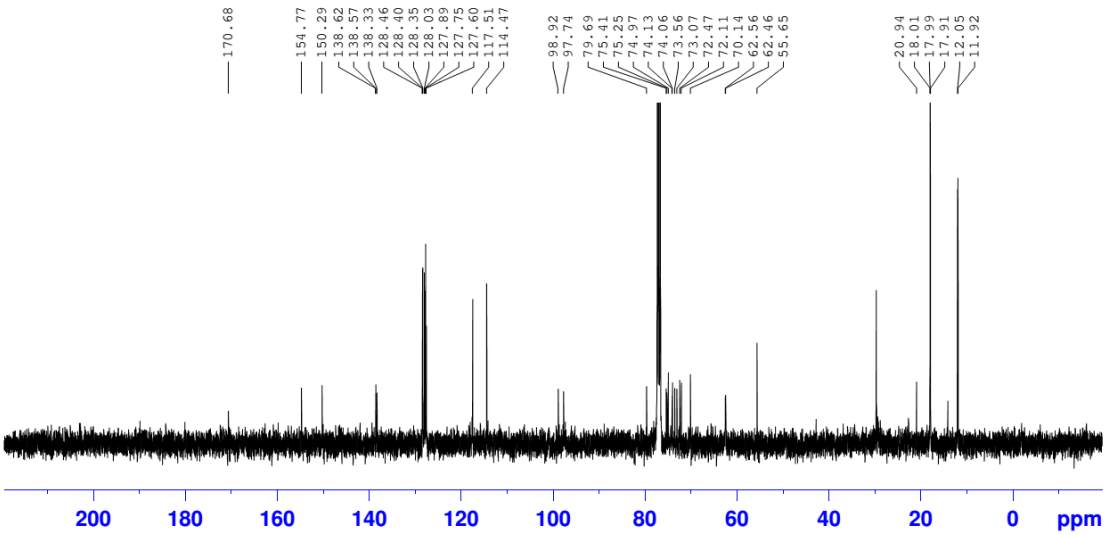



```
Current Data Parameters
NAME          JZ-N9-14-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_            20130201
Time                16.28
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     58
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ            3.9846387 sec
RG                 95.68
DW                60.800 usec
DE                 6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300382 MHz
WDW                    EM
SSB       0
LB                0.30 Hz
GB        0
PC                 1.00
```



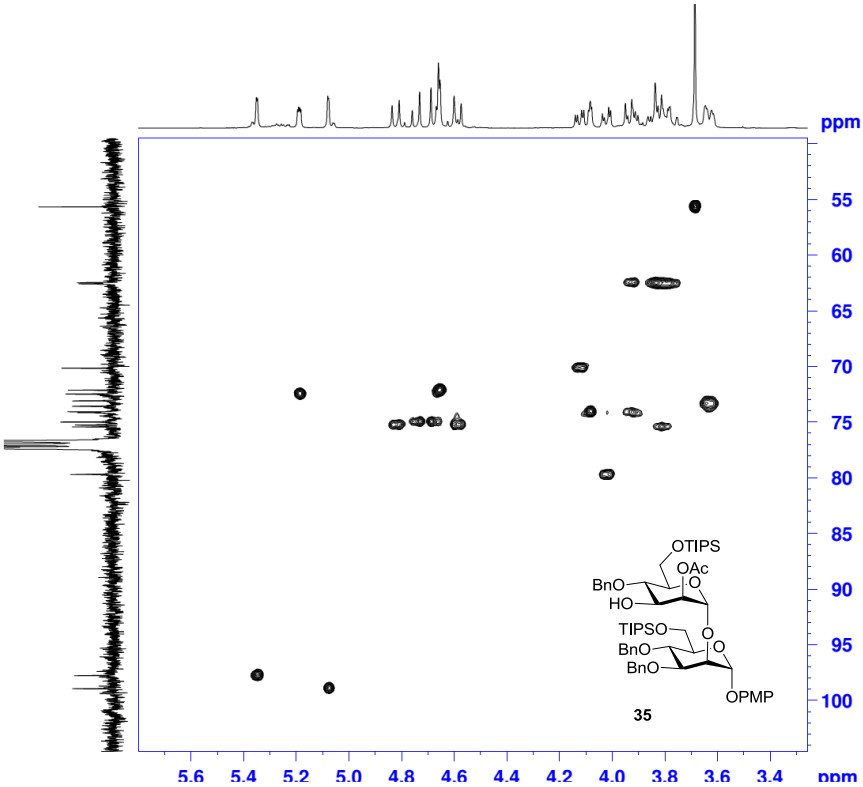

```
F2 - Acquisition Parameters
Date_            20130201
Time                17.34
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2048
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                189.81
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         73.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
PLW13         0.09920000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                    EM
SSB       0
LB                1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **35**




```
F2 - Acquisition Parameters
Date_            20130202
Time                11.17
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                   1024
SOLVENT             CDCl3
NS                     12
DS                     16
SWH             3289.474 Hz
FIDRES          3.212377 Hz
AQ             0.1556980 sec
RG                189.81
DW               152.000 usec
DE                 6.50 usec
TE                298.0 K
CNST2        145.00000000
D0            0.00000300 sec
D1            1.44040298 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28                0.10 usec
PLW1         16.00000000 W
SFO1        400.1316106 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2        100.6203124 MHz

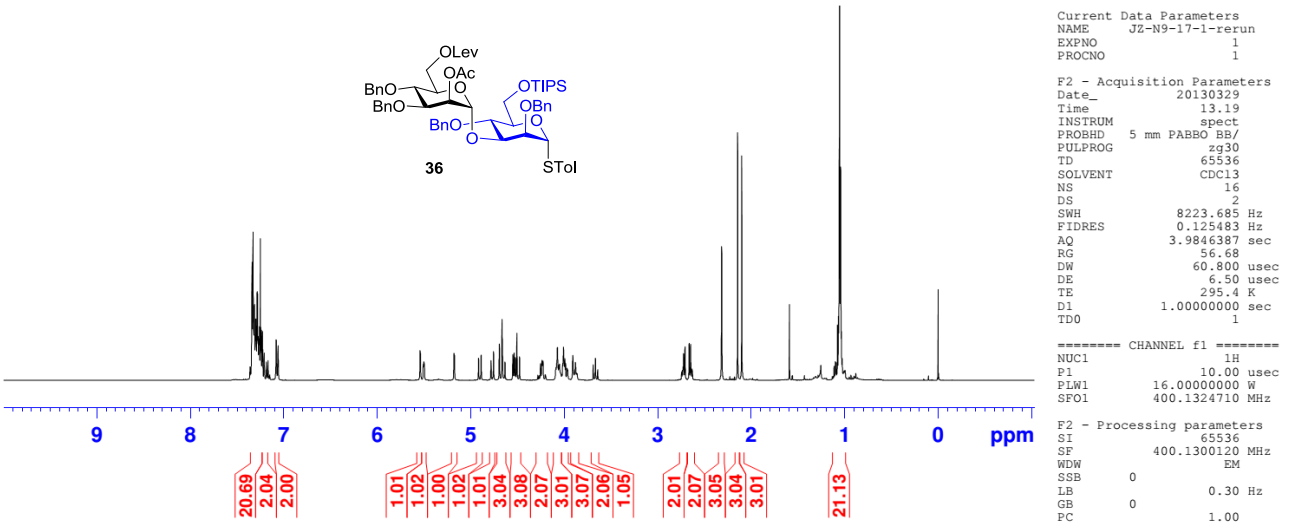
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPNAM4       SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

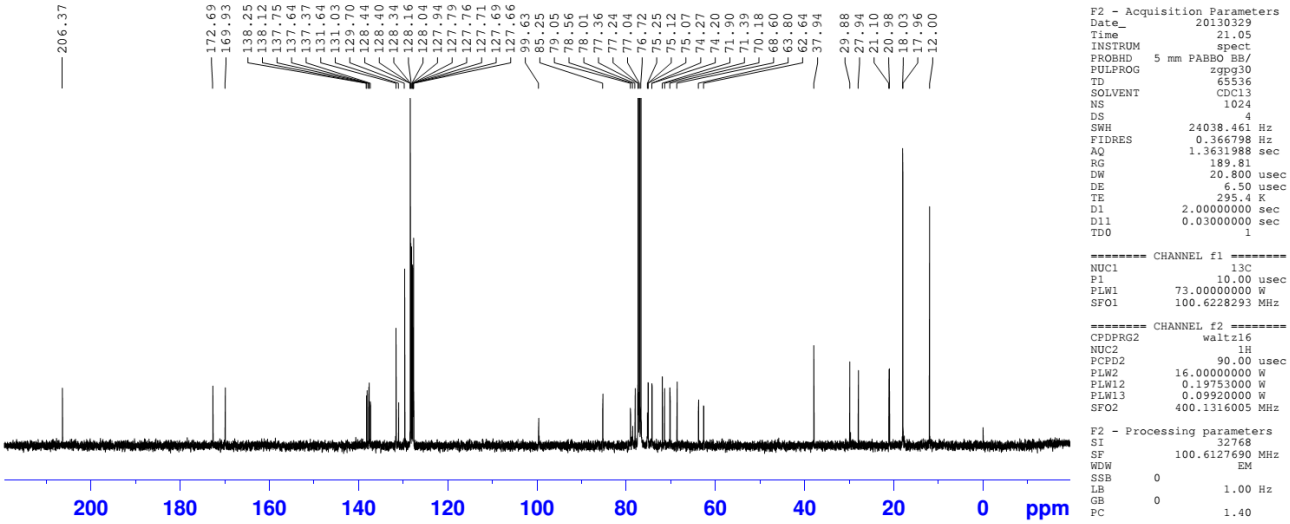
F1 - Acquisition parameters
TD                    256
SFO1            100.6203 MHz
FIDRES          65.108414 Hz
SW                165.650 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF          400.1300374 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                 1.40

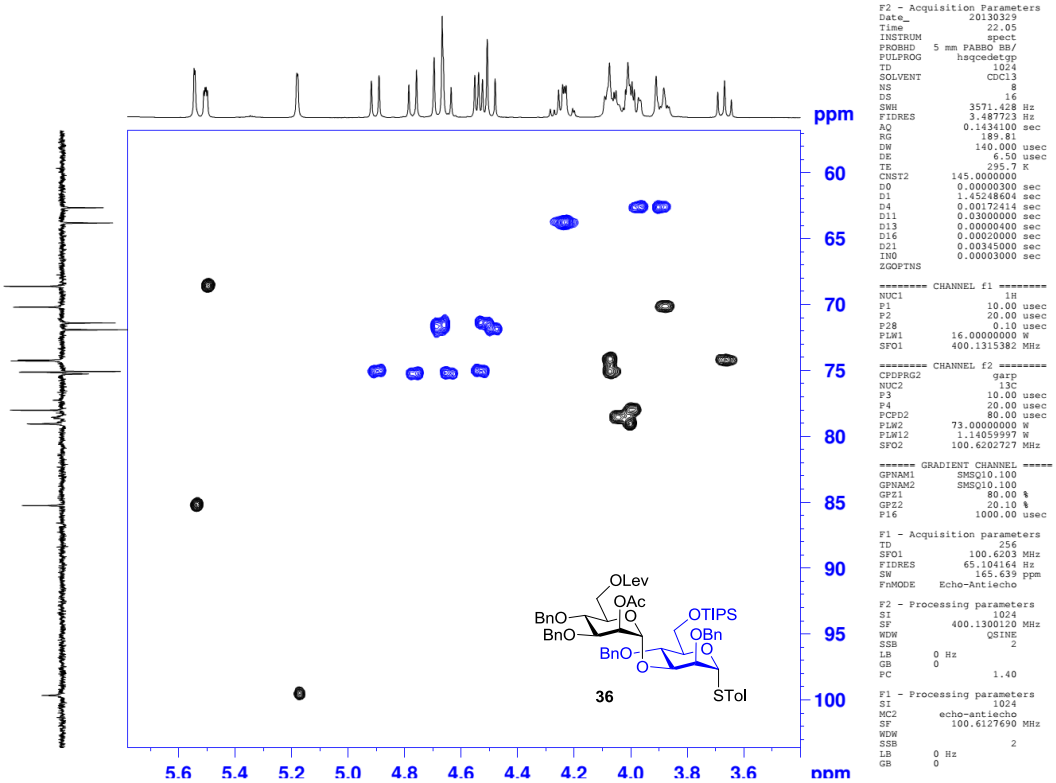
F1 - Processing parameters
SI                   1024
MC2          echo-antiecho
SF            100.6127690 MHz
WDW           States-TPPI
SSB                      2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **36**

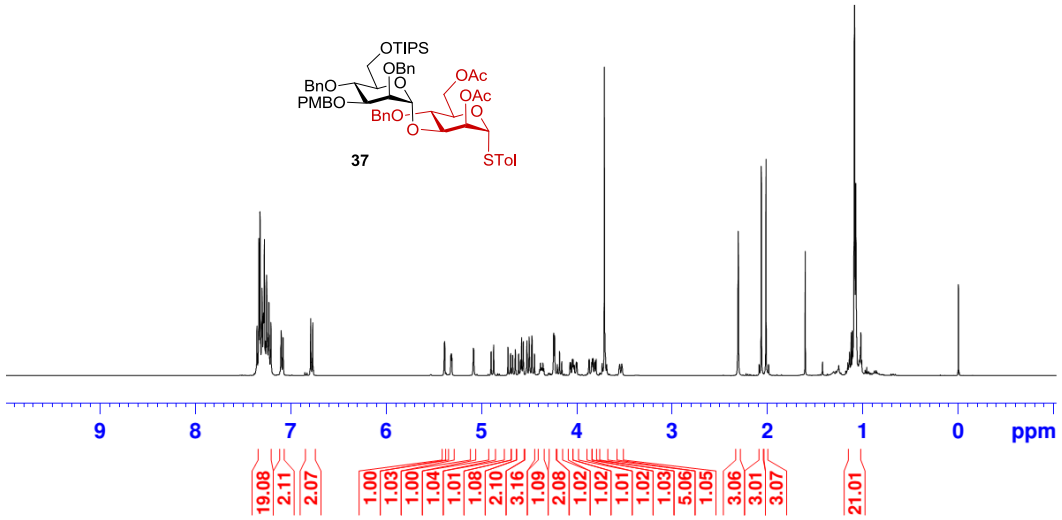




HSQC spectra (400 MHz, $CDCl_3$) for compound **36**



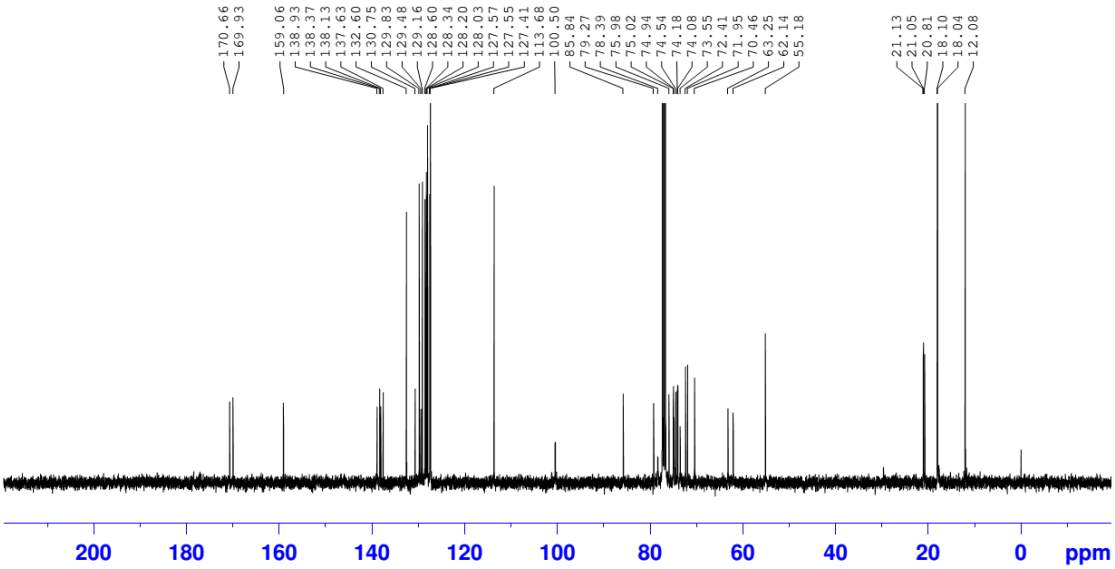
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **37**




```
F2 - Acquisition Parameters
Date_              20130327
Time                  20.42
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ               3.9846387 sec
RG                   31.69
DW                  60.800 usec
DE                    6.50 usec
TE                   294.5 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PLW1          16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300125 MHz
WDW                     EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.00
```



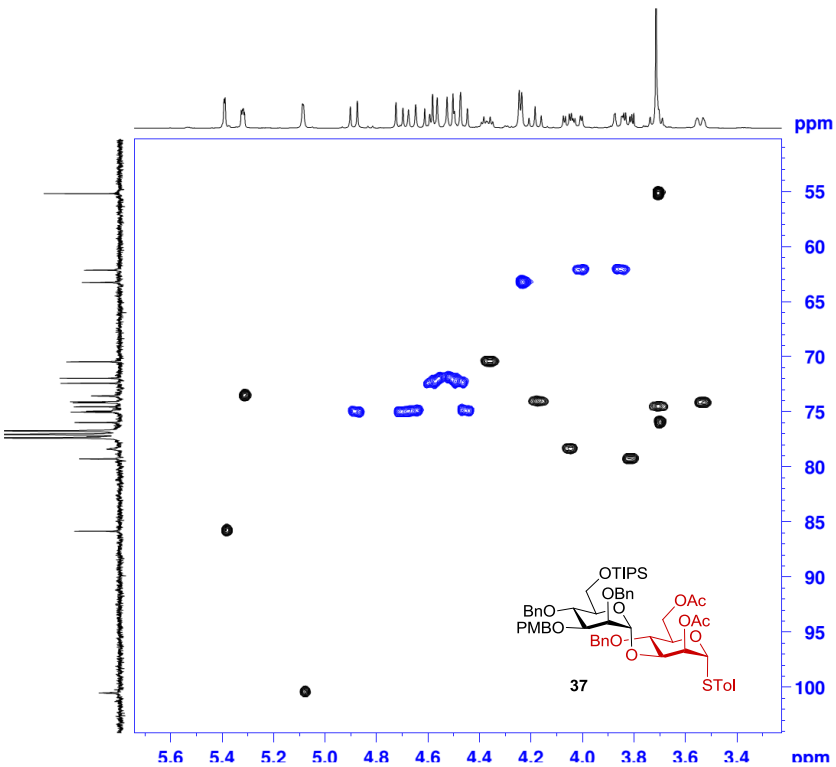

```
F2 - Acquisition Parameters
Date_              20130327
Time                  22.19
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                  189.81
DW                  20.800 usec
DE                    6.50 usec
TE                   294.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1          73.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PLW2          16.00000000 W
PLW12          0.19753000 W
PLW13          0.09920000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB        0
LB                    1.00 Hz
GB         0
PC                    1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **37**




```
F2 - Acquisition Parameters
Date_              20130327
Time                  23.03
INSTRUM               spect
PROBHD     5 mm PABBO BB/
PULPROG            hsqcedetgp
TD                    1024
SOLVENT              CDCl3
NS                       8
DS                      16
SWH               3521.127 Hz
FIDRES            3.438600 Hz
AQ               0.1454580 sec
RG                  189.81
DW                 142.000 usec
DE                    6.50 usec
TE                   294.9 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.45043802 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
P2                   20.00 usec
P28                   0.10 usec
PLW1          16.00000000 W
SFO1         400.1314808 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                   13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2         100.6202727 MHz

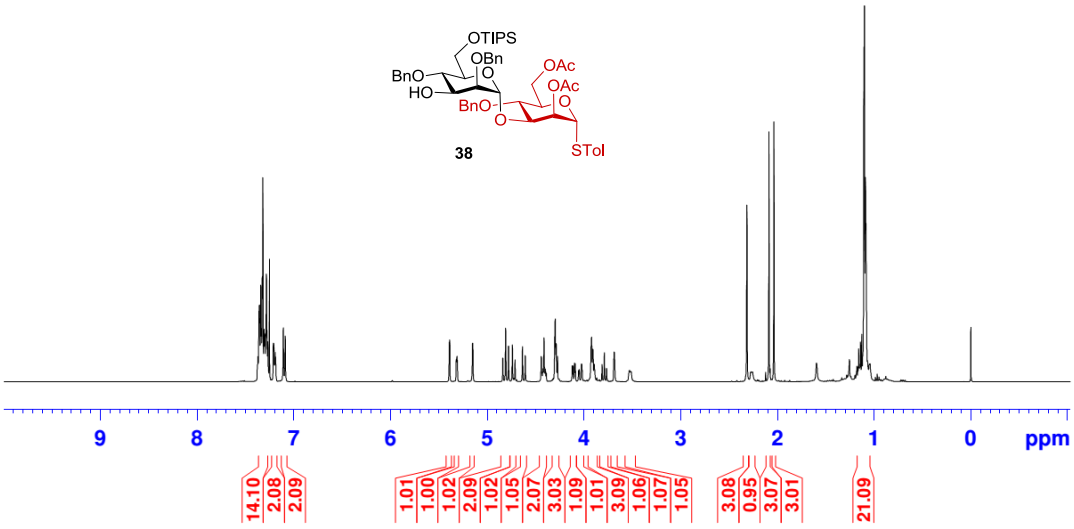
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW               165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF           400.1300125 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2         echo-antiecho
SF           100.6127690 MHz
WDW          States-TPPI
SSB                      2
LB         0 Hz
GB         0
```

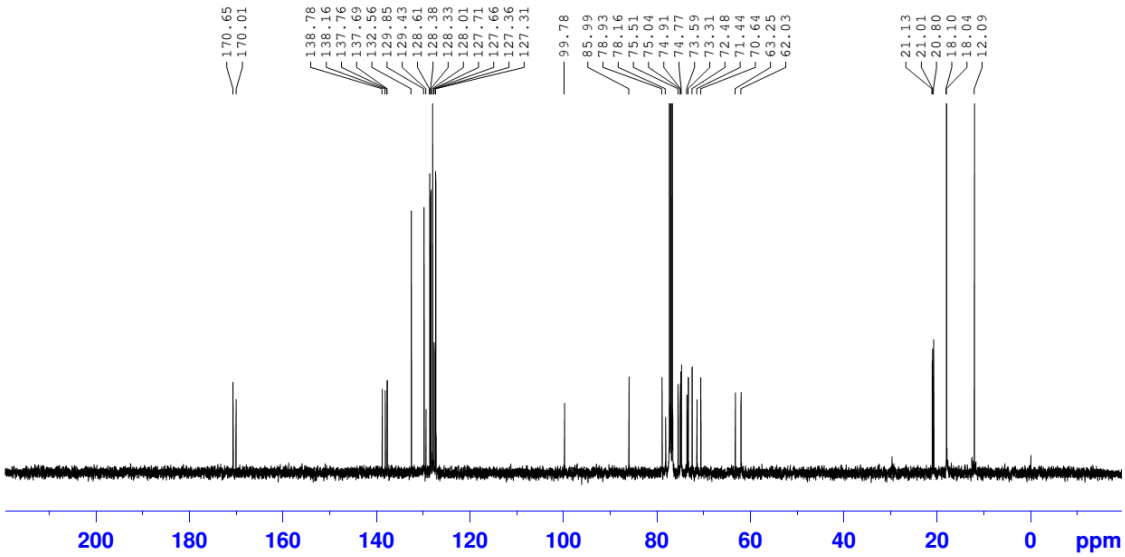
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **38**




```
F2 - Acquisition Parameters
Date_              20130331
Time                  13.43
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ               3.9846387 sec
RG                    56.68
DW                   60.800 usec
DE                     6.50 usec
TE                    296.8 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.00 usec
PLW1           16.00000000 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300121 MHz
WDW                      EM
SSB         0
LB                     0.30 Hz
GB          0
PC                     1.00
```



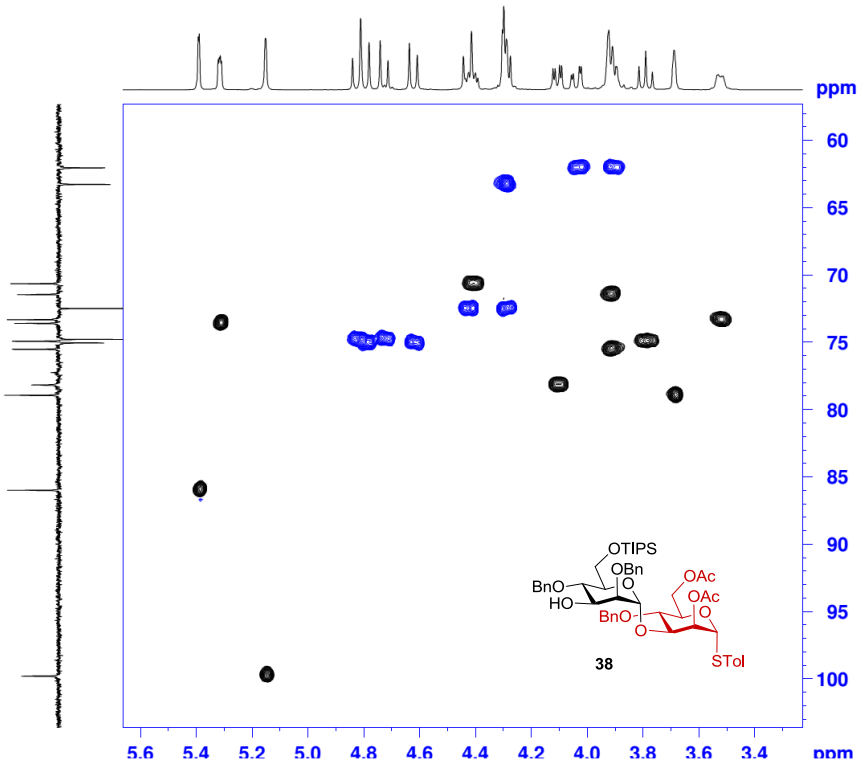

```
F2 - Acquisition Parameters
Date_              20130331
Time                  15.50
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                   189.81
DW                   20.800 usec
DE                     6.50 usec
TE                    296.8 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                    10.00 usec
PLW1           73.00000000 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2           16.00000000 W
PLW12           0.19753000 W
PLW13           0.09920000 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **38**




```
F2 - Acquisition Parameters
Date_              20130331
Time                  17.07
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG          hsqcedetgp
TD                     1024
SOLVENT               CDCl3
NS                        8
DS                       16
SWH               3649.635 Hz
FIDRES            3.564097 Hz
AQ               0.1403380 sec
RG                   189.81
DW                  137.000 usec
DE                     6.50 usec
TE                    298.0 K
CNST2          145.0000000
D0               0.00000300 sec
D1               1.45555794 sec
D4               0.00172414 sec
D11              0.03000000 sec
D13              0.00000400 sec
D16              0.00020000 sec
D21              0.00345000 sec
IN0              0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.00 usec
P2                    20.00 usec
P28                    0.10 usec
PLW1           16.00000000 W
SFO1           400.1315087 MHz

======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                     13C
P3                    10.00 usec
P4                    20.00 usec
PCPD2                 80.00 usec
PLW2           73.00000000 W
PLW12           1.14059997 W
SFO2           100.6202727 MHz

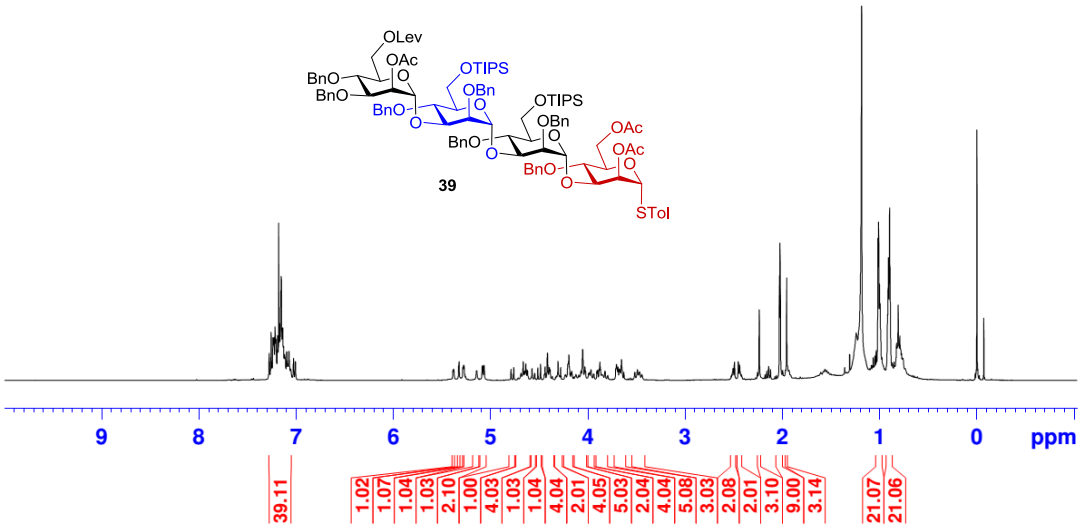
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                      256
SFO1             100.6203 MHz
FIDRES           65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF            400.1300121 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2          echo-antiecho
SF             100.6127690 MHz
WDW            States-TPPI
SSB                        2
LB          0 Hz
GB          0
```

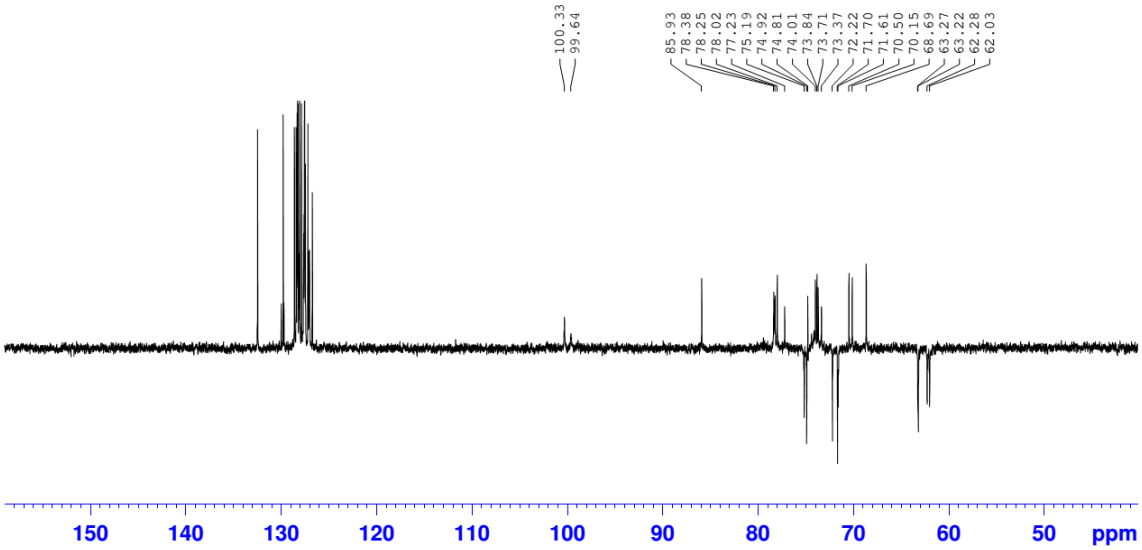
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **39**




```
F2 - Acquisition Parameters
Date_           20130407
Time               21.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                31.69
DW                60.800 usec
DE                 6.50 usec
TE                303.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300406 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



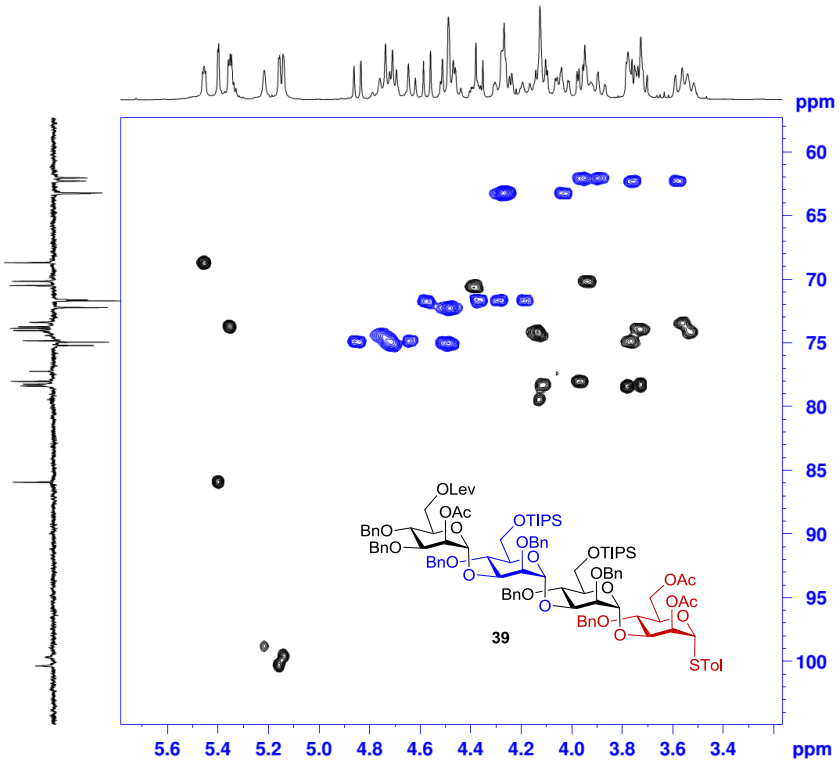

```
F2 - Acquisition Parameters
Date_           20130409
Time               2.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                  2048
DS                     4
SWH            16129.032 Hz
FIDRES          0.246110 Hz
AQ             2.0316660 sec
RG                189.81
DW                31.000 usec
DE                 6.50 usec
TE                298.0 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
P13             2000.00 usec
PLW0      0 W
PLW1         73.00000000 W
SFO1        100.6208171 MHz
SPNAM5       Crp60comp.4
SPOAL5             0.500
SPOFF85   0 Hz
SPW5         11.15400028 W

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
P3                10.00 usec
P4                20.00 usec
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2        400.1312797 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127697 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectrum (400 MHz, $CDCl_3$) for compound **39**




```
F2 - Acquisition Parameters
Date_           20130407
Time               23.03
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     8
DS                    16
SWH             4310.345 Hz
FIDRES          4.209321 Hz
AQ             0.1188340 sec
RG                189.81
DW               116.000 usec
DE                 6.50 usec
TE                303.0 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.47706199 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28                0.10 usec
PLW1         16.00000000 W
SFO1        400.1313619 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2        100.6202727 MHz

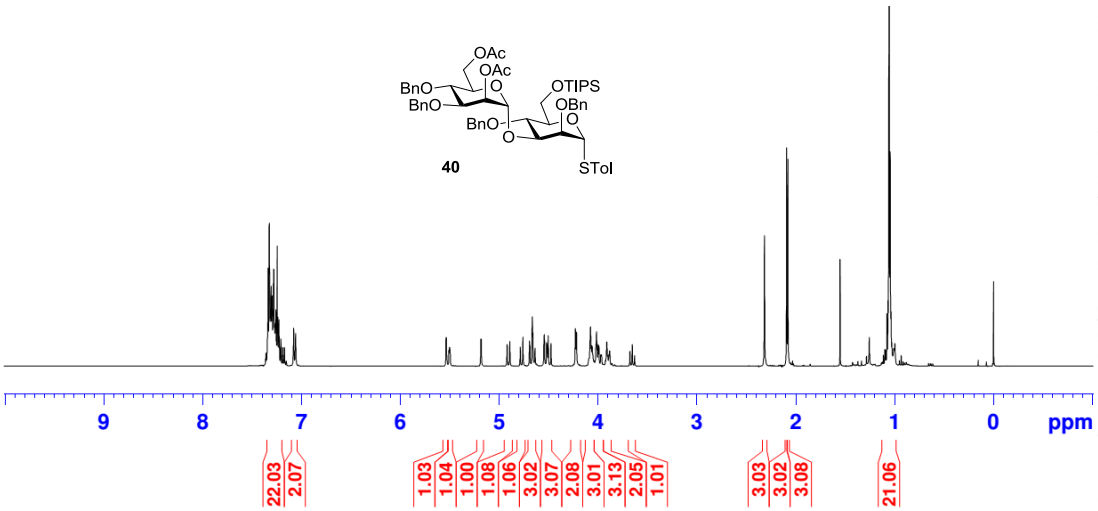
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW              165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF          400.1300098 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127660 MHz
WDW                    ;
SSB                    2
LB        0 Hz
GB        0
```

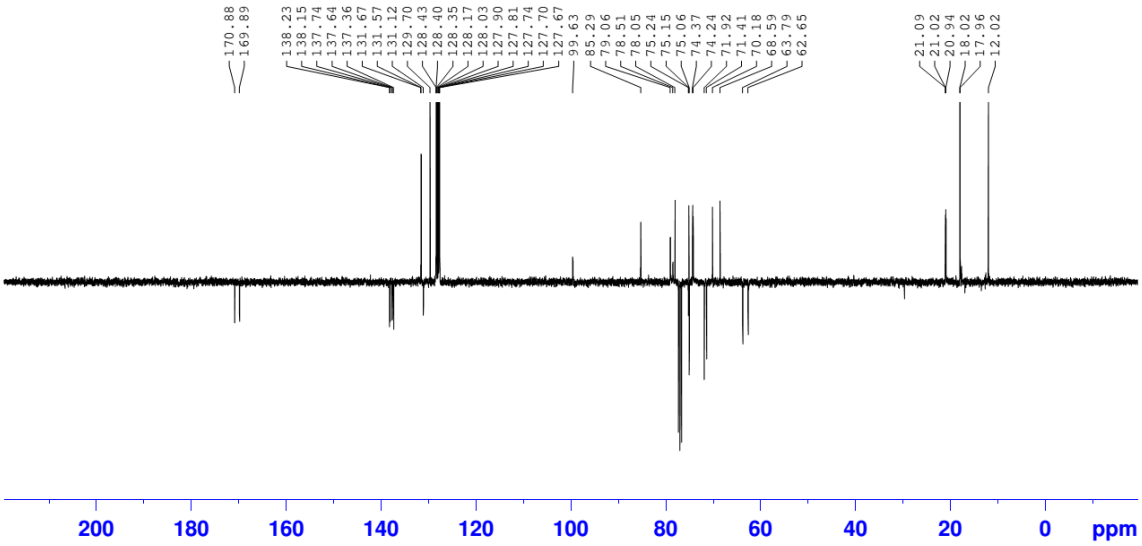
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **40**




```
F2 - Acquisition Parameters
Date_            20141022
Time               13.07
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                  62.9
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300138 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



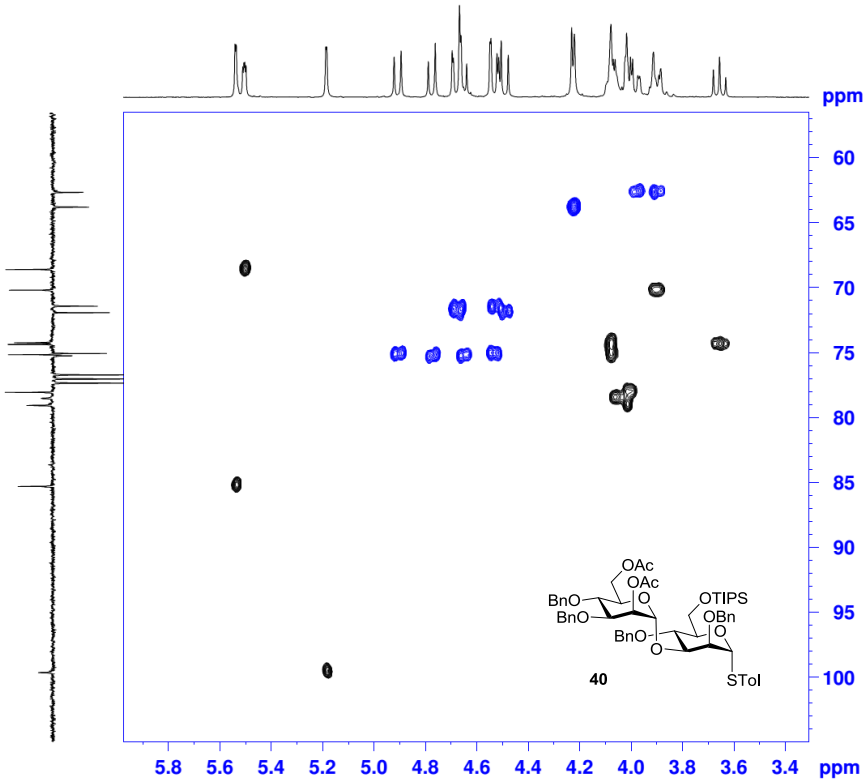

```
F2 - Acquisition Parameters
Date_            20141022
Time               14.45
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG            jmod
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                189.81
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         73.00000000 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **40**




```
F2 - Acquisition Parameters
Date_            20141022
Time               13.29
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             3378.378 Hz
FIDRES          3.299198 Hz
AQ             0.1516020 sec
RG                189.81
DW               148.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.44429398 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1         16.00000000 W
SFO1         400.1315982 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

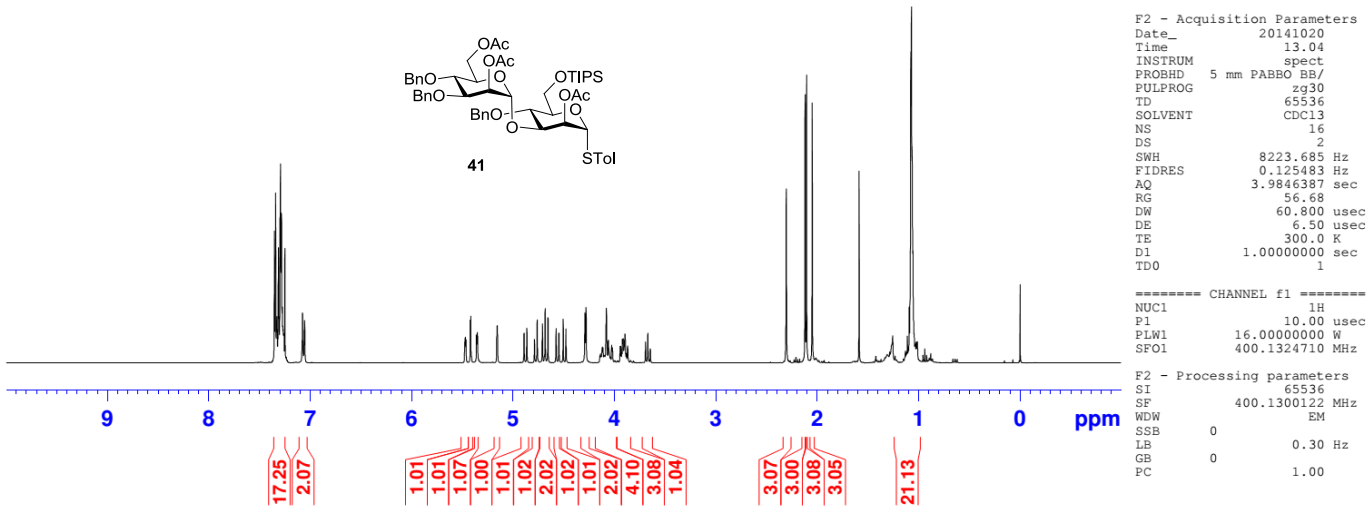
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

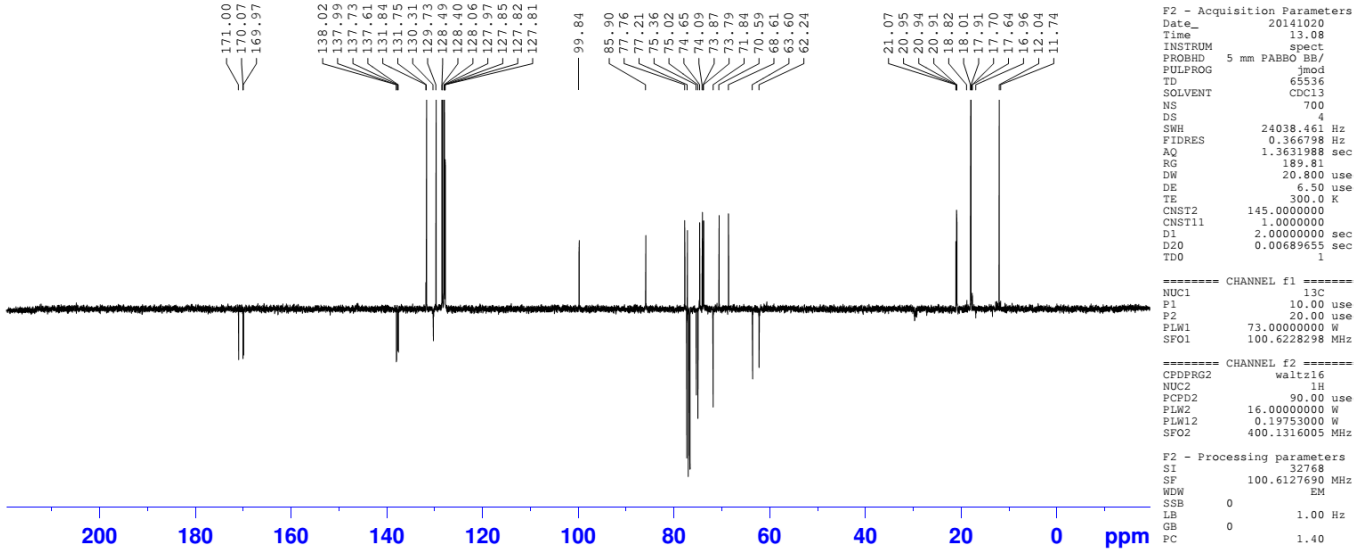
F1 - Acquisition parameters
TD                   210
SFO1          100.6203 MHz
FIDRES         79.365082 Hz
SW            165.639 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300138 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                 1.40

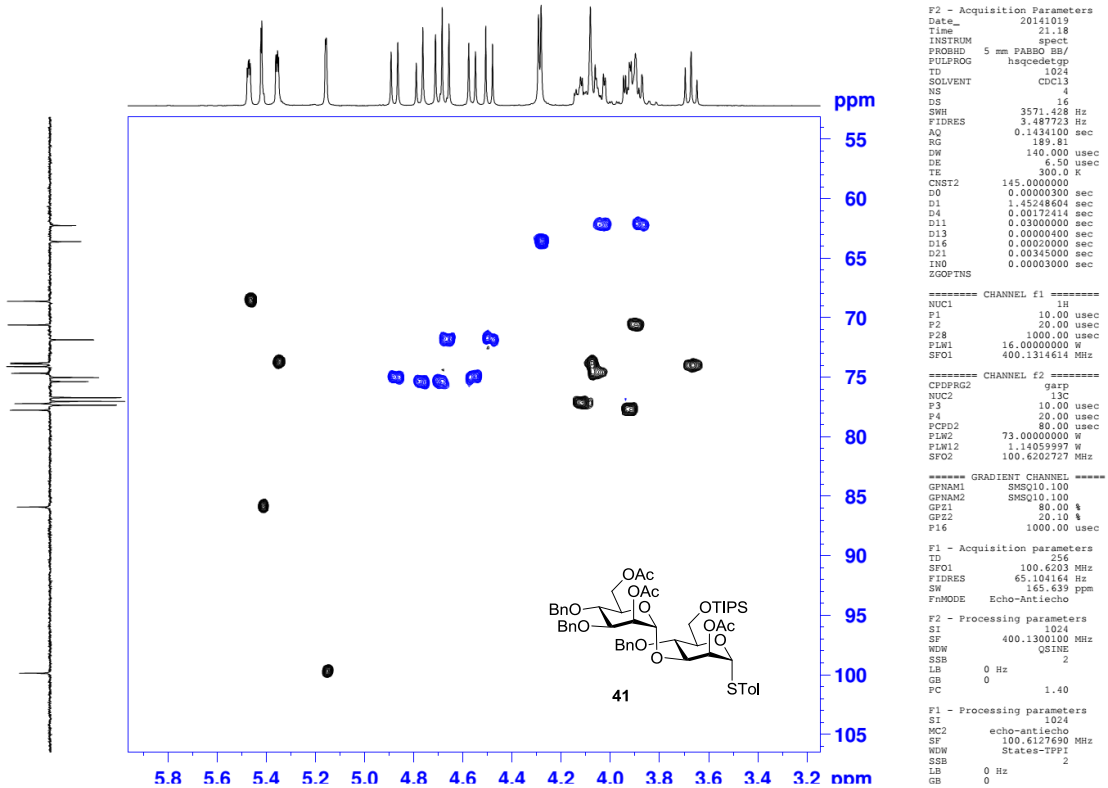
F1 - Processing parameters
SI                  1024
MC2         echo-antiecho
SF           100.6127690 MHz
WDW          States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **41**

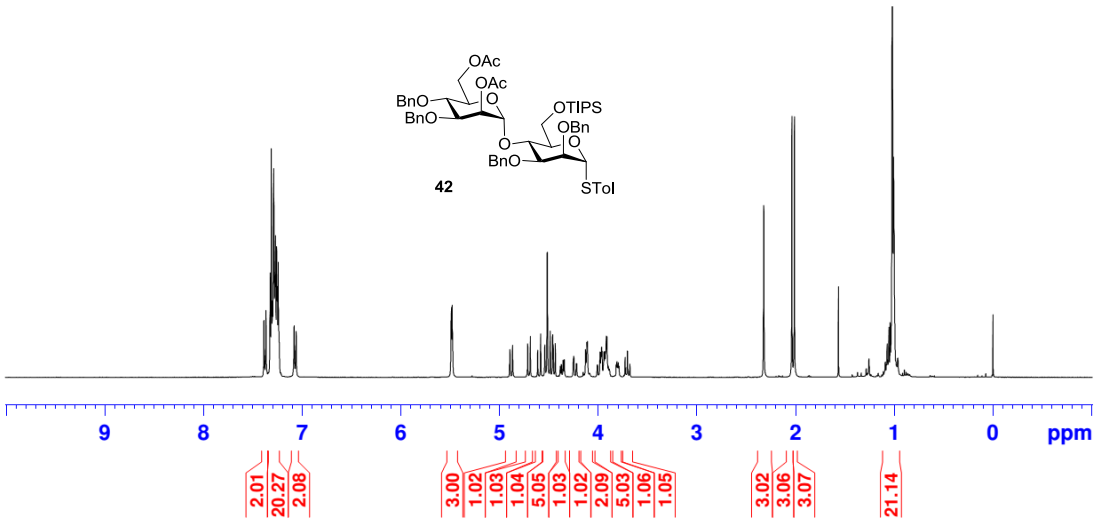




HSQC spectra (400 MHz, $CDCl_3$) for compound **41**



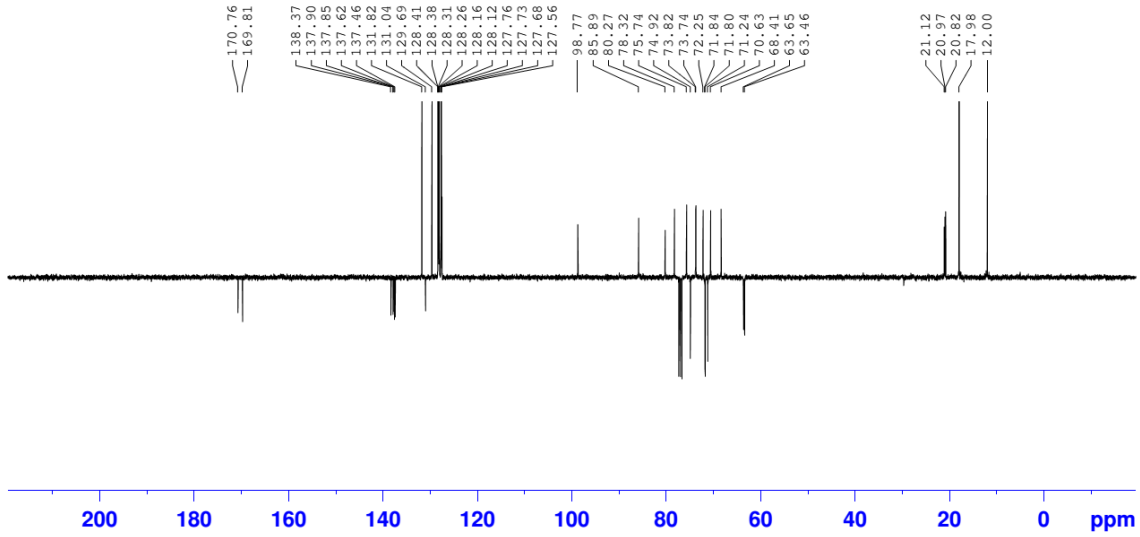
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **42**




```
F2 - Acquisition Parameters
Date_           20141022
Time               22.31
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 31.69
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300152 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



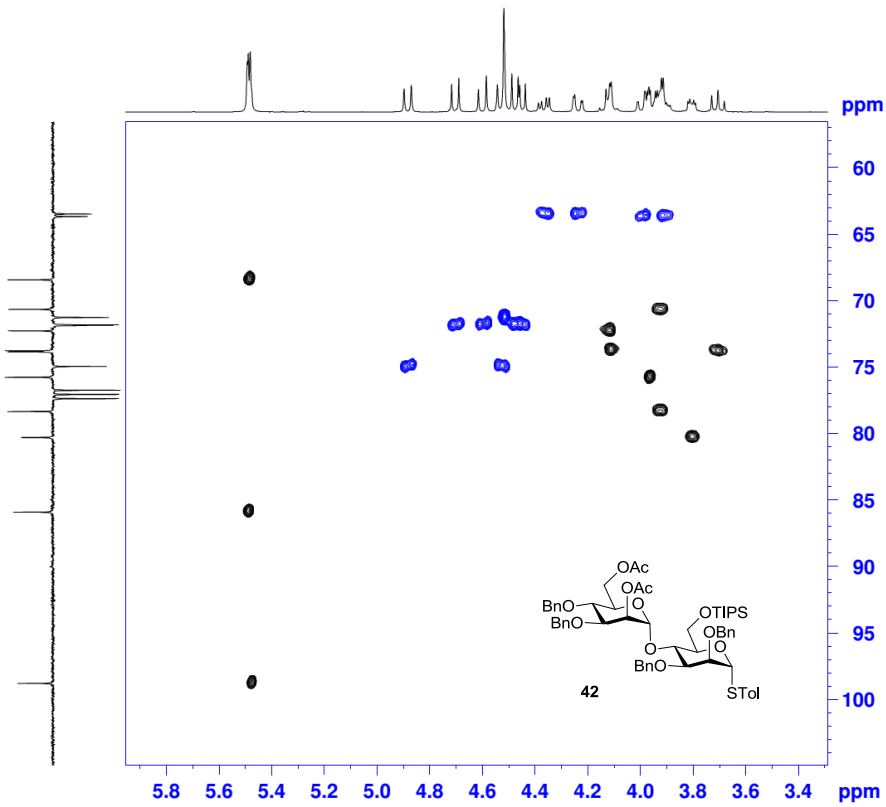

```
F2 - Acquisition Parameters
Date_           20141023
Time               0.15
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            jmod
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 189.81
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         73.00000000 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **42**




```
F2 - Acquisition Parameters
Date_           20141022
Time               22.51
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             3496.503 Hz
FIDRES          3.414554 Hz
AQ             0.1464820 sec
RG                 189.81
DW               143.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.00000000
D0            0.00000300 sec
D1            1.44941401 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1         16.00000000 W
SFO1         400.1315311 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

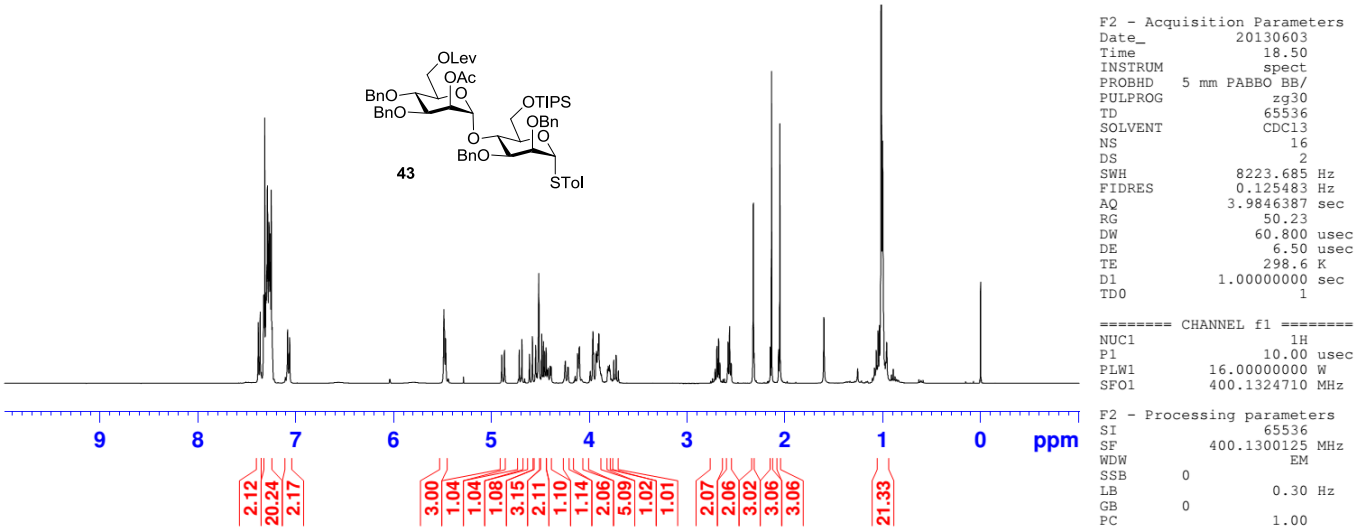
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1             80.00 %
GPZ2             20.10 %
P16             1000.00 usec

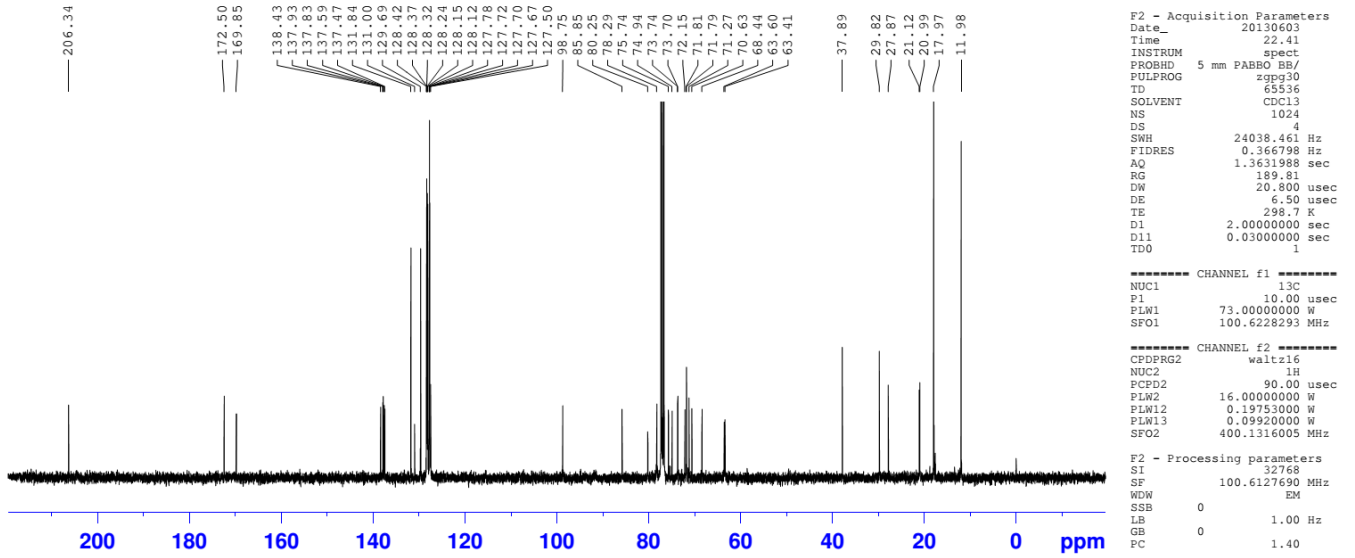
F1 - Acquisition parameters
TD                   256
SFO1           100.6203 MHz
FIDRES         65.104164 Hz
SW               165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF          400.1300152 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

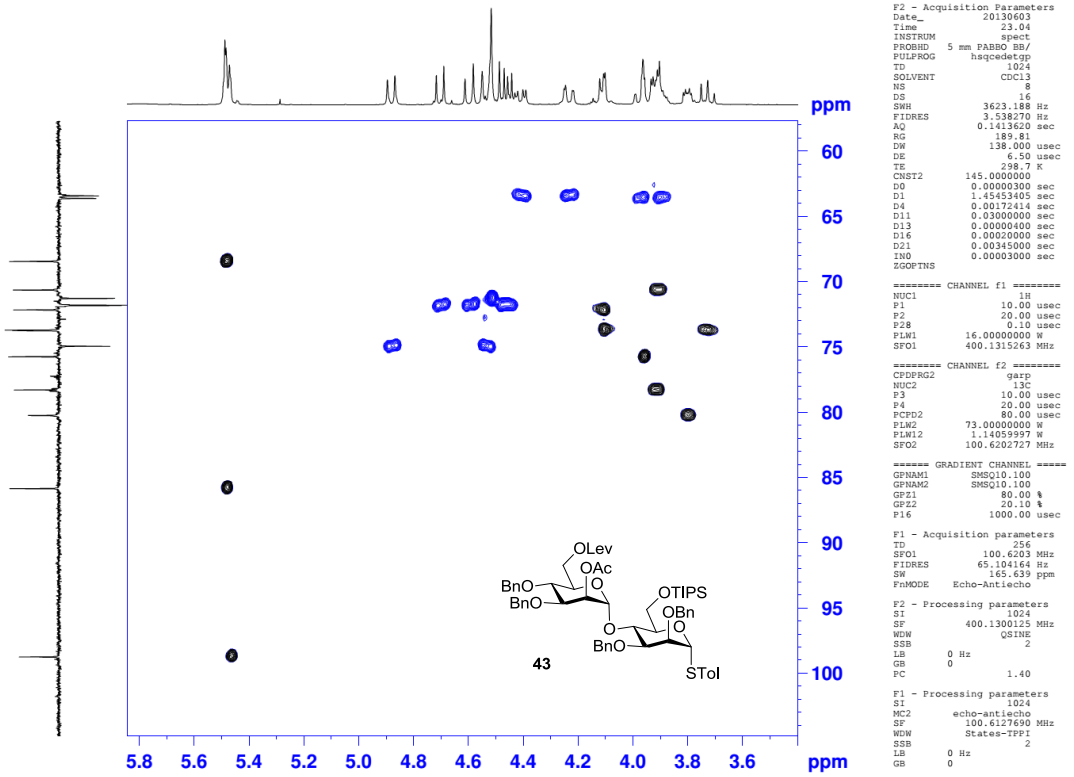
F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **43**

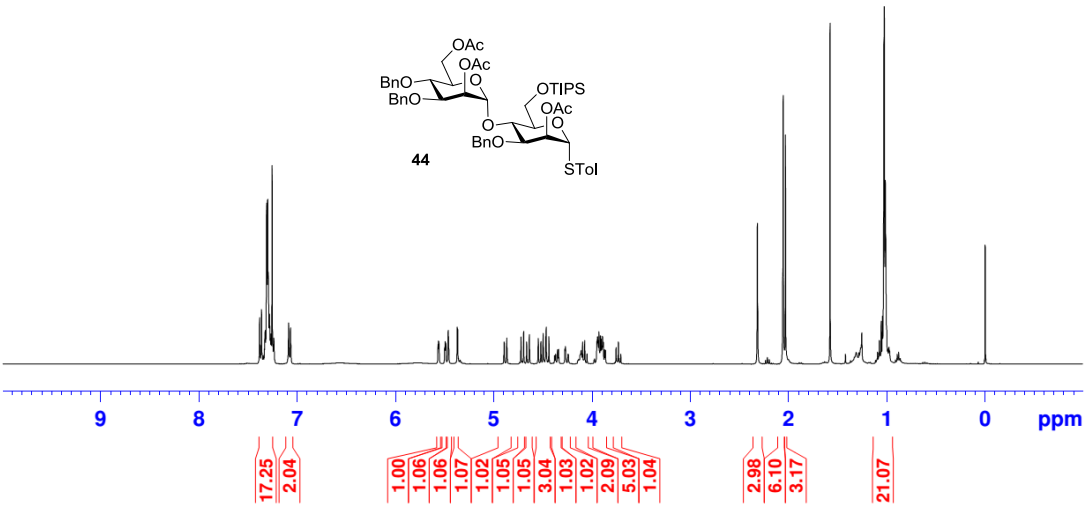




HSQC spectra (400 MHz, $CDCl_3$) for compound **43**



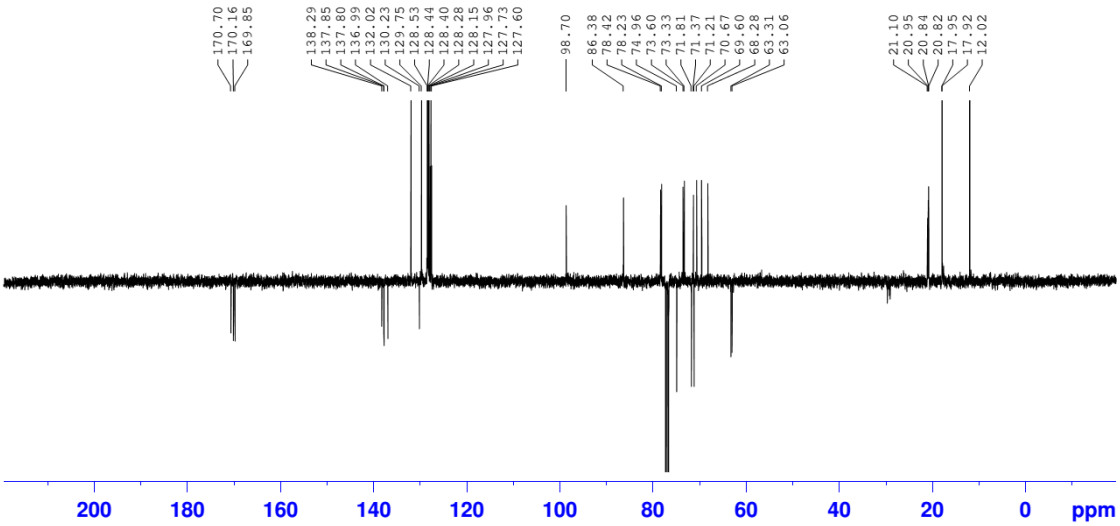
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **44**




```
F2 - Acquisition Parameters
Date_            20141019
Time                23.35
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 76.85
DW                60.800 usec
DE                  6.50 usec
TE                 300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PLW1          16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300102 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



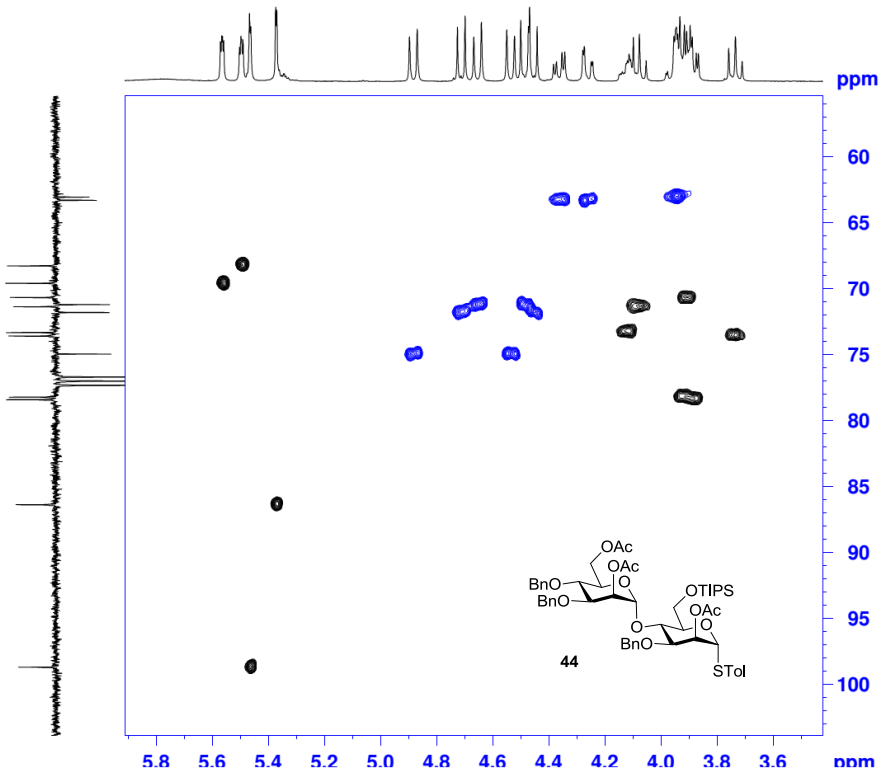

```
F2 - Acquisition Parameters
Date_            20141020
Time                12.46
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 189.81
DW                20.800 usec
DE                  6.50 usec
TE                 300.0 K
CNST2         145.0000000
CNST11          1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1          73.00000000 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PLW2          16.00000000 W
PLW12          0.19753000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **44**




```
F2 - Acquisition Parameters
Date_            20141020
Time                 0.35
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             3521.127 Hz
FIDRES          3.438600 Hz
AQ             0.1454580 sec
RG                 189.81
DW                142.000 usec
DE                  6.50 usec
TE                 300.0 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.45043802 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
P2                 20.00 usec
P28              1000.00 usec
PLW1          16.00000000 W
SFO1         400.1314979 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                  13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2         100.6202727 MHz

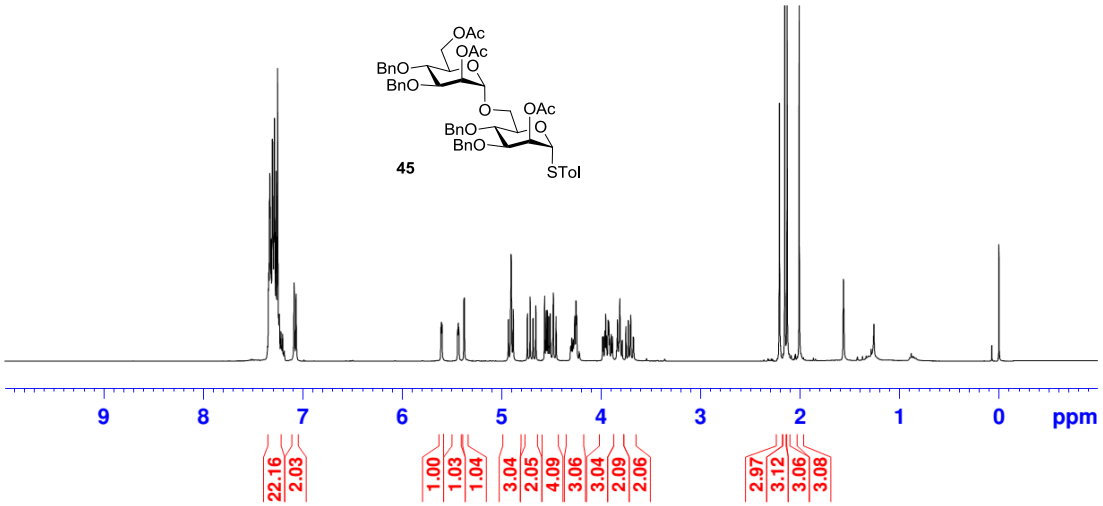
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF            400.1300102 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF            100.6127690 MHz
WDW           States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

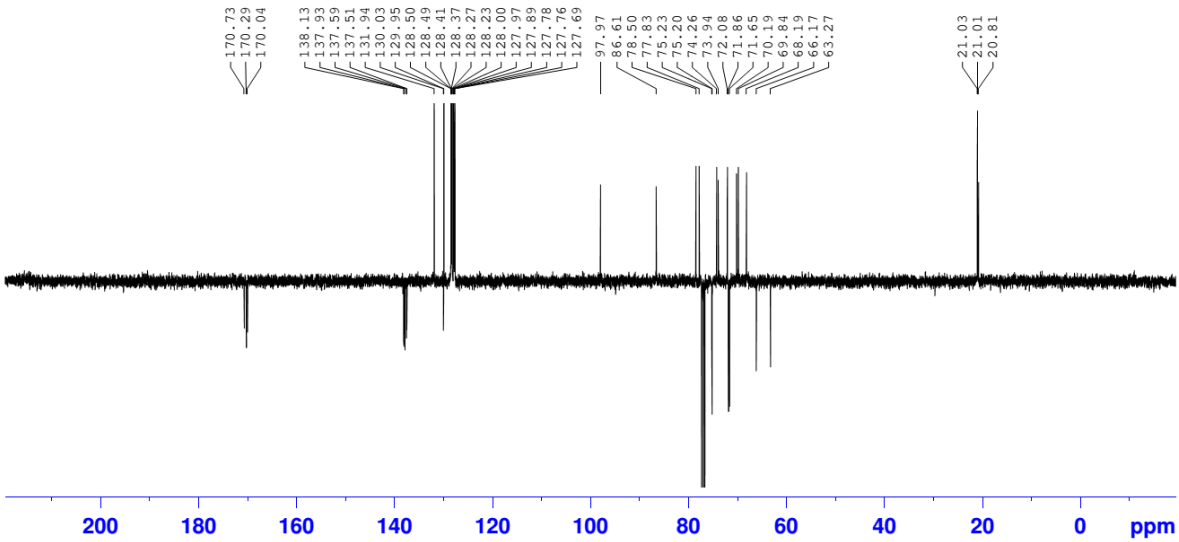
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **45**




```
F2 - Acquisition Parameters
Date_           20141021
Time               23.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 76.85
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300121 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



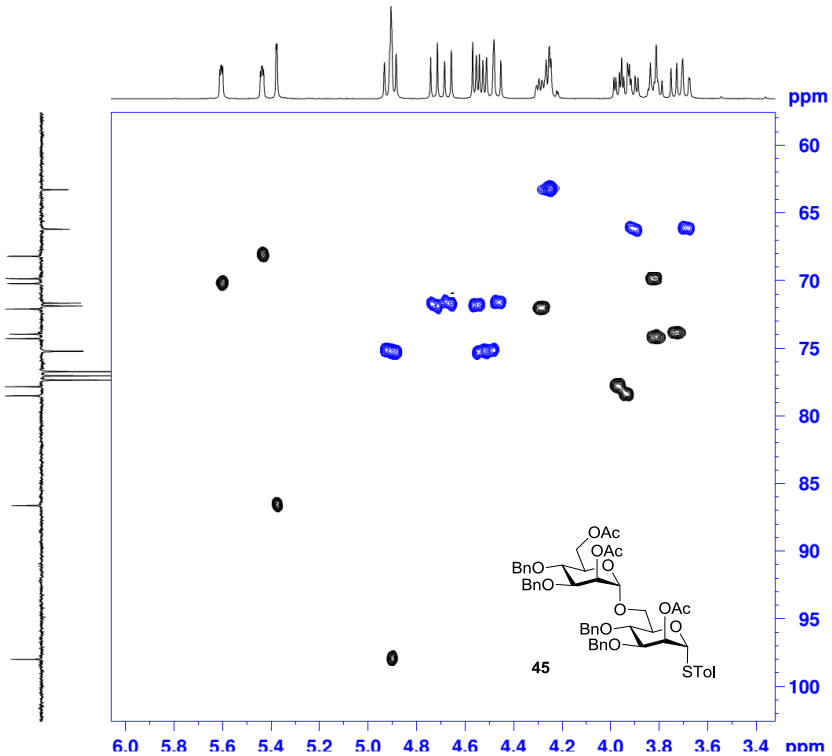

```
F2 - Acquisition Parameters
Date_           20141022
Time               0.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            jmod
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 189.81
DW                20.800 use
DE                 6.50 use
TE                300.0 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                 13C
P1                10.00 use
P2                20.00 use
PLW1         73.00000000 W
SFO1         100.6228298 MHz

======== CHANNEL f2 =======
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 use
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **45**




```
F2 - Acquisition Parameters
Date_           20141021
Time               0.53
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                 1024
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             3875.969 Hz
FIDRES          3.785126 Hz
AQ             0.1321460 sec
RG                 189.81
DW                129.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.46375000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1         16.00000000 W
SFO1         400.1316610 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

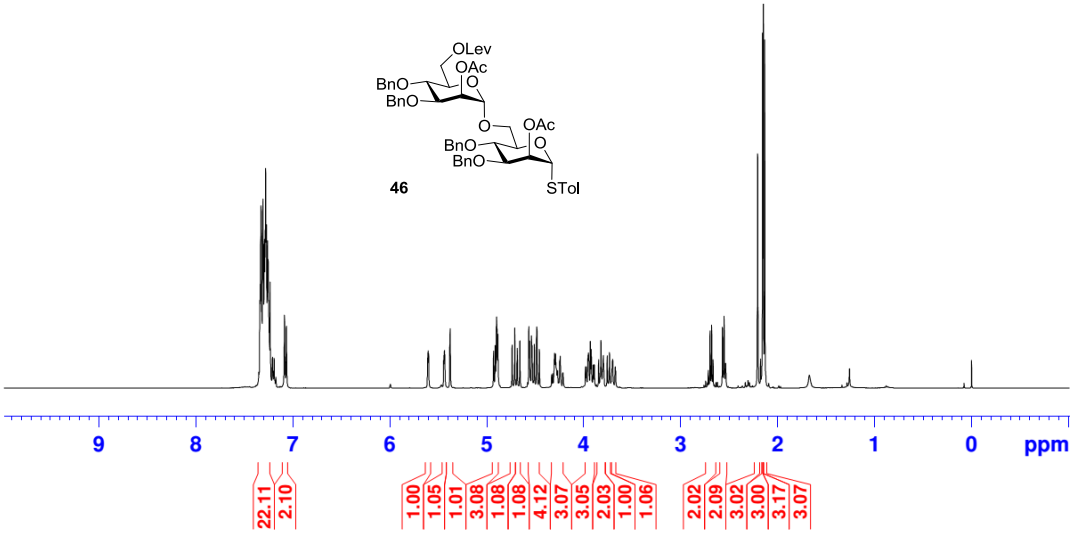
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  256
SFO1          100.6203 MHz
FIDRES        65.104164 Hz
SW            165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300125 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW          States-TPPI
SSB                    2
LB        0 Hz
GB        0
```

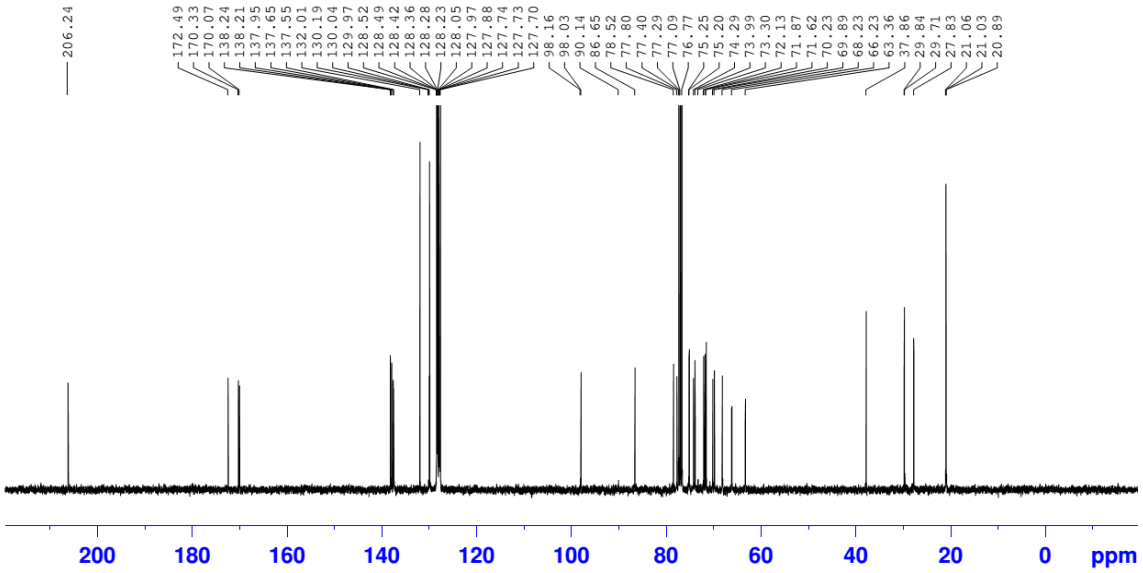
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **46**




```
F2 - Acquisition Parameters
Date_           20130719
Time               13.58
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 31.69
DW                60.800 usec
DE                 6.50 usec
TE                301.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PLW1          16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300186 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



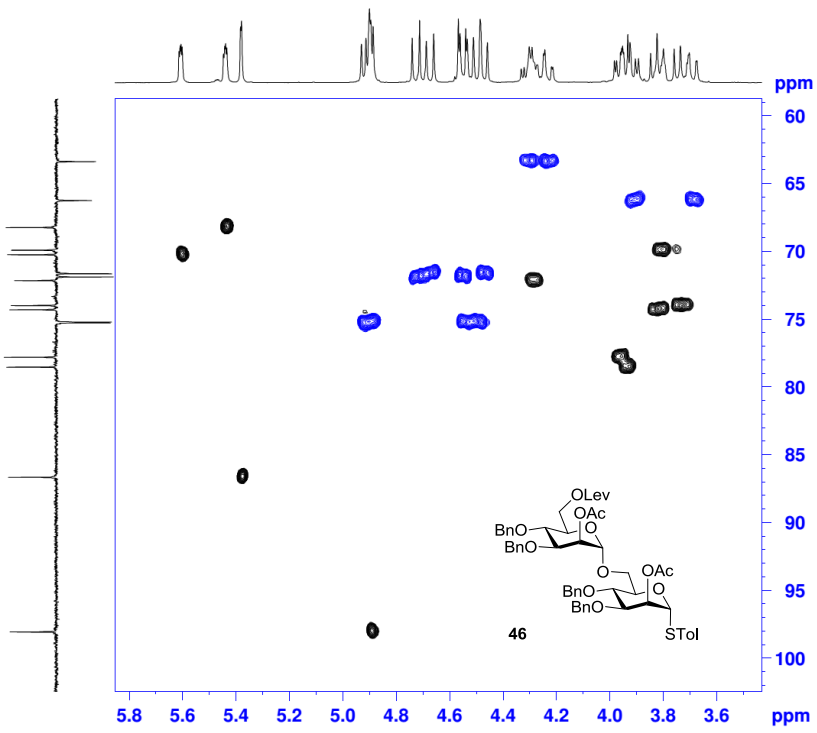

```
F2 - Acquisition Parameters
Date_           20130719
Time               22.10
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   470
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                189.81
DW                20.800 usec
DE                 6.50 usec
TE                301.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PLW1          73.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PLW2          16.00000000 W
PLW12          0.19753000 W
PLW13          0.09920000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **46**




```
F2 - Acquisition Parameters
Date_           20130719
Time               15.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     6
DS                    16
SWH             3333.333 Hz
FIDRES          3.255208 Hz
AQ             0.1536500 sec
RG                189.81
DW               150.000 usec
DE                 6.50 usec
TE                301.2 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.44224596 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
P2                 20.00 usec
P28                 0.10 usec
PLW1          16.00000000 W
SFO1         400.1317911 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                  13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2         100.6202727 MHz

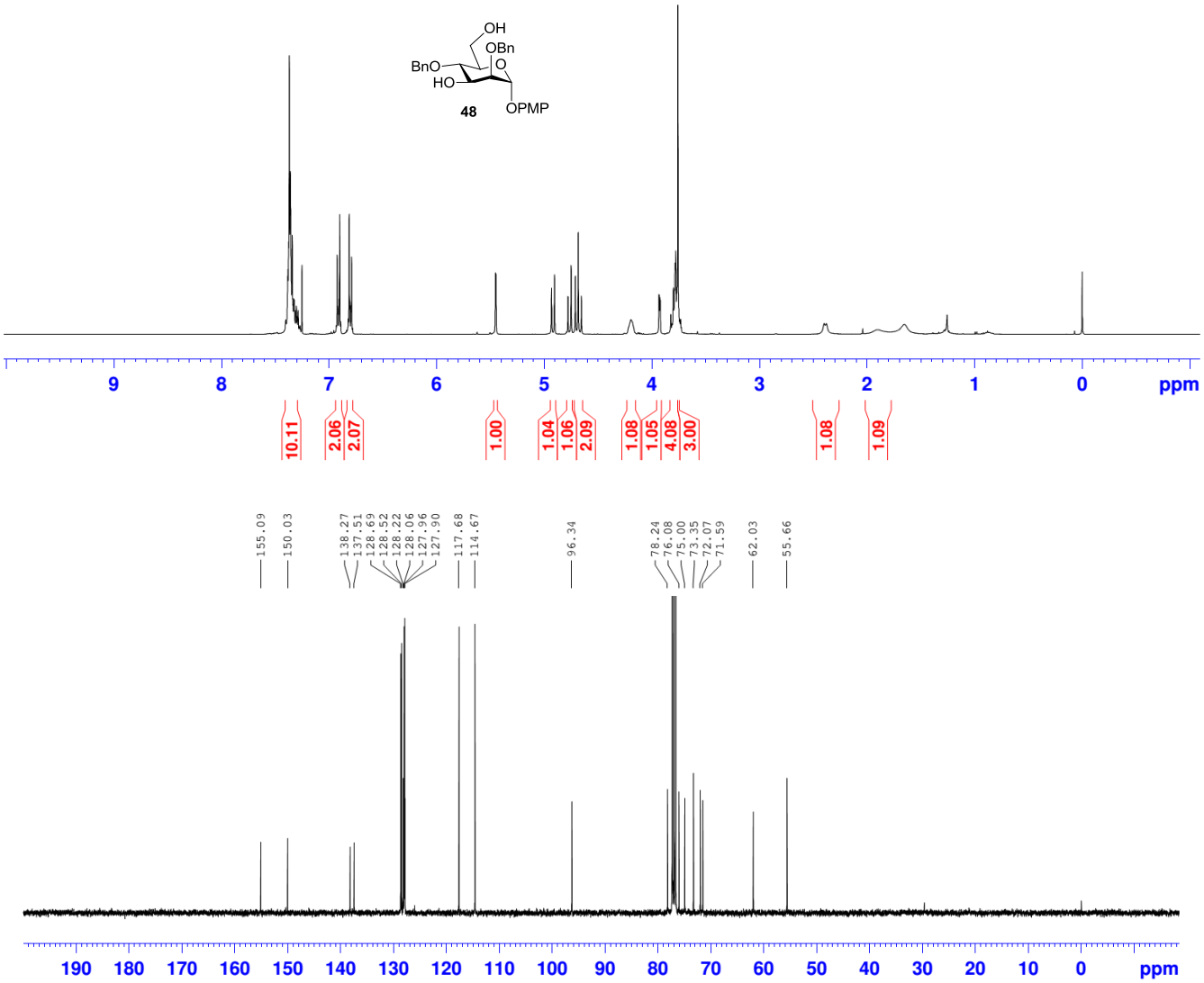
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

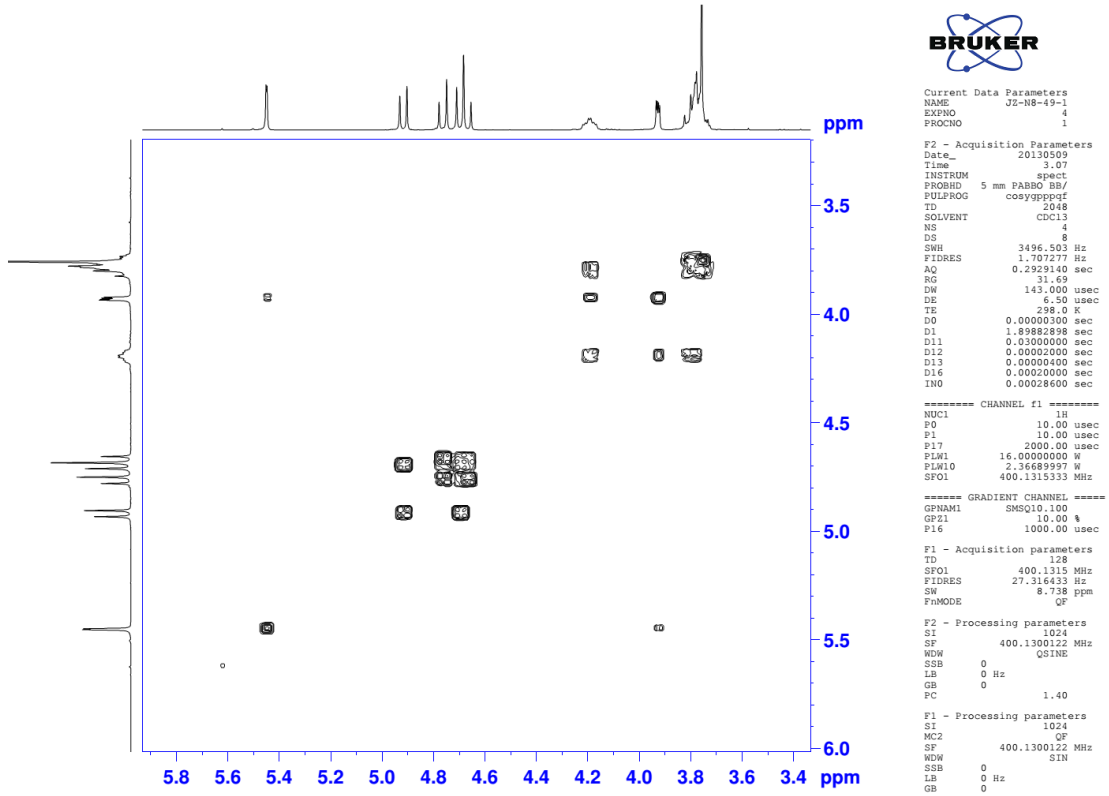
F2 - Processing parameters
SI                  1024
SF           400.1300186 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127690 MHz
WDW          States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **48**



COSY spectrum for Compound **48**




```
Current Data Parameters
NAME          JZ-N8-49-1
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130509
Time               3.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                  2048
SOLVENT            CDCl3
NS                     4
DS                     8
SWH             3496.503 Hz
FIDRES          1.707277 Hz
AQ             0.2929140 sec
RG                  31.69
DW                143.000 usec
DE                   6.50 usec
TE                  298.0 K
D0            0.00000300 sec
D1            1.89882898 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00028600 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                 10.00 usec
P1                 10.00 usec
P17              2000.00 usec
PLW1         16.00000000 W
PLW10         2.36689997 W
SFO1        400.1315333 MHz

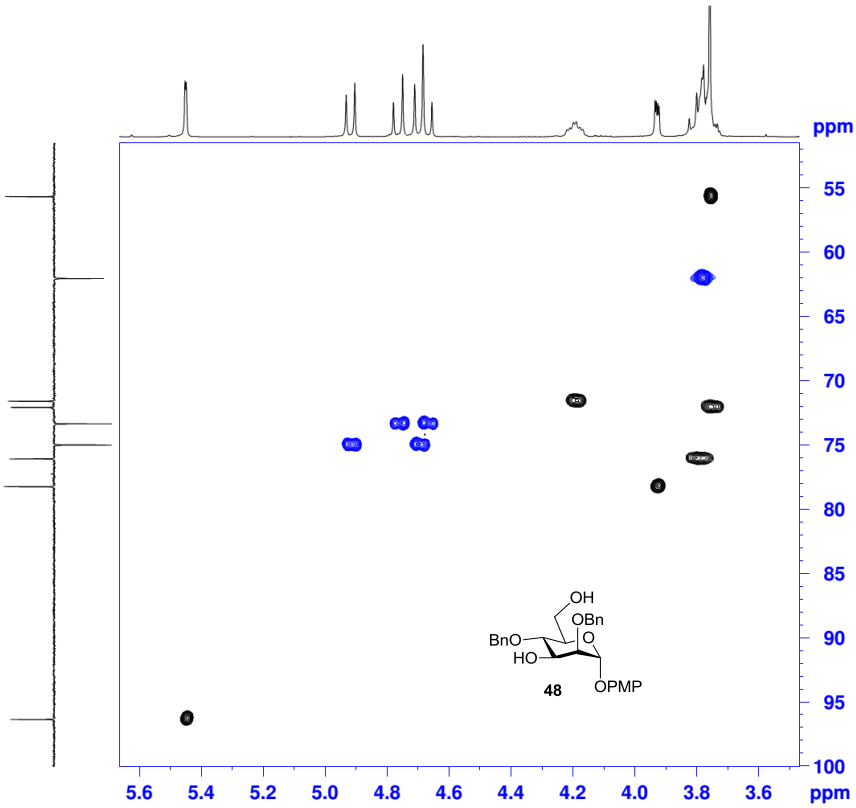
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            400.1315 MHz
FIDRES         27.316433 Hz
SW                 8.738 ppm
FnMODE                QF

F2 - Processing parameters
SI                    1024
SF            400.1300122 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            400.1300122 MHz
WDW                    SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for Compound **48**




```
Current Data Parameters
NAME                JZ-N8-49-1
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_             20130509
Time                      3.28
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                        1024
SOLVENT                   CDCl3
NS                           8
DS                          16
SWH                3496.503 Hz
FIDRES             3.414554 Hz
AQ                0.14648820 sec
RG                     189.81
DW                    143.000 usec
DE                       6.50 usec
TE                      298.0 K
CNST2            145.00000000
D0                0.00000300 sec
D1                1.44941401 sec
D4                0.00172414 sec
D11               0.03000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
D21               0.00345000 sec
IN0               0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.00 usec
P2                        20.00 usec
P28                        0.10 usec
PLW1             16.00000000 W
SFO1            400.1315333 MHz

======== CHANNEL f2 ========
CPDPRG2                    garp
NUC2                        13C
P3                        10.00 usec
P4                        20.00 usec
PCPD2                     80.00 usec
PLW2             73.00000000 W
PLW12             1.14059997 W
SFO2            100.6202727 MHz

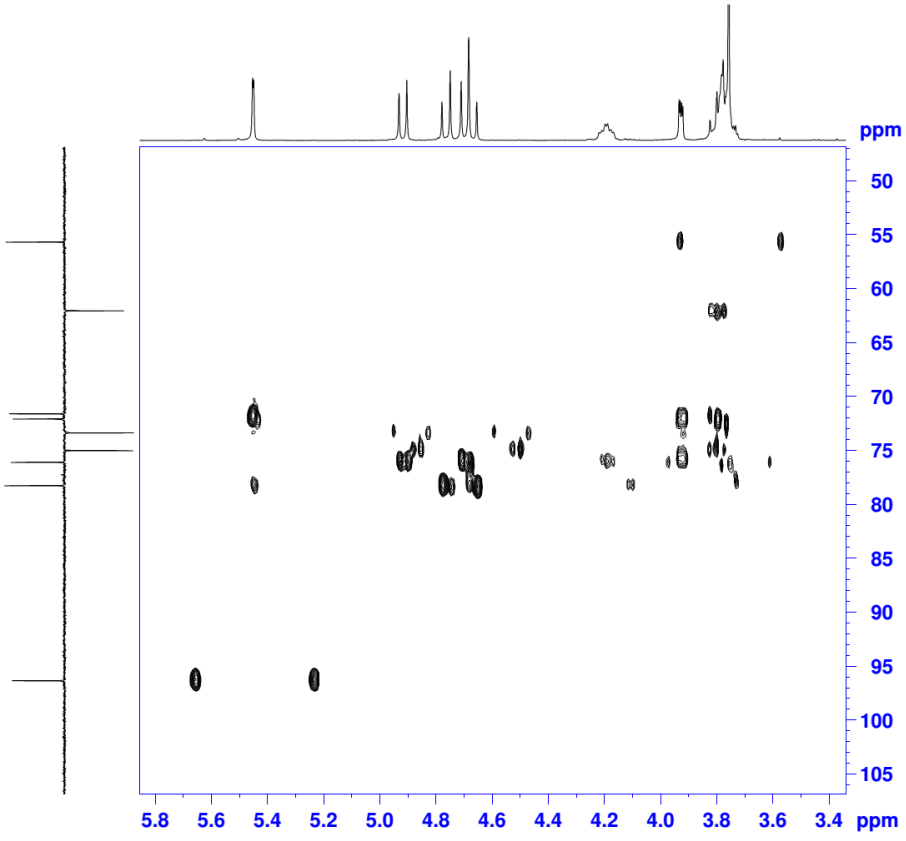
======= GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPZ1                     80.00 %
GPZ2                     20.10 %
P16                    1000.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                100.6203 MHz
FIDRES             65.104164 Hz
SW                    165.639 ppm
FnMODE       Echo-Antiecho

F2 - Processing parameters
SI                         1024
SF                400.1300122 MHz
WDW                       QSINE
SSB                           2
LB          0 Hz
GB          0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2            echo-antiecho
SF                100.6127690 MHz
WDW                States-TPPI
SSB                           2
LB          0 Hz
GB          0
```

HMBC spectrum for Compound **48**




```
Current Data Parameters
NAME                JZ-N8-49-1
EXPNO                        6
PROCNO                       1

F2 - Acquisition Parameters
Date_             20130509
Time                      4.25
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG        hmbcgpndqf
TD                        4096
SOLVENT                   CDCl3
NS                           32
DS                           16
SWH                3496.503 Hz
FIDRES             0.853639 Hz
AQ                0.5857780 sec
RG                     189.81
DW                    143.000 usec
DE                       6.50 usec
TE                      298.0 K
CNST13            8.00000000
D0                0.00000300 sec
D1                1.29847705 sec
D6                0.06250000 sec
D16               0.00020000 sec
IN0               0.00002235 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.00 usec
P2                        20.00 usec
PLW1             16.00000000 W
SFO1            400.1315333 MHz

======== CHANNEL f2 ========
NUC2                        13C
P3                        10.00 usec
PLW2             73.00000000 W
SFO2            100.6228138 MHz

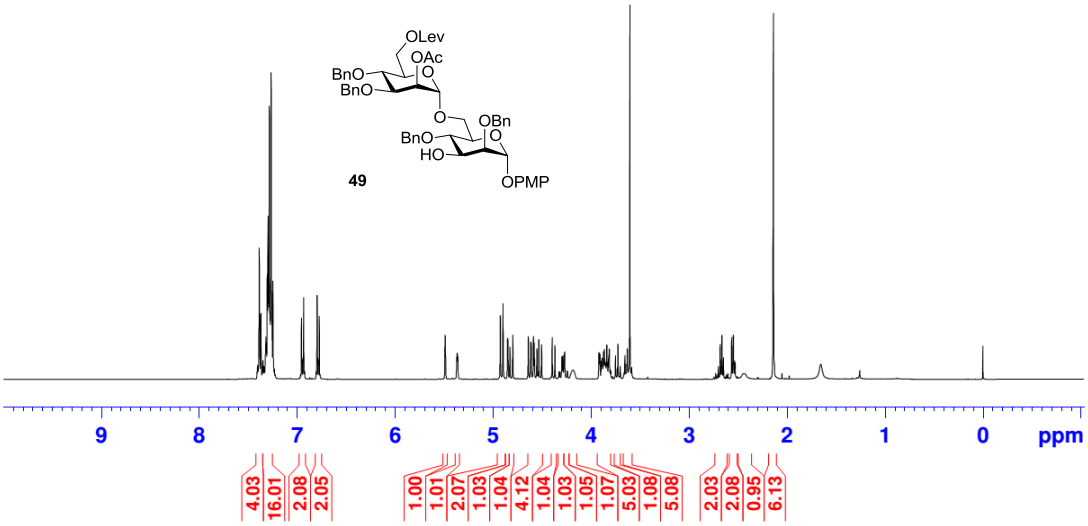
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPNAM3          SMSQ10.100
GPZ1                     50.00 %
GPZ2                     30.00 %
GPZ3                     40.10 %
P16                    1000.00 usec

F1 - Acquisition parameters
TD                          128
SFO1                100.6228 MHz
FIDRES            174.592422 Hz
SW                    222.095 ppm
FnMODE                       QF

F2 - Processing parameters
SI                         1024
SF                400.1300122 MHz
WDW                       SINE
SSB         0
LB          0 Hz
GB          0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2                          QF
SF                100.6127690 MHz
WDW                      States
SSB         0
LB          0 Hz
GB          0
```

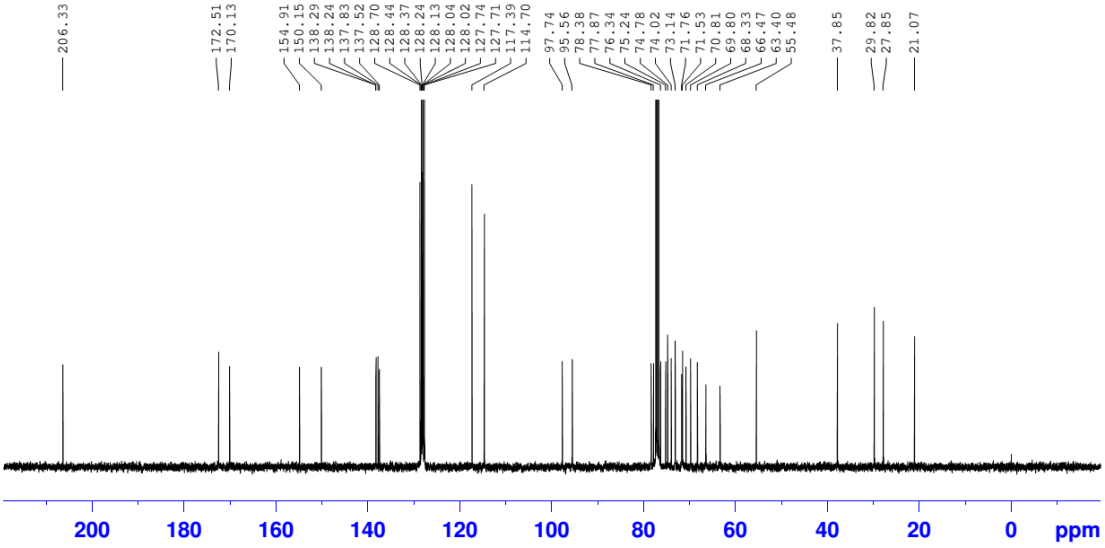
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **49**




```
F2 - Acquisition Parameters
Date_              20130701
Time                  21.10
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                3.9846387 sec
RG                    31.69
DW                   60.800 usec
DE                     6.50 usec
TE                    299.8 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.00 usec
PLW1            16.00000000 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF              400.1300136 MHz
WDW                      EM
SSB         0
LB                     0.30 Hz
GB          0
PC                     1.00
```



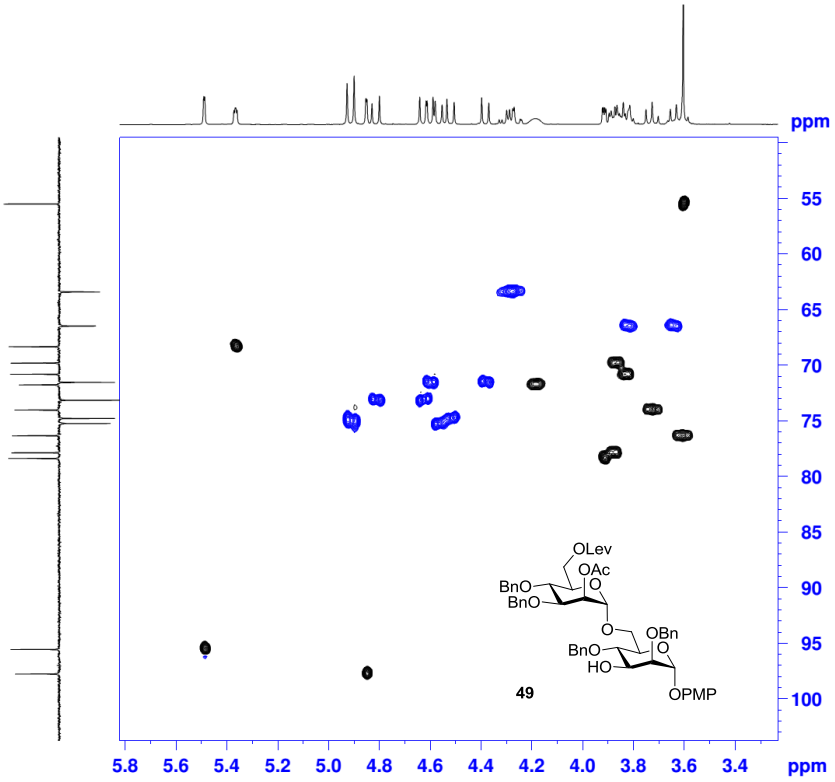

```
F2 - Acquisition Parameters
Date_              20130701
Time                  23.41
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631988 sec
RG                   189.81
DW                   20.800 usec
DE                     6.50 usec
TE                    300.2 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.00 usec
PLW1            73.00000000 W
SFO1            100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                     1H
PCPD2                 90.00 usec
PLW2            16.00000000 W
PLW12            0.19753000 W
PLW13            0.09920000 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF              100.6127690 MHz
WDW                      EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **49**




```
F2 - Acquisition Parameters
Date_              20130701
Time                  22.45
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG          hsqcedetgp
TD                     1024
SOLVENT               CDCl3
NS                         6
DS                        16
SWH                3164.557 Hz
FIDRES             3.090388 Hz
AQ                0.1618420 sec
RG                   189.81
DW                  158.000 usec
DE                     6.50 usec
TE                    300.0 K
CNST2           145.0000000
D0               0.00000300 sec
D1               1.43405402 sec
D4               0.00172414 sec
D11              0.03000000 sec
D13              0.00000400 sec
D16              0.00020000 sec
D21              0.00345000 sec
IN0              0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.00 usec
P2                    20.00 usec
P28                    0.10 usec
PLW1            16.00000000 W
SFO1            400.1316621 MHz

======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                    13C
P3                    10.00 usec
P4                    20.00 usec
PCPD2                 80.00 usec
PLW2            73.00000000 W
PLW12            1.14059997 W
SFO2            100.6202727 MHz

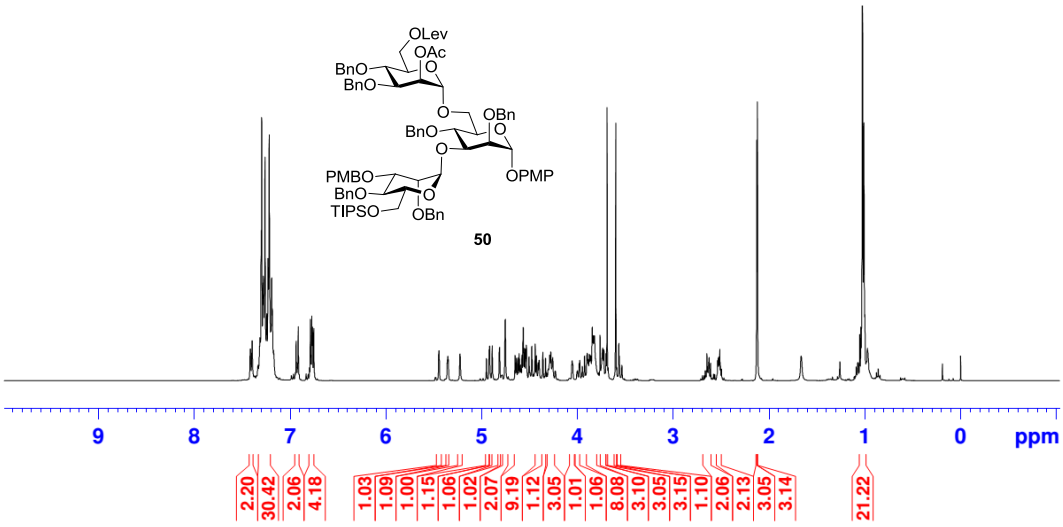
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                      256
SFO1                100.6203 MHz
FIDRES             65.104164 Hz
SW                   165.639 ppm
FnMODE        Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF              400.1300136 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2           echo-antiecho
SF              100.6127690 MHz
WDW             States-TPPI
SSB                        2
LB          0 Hz
GB          0
```

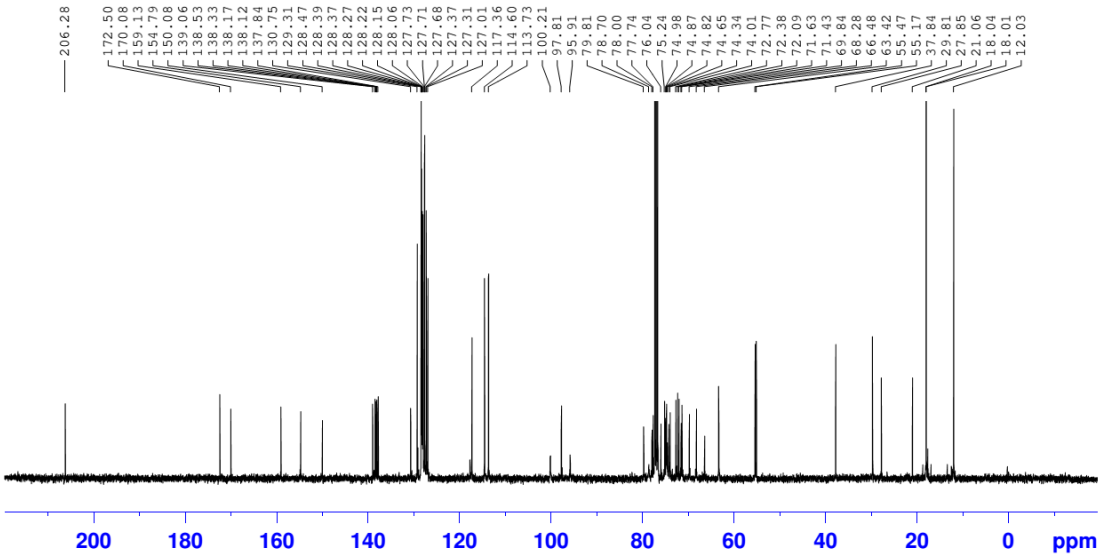
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **50**




```
F2 - Acquisition Parameters
Date_            20130716
Time                21.59
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ             3.9846387 sec
RG                 31.69
DW                60.800 usec
DE                 6.50 usec
TE                301.5 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                    1H
P1                  10.00 usec
PLW1          16.00000000 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF            400.1300195 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



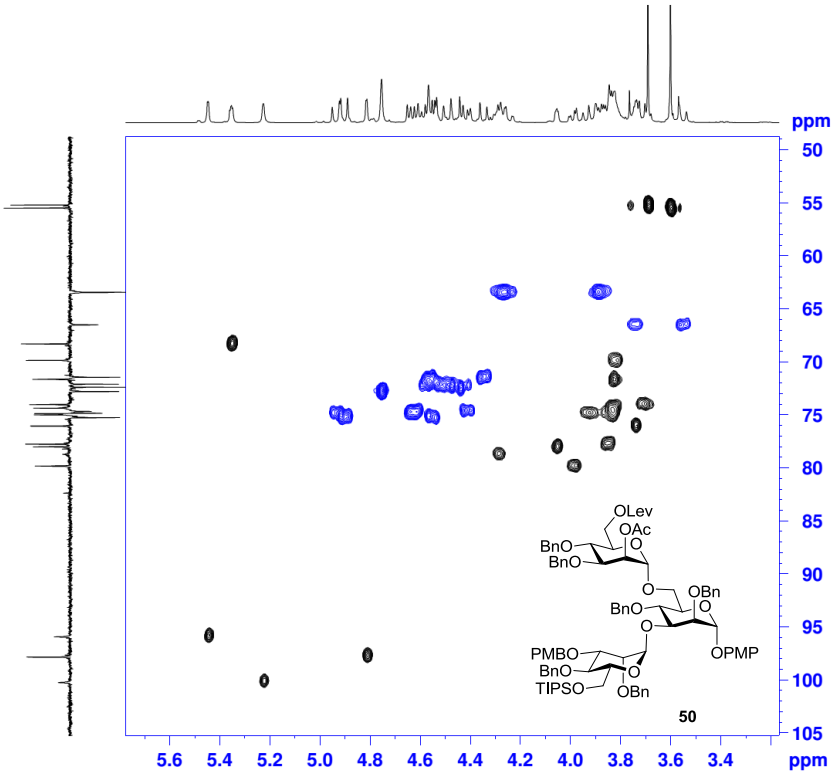

```
F2 - Acquisition Parameters
Date_            20130716
Time                22.54
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ             1.3631988 sec
RG                 189.81
DW                20.800 usec
DE                 6.50 usec
TE                301.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

========= CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PLW1          73.00000000 W
SFO1          100.6228293 MHz

========= CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               90.00 usec
PLW2          16.00000000 W
PLW12          0.19753000 W
PLW13          0.09920000 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **50**




```
F2 - Acquisition Parameters
Date_            20130716
Time                22.17
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                      8
DS                     16
SWH              3496.503 Hz
FIDRES           3.414554 Hz
AQ             0.1464820 sec
RG                 189.81
DW                143.000 usec
DE                 6.50 usec
TE                301.7 K
CNST2        145.00000000
D0            0.00000300 sec
D1            1.44941401 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1          16.00000000 W
SFO1          400.1315217 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                   13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

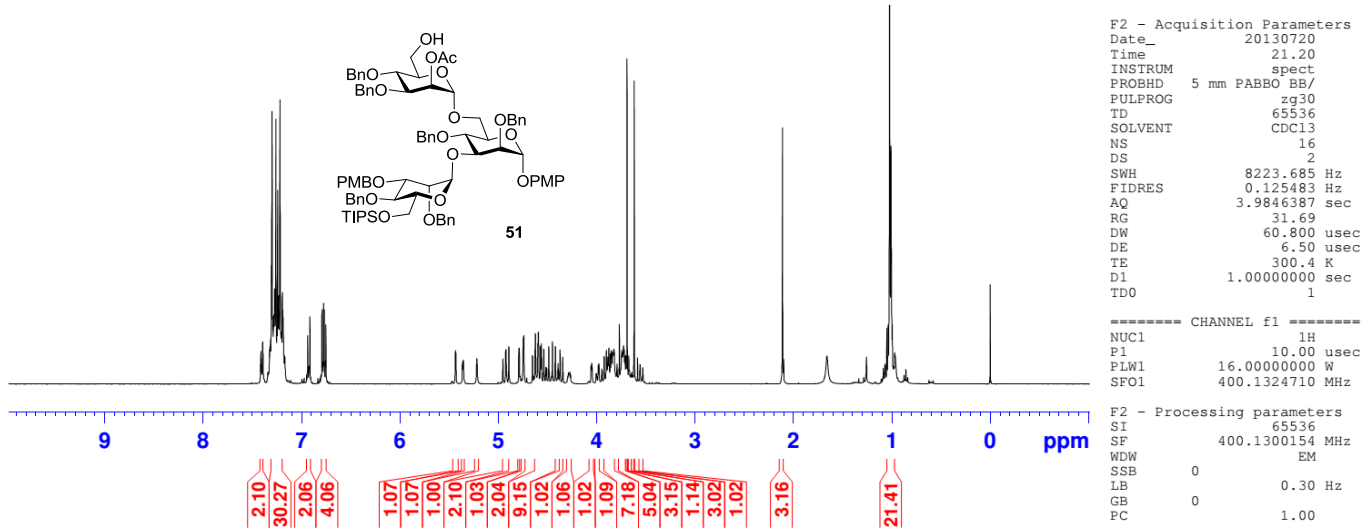
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16                1000.00 usec

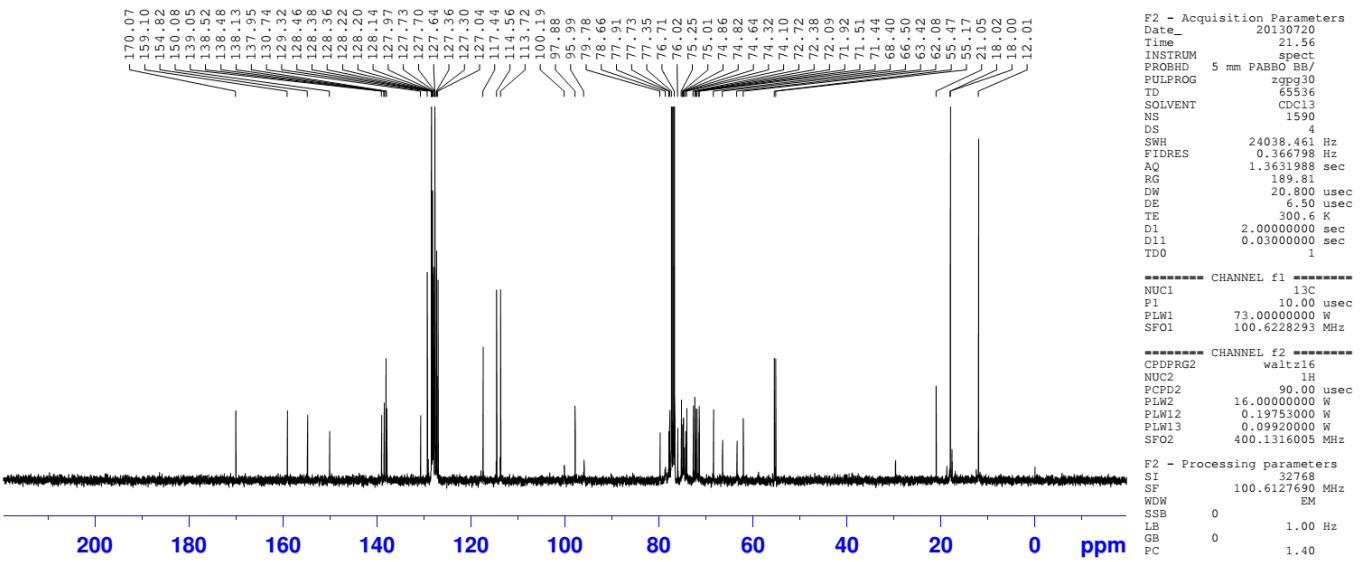
F1 - Acquisition parameters
TD                    170
SFO1            100.6203 MHz
FIDRES          98.039215 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF            400.1300195 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                  1.40

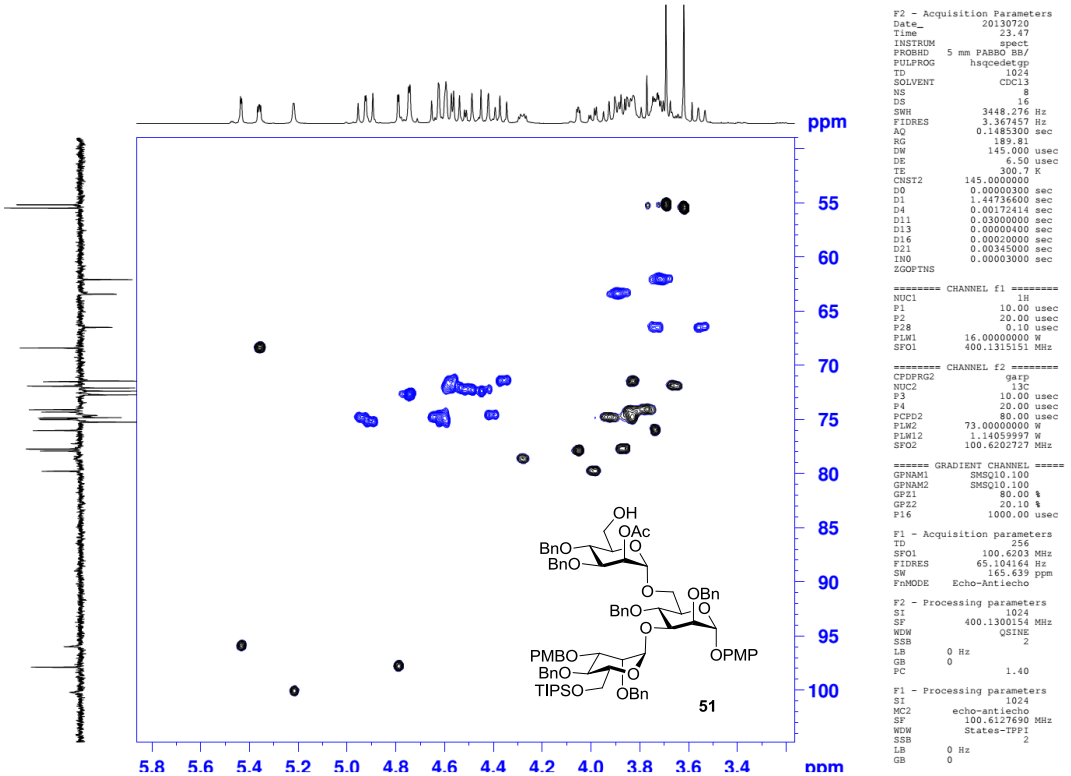
F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF            100.6127690 MHz
WDW           States-TPPI
SSB                      2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **51**

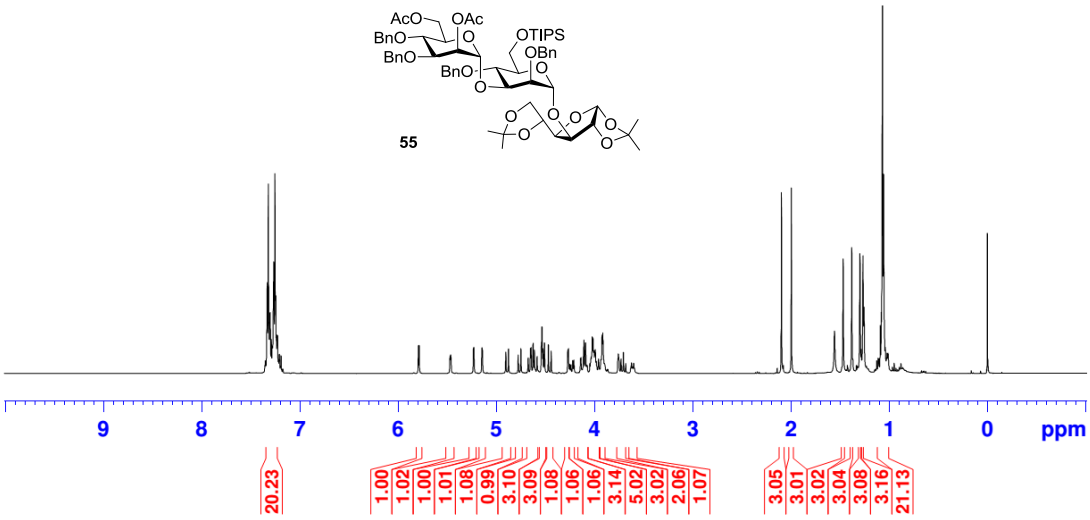




HSQC spectra (400 MHz, $CDCl_3$) for compound **51**



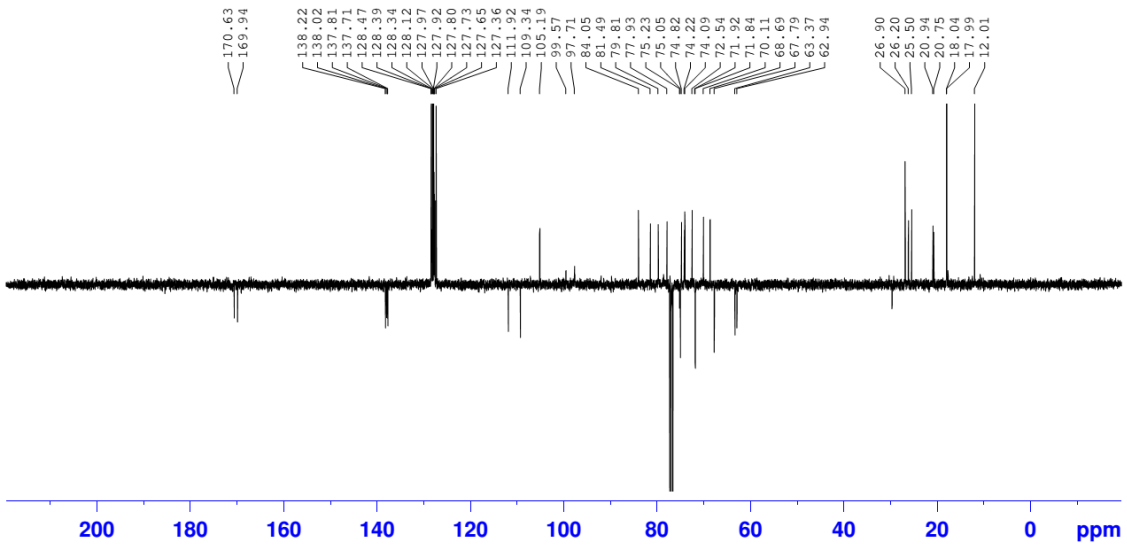
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **55**




```
F2 - Acquisition Parameters
Date_           20141025
Time               22.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ            3.9846387 sec
RG                76.85
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300107 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



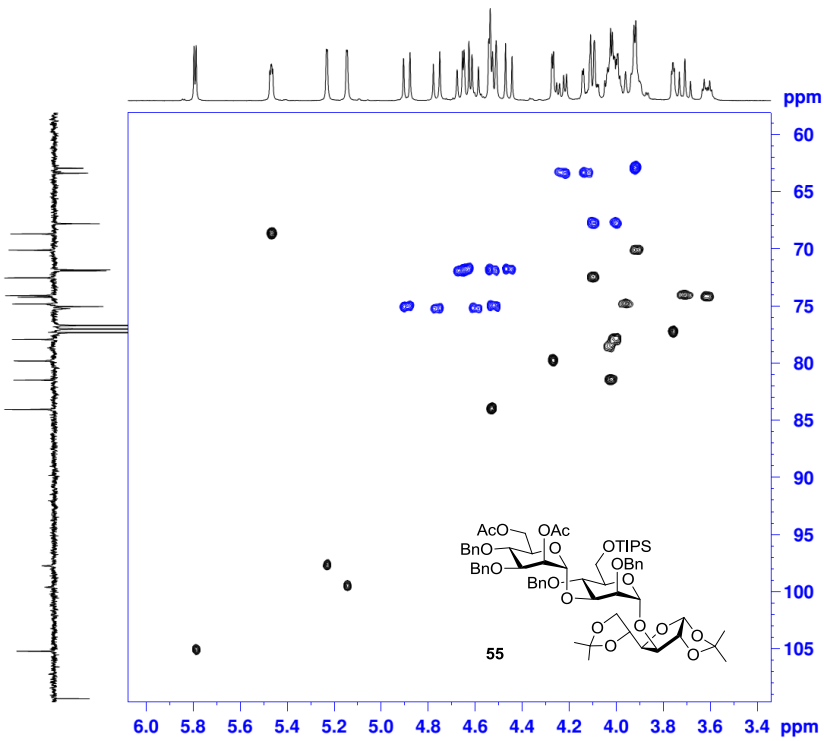

```
F2 - Acquisition Parameters
Date_           20141025
Time               23.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            jmod
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               189.81
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
CNST11         1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         73.00000000 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **55**




```
F2 - Acquisition Parameters
Date_           20141026
Time               12.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     6
DS                    16
SWH            3571.428 Hz
FIDRES         3.487723 Hz
AQ            0.1434100 sec
RG               189.81
DW               140.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.45248604 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1         16.00000000 W
SFO1         400.1315049 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

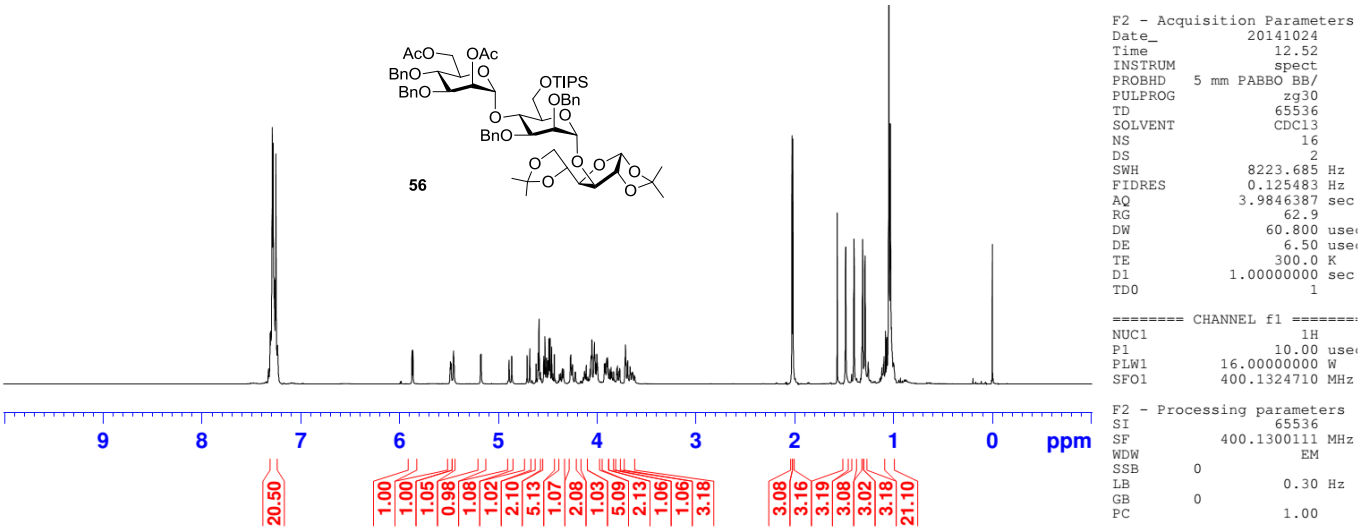
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

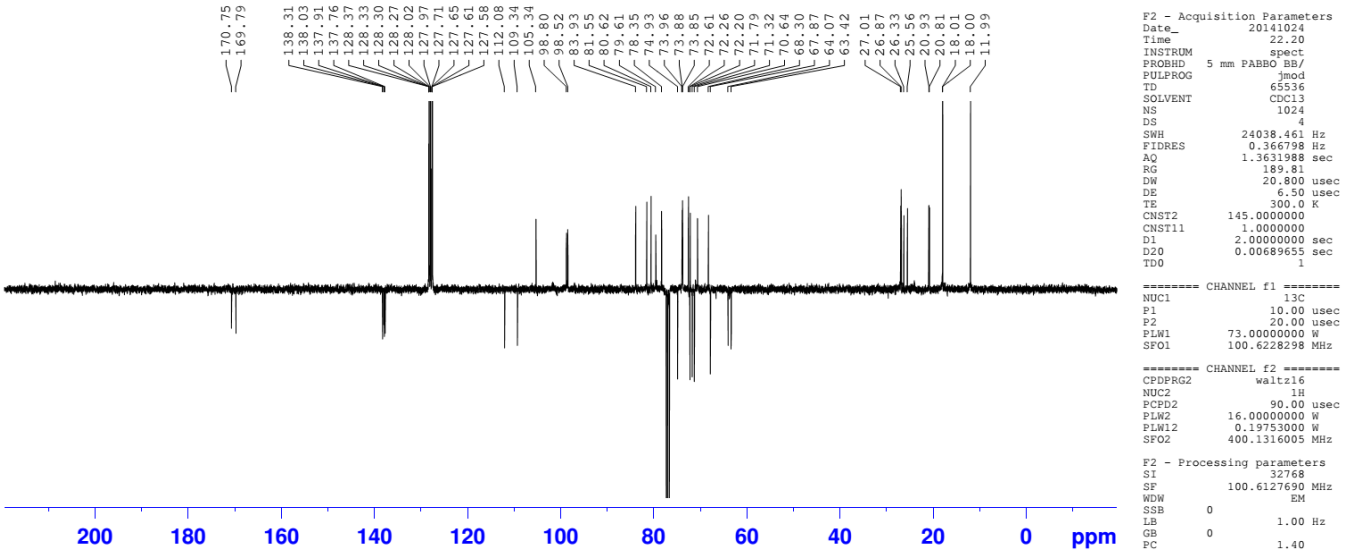
F1 - Acquisition parameters
TD                   256
SFO1           100.6203 MHz
FIDRES         65.104164 Hz
SW               165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF          400.1300107 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                 1.40

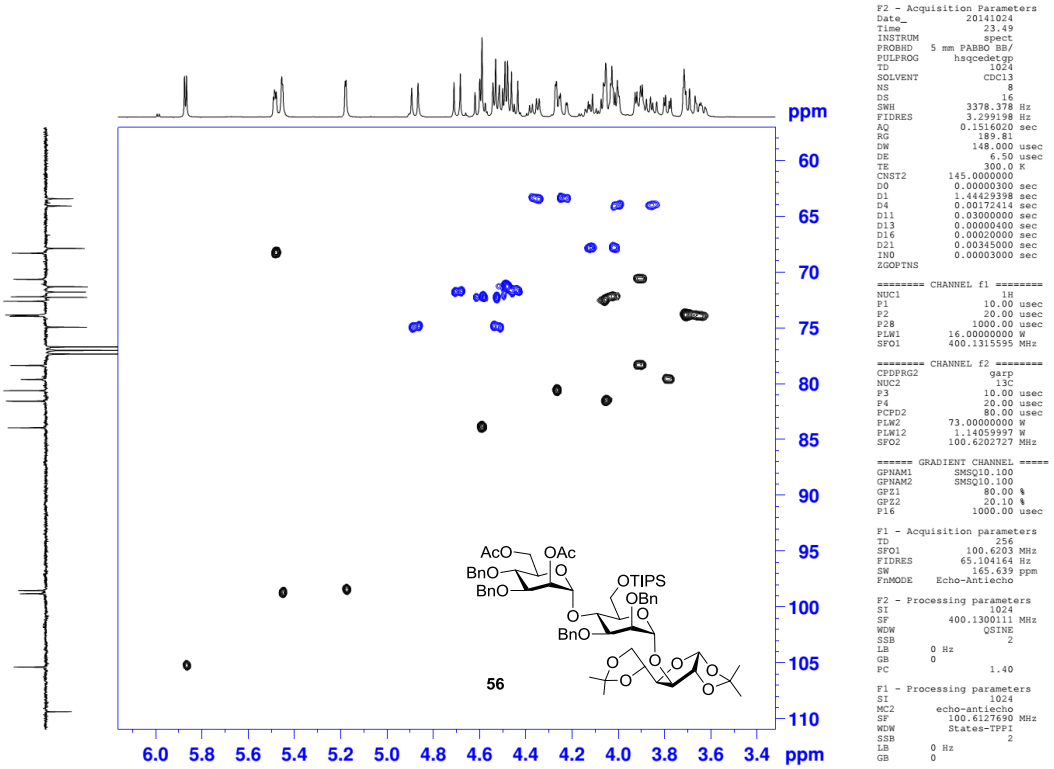
F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **56**

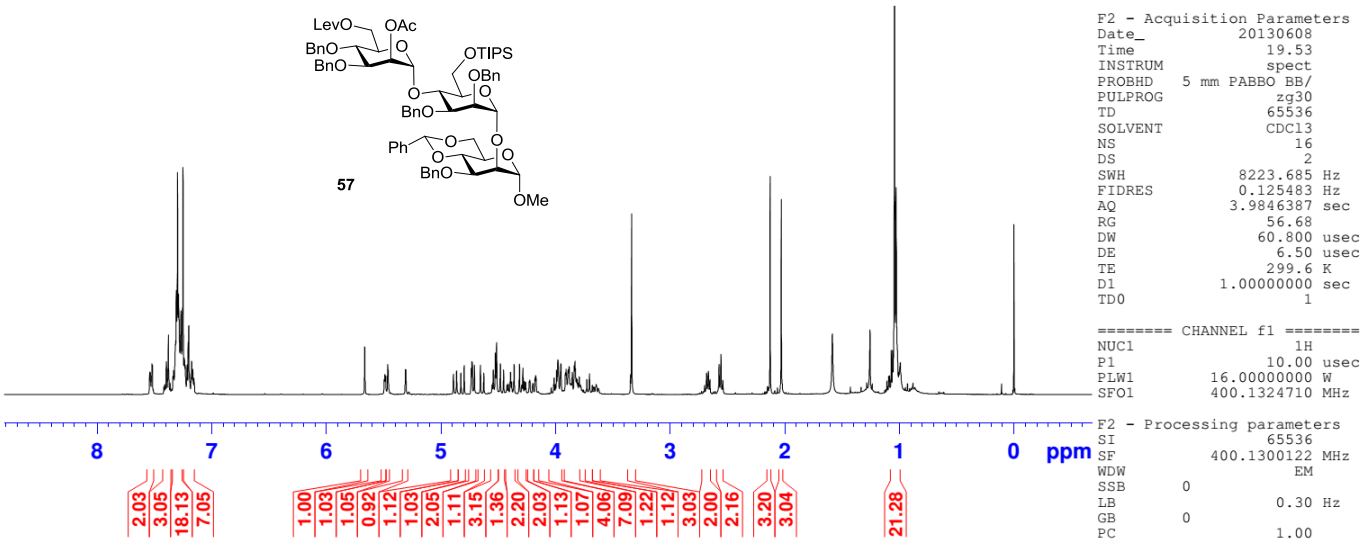


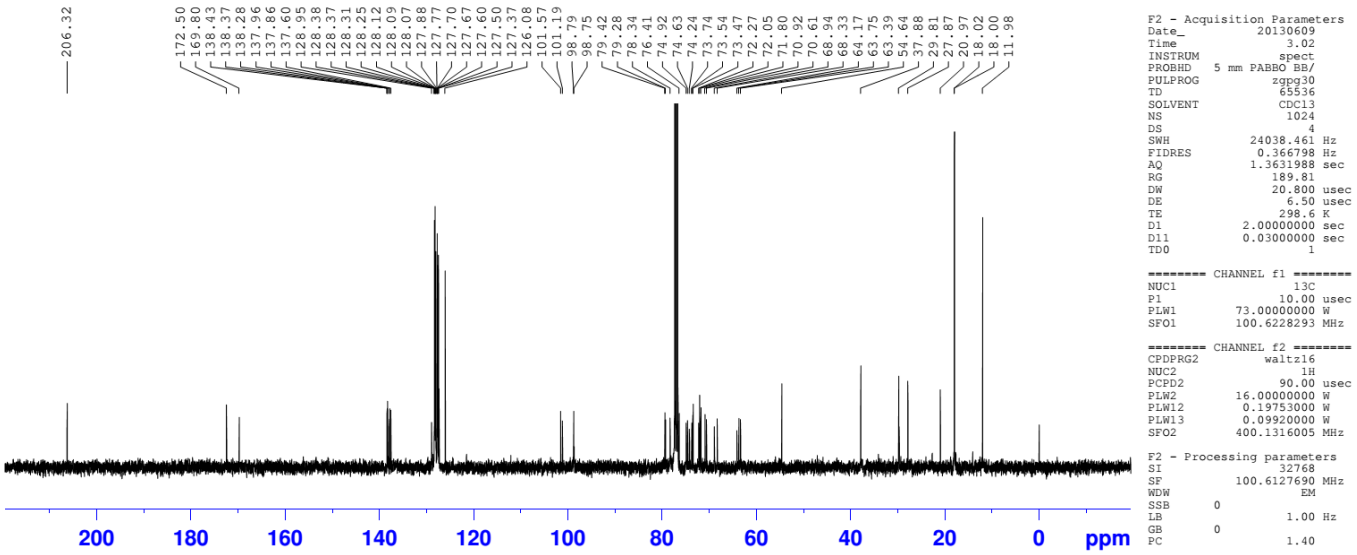


HSQC spectra (400 MHz, $CDCl_3$) for compound **56**

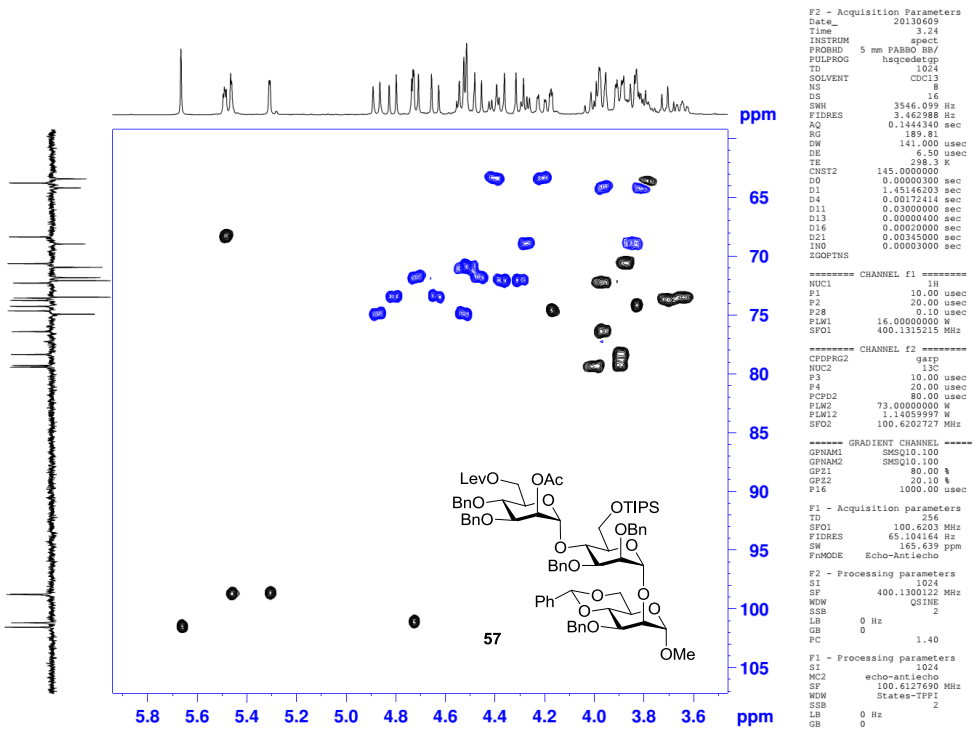


^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **57**

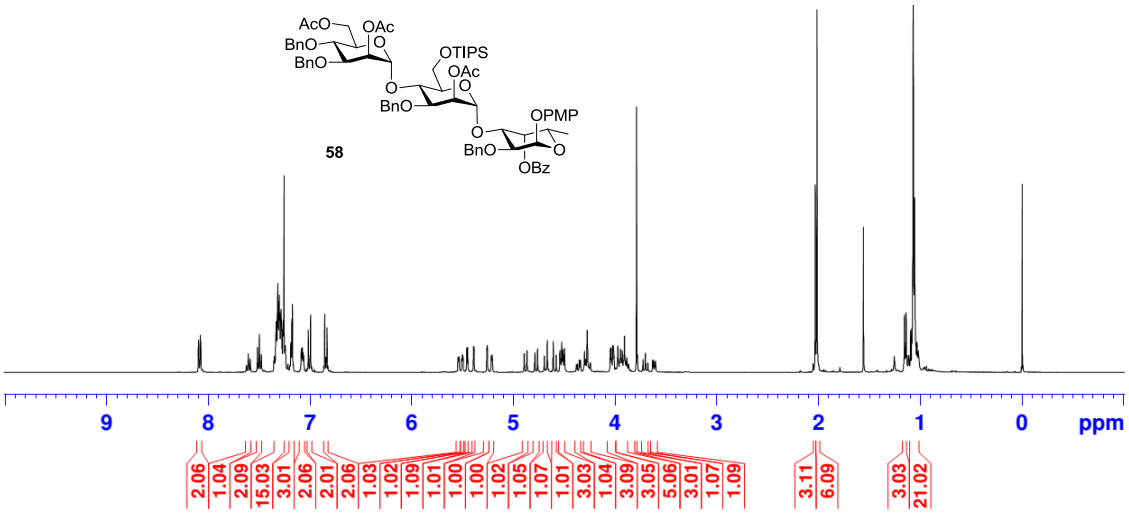




HSQC spectra (400 MHz, $CDCl_3$) for compound **57**



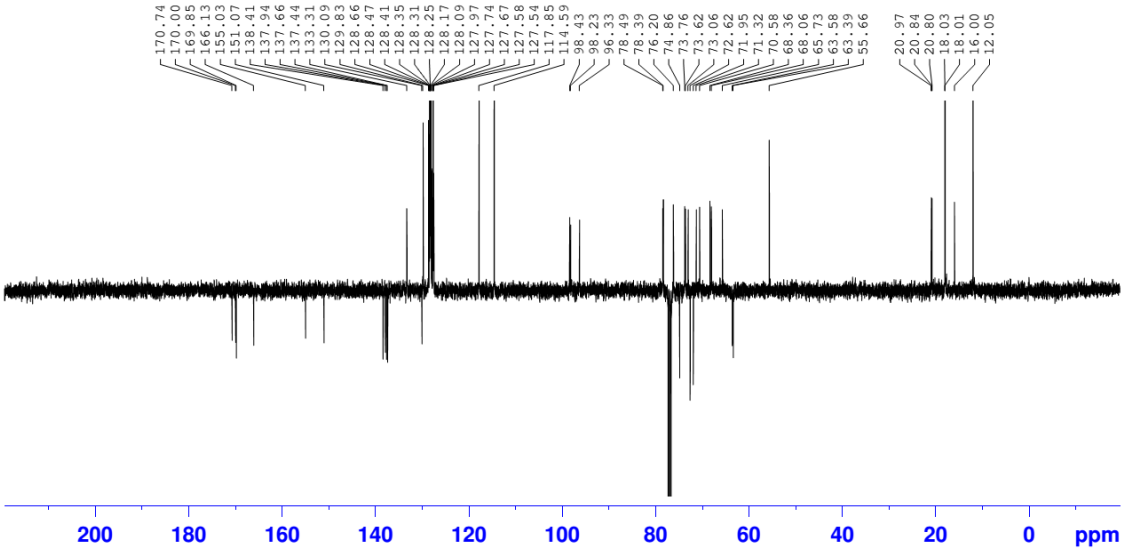
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **58**




```
F2 - Acquisition Parameters
Date_           20141106
Time                17.31
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 76.85
DW                60.800 usec
DE                 6.50 usec
TE                298.9 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300109 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



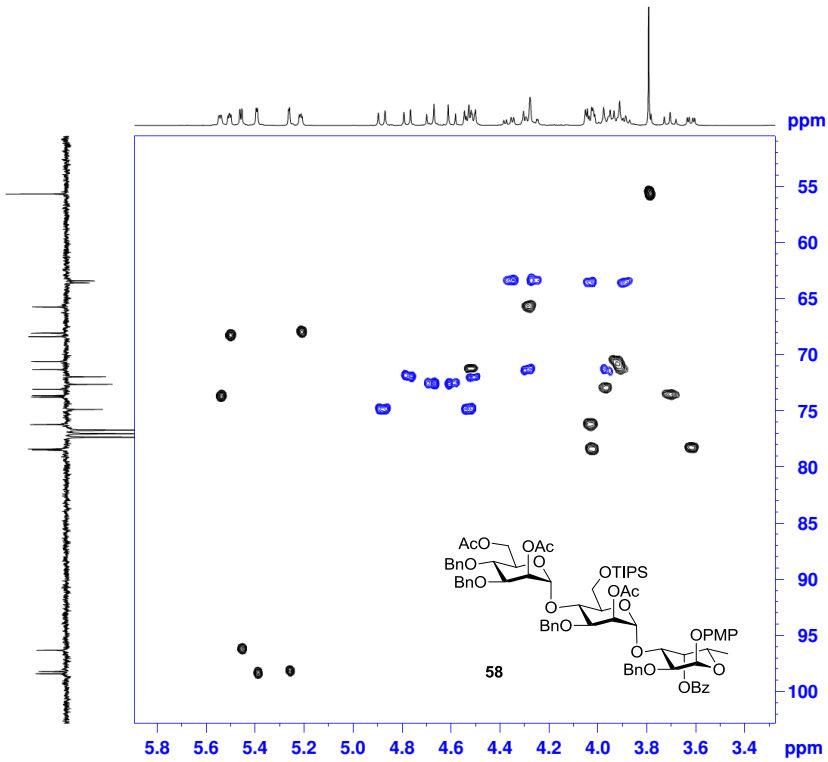

```
F2 - Acquisition Parameters
Date_           20141107
Time                3.31
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                189.81
DW                20.800 usec
DE                 6.50 usec
TE                297.5 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         73.00000000 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **58**




```
F2 - Acquisition Parameters
Date_           20141106
Time               18.28
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             3703.704 Hz
FIDRES          3.616898 Hz
AQ             0.1382900 sec
RG                189.81
DW               135.000 usec
DE                 6.50 usec
TE                298.8 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.45760596 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1         16.00000000 W
SFO1        400.1316256 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2        100.6202727 MHz

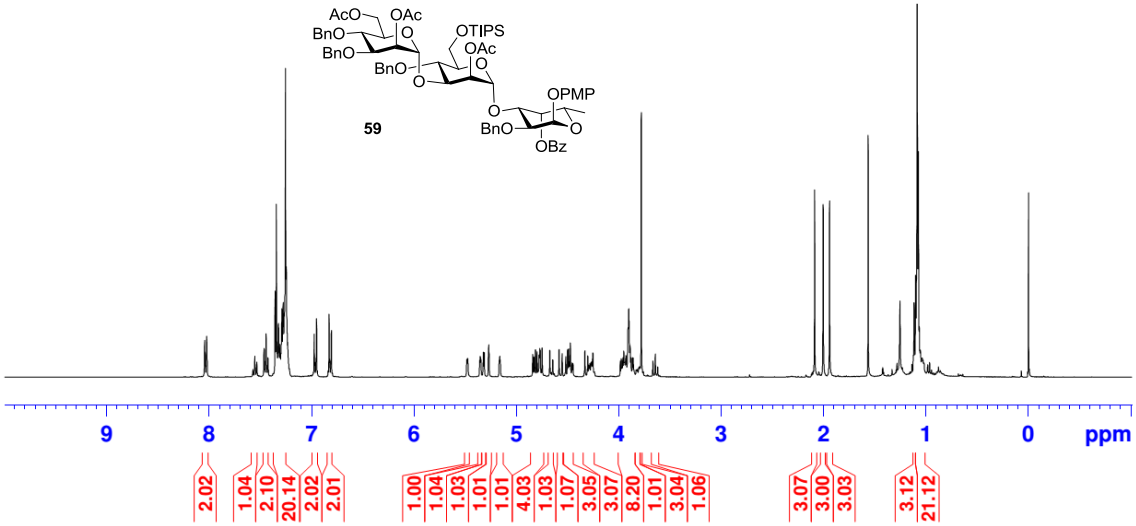
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   240
SFO1            100.6203 MHz
FIDRES          69.444443 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF          400.1300109 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

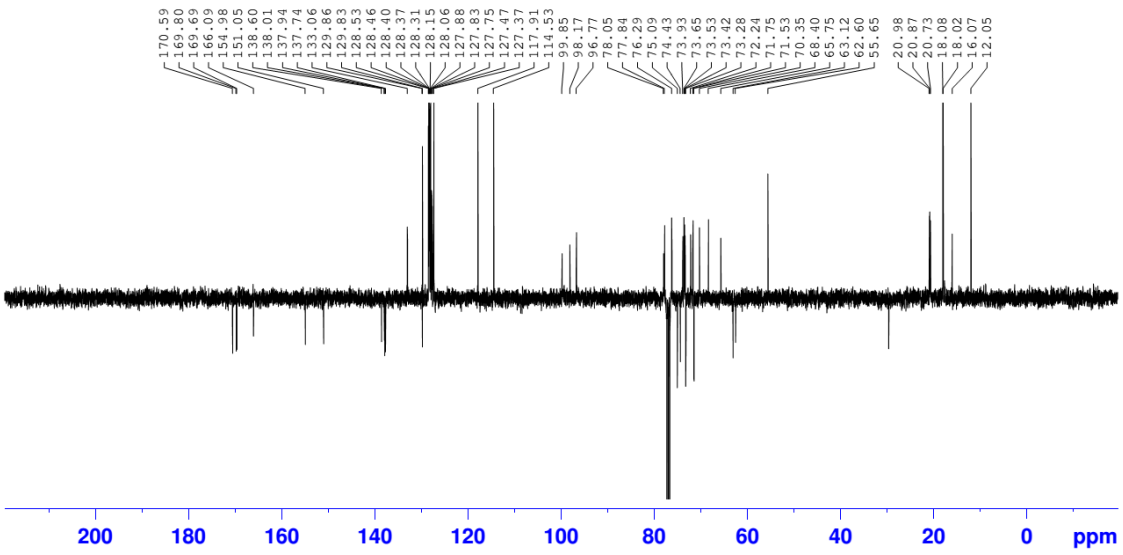
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **59**




```
F2 - Acquisition Parameters
Date_            20141106
Time                18.58
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 84.85
DW                60.800 usec
DE                 6.50 usec
TE                298.7 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PLW1         16.00000000 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300105 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



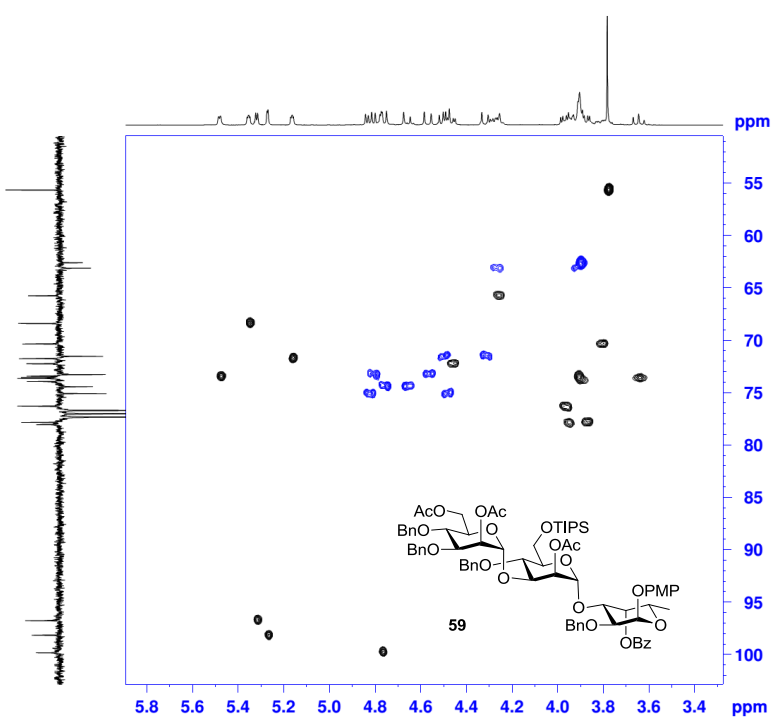

```
F2 - Acquisition Parameters
Date_            20141107
Time                 5.01
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             jmod
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 189.81
DW                20.800 usec
DE                 6.50 usec
TE                297.2 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1         73.00000000 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **59**




```
F2 - Acquisition Parameters
Date_            20141106
Time                23.31
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG         hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                      4
DS                     16
SWH             3546.099 Hz
FIDRES          3.462988 Hz
AQ             0.1444340 sec
RG                 189.81
DW                141.000 usec
DE                 6.50 usec
TE                298.1 K
CNST2        145.00000000
D0             0.00000300 sec
D1             1.45146203 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
P2                 20.00 usec
P28              1000.00 usec
PLW1         16.00000000 W
SFO1         400.1316976 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                  13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

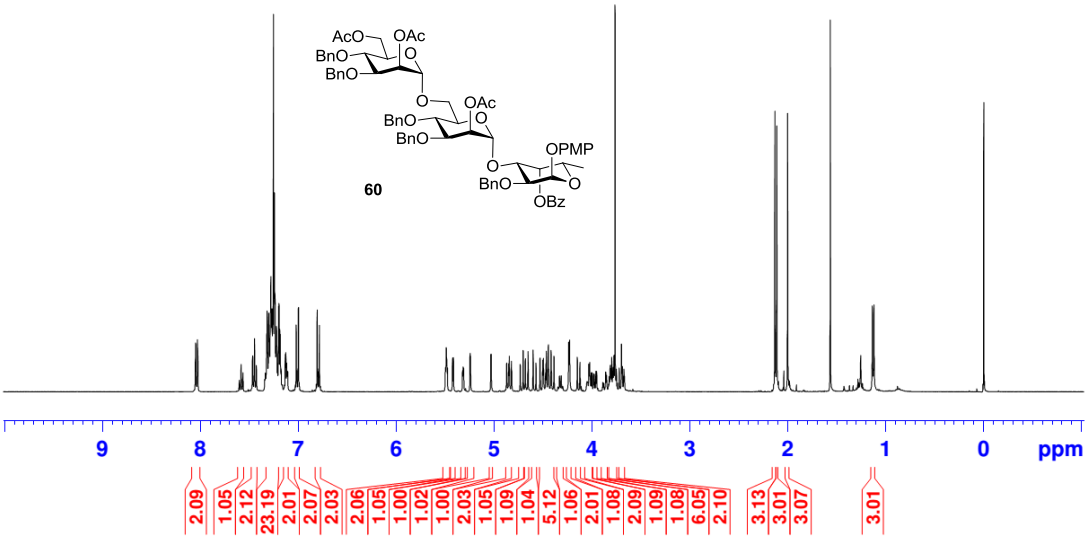
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1          100.6203 MHz
FIDRES       65.104164 Hz
SW              165.639 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF           400.1300105 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF           100.6127690 MHz
WDW          States-TPPI
SSB                      2
LB        0 Hz
GB        0
```

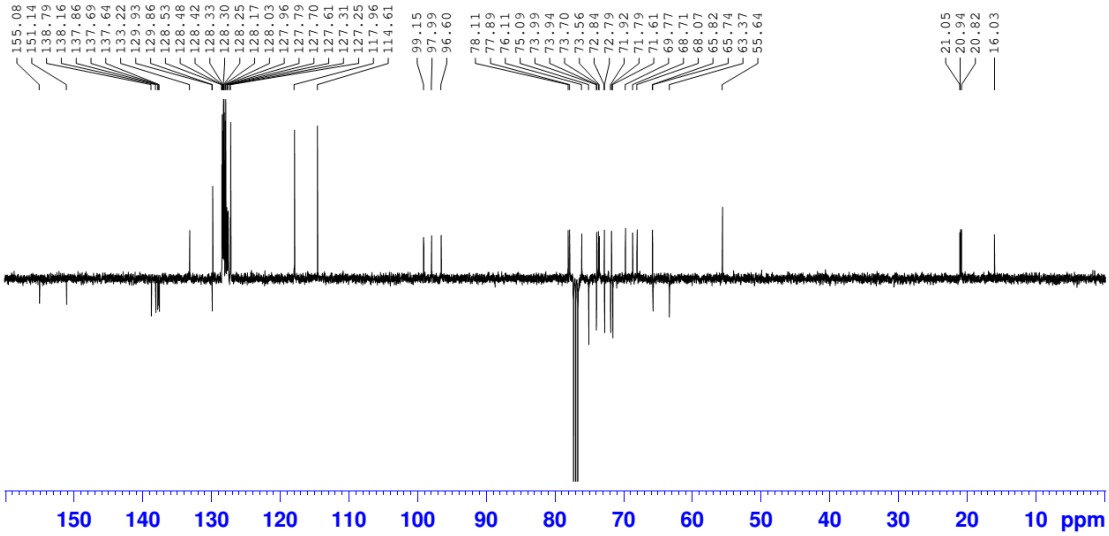
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **60**




```
F2 - Acquisition Parameters
Date_            20141027
Time               20.34
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ            3.9846387 sec
RG                 84.85
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300111 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



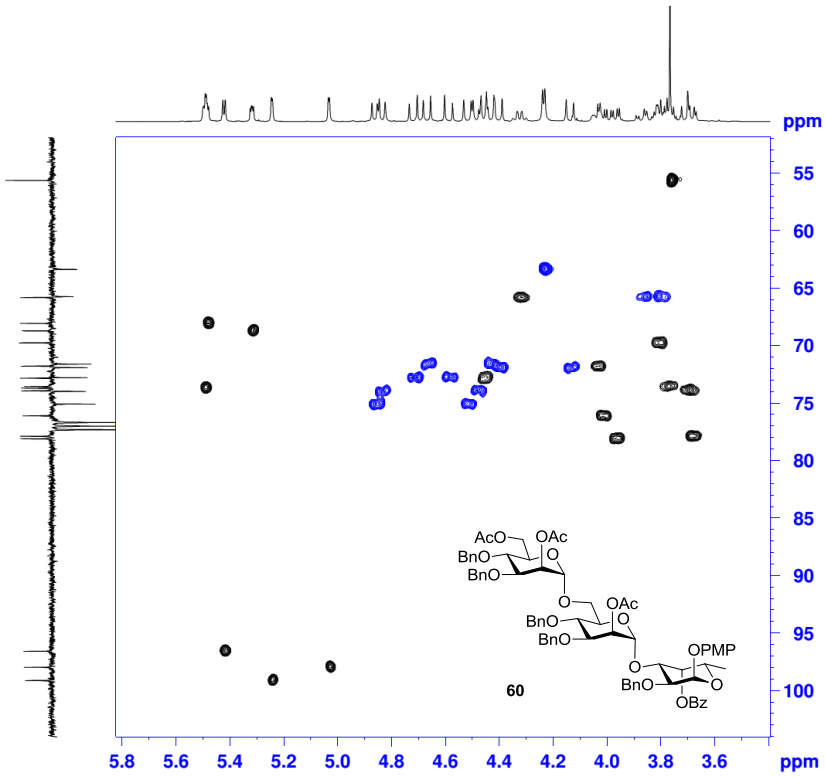

```
F2 - Acquisition Parameters
Date_            20141028
Time               0.10
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            jmod
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ            1.3631988 sec
RG                189.81
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
CNST11         1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         73.00000000 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **60**




```
F2 - Acquisition Parameters
Date_            20141027
Time               22.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     6
DS                    16
SWH            3378.378 Hz
FIDRES         3.299198 Hz
AQ             0.1516020 sec
RG                189.81
DW               148.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.44429398 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1         16.00000000 W
SFO1        400.1317675 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2        100.6202727 MHz

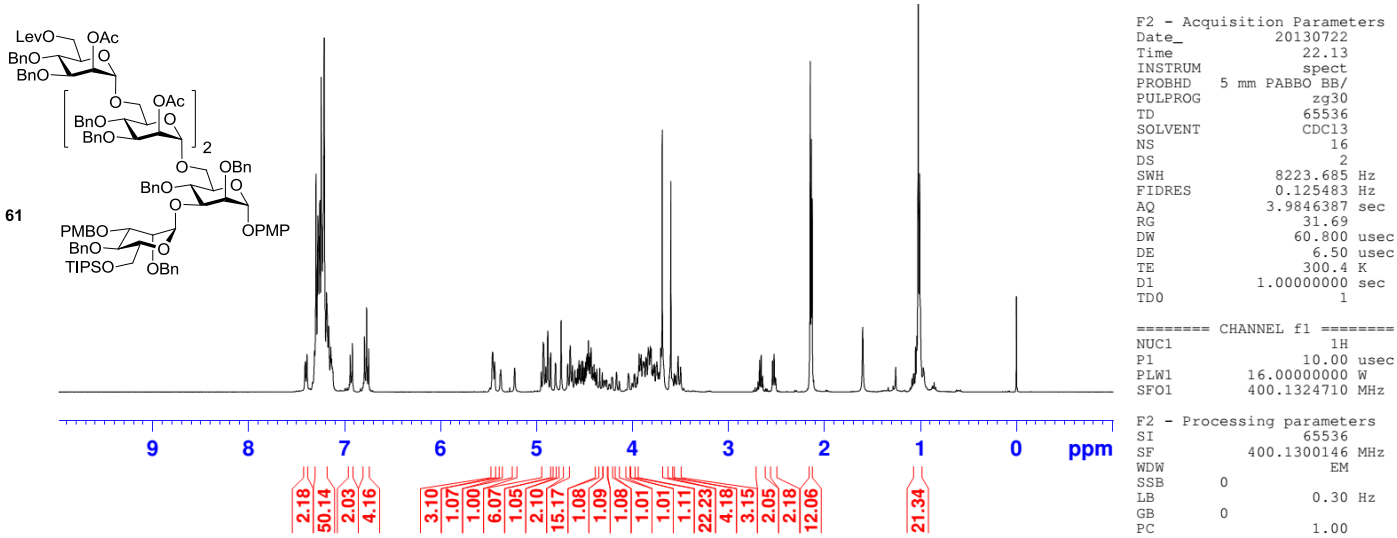
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES        65.104164 Hz
SW              165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF          400.1300111 MHz
WDW               QSINE
SSB                    2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW          States-TPPI
SSB                    2
LB        0 Hz
GB        0
```

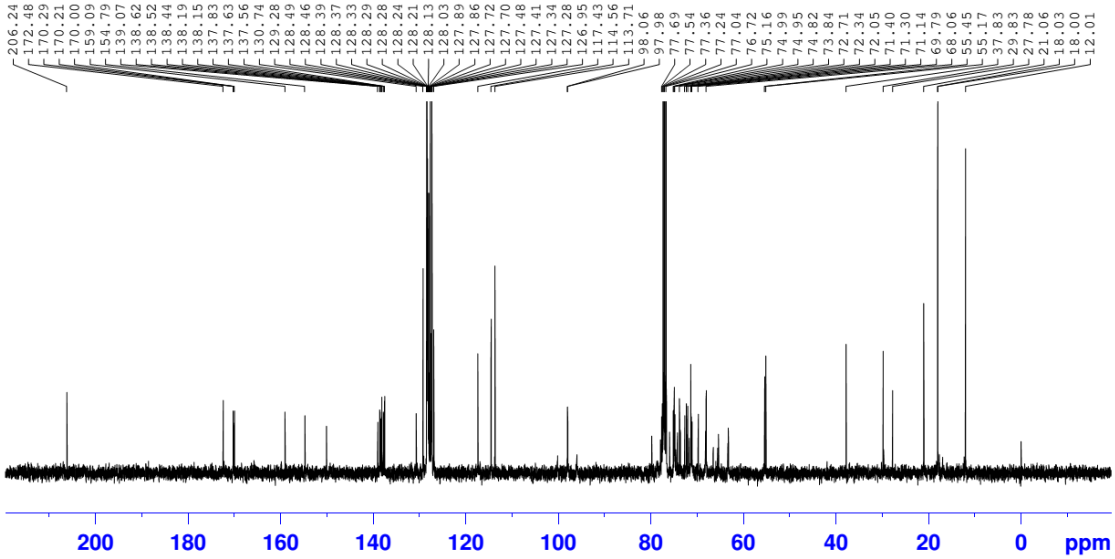
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra for compound **61**




```
F2 - Acquisition Parameters
Date_            20130722
Time               22.13
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 31.69
DW                60.800 usec
DE                 6.50 usec
TE                 300.4 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1         16.00000000 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300146 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



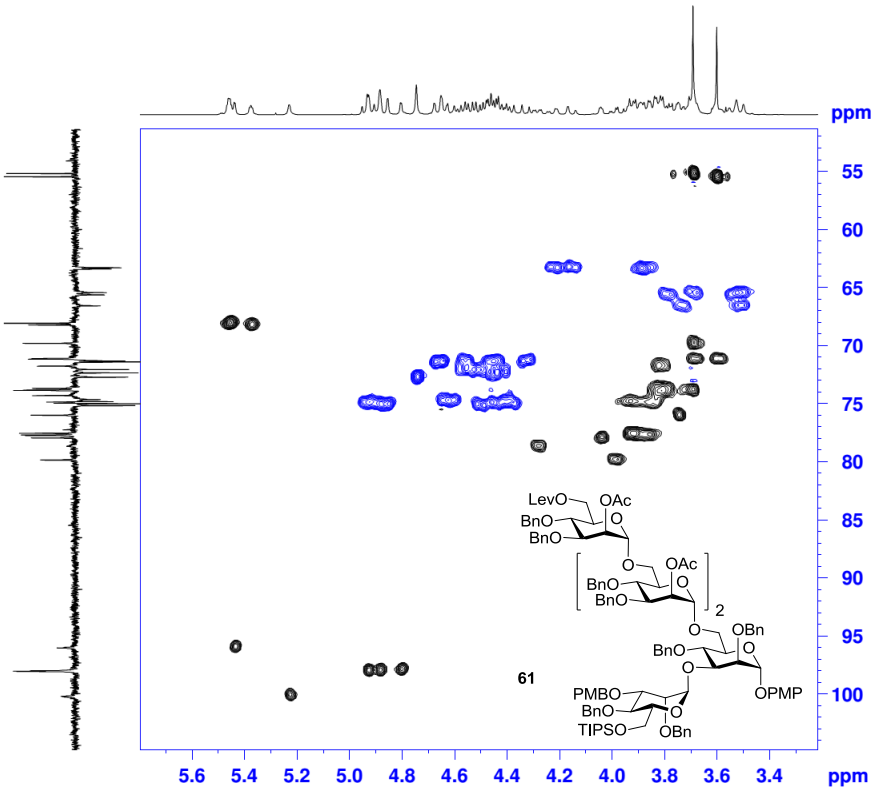

```
F2 - Acquisition Parameters
Date_            20130723
Time                4.09
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1500
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                189.81
DW                20.800 usec
DE                 6.50 usec
TE                 299.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         73.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.19753000 W
PLW13         0.09920000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **61**




```
F2 - Acquisition Parameters
Date_            20130722
Time               23.33
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                 1024
SOLVENT            CDCl3
NS                     8
DS                    16
SWH             3401.361 Hz
FIDRES          3.321641 Hz
AQ             0.1505780 sec
RG                189.81
DW               147.000 usec
DE                 6.50 usec
TE                 300.3 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.44531798 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28                0.10 usec
PLW1         16.00000000 W
SFO1        400.1315672 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2        100.6202727 MHz

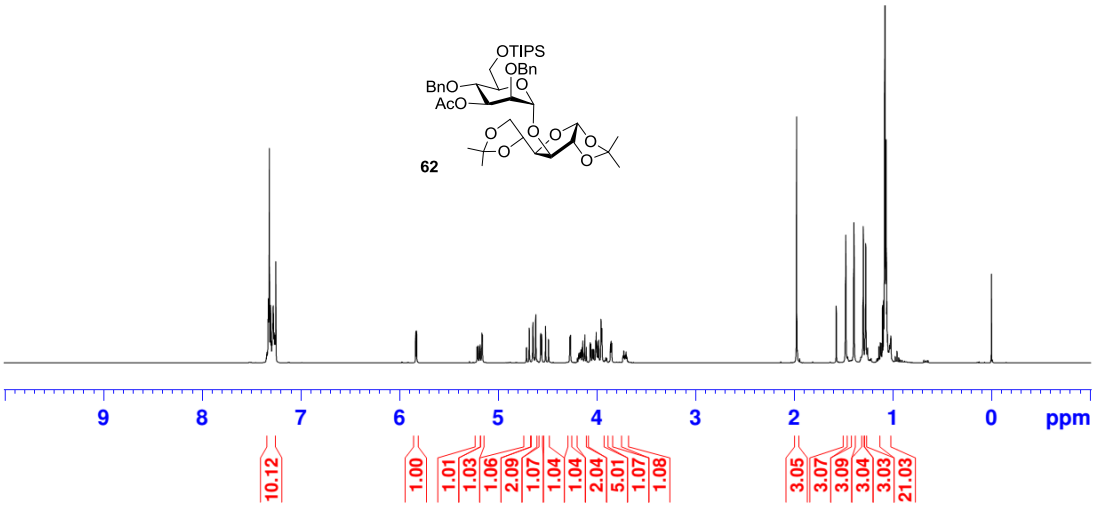
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW              165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300146 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2         echo-antiecho
SF          100.6127690 MHz
WDW         States-TPPI
SSB                    2
LB        0 Hz
GB        0
```

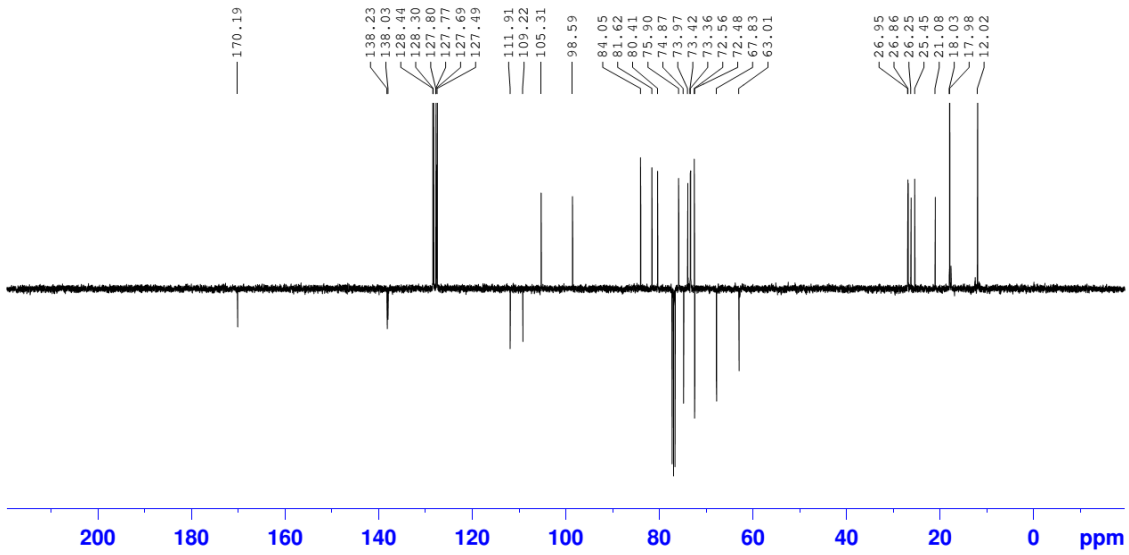
^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **62**




```
F2 - Acquisition Parameters
Date_            20141102
Time                22.03
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                  62.9
DW                60.800 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PLW1        16.00000000 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300107 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



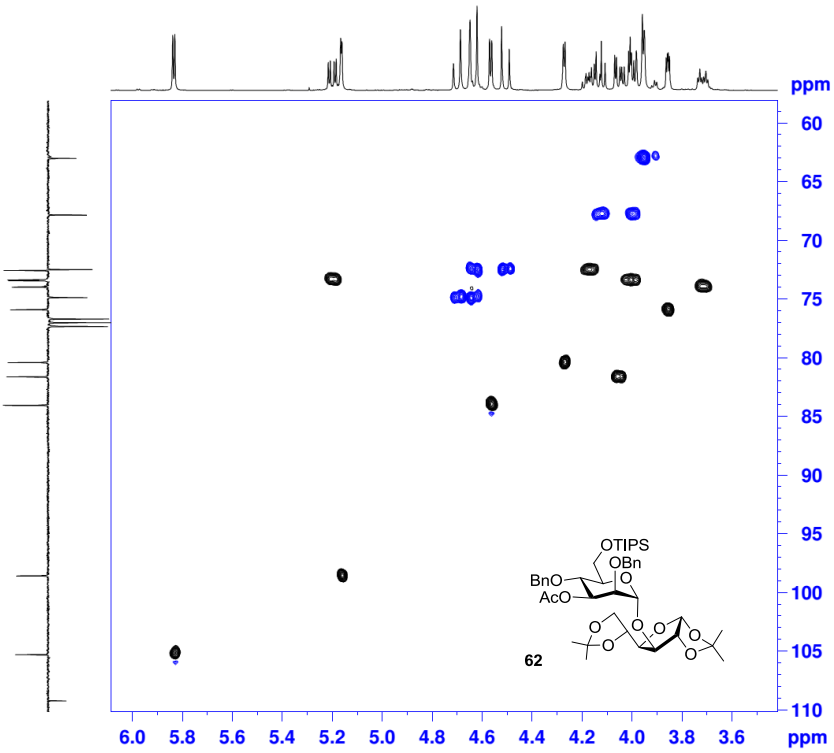

```
F2 - Acquisition Parameters
Date_            20141103
Time                 1.19
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                   800
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 189.81
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
CNST11         1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1        73.00000000 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2        16.00000000 W
PLW12        0.19753000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HSQC spectra (400 MHz, $CDCl_3$) for compound **62**




```
F2 - Acquisition Parameters
Date_            20141102
Time                23.43
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                  1024
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             3205.128 Hz
FIDRES          3.130008 Hz
AQ             0.1597940 sec
RG                 189.81
DW                156.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.43610203 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1        16.00000000 W
SFO1        400.1316205 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2        73.00000000 W
PLW12        1.14059997 W
SFO2        100.6202727 MHz

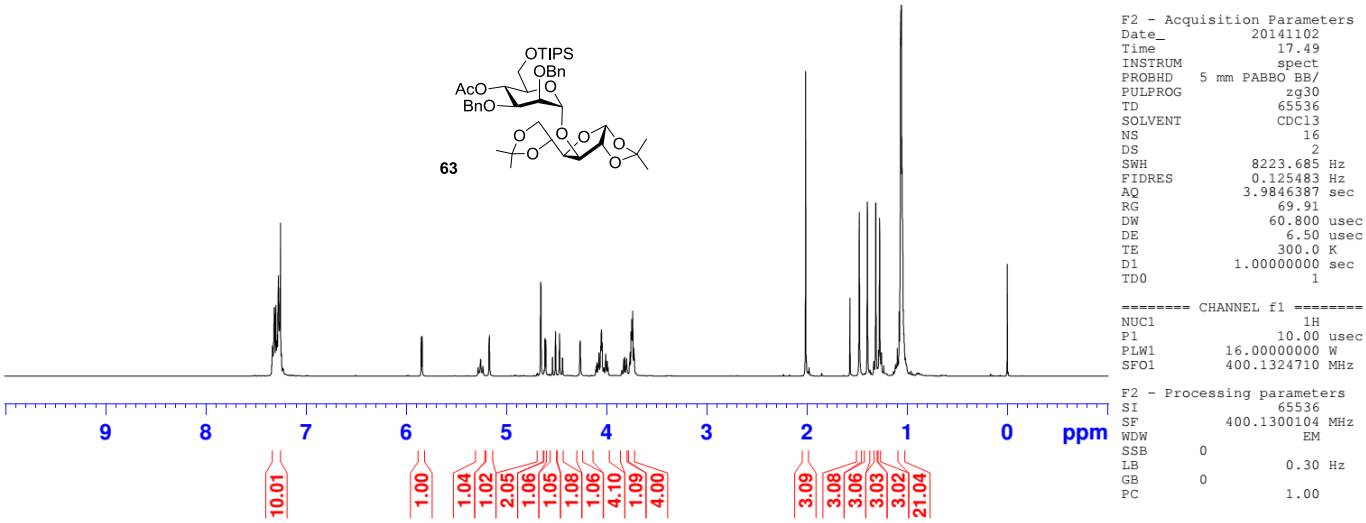
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16             1000.00 usec

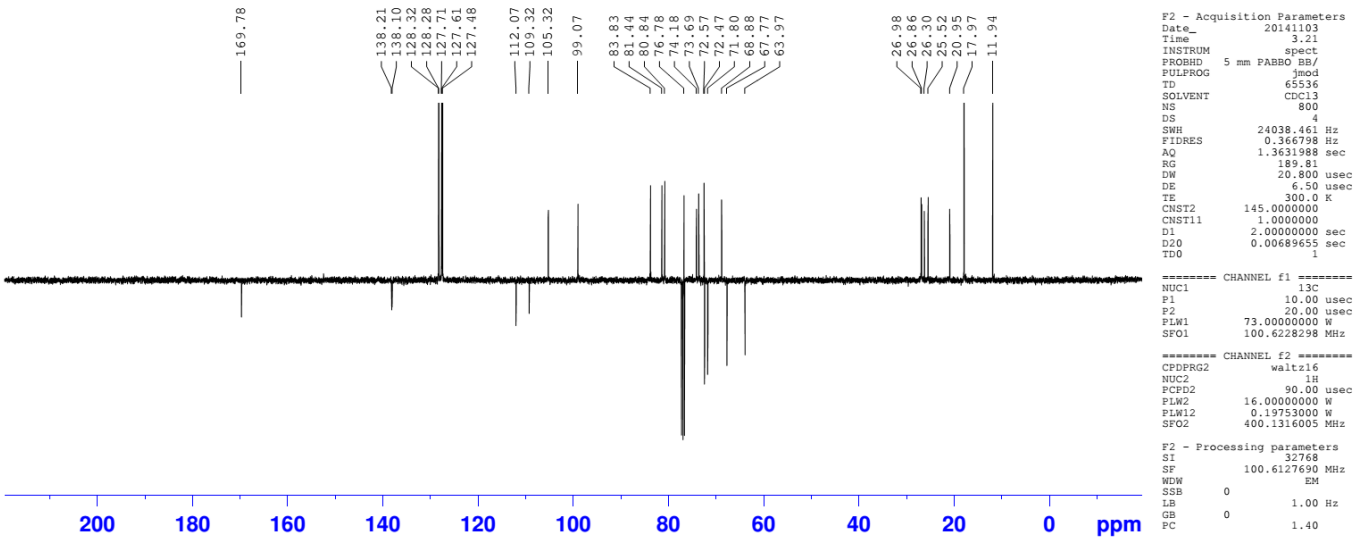
F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF          400.1300107 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                 1.40

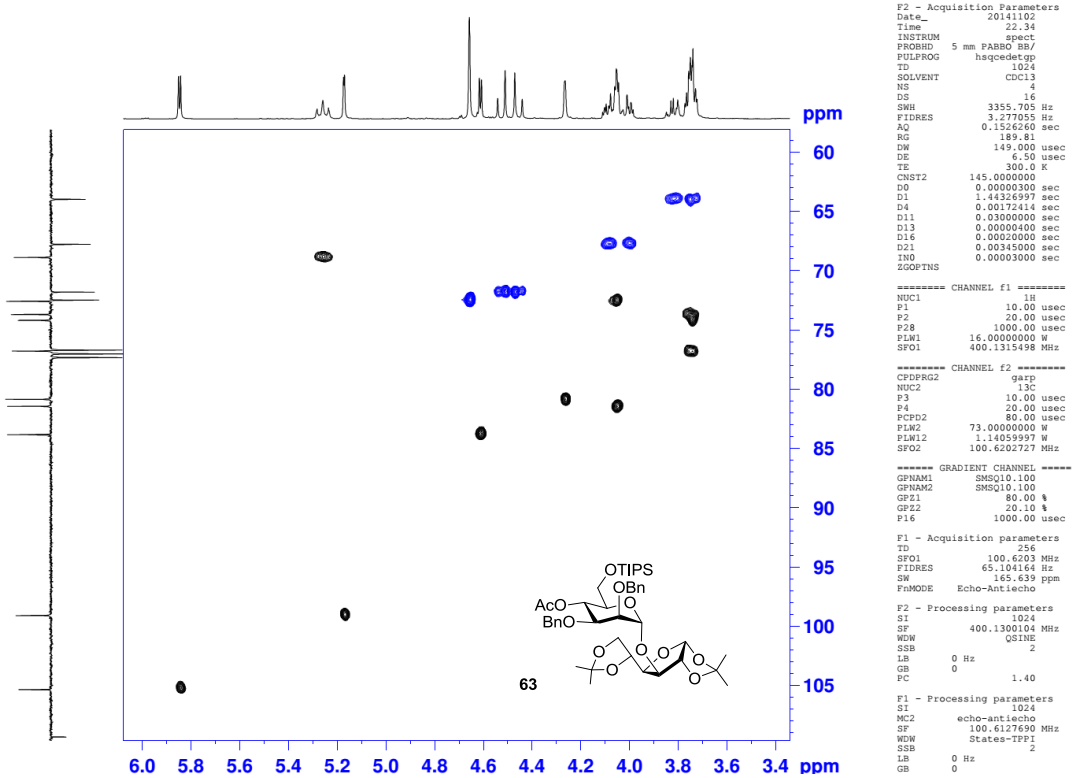
F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **63**

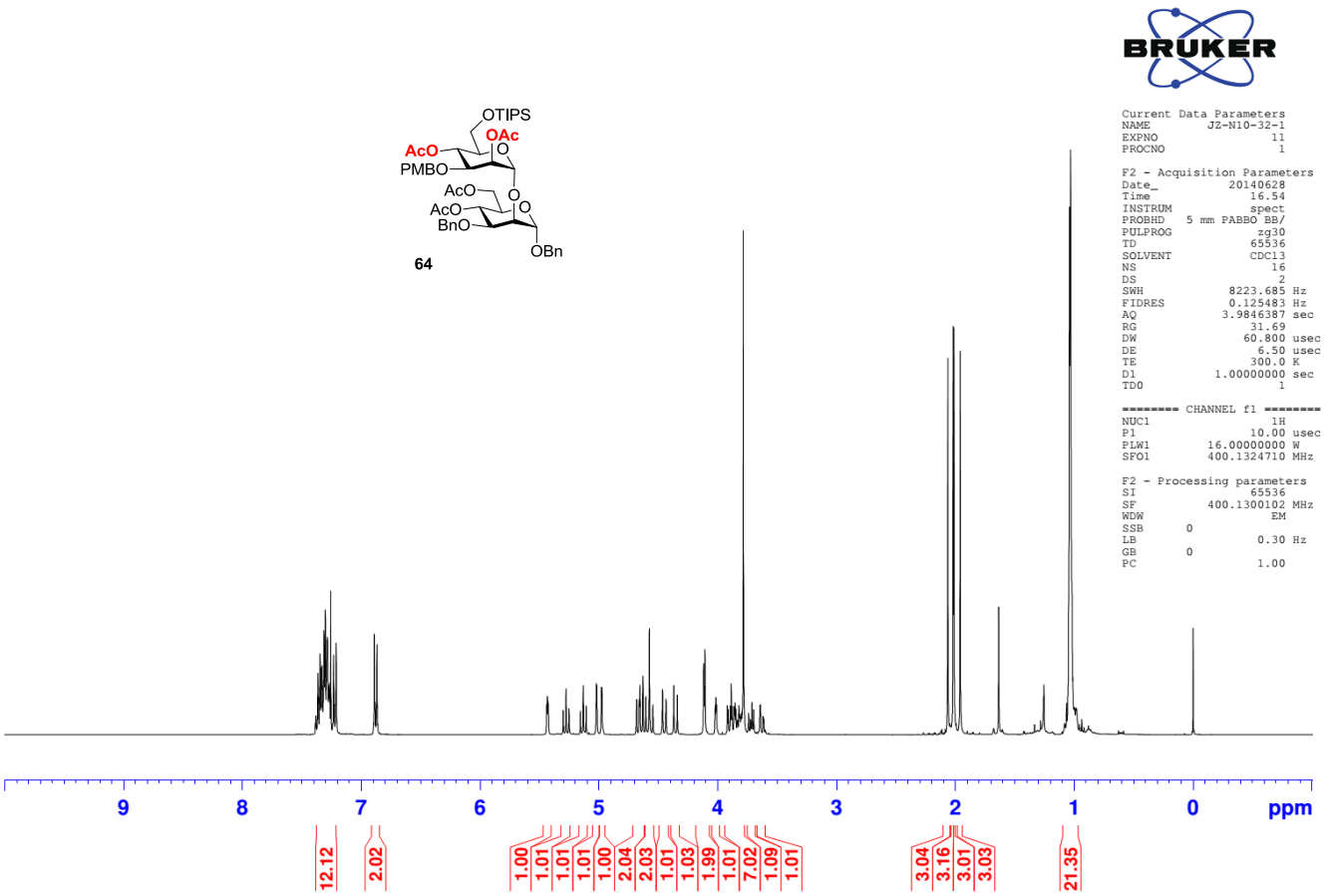




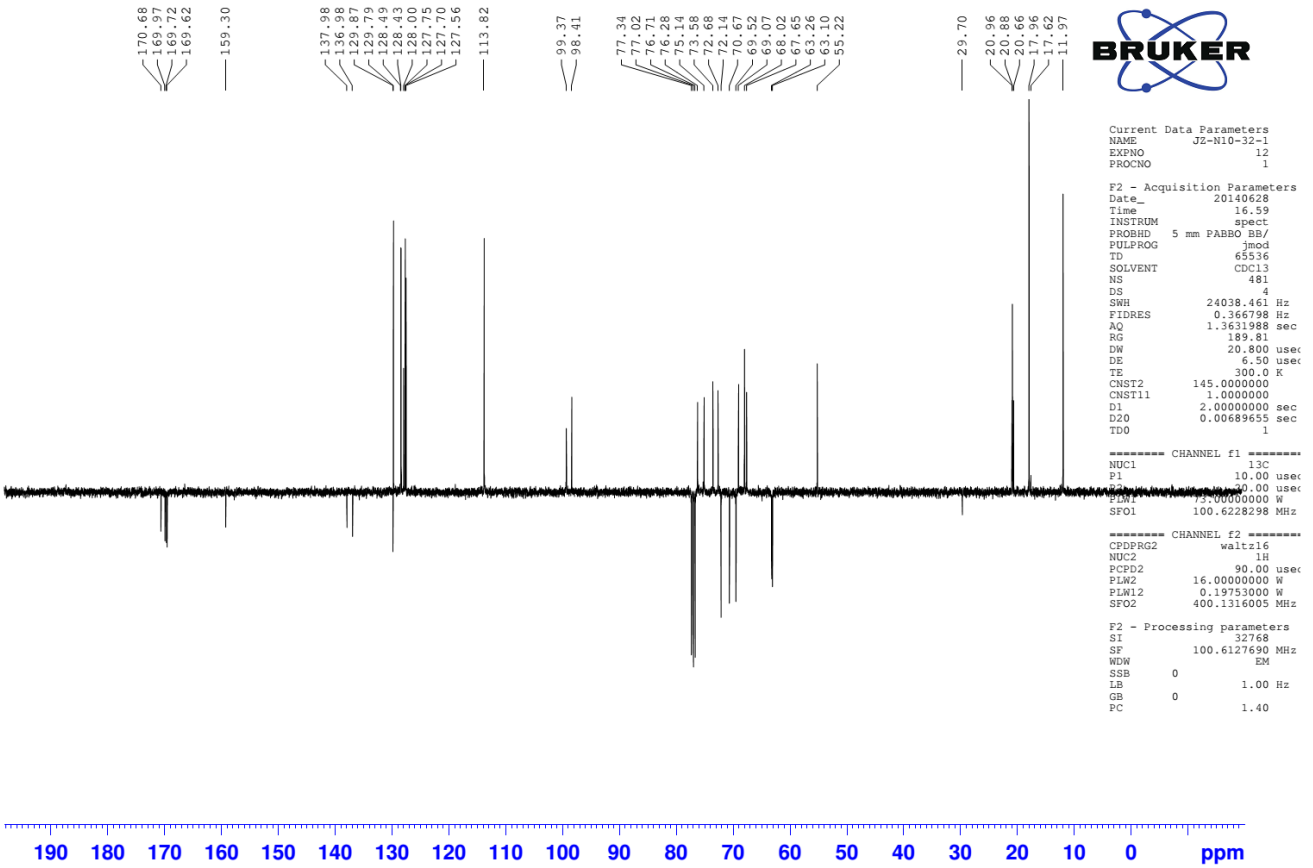
HSQC spectra (400 MHz, $CDCl_3$) for compound **63**



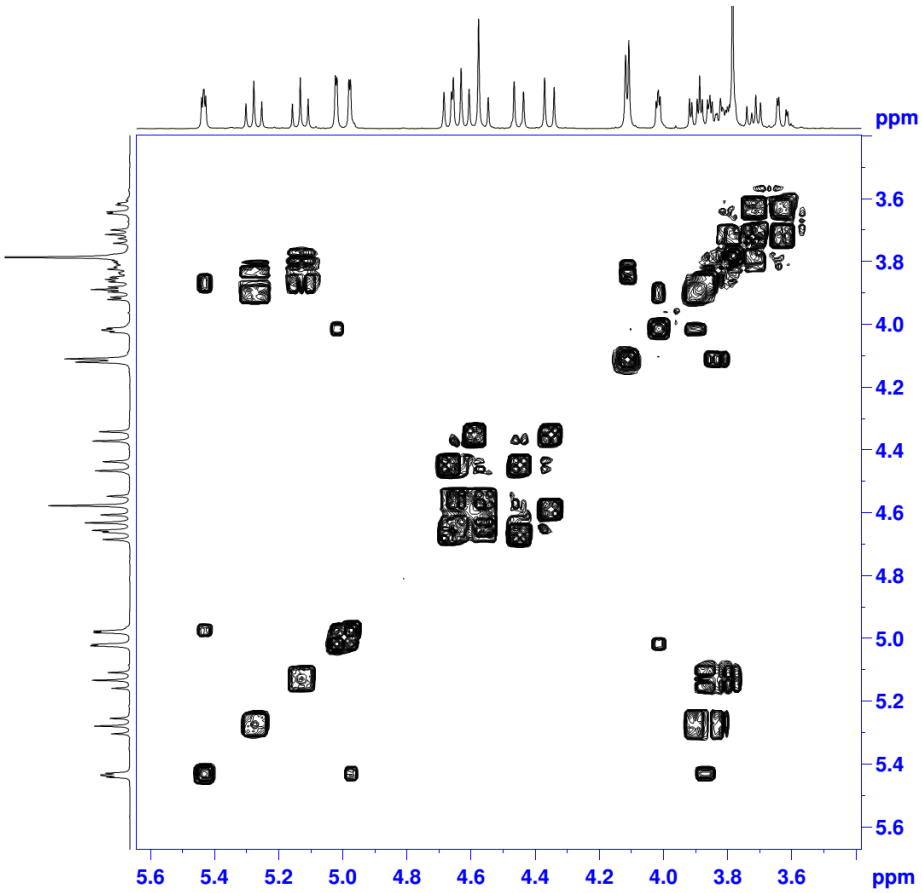
^{1}H NMR spectrum for compound **64**



^{13}C-APT NMR spectrum for compound **64**



COSY spectrum for compound **64**




```
Current Data Parameters
NAME         JZ-N10-32-1
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140628
Time               18.32
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT           CDCl3
NS                    4
DS                    8
SWH            3623.188 Hz
FIDRES         1.769135 Hz
AQ           0.2826740 sec
RG               26.04
DW             138.000 usec
DE                6.50 usec
TE               300.0 K
D0           0.00000300 sec
D1           1.90906894 sec
D11          0.03000000 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00027600 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                10.00 usec
P1                10.00 usec
P17             2000.00 usec
PLW1        16.00000000 W
PLW10        2.36689997 W
SFO1       400.1314441 MHz

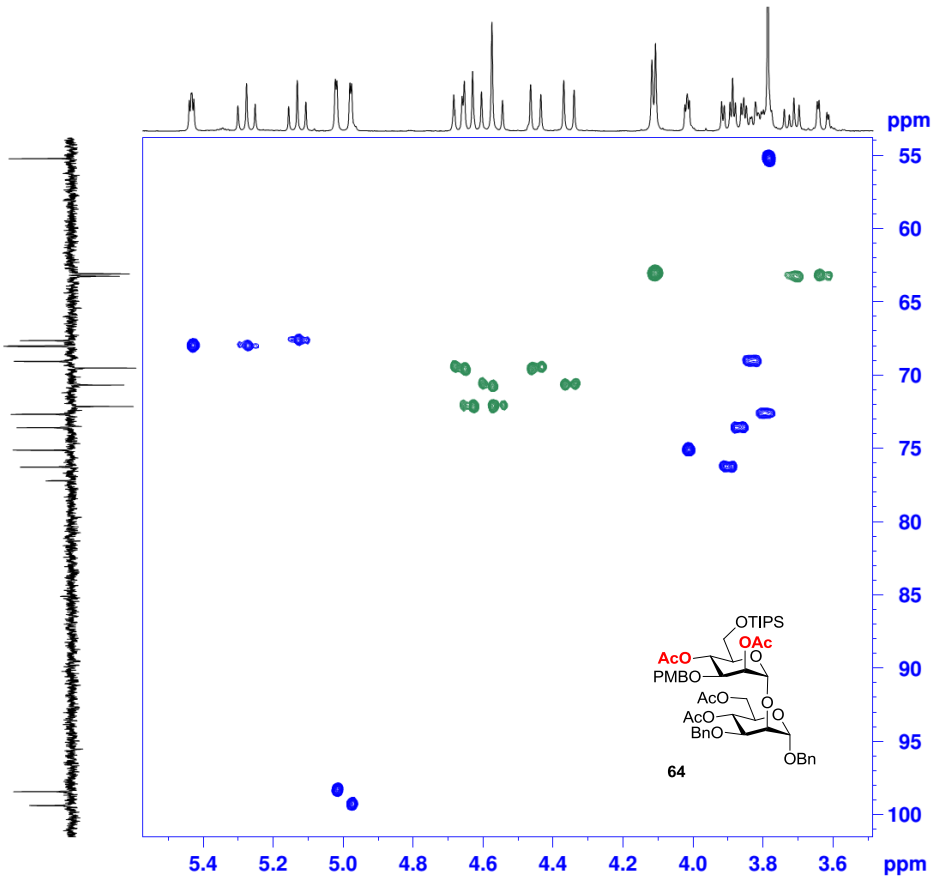
====== GRADIENT CHANNEL =====
GPNAM1      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1           400.1314 MHz
FIDRES        28.306160 Hz
SW                9.055 ppm
FnMODE               QF

F2 - Processing parameters
SI                 1024
SF          400.1300102 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2                  QF
SF          400.1300102 MHz
WDW                 SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **64**




```
Current Data Parameters
NAME         JZ-N10-32-1
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140628
Time               3.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                 1024
SOLVENT           CDCl3
NS                    8
DS                   16
SWH            3205.128 Hz
FIDRES         3.130008 Hz
AQ           0.1597940 sec
RG               189.81
DW             156.000 usec
DE                6.50 usec
TE               300.0 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.43610203 sec
D4           0.00172414 sec
D11          0.03000000 sec
D13          0.00000400 sec
D16          0.00020000 sec
D21          0.00345000 sec
IN0          0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28                0.10 usec
PLW1        16.00000000 W
SFO1       400.1316197 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2        73.00000000 W
PLW12        1.14059997 W
SFO2       100.6202727 MHz

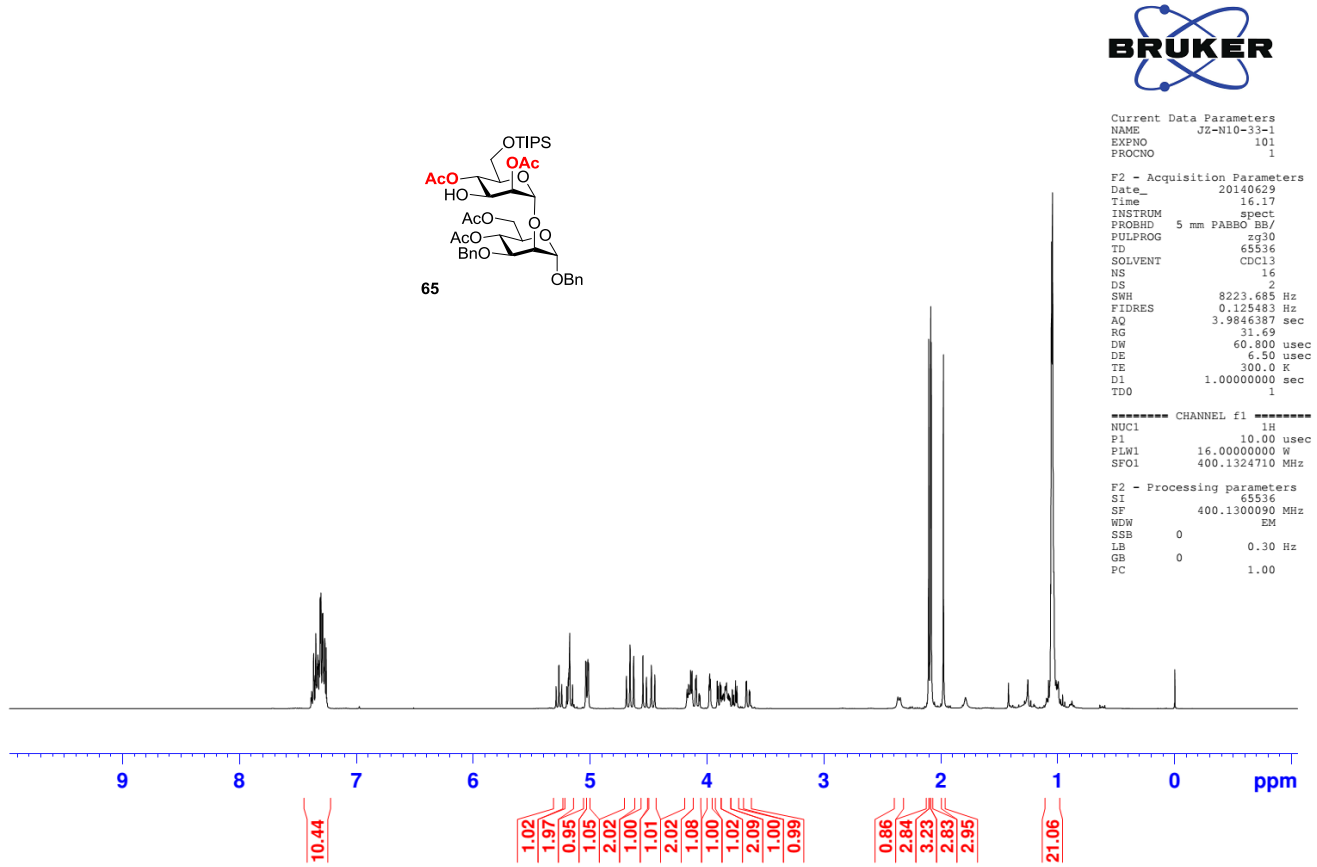
====== GRADIENT CHANNEL =====
GPNAM1      SMSQ10.100
GPNAM2      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  256
SFO1           100.6203 MHz
FIDRES         65.104164 Hz
SW               165.639 ppm
FnMODE     Echo-Antiecho

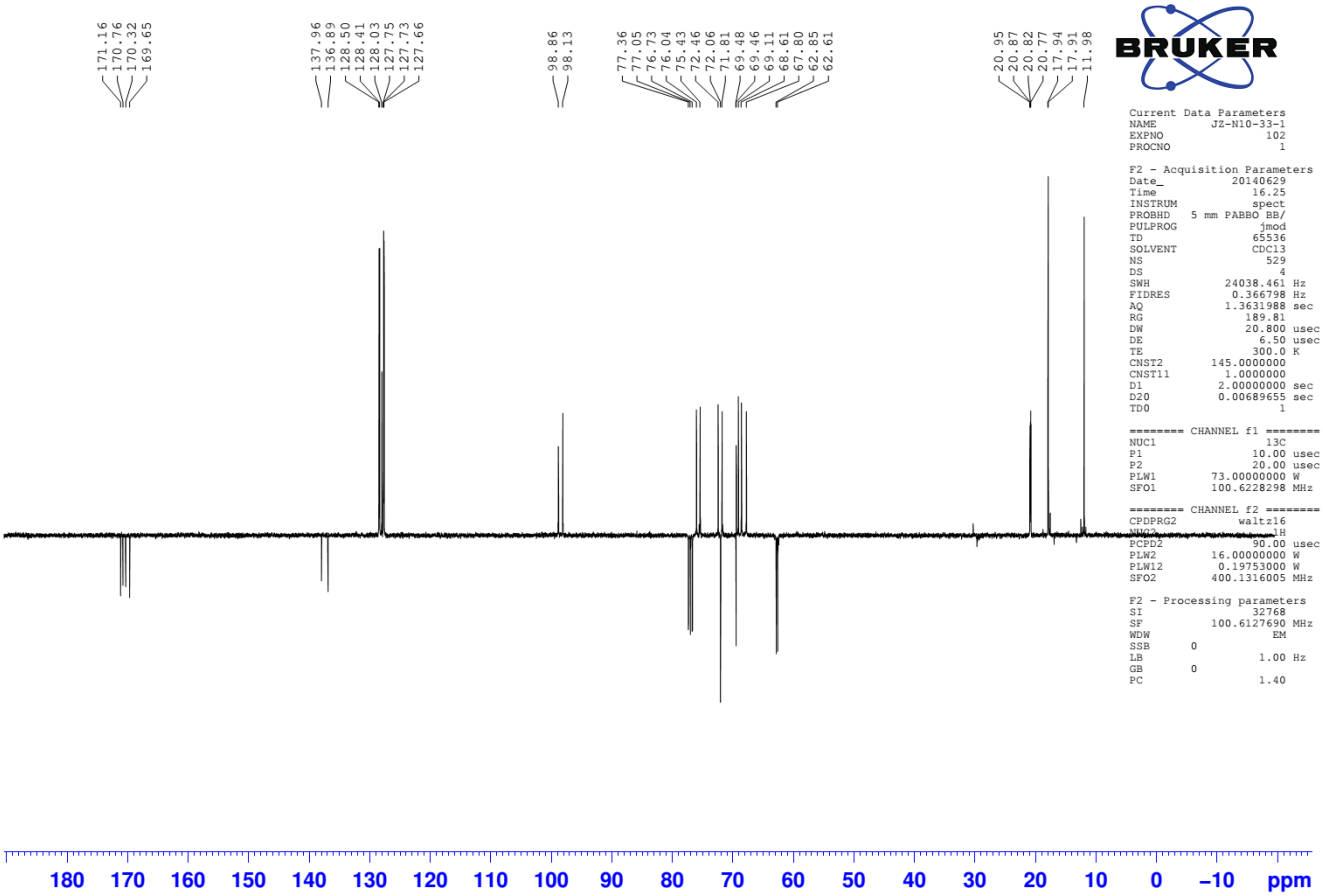
F2 - Processing parameters
SI                 1024
SF          400.1300095 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW                 SINE
SSB                    2
LB        0 Hz
GB        0
```

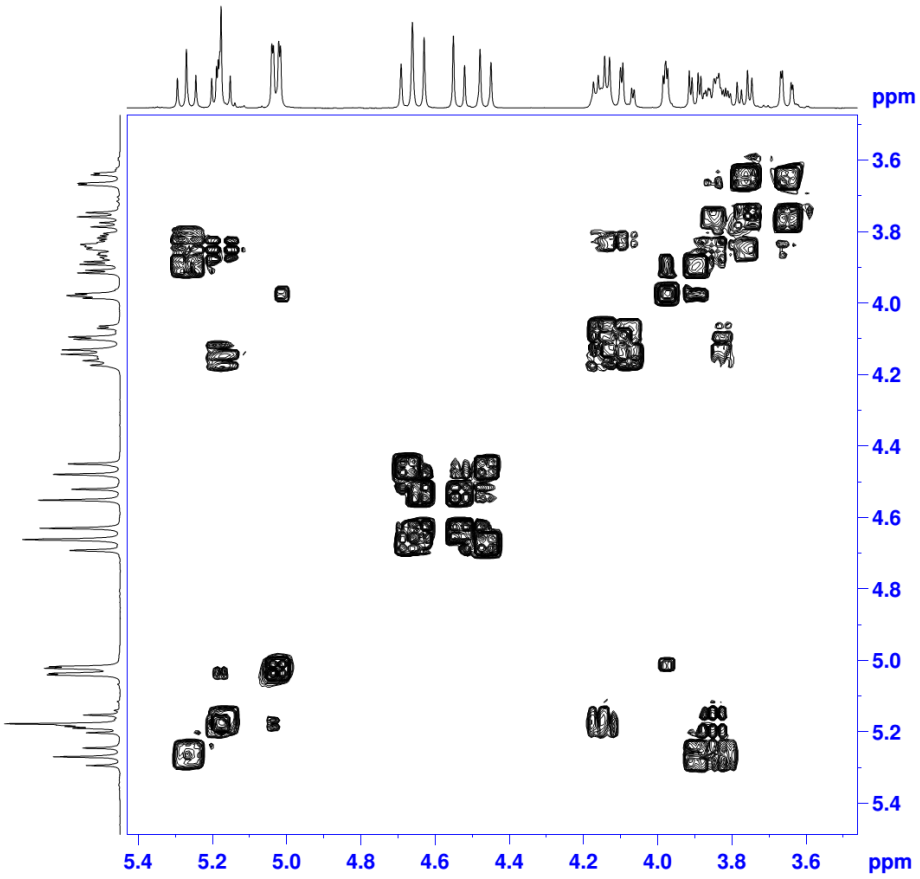
^{1}H NMR spectrum for compound **65**



^{13}C-APT NMR spectrum for compound **65**



COSY spectrum for compound **65**




```
Current Data Parameters
NAME          JZ-N10-33-1
EXPNO                 104
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140629
Time                16.50
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                    2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             3496.503 Hz
FIDRES          1.707277 Hz
AQ             0.2929140 sec
RG                 14.37
DW               143.000 usec
DE                 6.50 usec
TE                300.0 K
D0            0.00000300 sec
D1            1.89882898 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00028600 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                  10.00 usec
P1                  10.00 usec
P17                2000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1         400.1315766 MHz

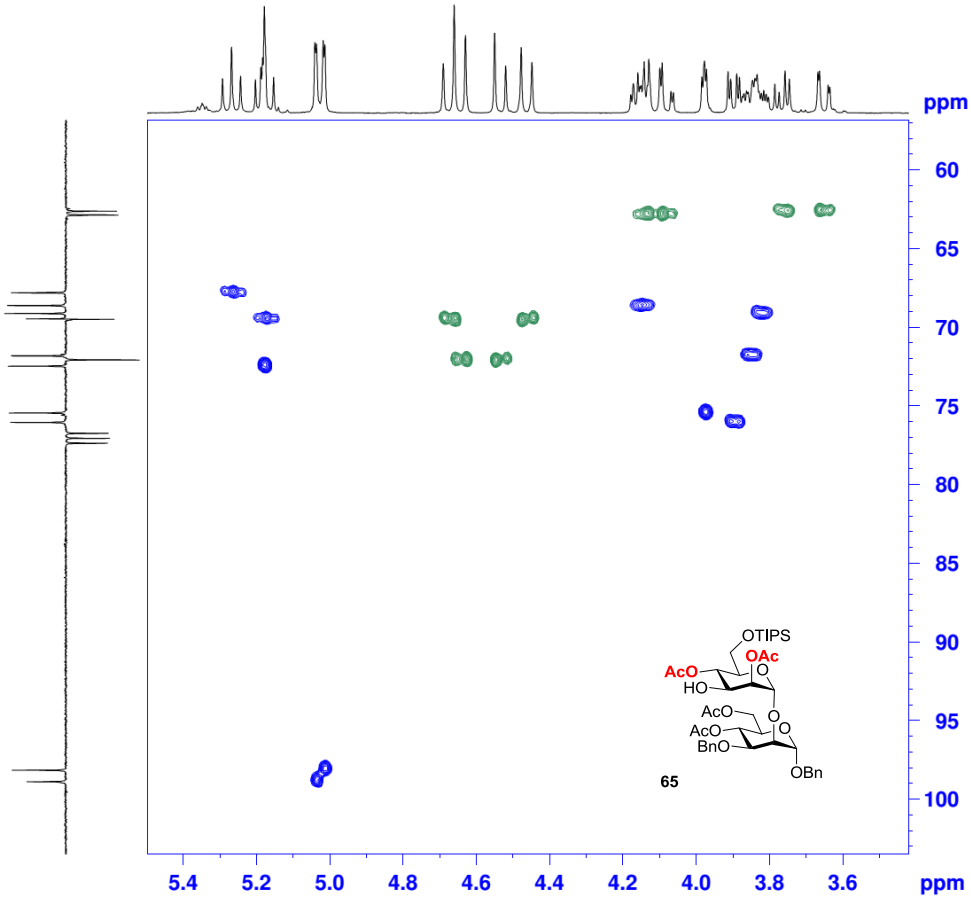
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            400.1316 MHz
FIDRES          27.316433 Hz
SW                   8.738 ppm
FnMODE                  QF

F2 - Processing parameters
SI                     1024
SF           400.1300090 MHz
WDW                   QSINE
SSB       0
LB        0 Hz
GB        0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF           400.1300090 MHz
WDW                     SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **65**




```
Current Data Parameters
NAME          JZ-N10-33-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140629
Time                 4.43
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                    1024
SOLVENT             CDCl3
NS                      8
DS                     16
SWH             3267.974 Hz
FIDRES          3.191381 Hz
AQ             0.1567220 sec
RG                 189.81
DW               153.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.43917406 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1          16.00000000 W
SFO1         400.1316022 MHz

======== CHANNEL f2 ========
CPDPRG2               garp
NUC2                   13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2         100.6202727 MHz

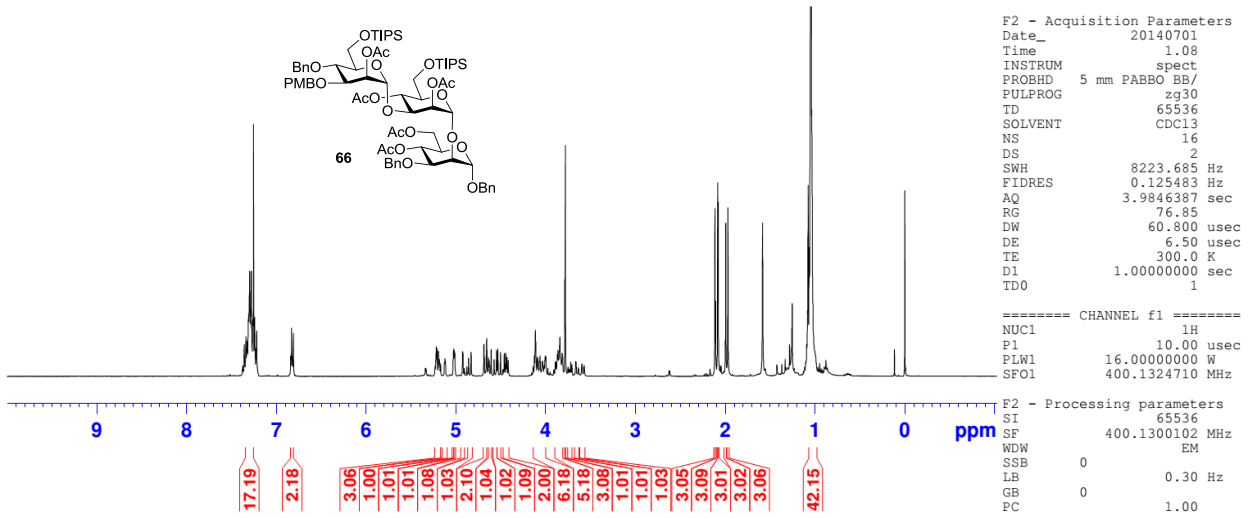
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

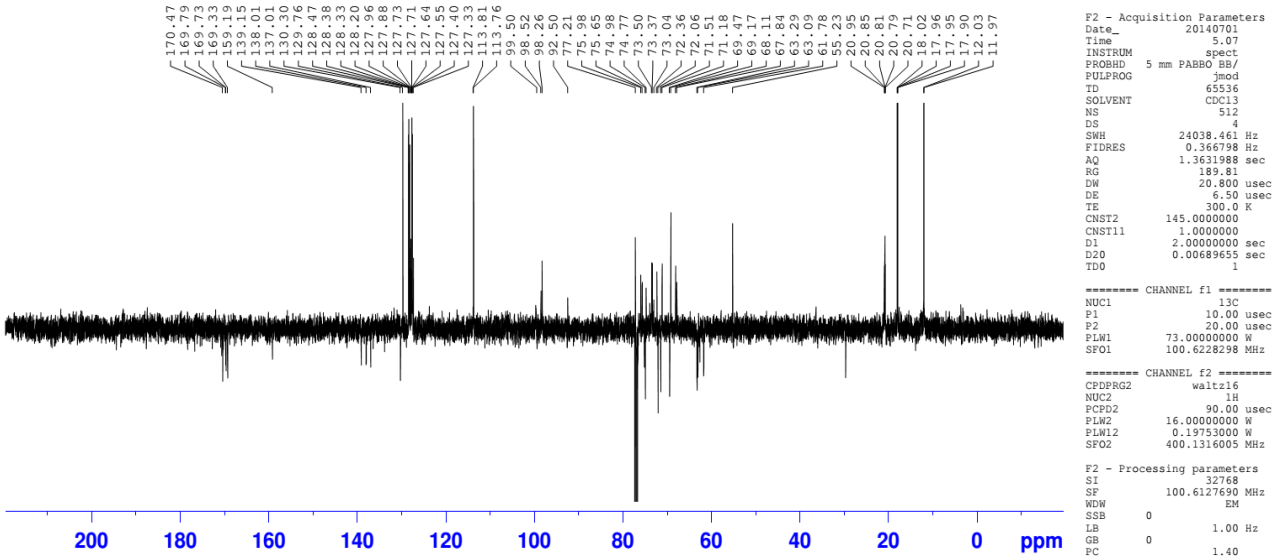
F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF           400.1300092 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                     1.40

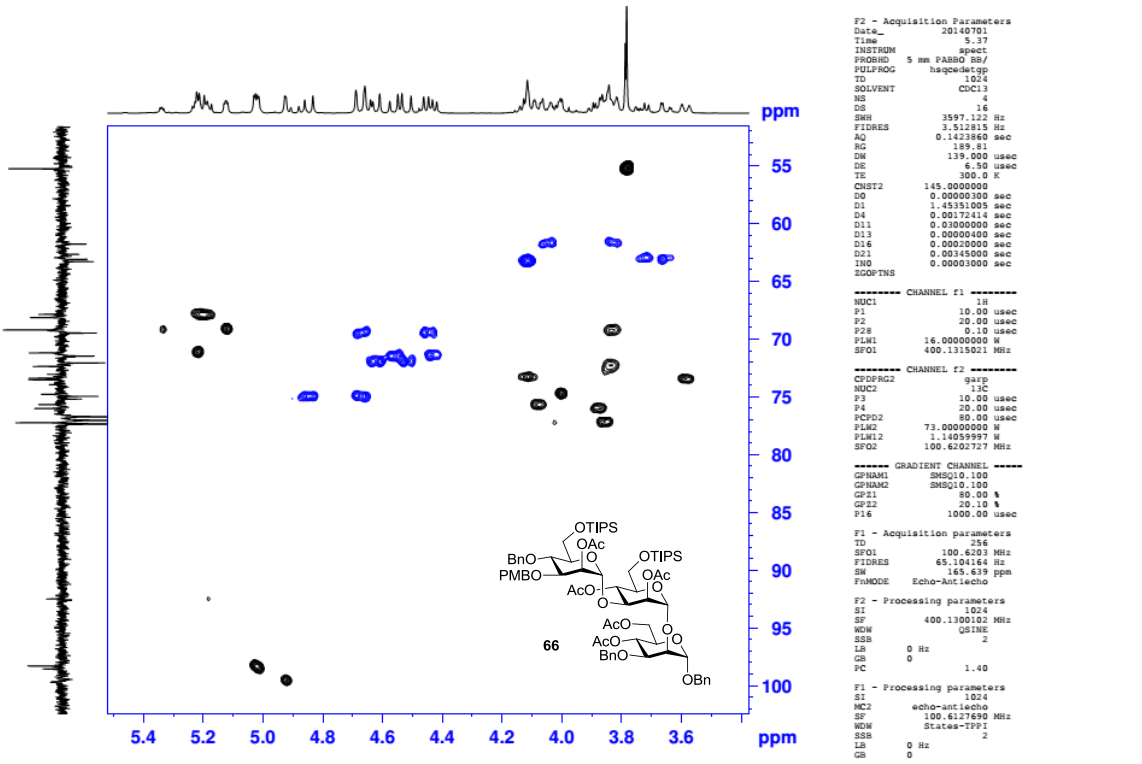
F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF           100.6127690 MHz
WDW          States-TPPI
SSB                       2
LB        0 Hz
GB        0
```

^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C-APT NMR (100 MHz, $CDCl_3$) spectra for compound **66**

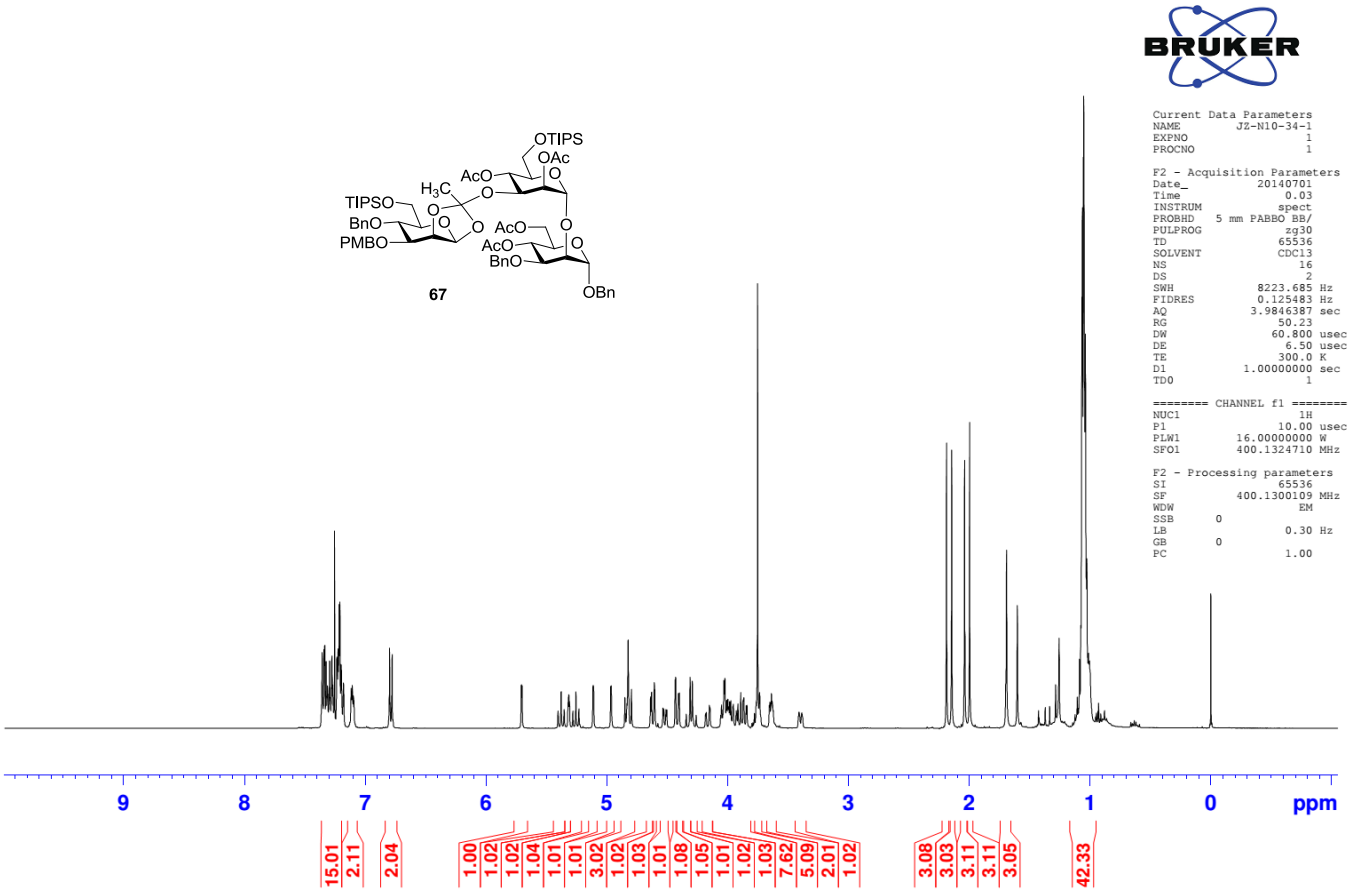




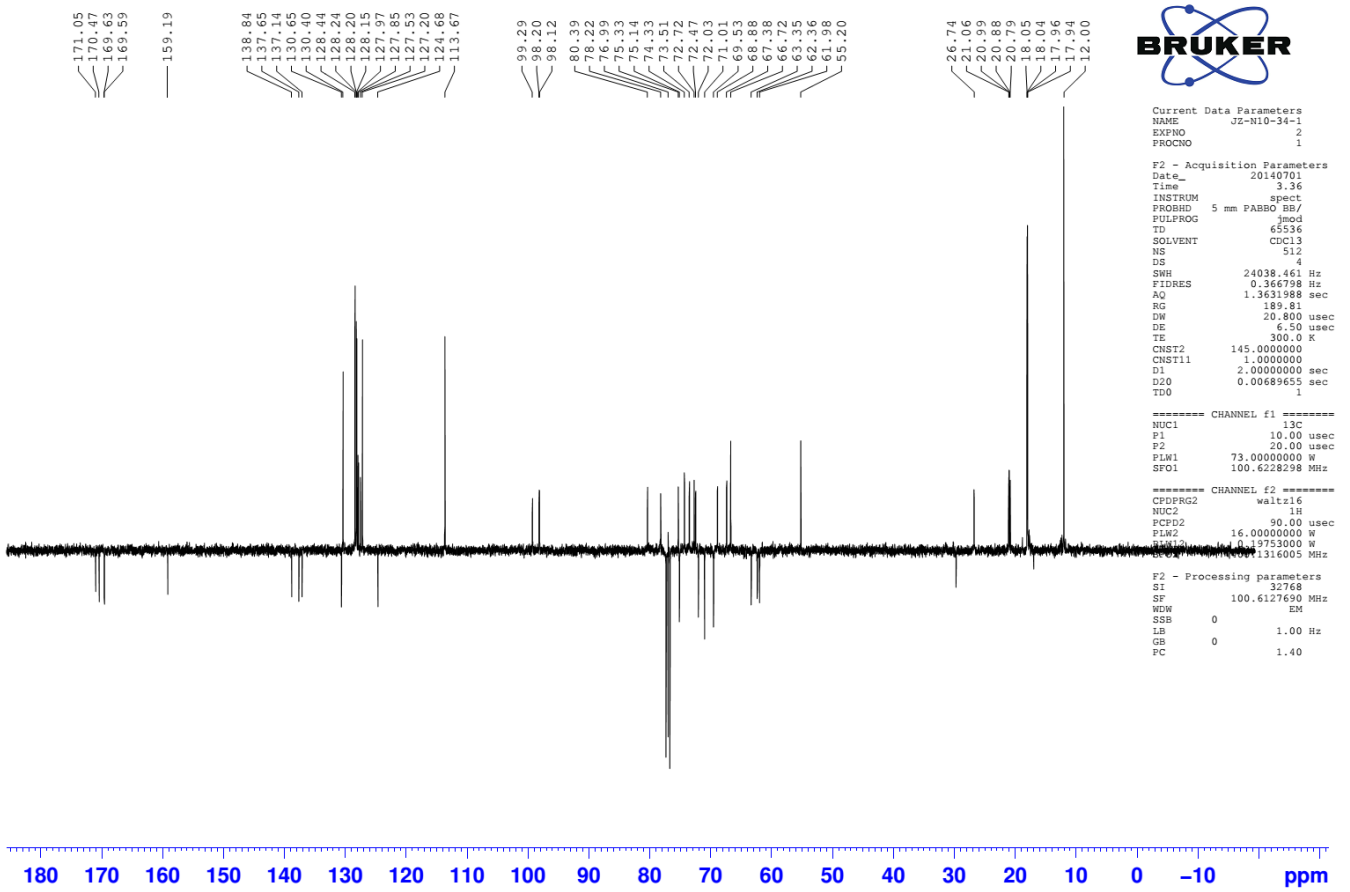
HSQC spectra (400 MHz, $CDCl_3$) for compound **66**



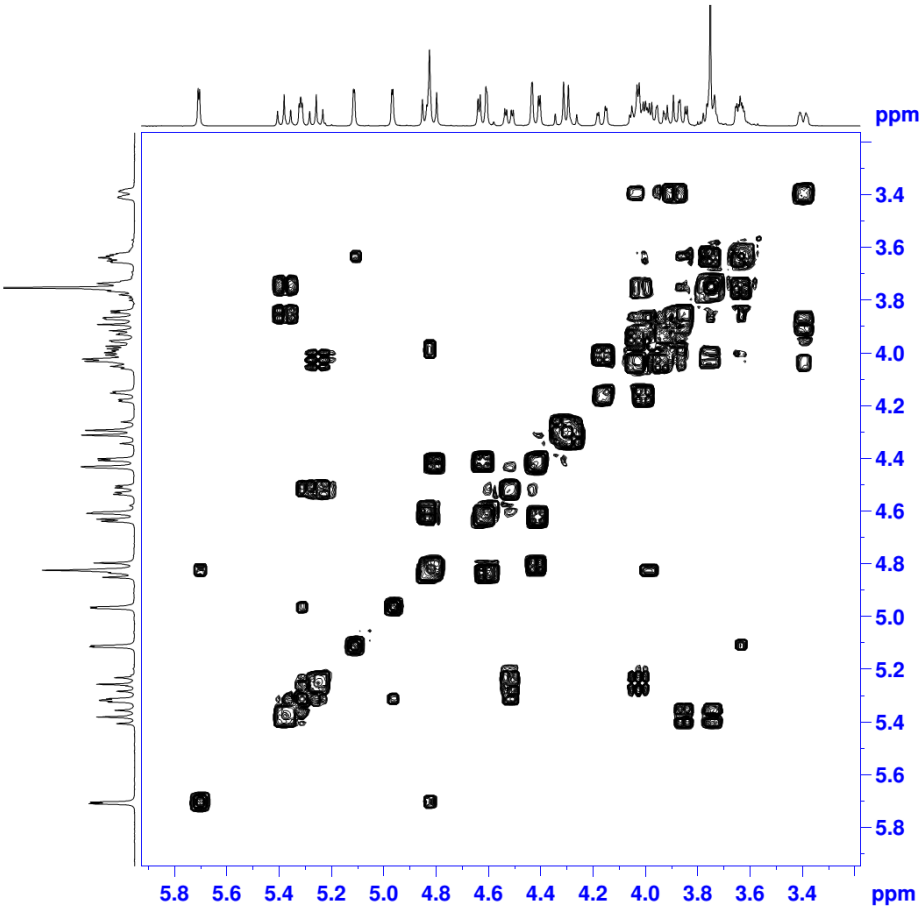
^{1}H NMR spectrum for compound **67**



^{13}C-APT NMR spectrum for compound **67**



COSY spectrum for compound **67**




```
Current Data Parameters
NAME          JZ-N10-34-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140701
Time                 0.05
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             3846.154 Hz
FIDRES          1.878005 Hz
AQ             0.2662900 sec
RG                 18.47
DW               130.000 usec
DE                 6.50 usec
TE                300.0 K
D0            0.00000300 sec
D1            1.92545295 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00026000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17                2000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1          400.1313398 MHz

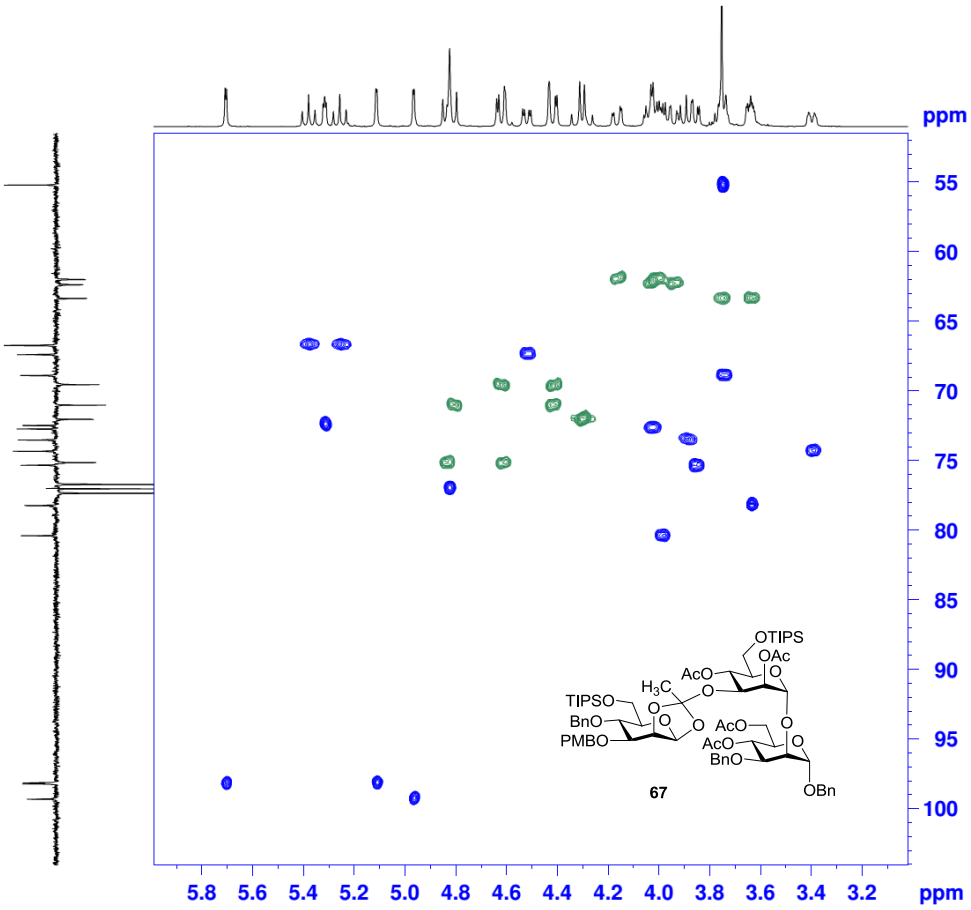
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            400.1313 MHz
FIDRES         30.048077 Hz
SW                  9.612 ppm
FnMODE                 QF

F2 - Processing parameters
SI                     1024
SF            400.1300109 MHz
WDW                   QSINE
SSB       0
LB        0 Hz
GB        0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            400.1300109 MHz
WDW                     SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **67**




```
Current Data Parameters
NAME          JZ-N10-34-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140701
Time                 1.13
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                      4
DS                     16
SWH             3846.154 Hz
FIDRES          3.756010 Hz
AQ             0.1331700 sec
RG                189.81
DW               130.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.46272600 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1          16.00000000 W
SFO1          400.1313398 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

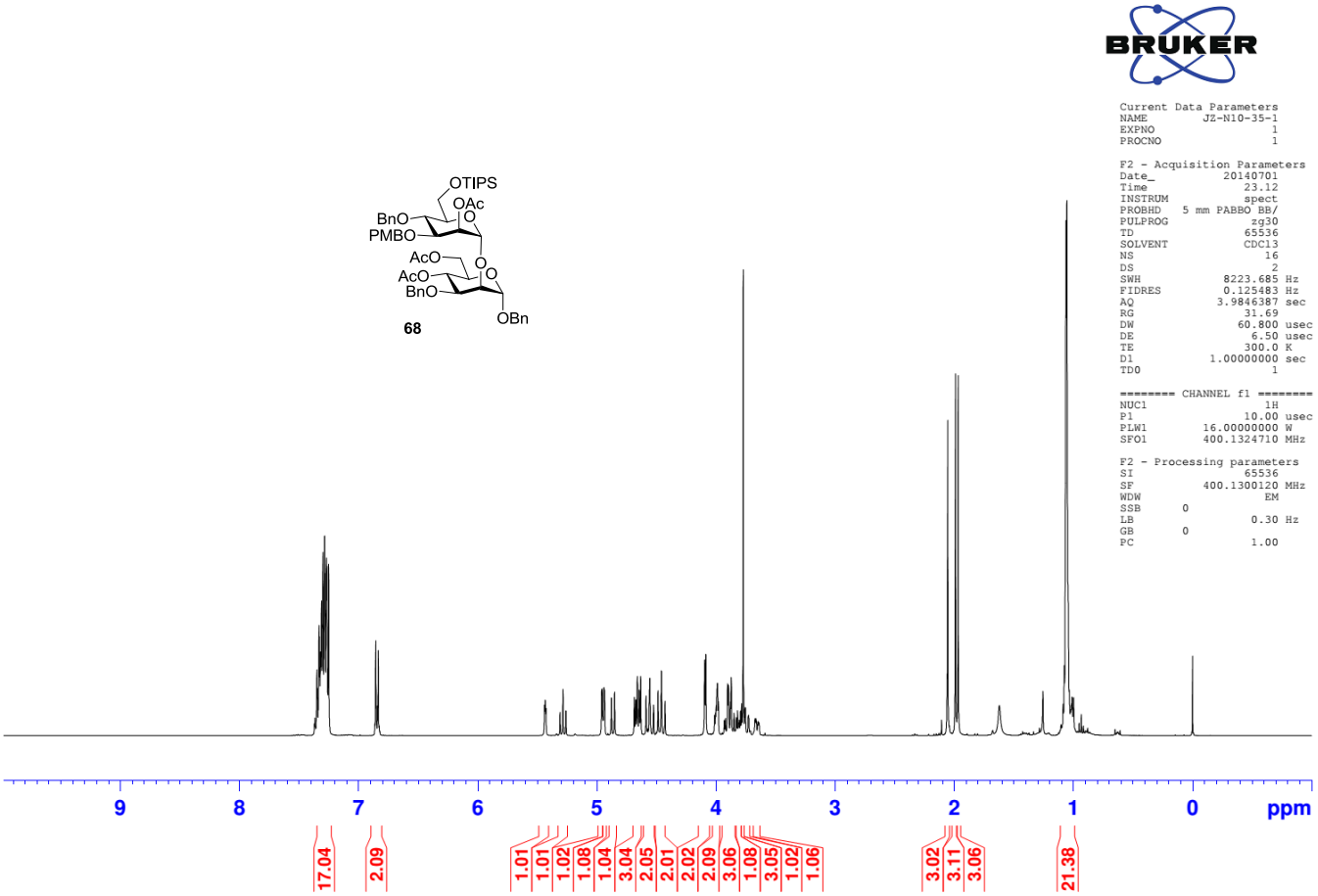
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

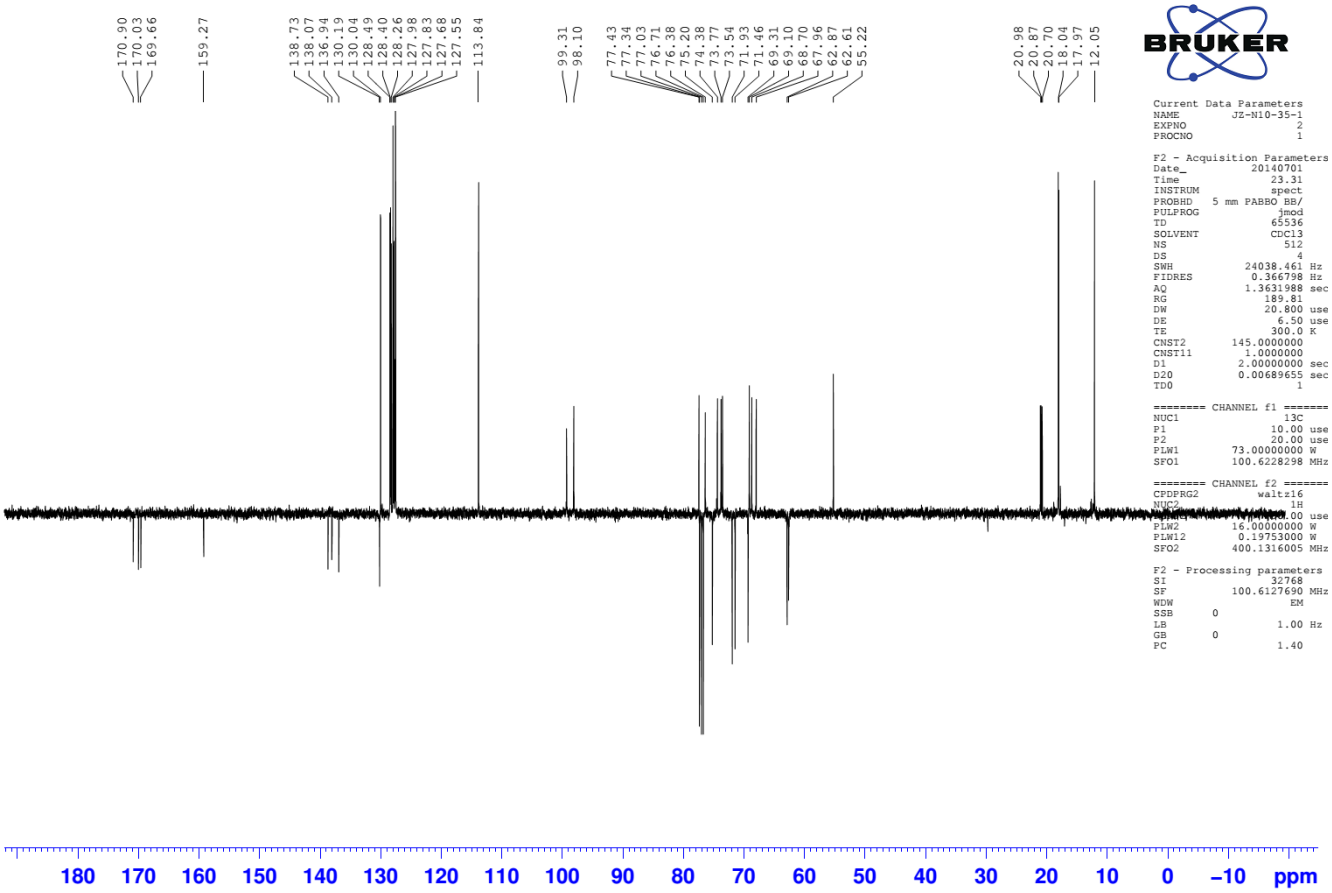
F2 - Processing parameters
SI                     1024
SF            400.1300109 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2        echo-antiecho
SF             100.6127690 MHz
WDW          States-TPPI
SSB                       2
LB        0 Hz
GB        0
```

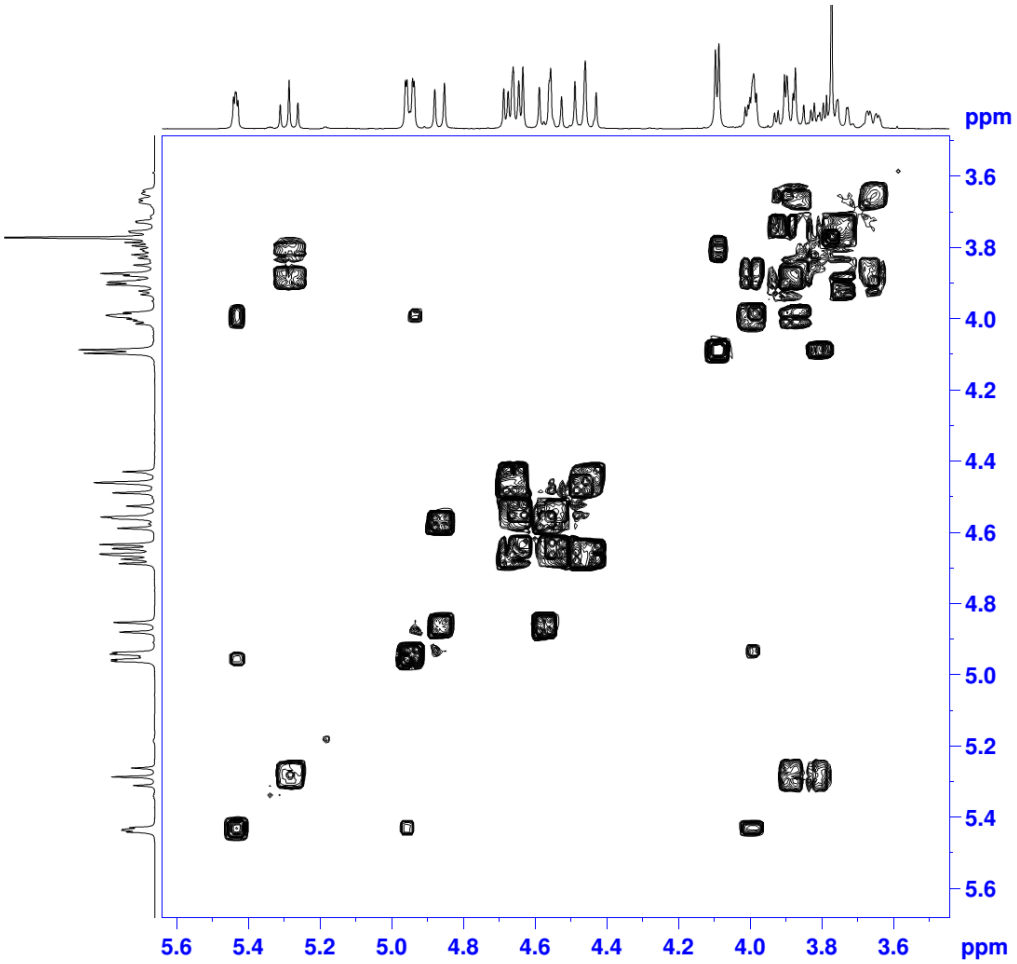
^{1}H NMR spectrum for compound **68**



^{13}C-APT NMR spectrum for compound **68**



COSY spectrum for compound **68**




```
Current Data Parameters
NAME          JZ-N10-35-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_              20140702
Time                   0.01
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                     2048
SOLVENT               CDCl3
NS                      4
DS                      8
SWH              3521.127 Hz
FIDRES           1.719300 Hz
AQ              0.2908660 sec
RG                  19.91
DW                142.000 usec
DE                   6.50 usec
TE                  300.0 K
D0             0.00000300 sec
D1             1.90087700 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00028400 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                   10.00 usec
P1                   10.00 usec
P17                2000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1          400.1314993 MHz

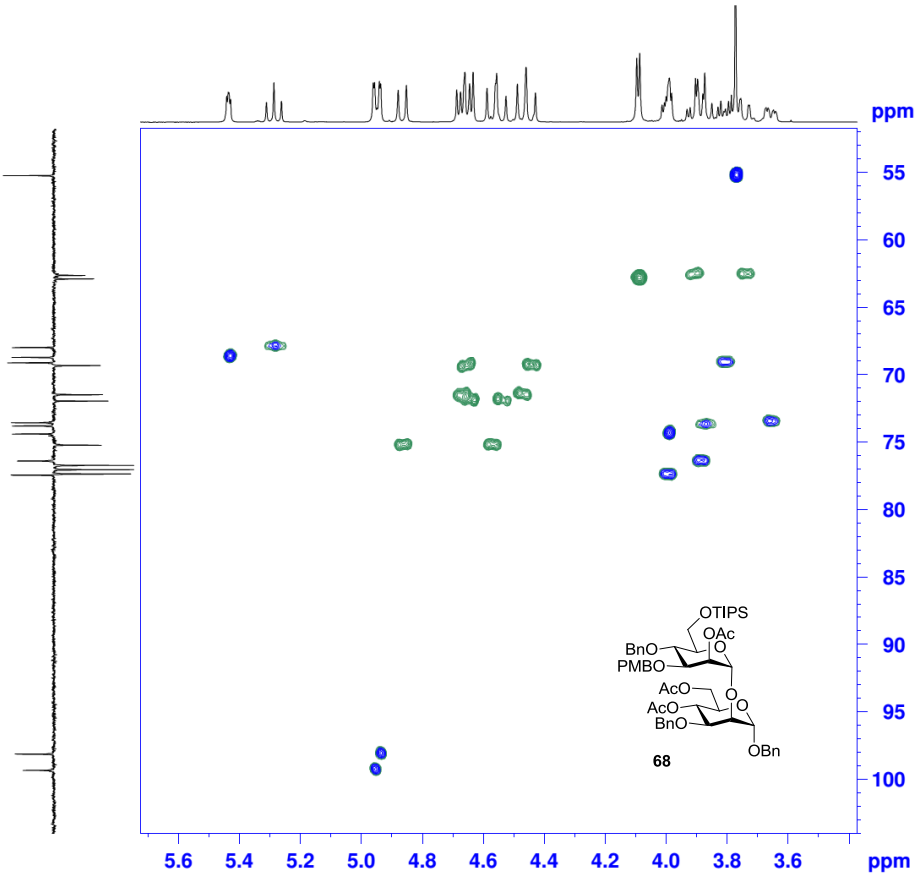
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            400.1315 MHz
FIDRES         27.508802 Hz
SW                  8.800 ppm
FnMODE                 QF

F2 - Processing parameters
SI                     1024
SF            400.1300120 MHz
WDW                   QSINE
SSB        0
LB         0 Hz
GB         0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            400.1300120 MHz
WDW                     SIN
SSB        0
LB         0 Hz
GB         0
```

HSQC spectrum for compound **68**




```
Current Data Parameters
NAME          JZ-N10-35-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_              20140702
Time                   0.21
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                     1024
SOLVENT               CDCl3
NS                      4
DS                     16
SWH              3521.127 Hz
FIDRES           3.438600 Hz
AQ              0.1454580 sec
RG                 189.81
DW                142.000 usec
DE                   6.50 usec
TE                  300.0 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.45043802 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
P2                   20.00 usec
P28                   0.10 usec
PLW1          16.00000000 W
SFO1          400.1314993 MHz

======== CHANNEL f2 ========
CPDPRG2               garp
NUC2                   13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

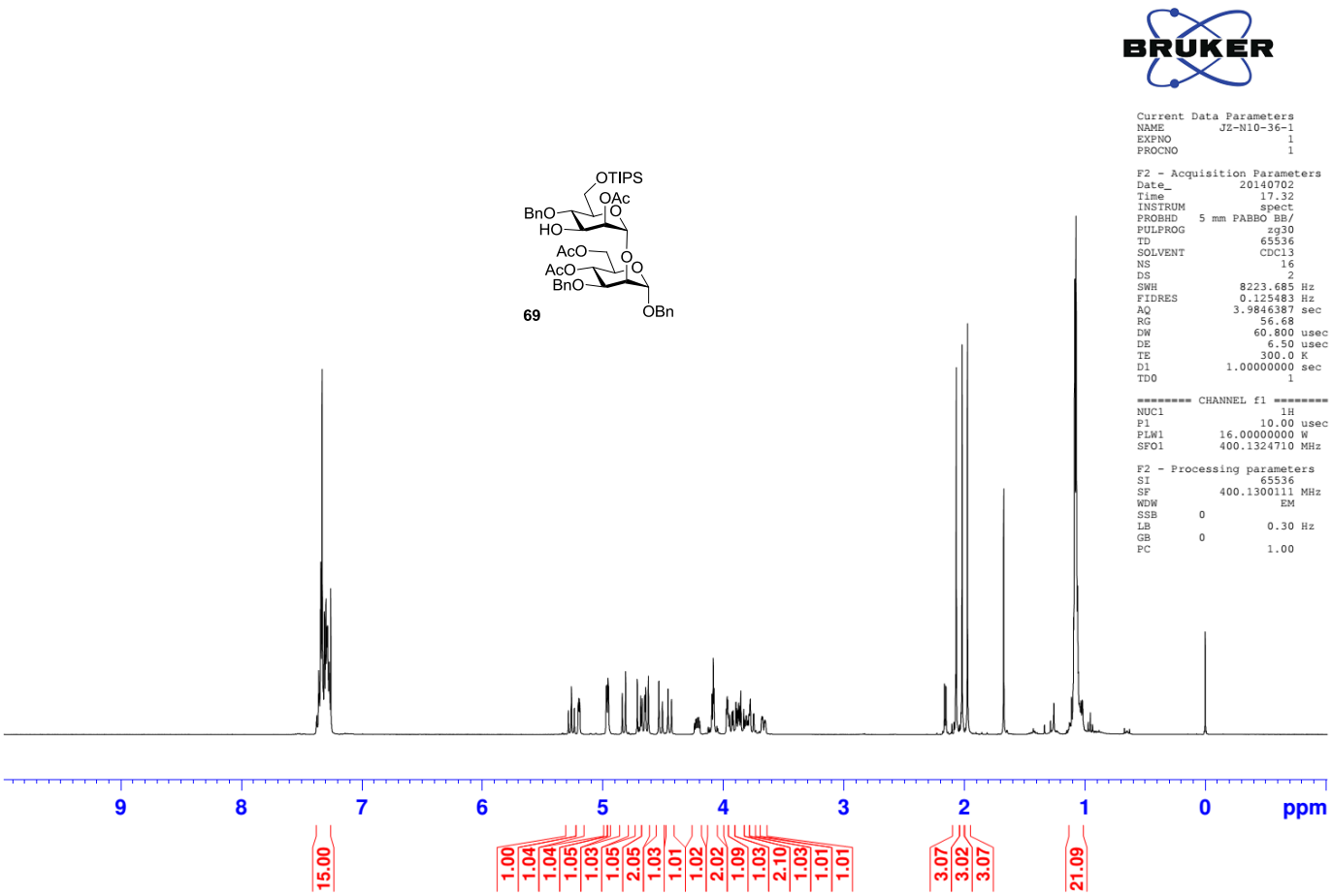
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPNAM2         SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                      256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho

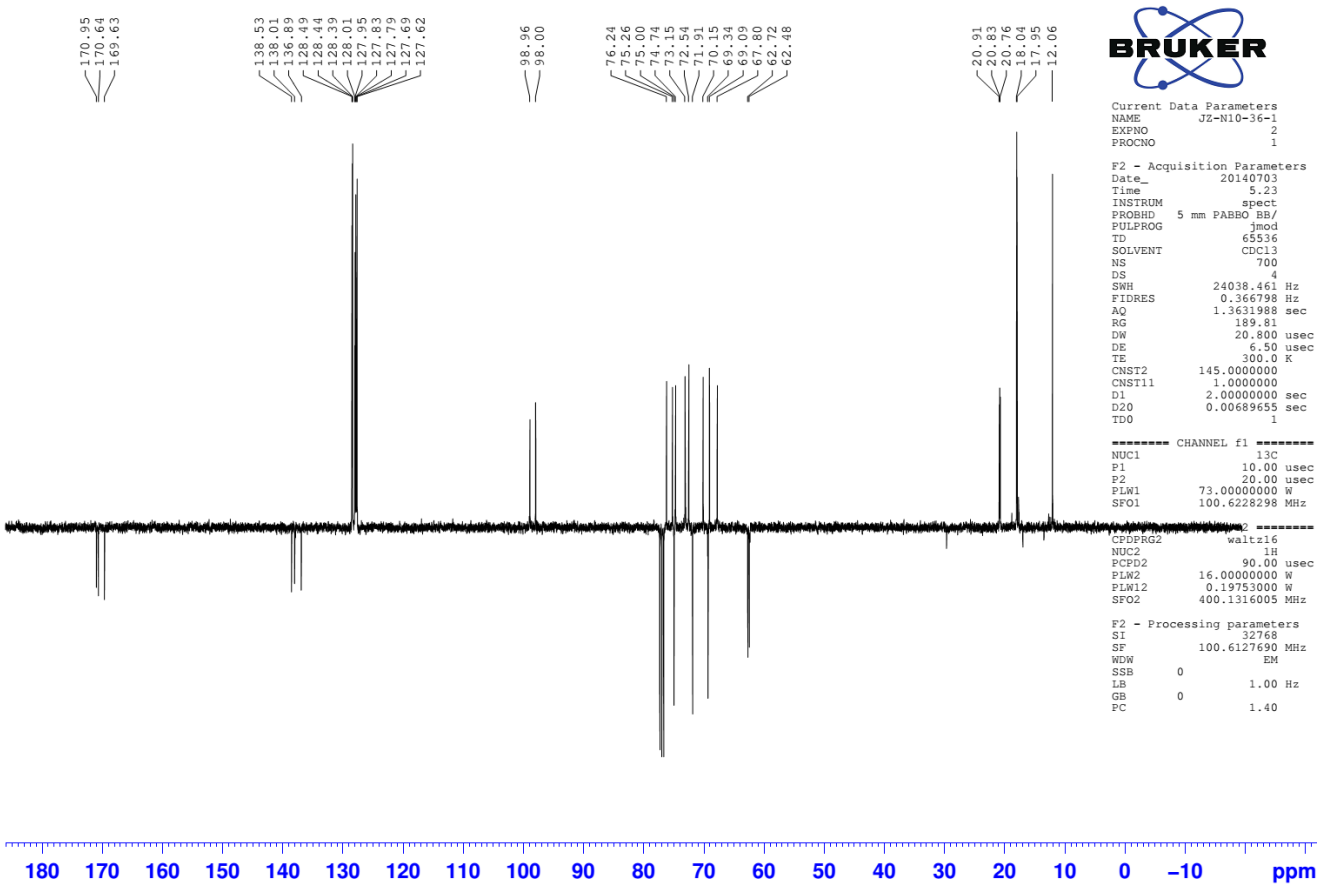
F2 - Processing parameters
SI                     1024
SF            400.1300120 MHz
WDW                   QSINE
SSB                        2
LB         0 Hz
GB         0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2        echo-antiecho
SF             100.6127690 MHz
WDW           States-TPPI
SSB                        2
LB         0 Hz
GB         0
```

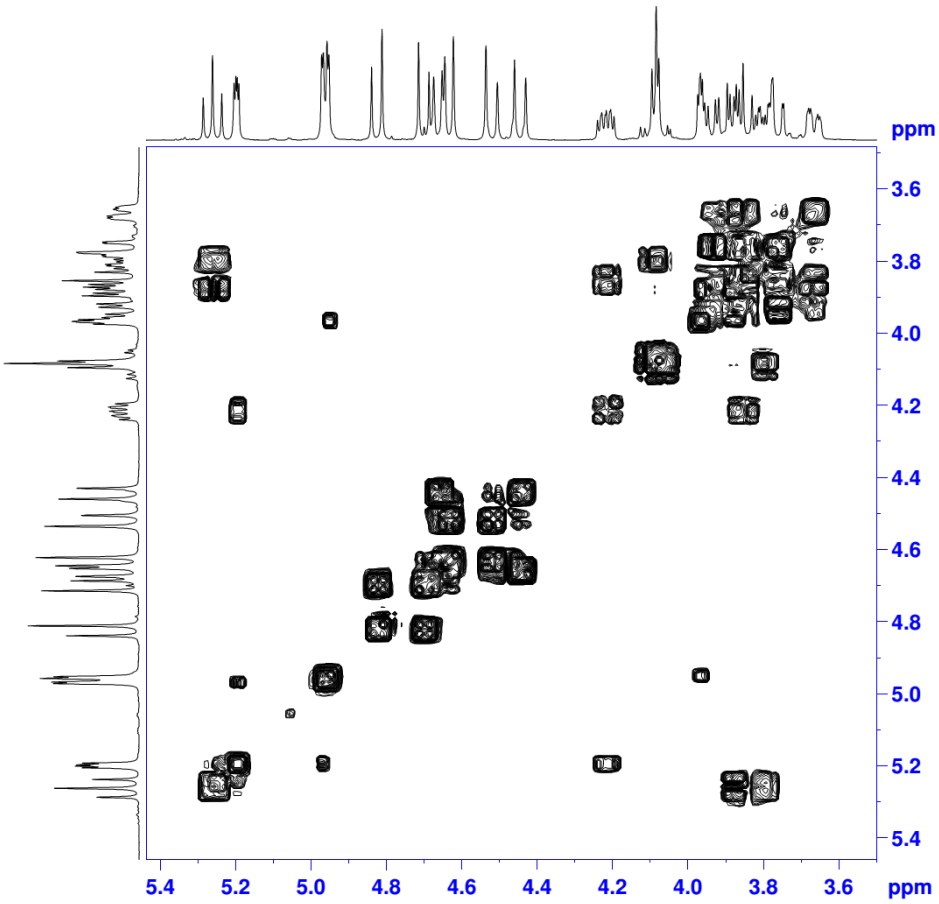
^{1}H NMR spectrum for compound **69**



^{13}C-APT NMR spectrum for compound **69**



COSY spectrum for compound **69**




```
Current Data Parameters
NAME          JZ-N10-36-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140702
Time               17.38
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG      cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             3571.428 Hz
FIDRES          1.743862 Hz
AQ             0.2867700 sec
RG                 19.91
DW               140.000 usec
DE                  6.50 usec
TE                 300.0 K
D0             0.00000300 sec
D1             1.90497303 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00028000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17               2000.00 usec
PLW1         16.00000000 W
PLW10         2.36689997 W
SFO1        400.1314565 MHz

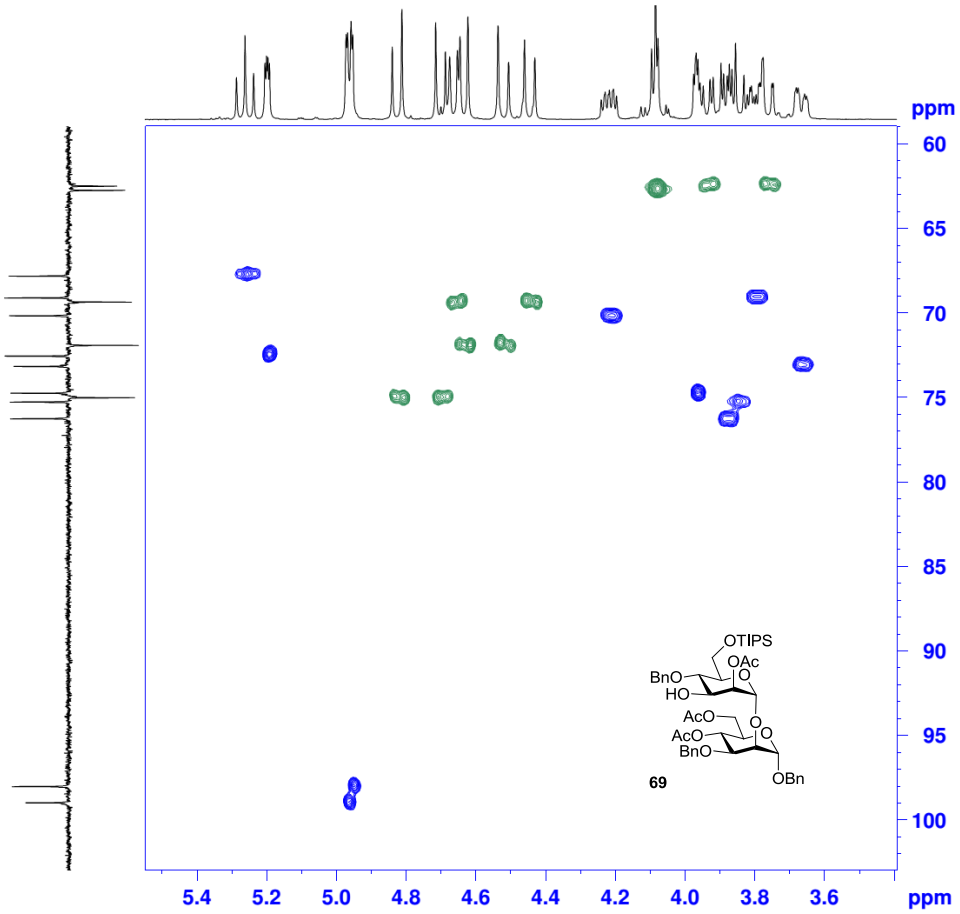
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            400.1315 MHz
FIDRES         27.901785 Hz
SW                  8.926 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF           400.1300111 MHz
WDW                  QSINE
SSB        0
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF           400.1300111 MHz
WDW                    SIN
SSB        0
LB         0 Hz
GB         0
```

HSQC spectrum for compound **69**




```
Current Data Parameters
NAME          JZ-N10-36-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140702
Time               18.47
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG     hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                      4
DS                     16
SWH             3571.428 Hz
FIDRES          3.487723 Hz
AQ             0.1434100 sec
RG                 189.81
DW               140.000 usec
DE                  6.50 usec
TE                 300.0 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.45248604 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1         16.00000000 W
SFO1        400.1314565 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                   13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2        100.6202727 MHz

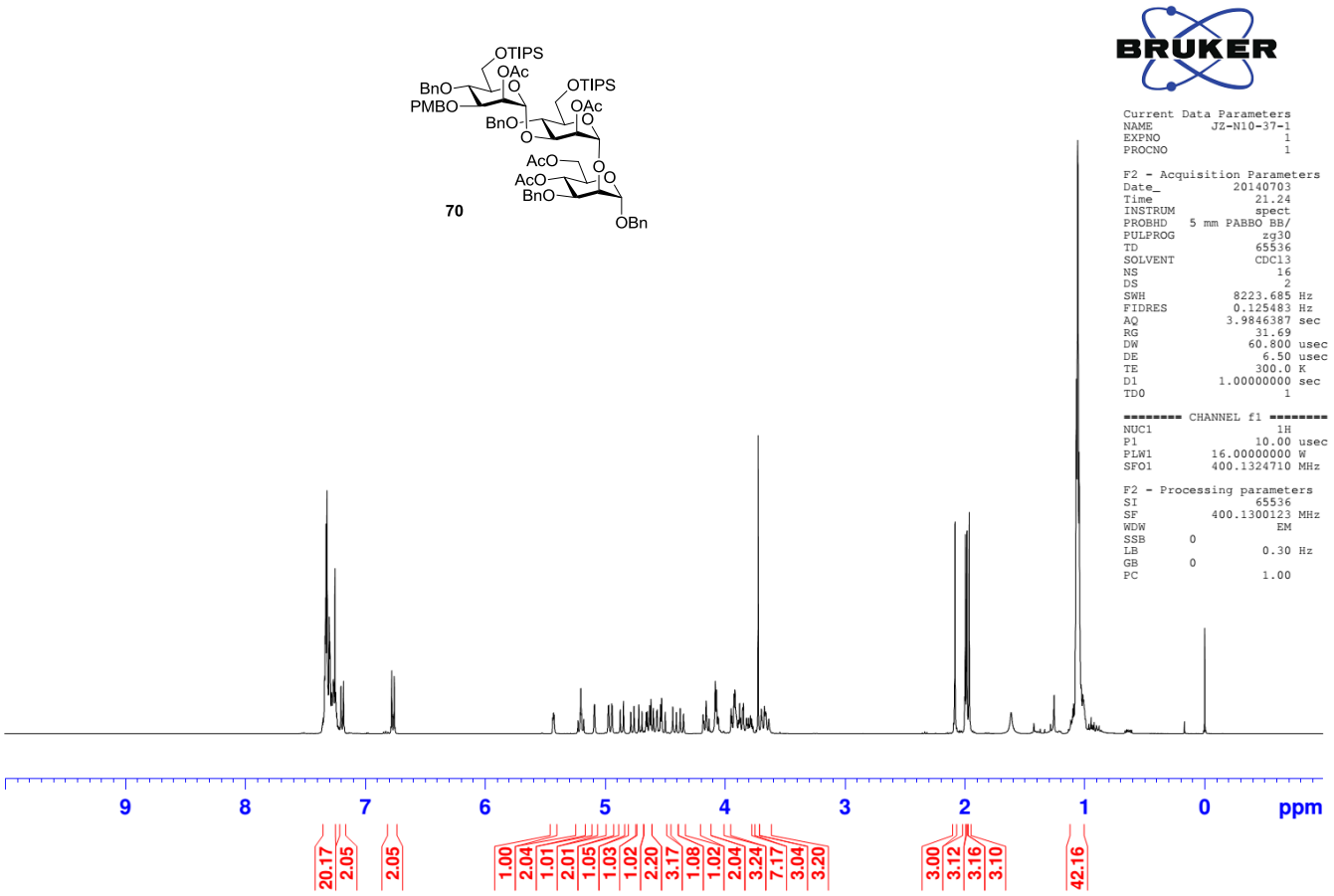
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

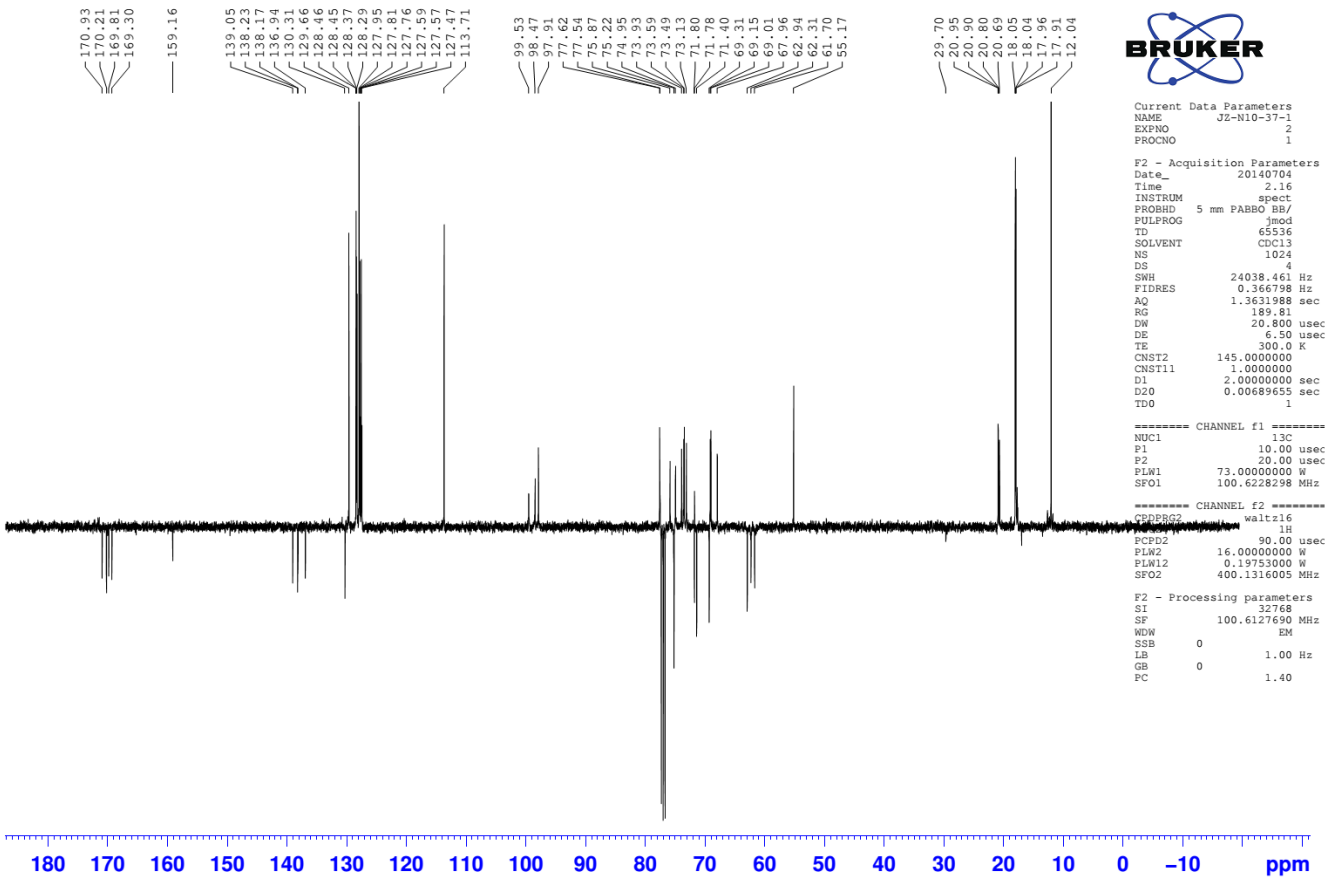
F2 - Processing parameters
SI                    1024
SF           400.1300111 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF            100.6127690 MHz
WDW          States-TPPI
SSB                      2
LB         0 Hz
GB         0
```

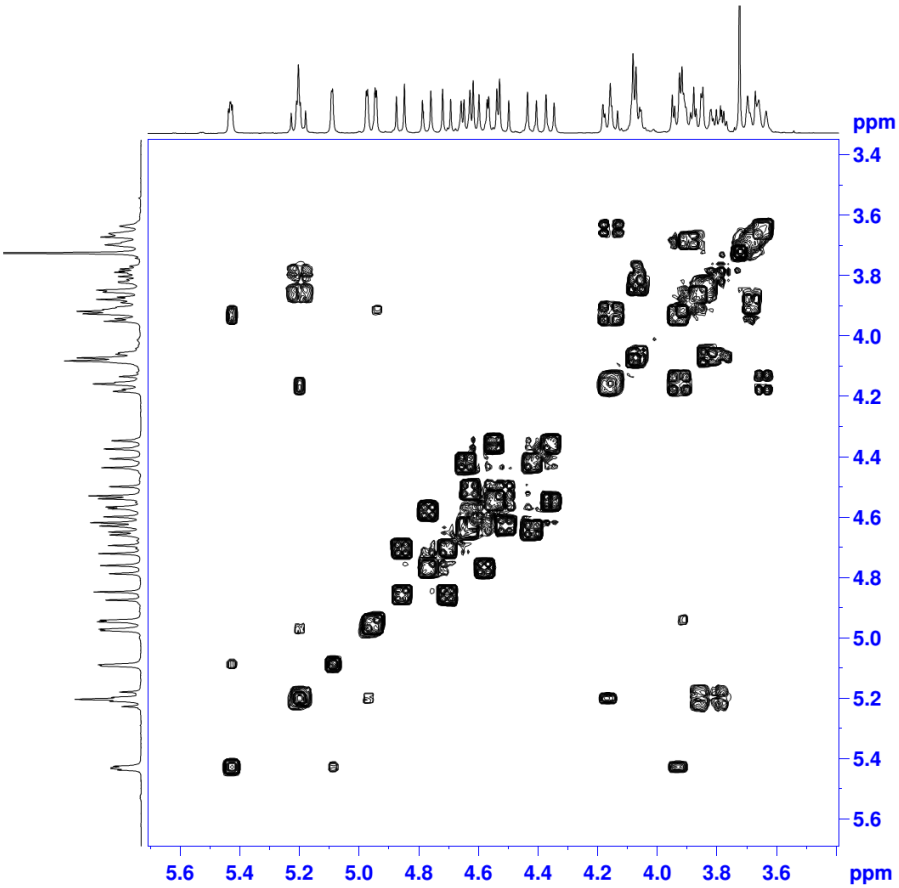
^{1}H NMR spectrum for compound **70**



^{13}C-APT NMR spectrum for compound **70**



COSY spectrum for compound **70**




```
Current Data Parameters
NAME          JZ-N10-37-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140703
Time               21.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG     cosygpppqf
TD                 2048
SOLVENT           CDCl3
NS                     4
DS                     8
SWH            3649.635 Hz
FIDRES         1.782048 Hz
AQ           0.2806260 sec
RG                18.47
DW             137.000 usec
DE                6.50 usec
TE               300.0 K
D0           0.00000300 sec
D1           1.91111696 sec
D11          0.03000000 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00027400 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                 10.00 usec
P1                 10.00 usec
P17              2000.00 usec
PLW1        16.00000000 W
PLW10        2.36689997 W
SFO1        400.1314220 MHz

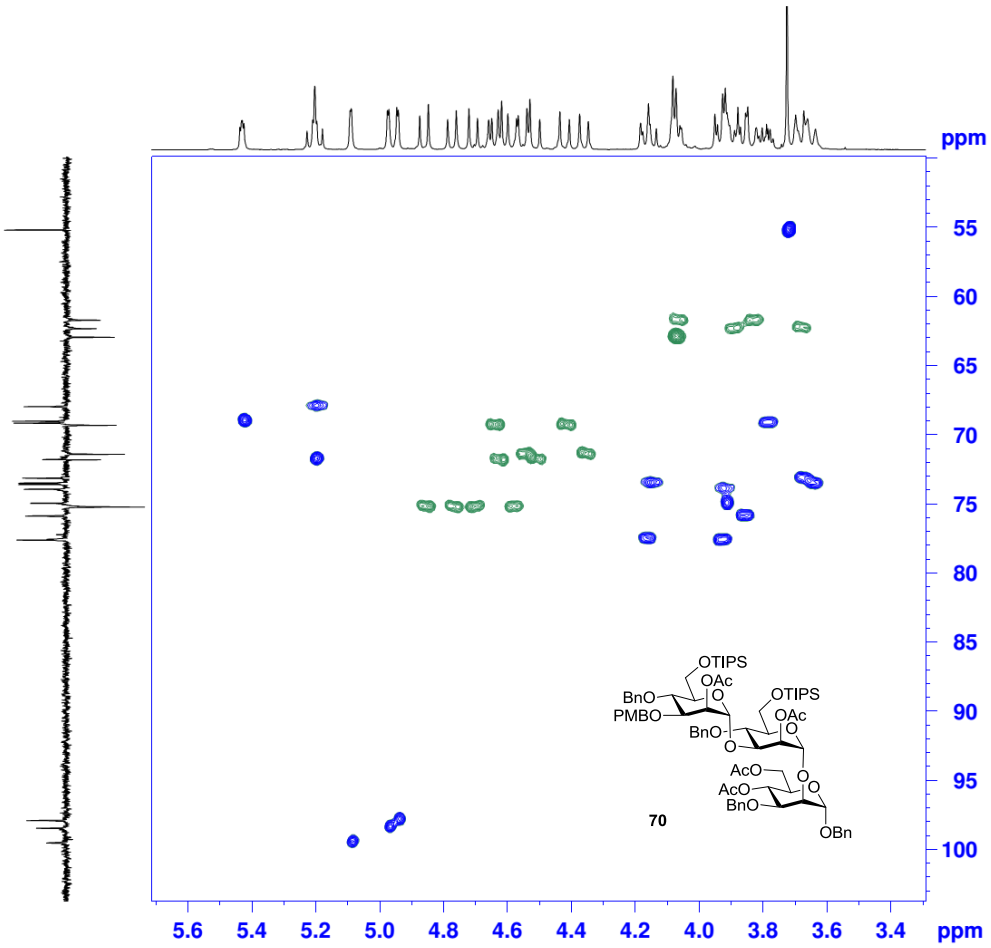
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1            400.1314 MHz
FIDRES         28.512774 Hz
SW                 9.121 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF          400.1300123 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF          400.1300123 MHz
WDW                  SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **70**




```
Current Data Parameters
NAME          JZ-N10-37-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140704
Time               0.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                 1024
SOLVENT           CDCl3
NS                     8
DS                    16
SWH            3649.635 Hz
FIDRES         3.564097 Hz
AQ           0.1403380 sec
RG               189.81
DW             137.000 usec
DE                6.50 usec
TE               300.0 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.45555794 sec
D4           0.00172414 sec
D11          0.03000000 sec
D13          0.00000400 sec
D16          0.00020000 sec
D21          0.00345000 sec
IN0          0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
P2                 20.00 usec
P28                 0.10 usec
PLW1        16.00000000 W
SFO1        400.1314220 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              80.00 usec
PLW2        73.00000000 W
PLW12        1.14059997 W
SFO2        100.6202727 MHz

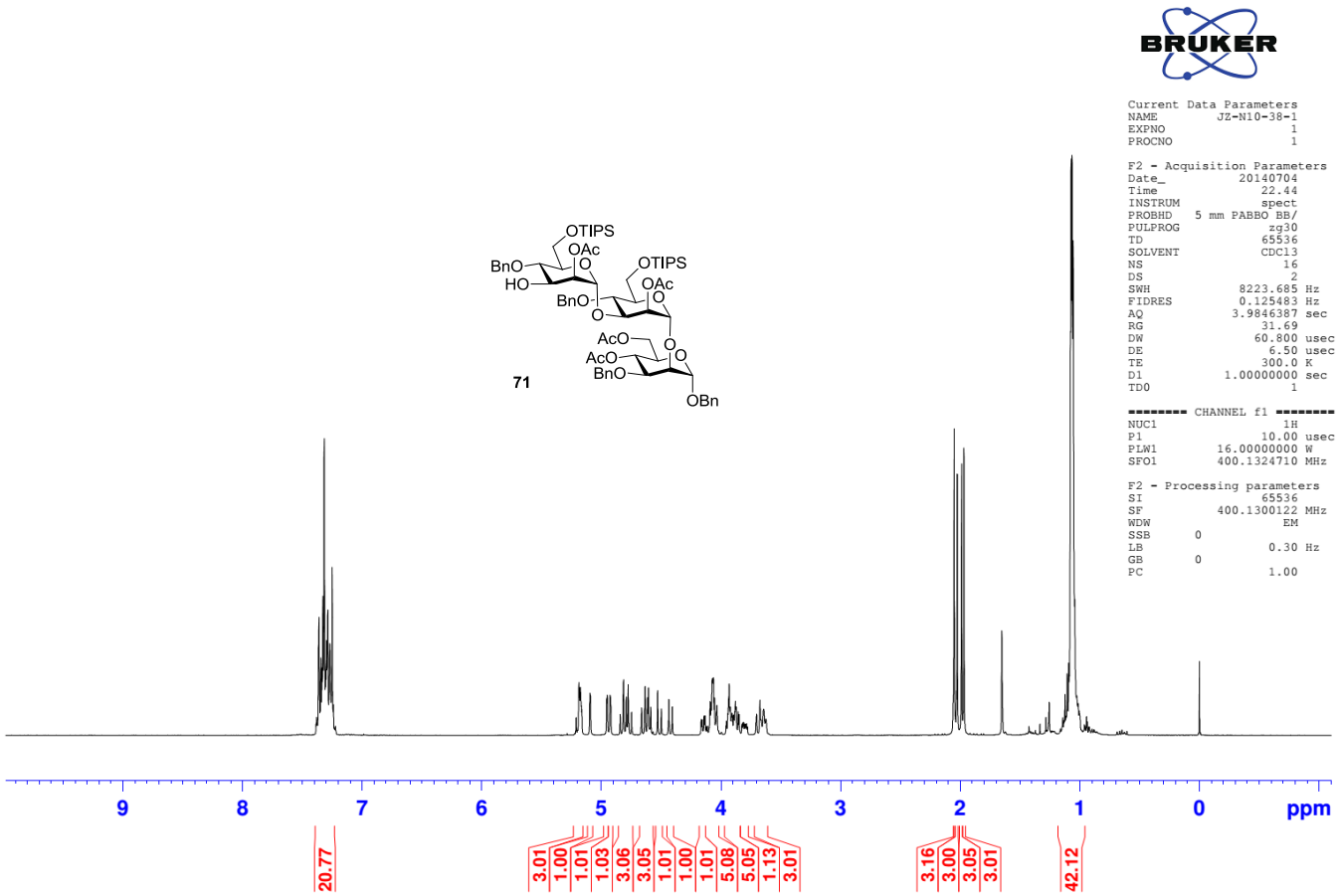
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW               165.639 ppm
FnMODE     Echo-Antiecho

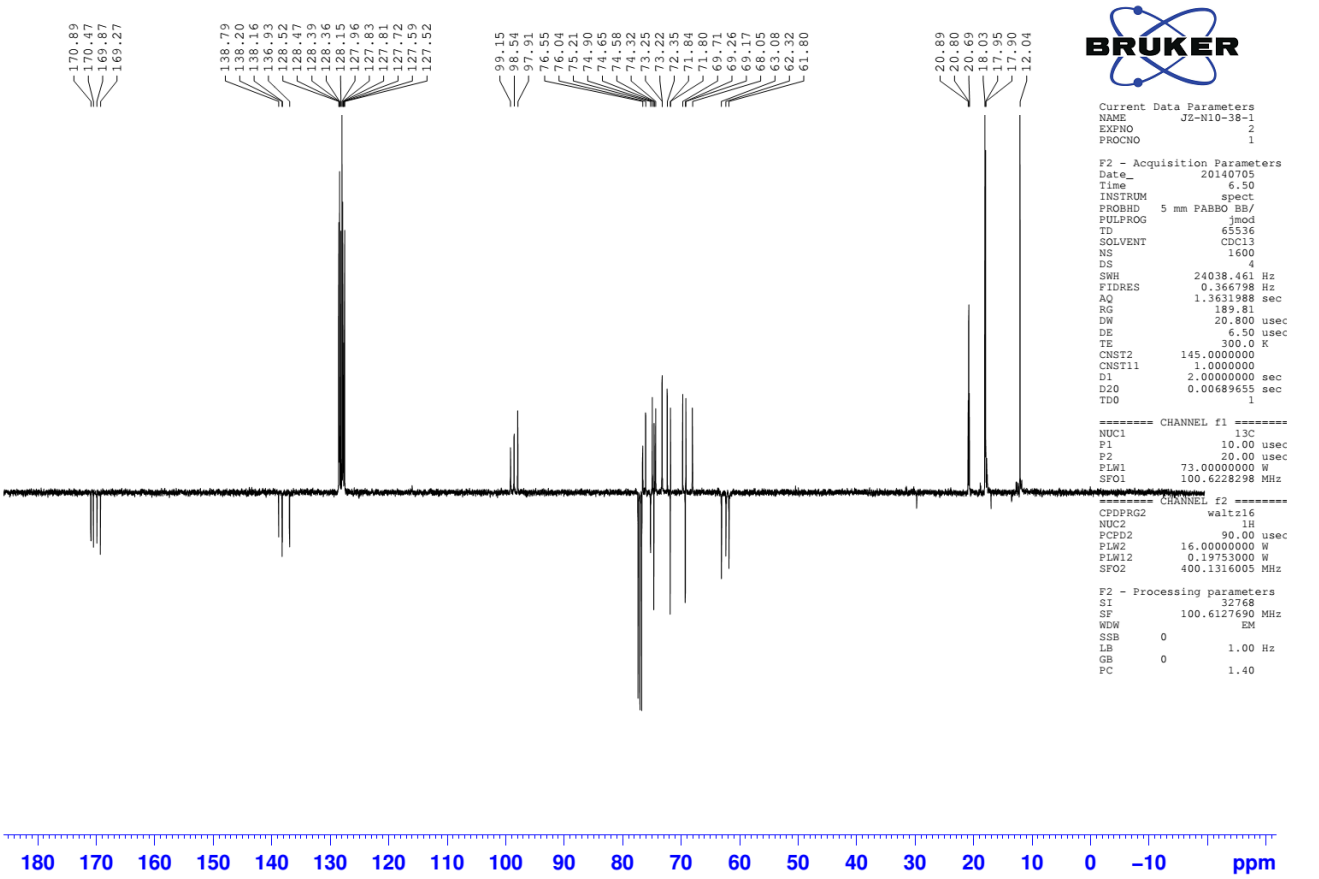
F2 - Processing parameters
SI                   1024
SF          400.1300123 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW                  SINE
SSB                     2
LB        0 Hz
GB        0
```

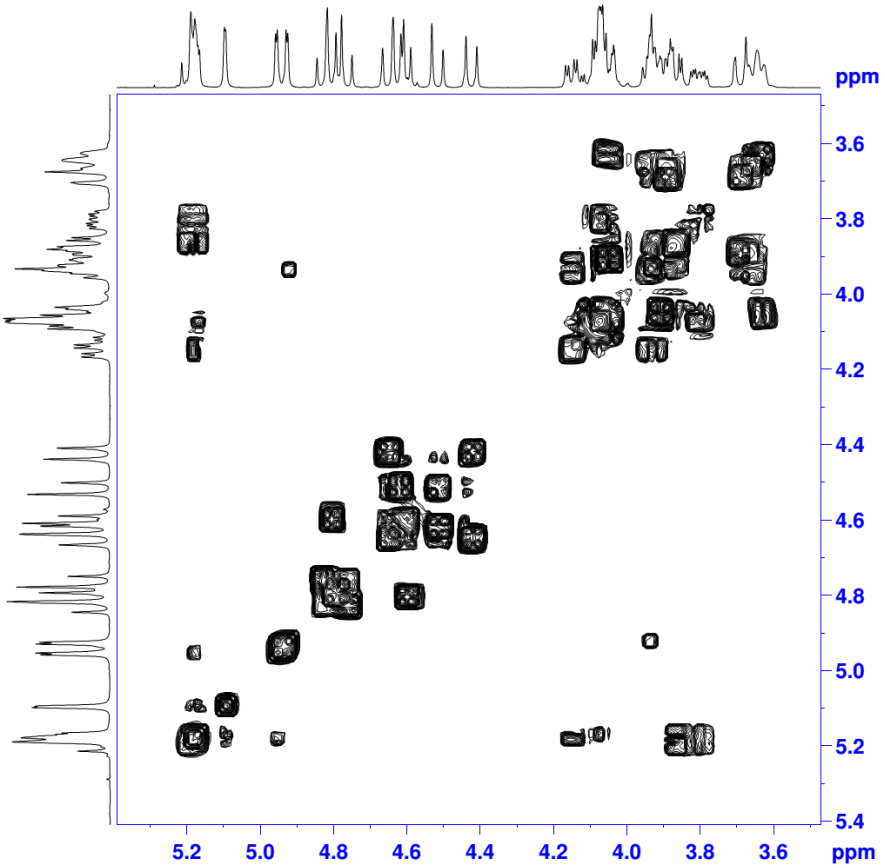
^{1}H NMR spectrum for compound **71**



^{13}C-APT NMR spectrum for compound **71**



COSY spectrum for compound **71**




```
Current Data Parameters
NAME          JZ-N10-38-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140704
Time              22.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             3521.127 Hz
FIDRES          1.719300 Hz
AQ             0.2908660 sec
RG                 18.47
DW              142.000 usec
DE                 6.50 usec
TE                300.0 K
D0             0.00000300 sec
D1             1.90087700 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00028400 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                  10.00 usec
P1                  10.00 usec
P17               20000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1          400.1315028 MHz

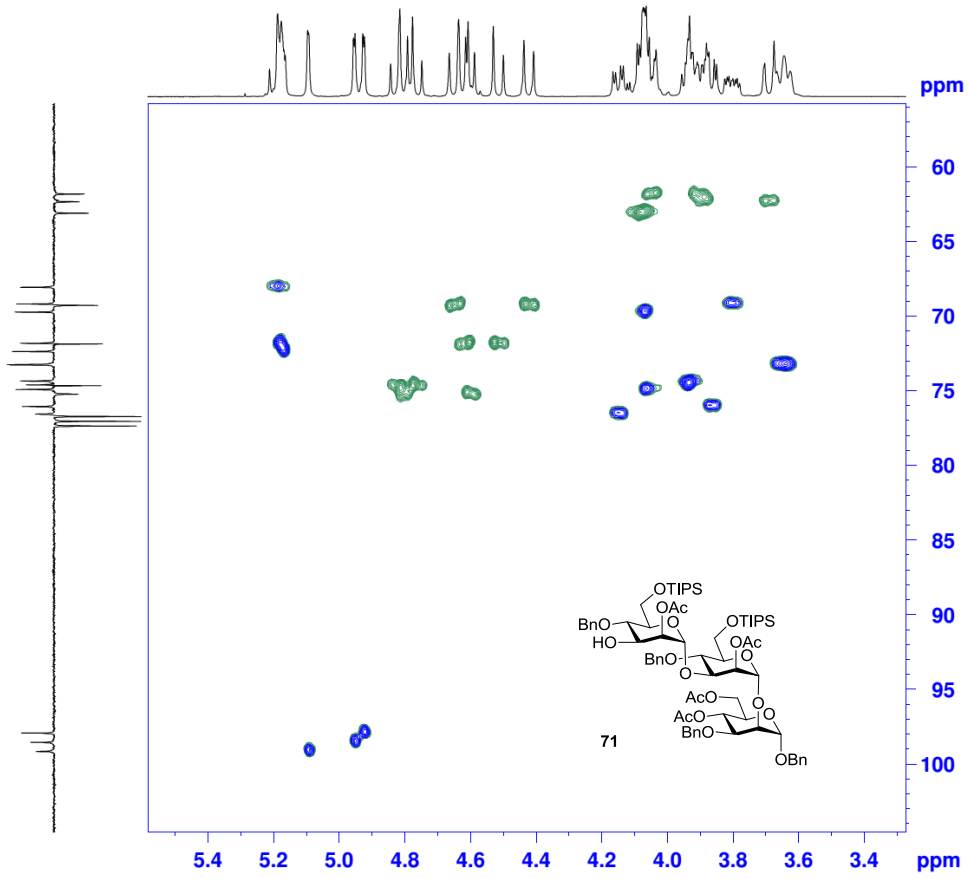
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            400.1315 MHz
FIDRES         27.508802 Hz
SW                  8.800 ppm
FnMODE                 QF

F2 - Processing parameters
SI                     1024
SF            400.1300122 MHz
WDW                   QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            400.1300122 MHz
WDW                     SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **71**




```
Current Data Parameters
NAME          JZ-N10-38-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140704
Time              23.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                      8
DS                     16
SWH             3521.127 Hz
FIDRES          3.438600 Hz
AQ             0.1454580 sec
RG                 189.81
DW              142.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.45043802 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1          16.00000000 W
SFO1          400.1315028 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                   13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

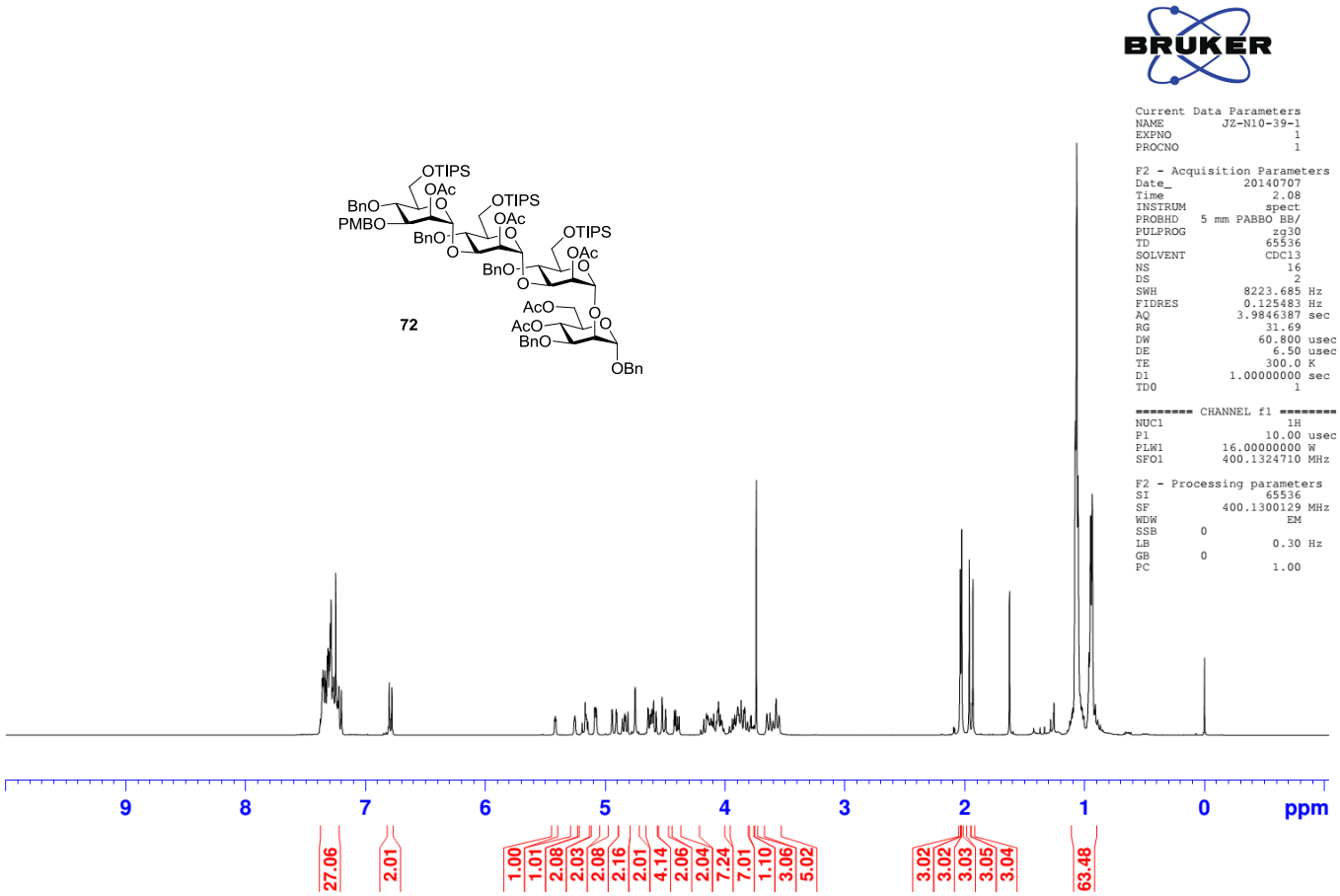
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPNAM2         SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

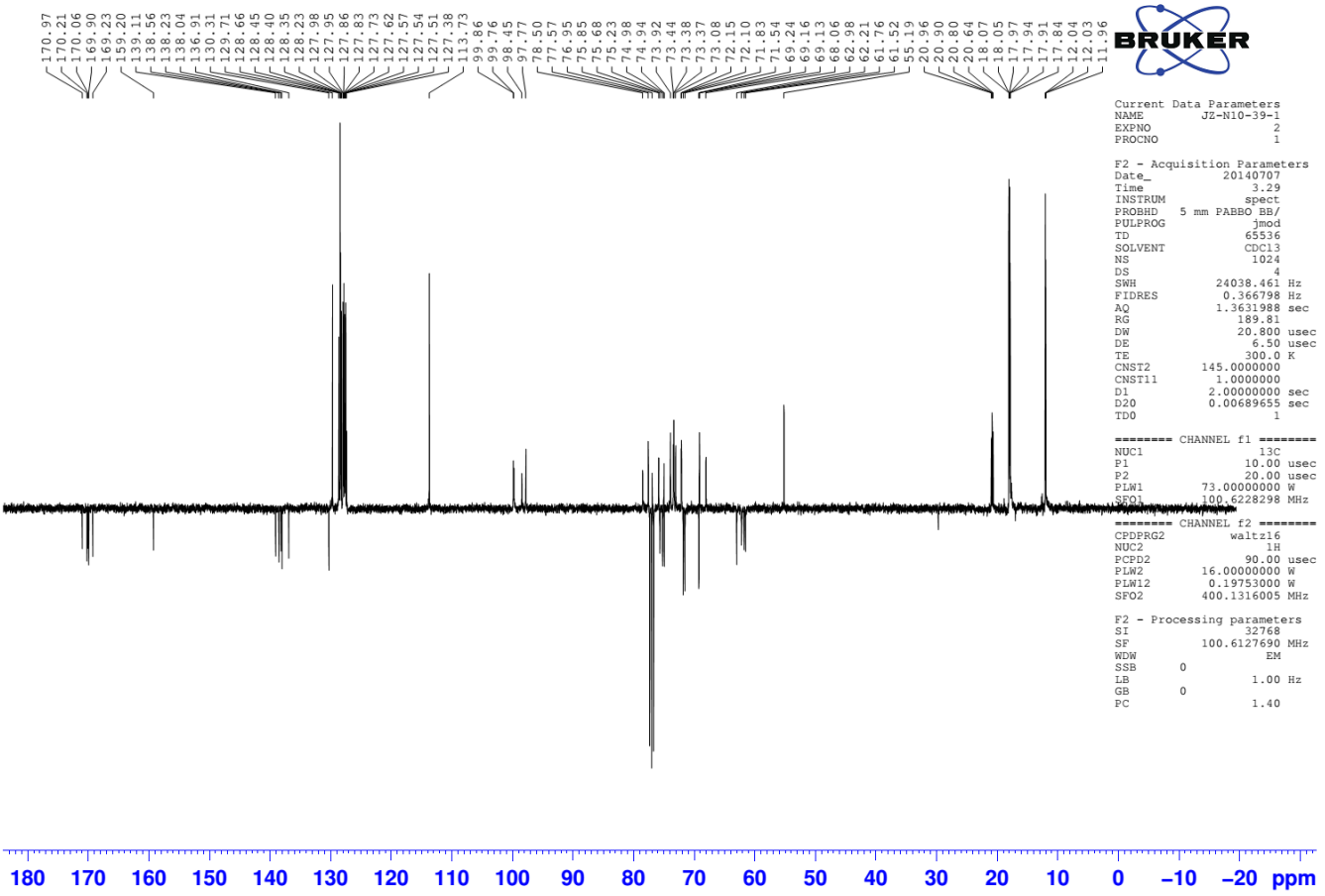
F2 - Processing parameters
SI                     1024
SF            400.1300122 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF            100.6127690 MHz
WDW           States-TPPI
SSB                       2
LB        0 Hz
GB        0
```

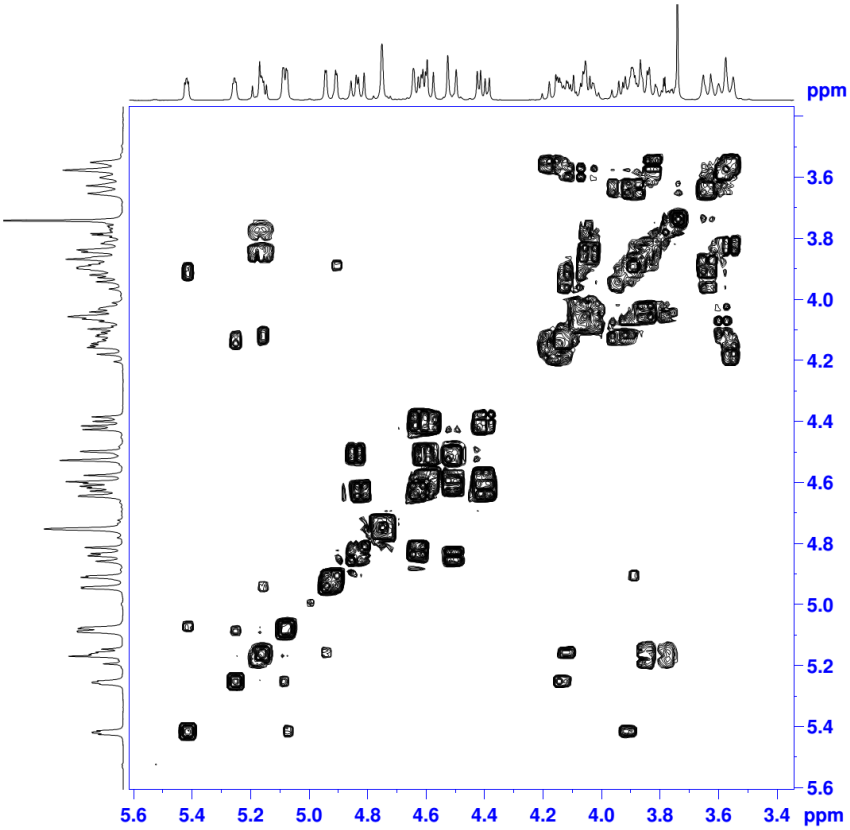
^{1}H NMR spectrum for compound **72**



^{13}C-APT NMR spectrum for compound **72**



COSY spectrum for compound **72**




```
Current Data Parameters
NAME          JZ-N10-39-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_              20140707
Time                   2.10
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG        cosygpppqf
TD                     2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             3546.099 Hz
FIDRES          1.731494 Hz
AQ             0.2888180 sec
RG                  18.47
DW                141.000 usec
DE                   6.50 usec
TE                  300.0 K
D0             0.00000300 sec
D1             1.90292501 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00028200 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                   10.00 usec
P1                   10.00 usec
P17                2000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1          400.1315558 MHz

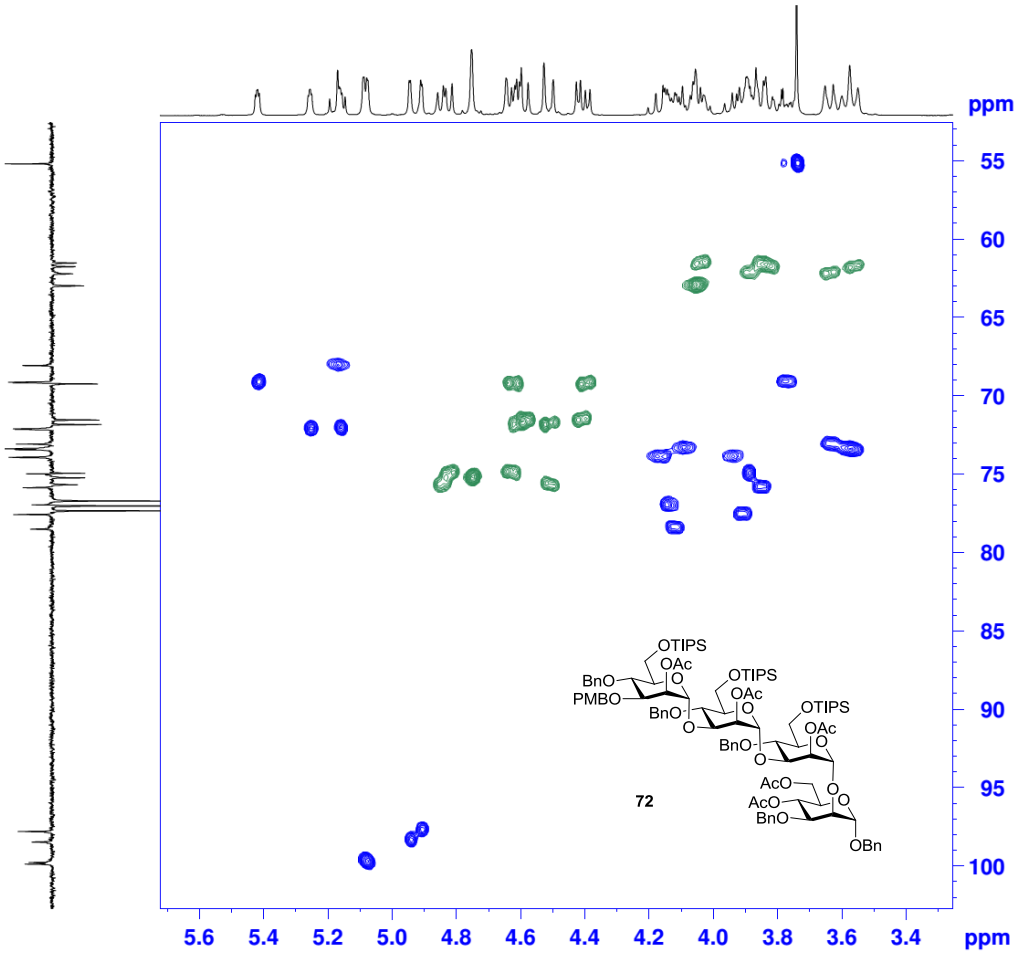
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            400.1316 MHz
FIDRES          27.703901 Hz
SW                  8.862 ppm
FnMODE                 QF

F2 - Processing parameters
SI                     1024
SF            400.1300129 MHz
WDW                   QSINE
SSB        0
LB         0 Hz
GB         0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            400.1300129 MHz
WDW                     SIN
SSB        0
LB         0 Hz
GB         0
```

HSQC spectrum for compound **72**




```
Current Data Parameters
NAME          JZ-N10-39-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_              20140707
Time                   3.30
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG        hsqcedetgp
TD                     1024
SOLVENT             CDCl3
NS                      8
DS                     16
SWH             3546.099 Hz
FIDRES          3.462988 Hz
AQ             0.1444340 sec
RG                  189.81
DW                141.000 usec
DE                   6.50 usec
TE                  300.0 K
CNST2          145.0000000
D0             0.00000300 sec
D1             1.45146203 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
P2                   20.00 usec
P28                   0.10 usec
PLW1          16.00000000 W
SFO1          400.1315558 MHz

======== CHANNEL f2 ========
CPDPRG2               garp
NUC2                   13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

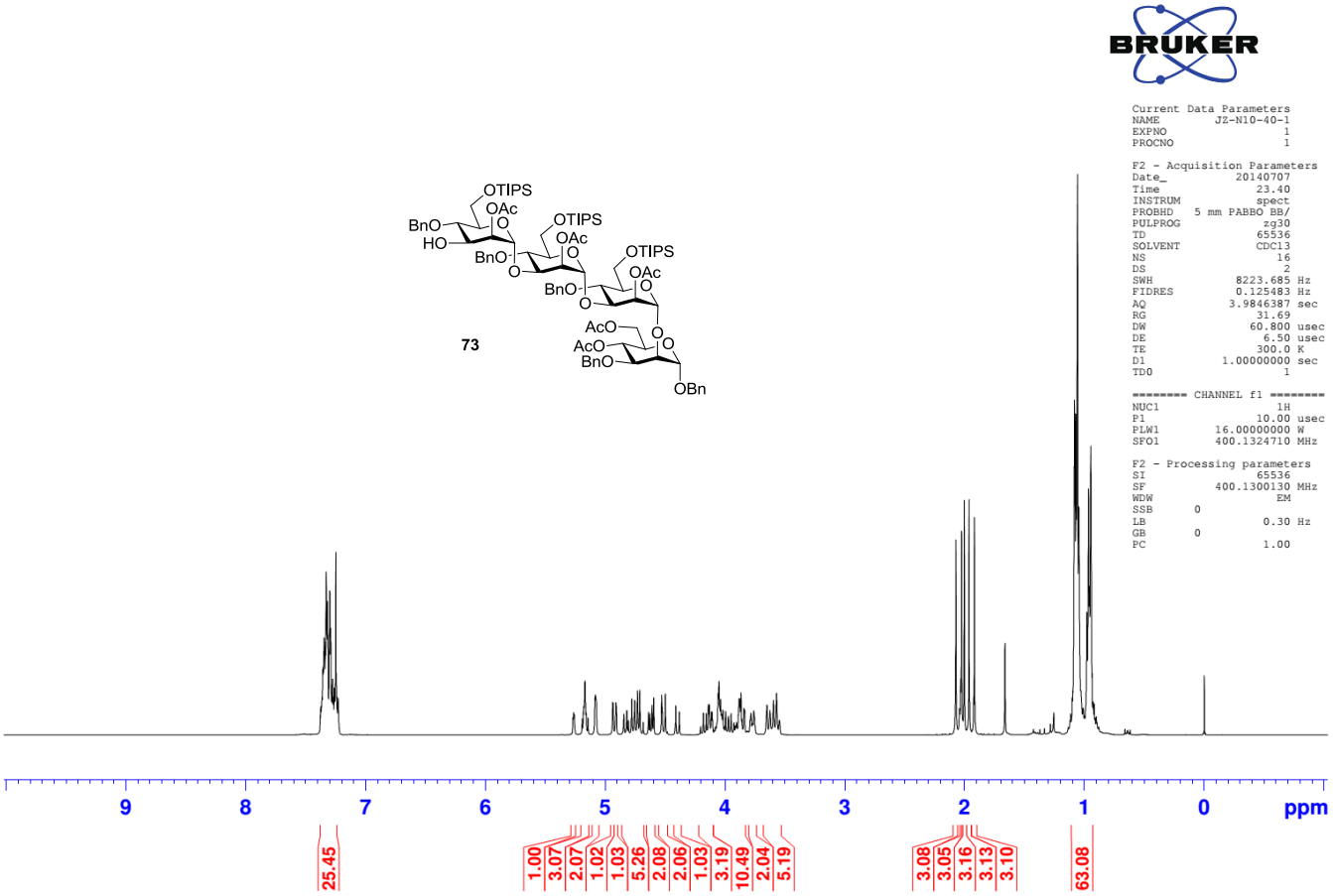
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPNAM2         SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                 165.639 ppm
FnMODE      Echo-Antiecho

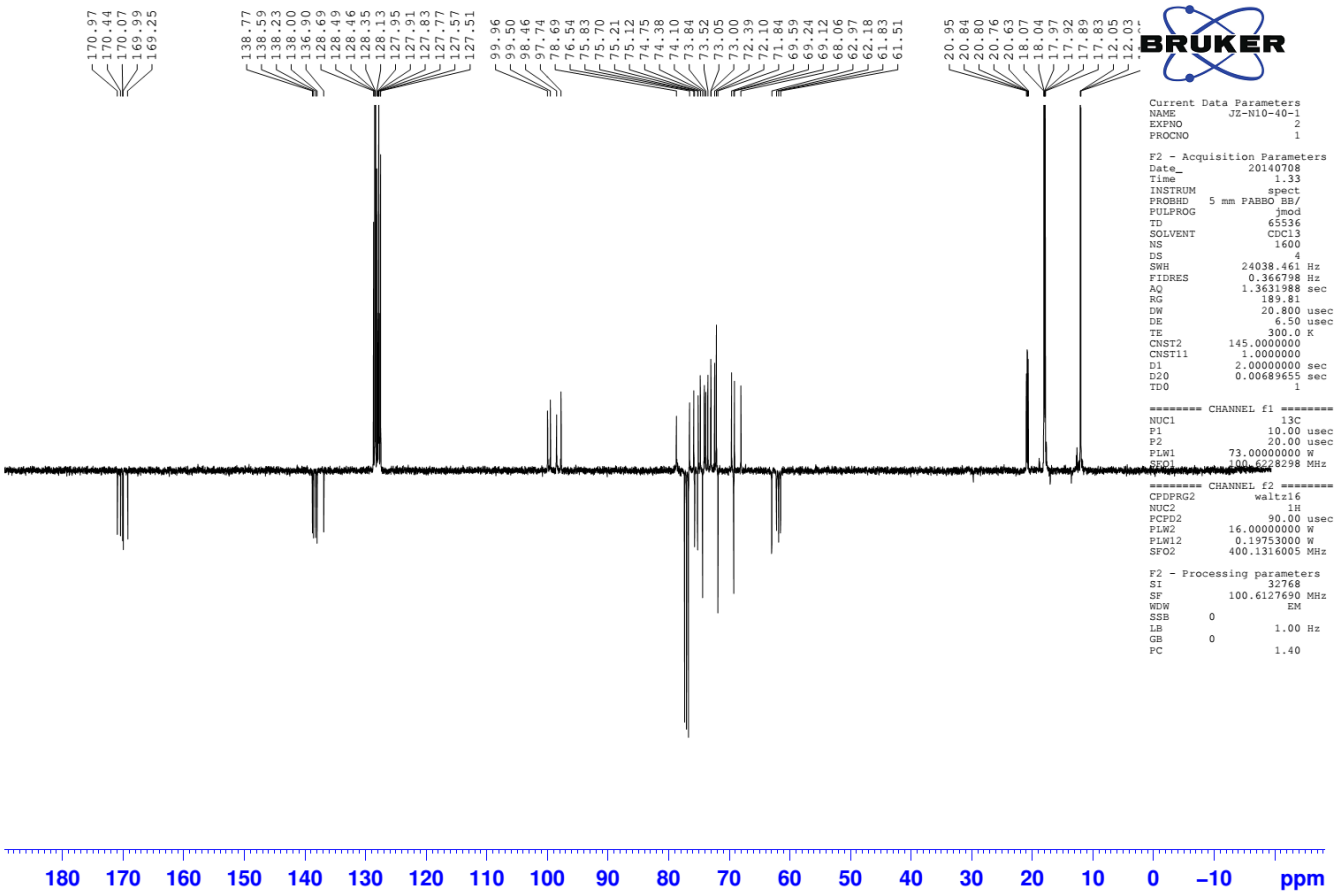
F2 - Processing parameters
SI                     1024
SF            400.1300129 MHz
WDW                   QSINE
SSB                        2
LB         0 Hz
GB         0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2          echo-antiecho
SF            100.6127690 MHz
WDW           States-TPPI
SSB                        2
LB         0 Hz
GB         0
```

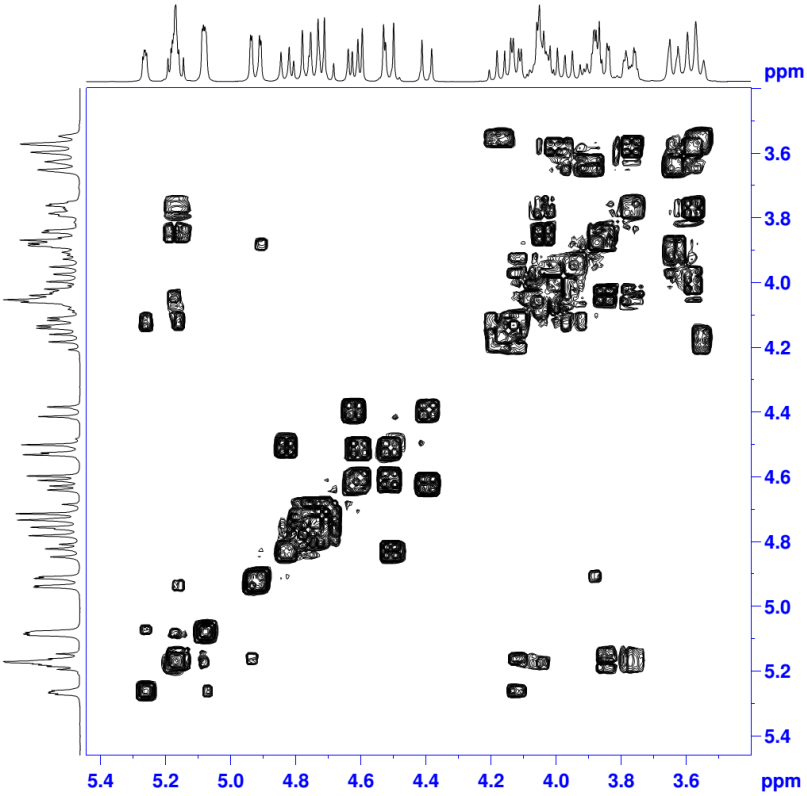
^{1}H NMR spectrum for compound **73**



^{13}C-APT NMR spectrum for compound **73**



COSY spectrum for compound **73**




```
Current Data Parameters
NAME          JZ-N10-40-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140707
Time                23.42
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH            3448.276 Hz
FIDRES         1.683728 Hz
AQ           0.2970100 sec
RG               15.91
DW             145.000 usec
DE               6.50 usec
TE              300.0 K
D0           0.00000300 sec
D1           1.89473295 sec
D11          0.03000000 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00029000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17                2000.00 usec
PLW1         16.000000000 W
PLW10         2.36689997 W
SFO1         400.1316266 MHz

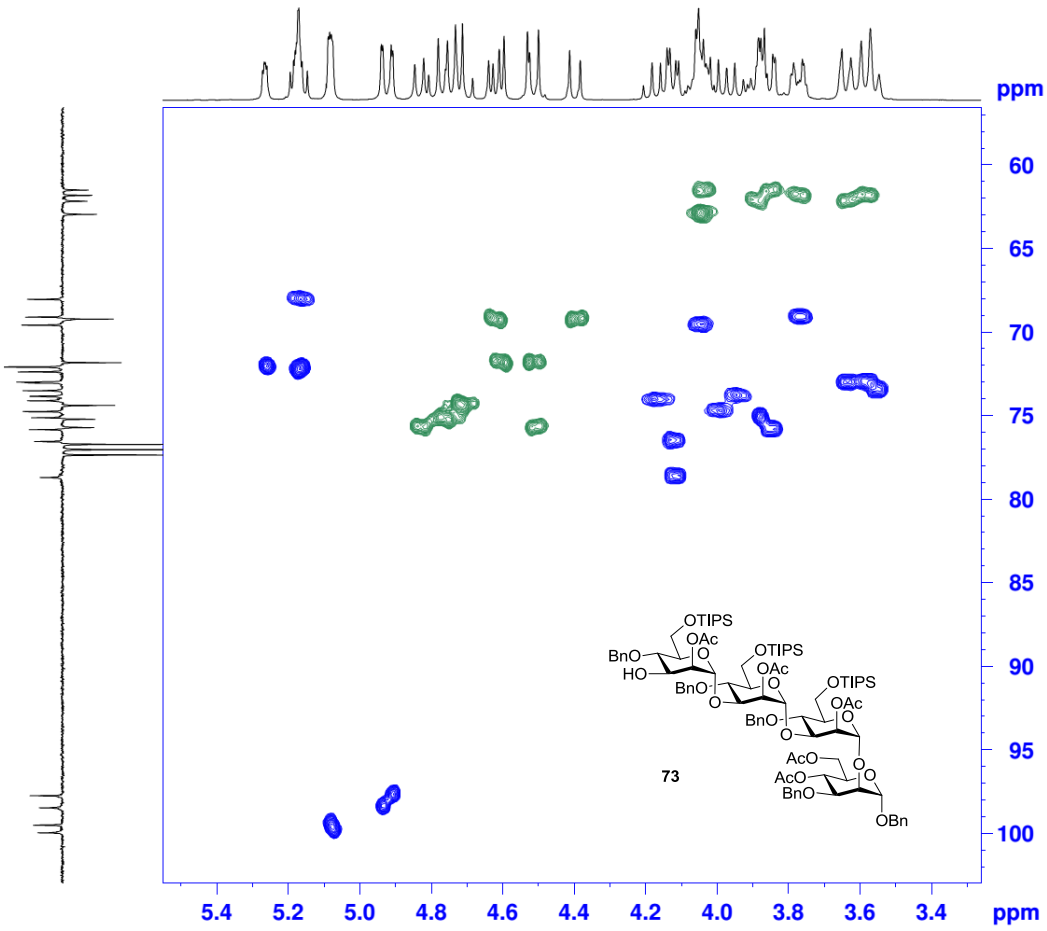
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPZ1                10.00 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            400.1316 MHz
FIDRES          26.939655 Hz
SW                  8.618 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF            400.1300130 MHz
WDW                   QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            400.1300130 MHz
WDW                    SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **73**




```
Current Data Parameters
NAME          JZ-N10-40-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140708
Time                 1.34
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                     13
DS                     16
SWH            3448.276 Hz
FIDRES         3.367457 Hz
AQ           0.1485300 sec
RG               189.81
DW             145.000 usec
DE               6.50 usec
TE              300.0 K
CNST2        145.00000000
D0           0.00000300 sec
D1           1.44736600 sec
D4           0.00172414 sec
D11          0.03000000 sec
D13          0.00000400 sec
D16          0.00020000 sec
D21          0.00345000 sec
IN0          0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1         16.00000000 W
SFO1         400.1316266 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                 13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

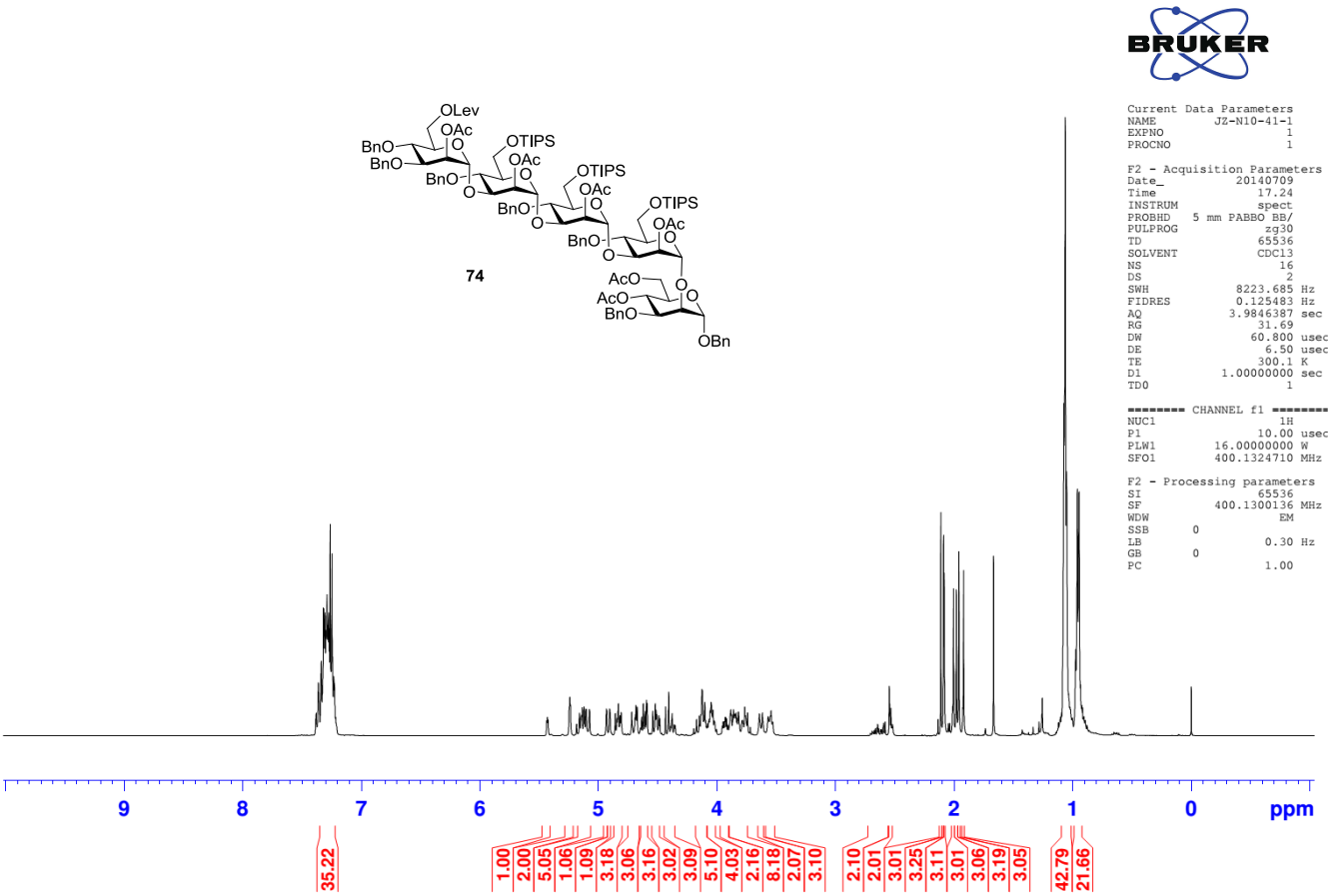
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho

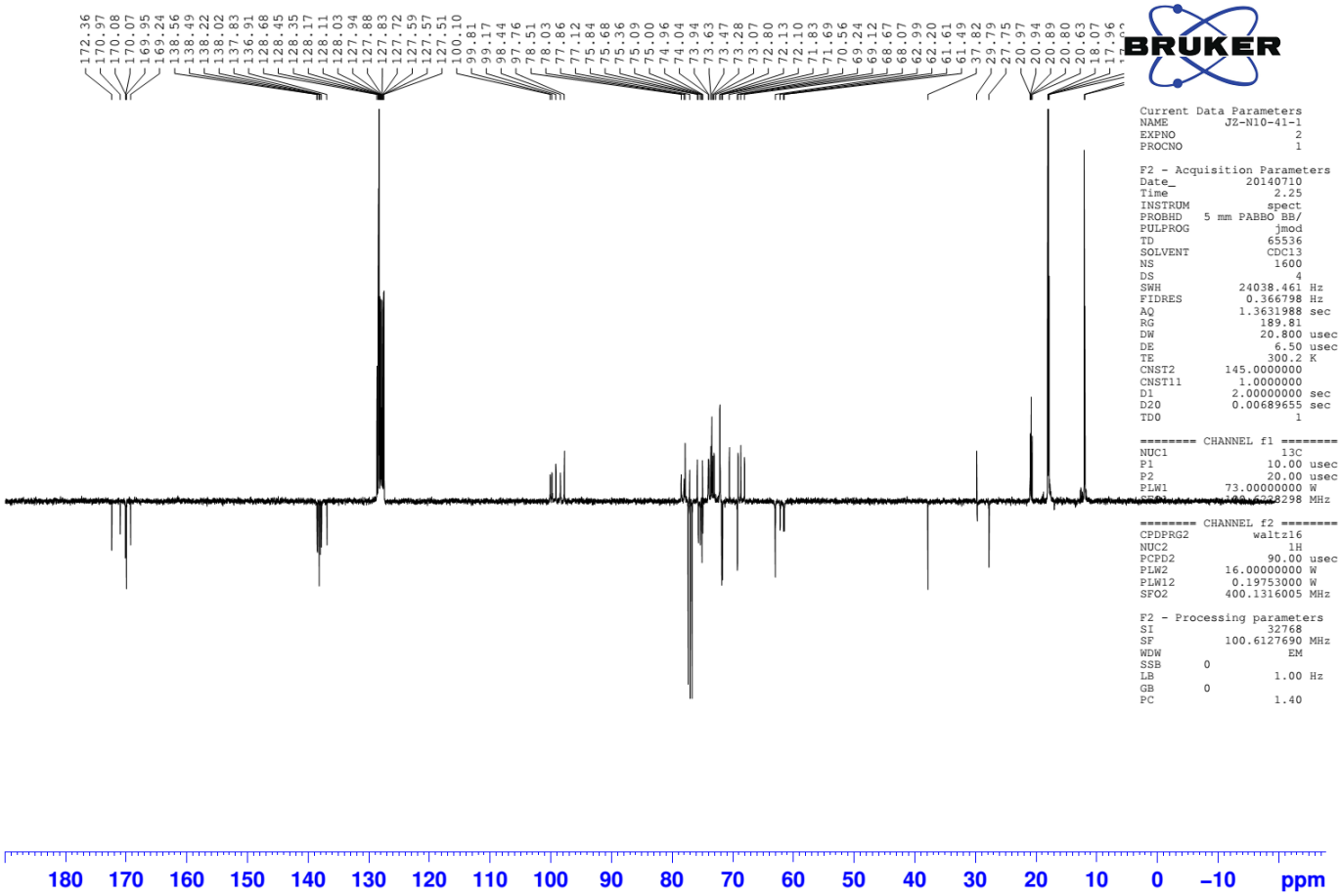
F2 - Processing parameters
SI                    1024
SF            400.1300130 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF             100.6127690 MHz
WDW            States-TPPI
SSB                       2
LB        0 Hz
GB        0
```

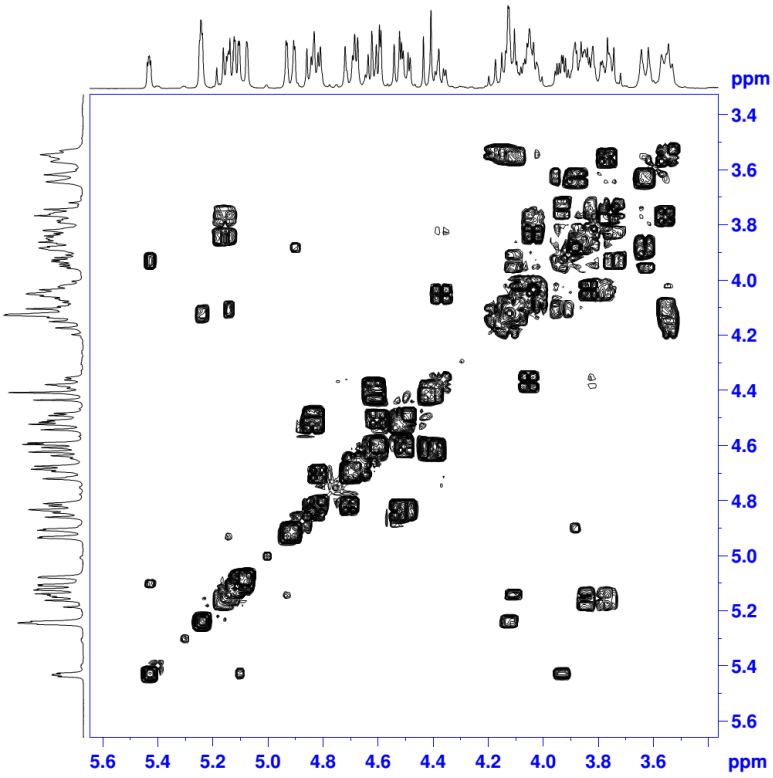
^{1}H NMR spectrum for compound **74**



^{13}C-APT NMR spectrum for compound **74**



COSY spectrum for compound **74**




```
Current Data Parameters
NAME          JZ-N10-41-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140709
Time                17.44
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDC13
NS                      4
DS                      8
SWH             3703.704 Hz
FIDRES          1.808449 Hz
AQ             0.2765300 sec
RG                  14.37
DW               135.000 usec
DE                  6.50 usec
TE                 300.3 K
D0             0.00000300 sec
D1             1.91521299 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00027000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17               2000.00 usec
PLW1          16.000000000 W
PLW10          2.36689997 W
SFO1          400.1314158 MHz

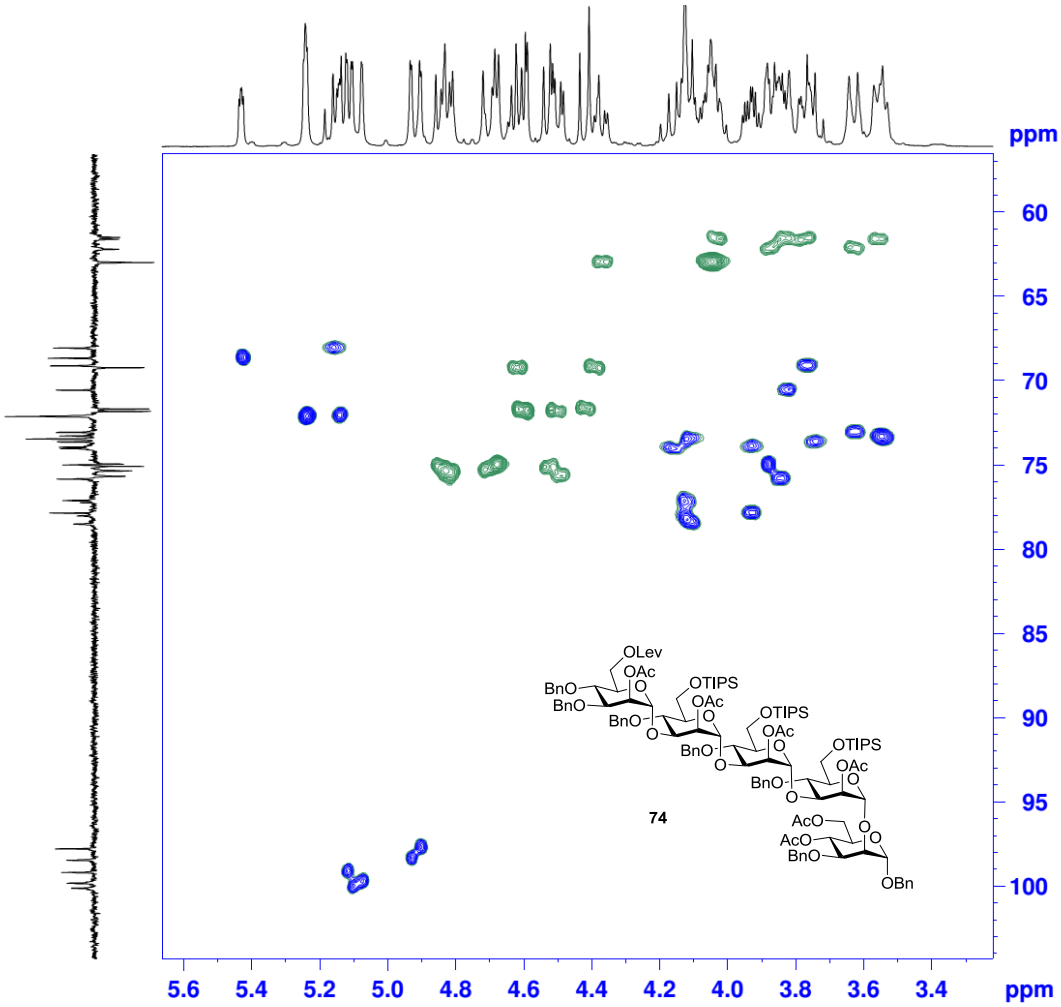
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            400.1314 MHz
FIDRES         28.935184 Hz
SW                  9.256 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF            400.1300136 MHz
WDW                   QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            400.1300136 MHz
WDW                    SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **74**




```
Current Data Parameters
NAME          JZ-N10-41-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140709
Time                23.03
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                   1024
SOLVENT             CDC13
NS                     16
DS                     16
SWH             3703.704 Hz
FIDRES          3.616898 Hz
AQ             0.1382900 sec
RG                 189.81
DW               135.000 usec
DE                  6.50 usec
TE                 300.1 K
CNST2          145.0000000
D0             0.00000300 sec
D1             1.45760596 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1          16.000000000 W
SFO1          400.1314158 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

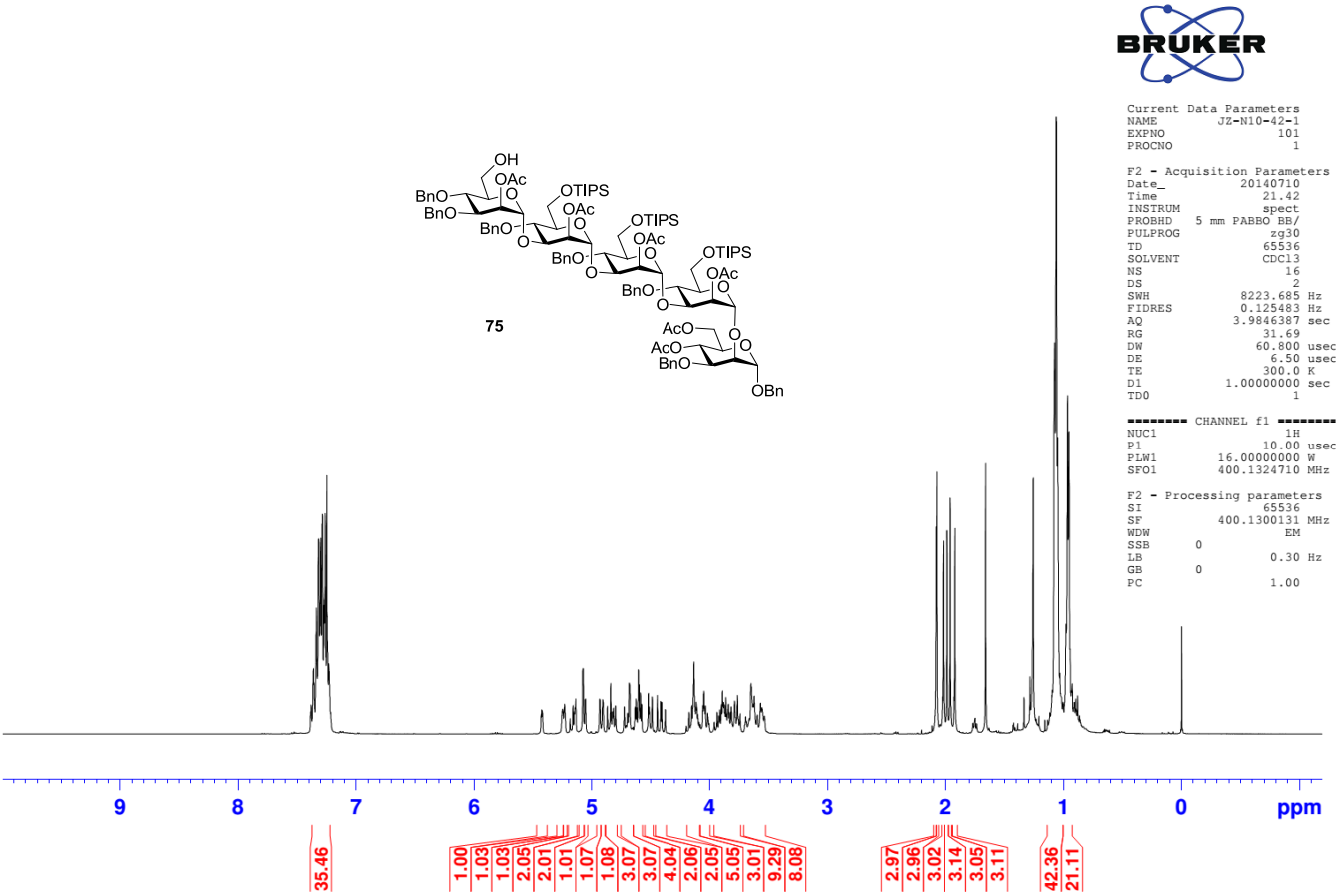
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPNAM2         SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

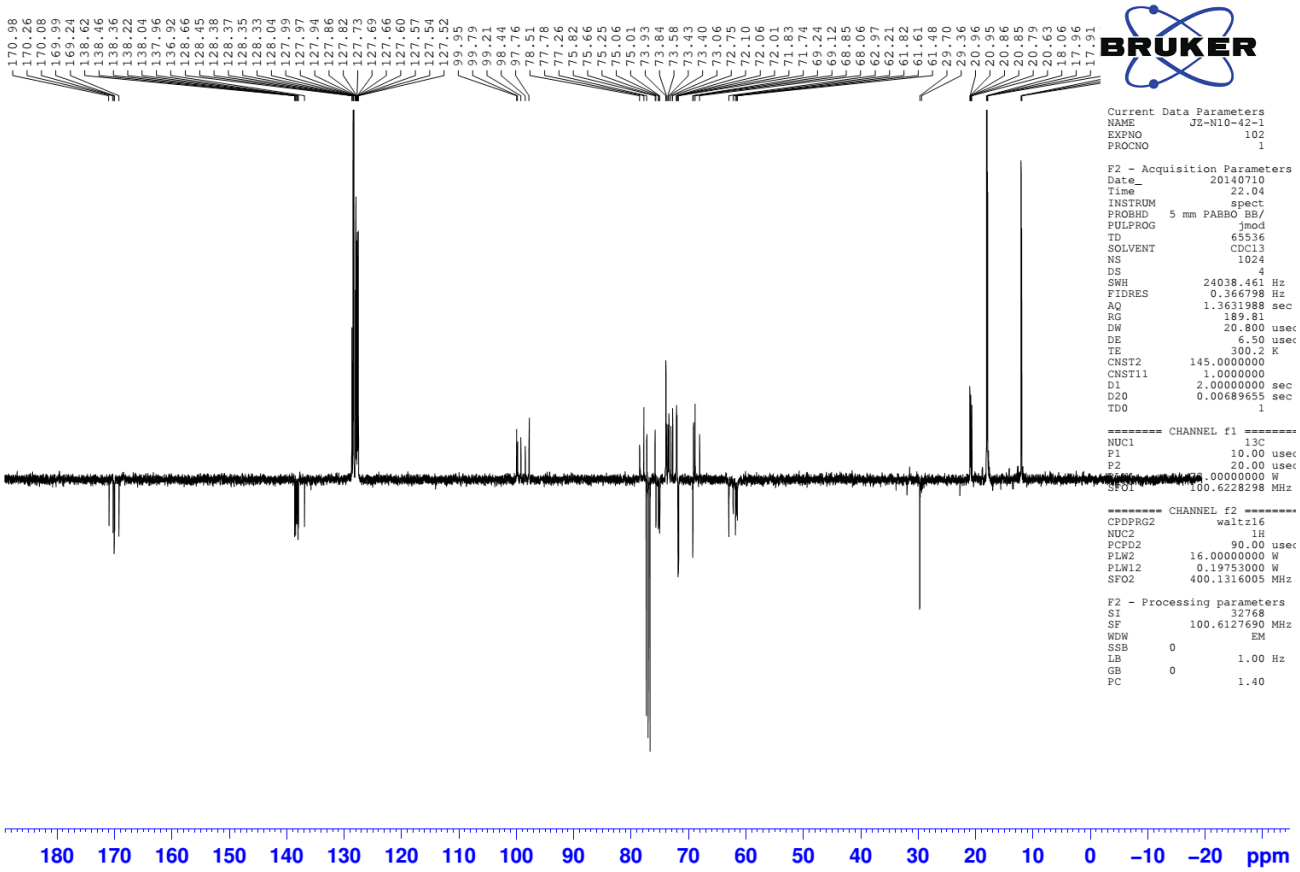
F2 - Processing parameters
SI                    1024
SF            400.1300136 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2         echo-antiecho
SF            100.6127690 MHz
WDW           States-TPPI
SSB                       2
LB        0 Hz
GB        0
```

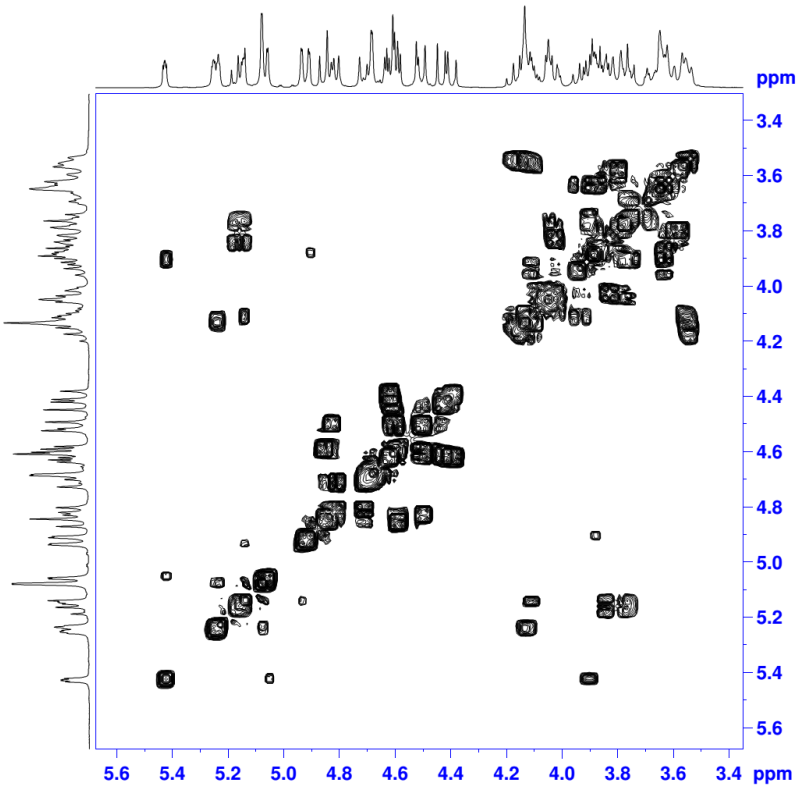
^{1}H NMR spectrum for compound **75**



^{13}C-APT NMR spectrum for compound **75**



COSY spectrum for compound **75**




```
Current Data Parameters
NAME          JZ-N10-42-1
EXPNO                 104
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140710
Time                21.44
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             3731.343 Hz
FIDRES          1.821945 Hz
AQ             0.2744820 sec
RG                 15.91
DW               134.000 usec
DE                 6.50 usec
TE                300.0 K
D0             0.00000300 sec
D1             1.91726100 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00026800 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17                2000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1          400.1313938 MHz

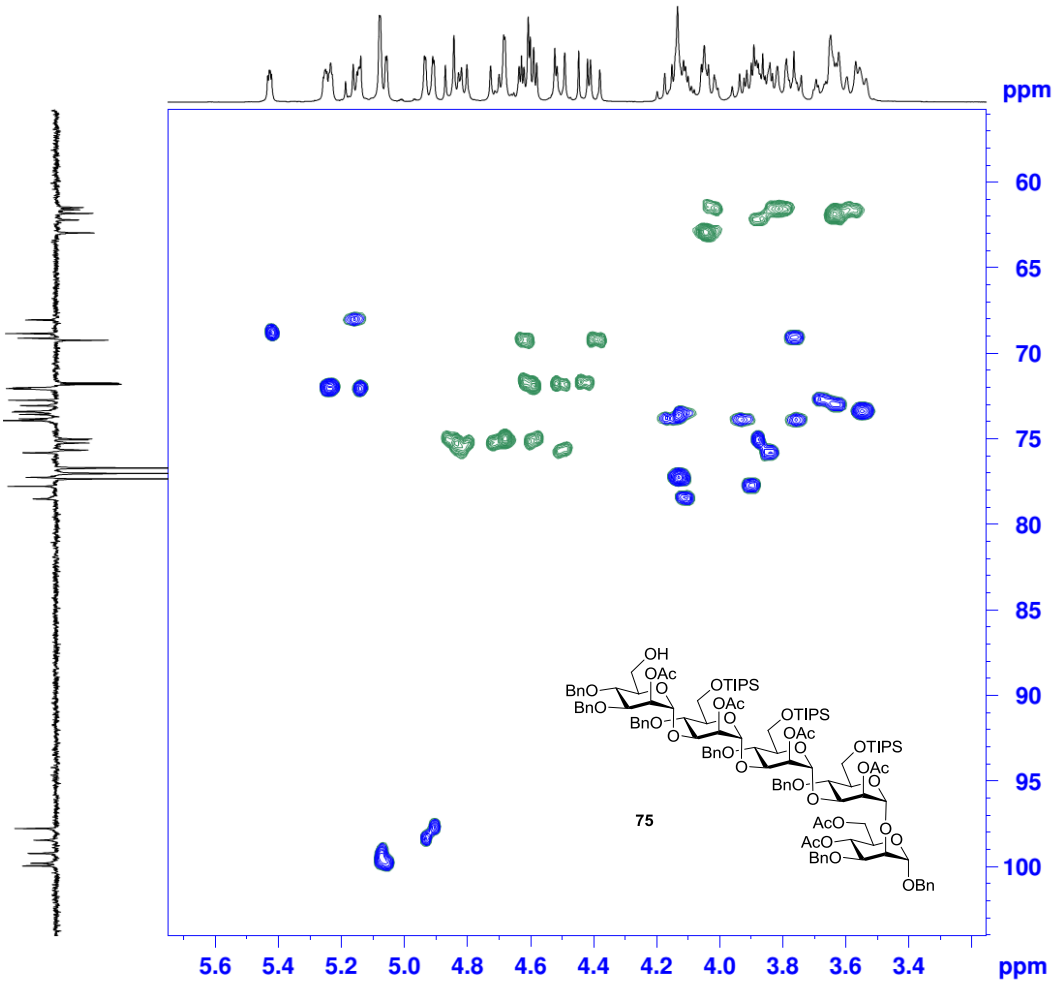
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1             400.1314 MHz
FIDRES          29.151119 Hz
SW                   9.325 ppm
FnMODE                  QF

F2 - Processing parameters
SI                     1024
SF            400.1300131 MHz
WDW                    QSINE
SSB         0
LB          0 Hz
GB          0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            400.1300131 MHz
WDW                     SIN
SSB         0
LB          0 Hz
GB          0
```

HSQC spectrum for compound **75**




```
Current Data Parameters
NAME          JZ-N10-42-1
EXPNO                 105
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140710
Time                23.04
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                     13
DS                     16
SWH             3731.343 Hz
FIDRES          3.643890 Hz
AQ             0.1372660 sec
RG                 189.81
DW               134.000 usec
DE                 6.50 usec
TE                300.2 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.45862997 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D21            0.00345000 sec
IN0            0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1          16.00000000 W
SFO1          400.1313938 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2          100.6202727 MHz

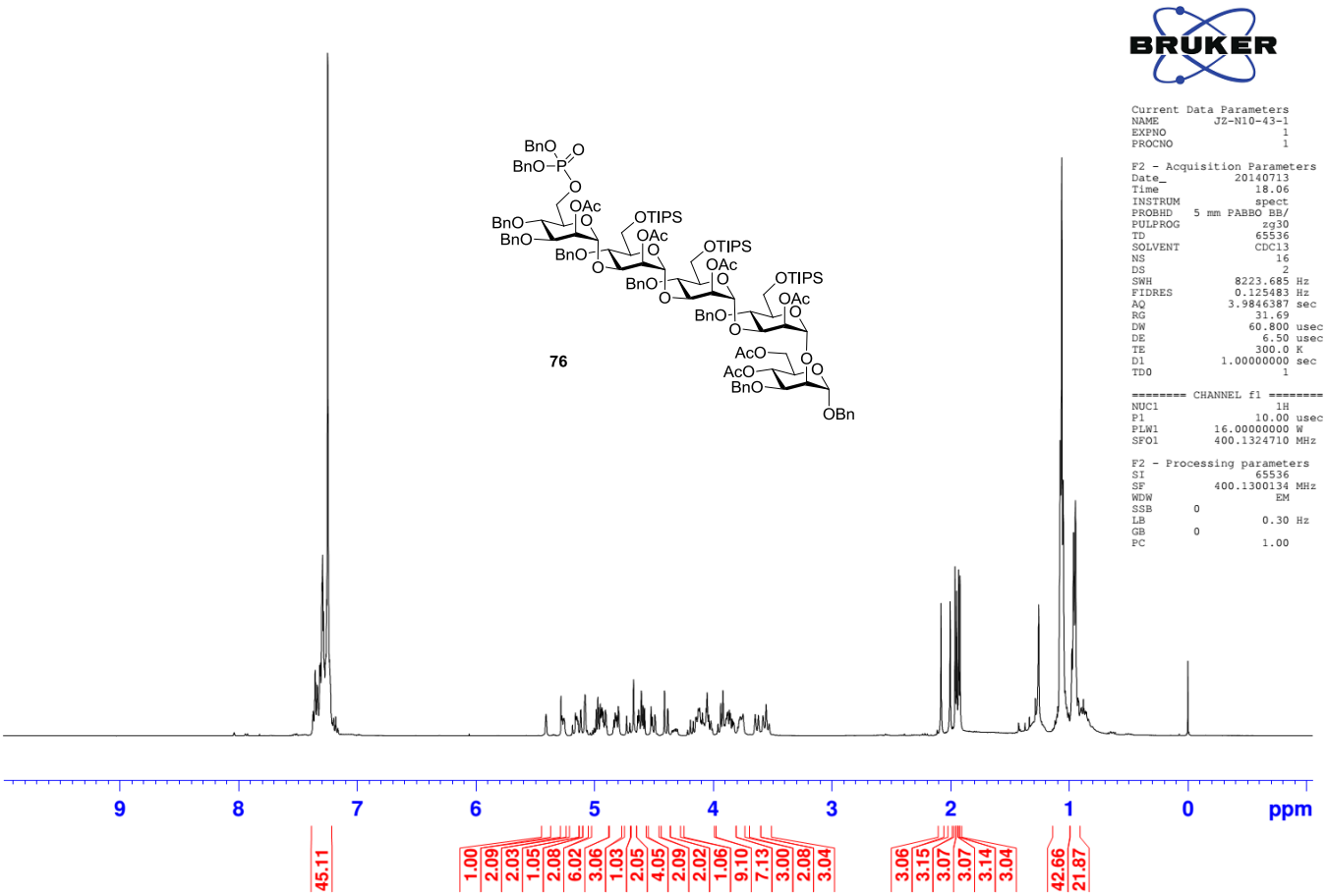
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPNAM2         SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1             100.6203 MHz
FIDRES          65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho

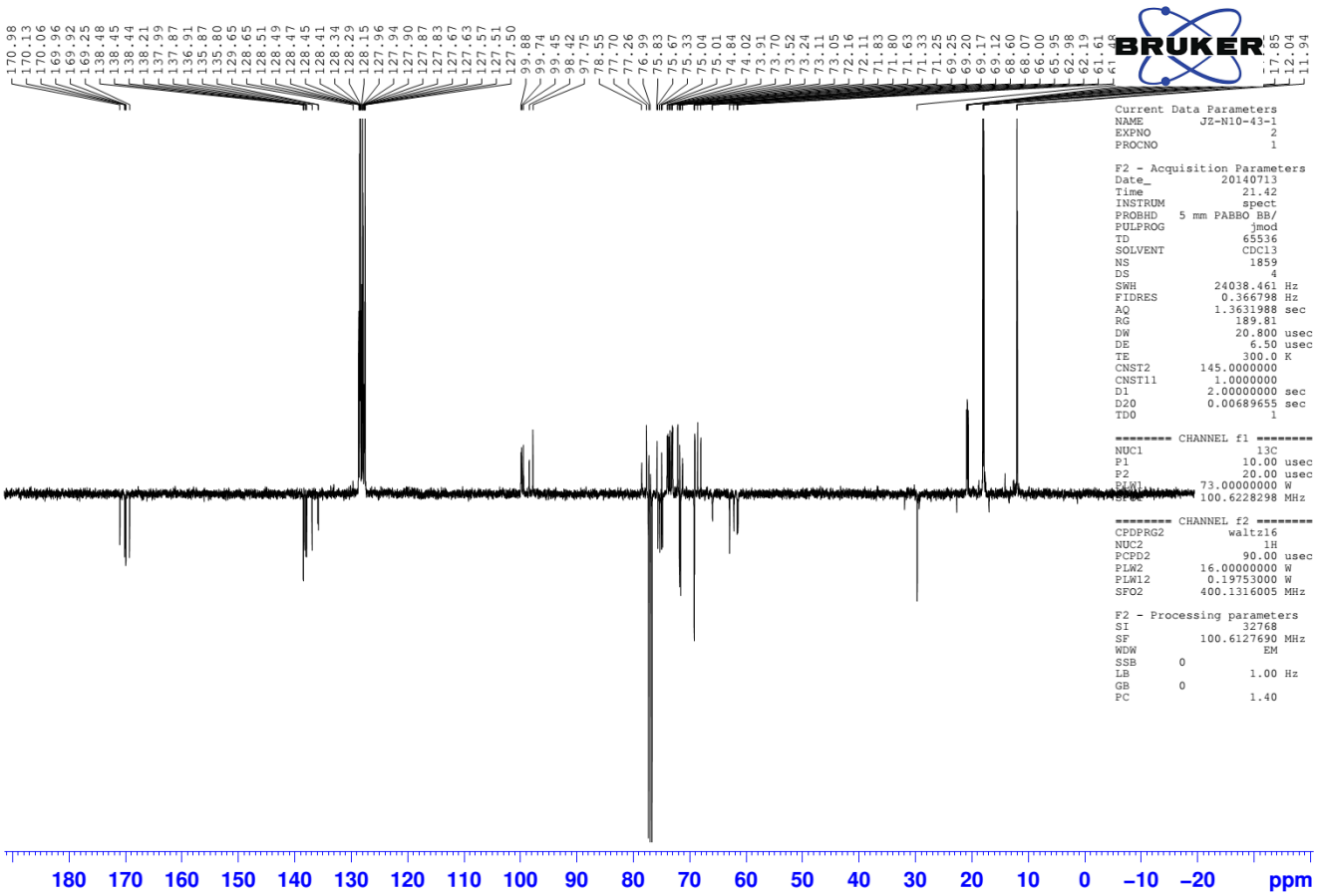
F2 - Processing parameters
SI                     1024
SF            400.1300131 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF            100.6127690 MHz
WDW            States-TPPI
SSB                        2
LB          0 Hz
GB          0
```

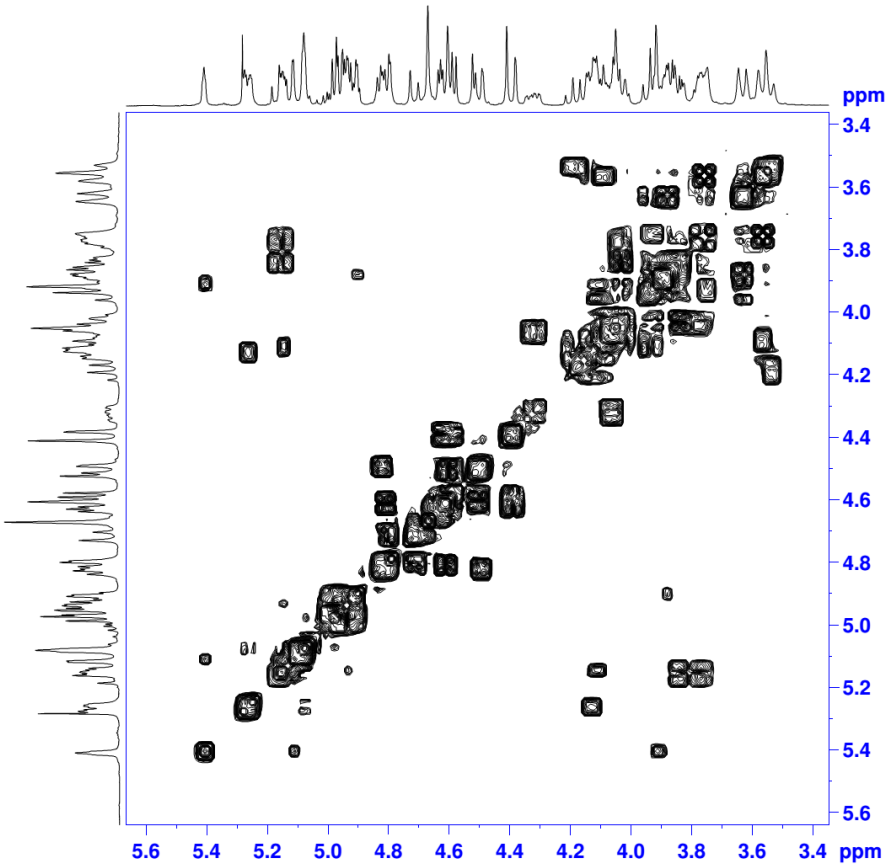
^{1}H NMR spectrum for compound **76**



^{13}C-APT NMR spectrum for compound **76**



COSY spectrum for compound **76**




```
Current Data Parameters
NAME          JZ-N10-43-1
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140713
Time               18.14
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG      cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH             4166.667 Hz
FIDRES          2.034505 Hz
AQ            0.2458100 sec
RG                 18.47
DW               120.000 usec
DE                 6.50 usec
TE                300.0 K
D0            0.00000300 sec
D1            1.94593298 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00024000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17               2000.00 usec
PLW1         16.00000000 W
PLW10         2.36689997 W
SFO1         400.1313680 MHz

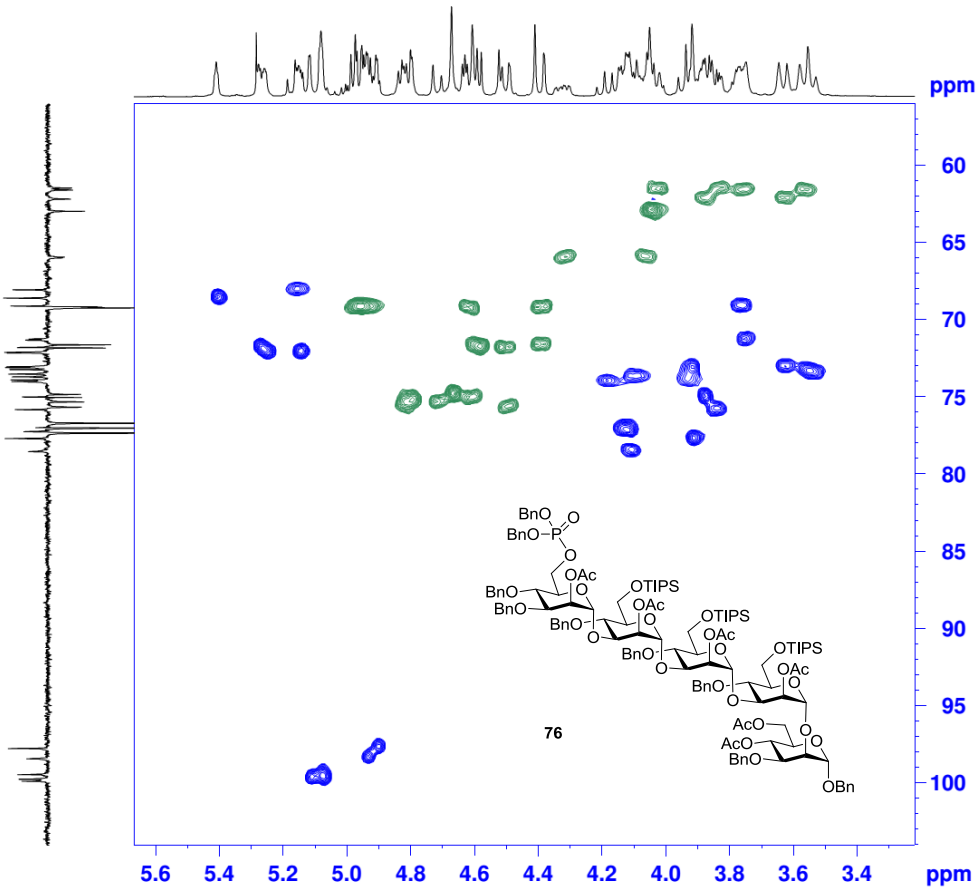
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            400.1314 MHz
FIDRES         32.552082 Hz
SW                 10.413 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF           400.1300134 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                    QF
SF           400.1300134 MHz
WDW                   SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **76**




```
Current Data Parameters
NAME          JZ-N10-43-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140713
Time               23.27
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG       hsqcedetgp
TD                   1024
SOLVENT             CDCl3
NS                     16
DS                     16
SWH             4166.667 Hz
FIDRES          4.069010 Hz
AQ            0.1229300 sec
RG                 189.81
DW               120.000 usec
DE                 6.50 usec
TE                300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.47296596 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28                  0.10 usec
PLW1         16.00000000 W
SFO1         400.1313680 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

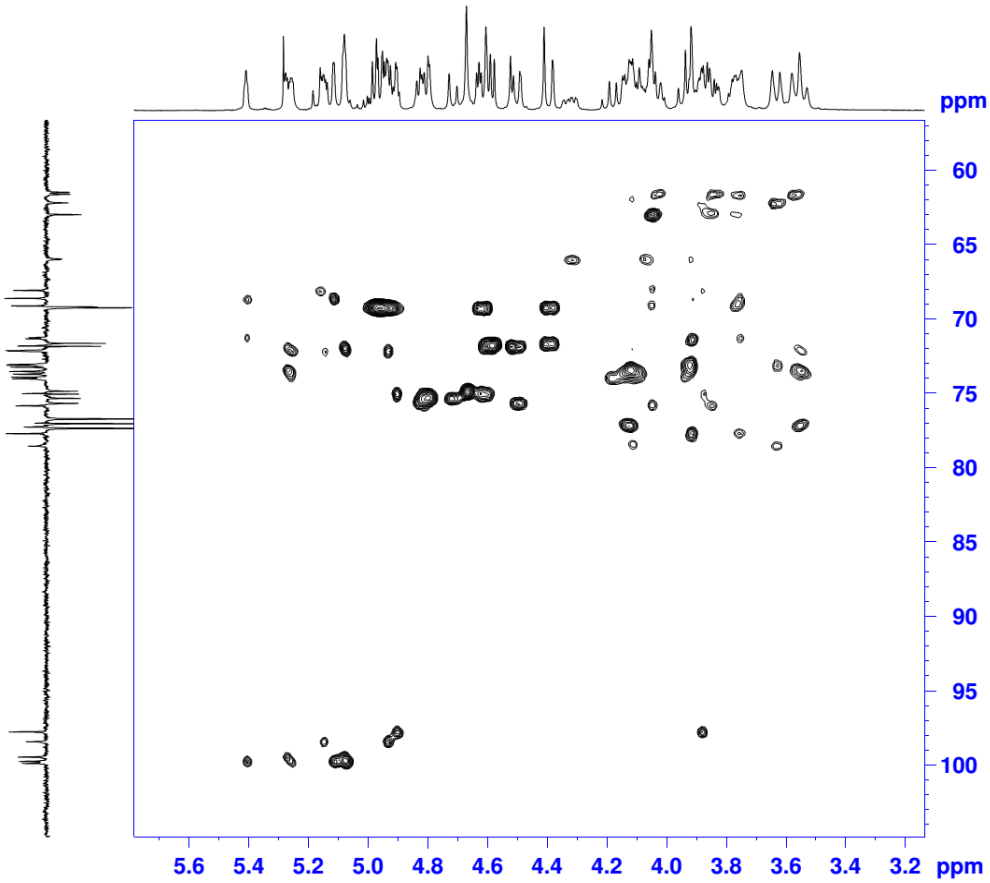
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            100.6203 MHz
FIDRES         65.104164 Hz
SW                165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF           400.1300134 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF           100.6127690 MHz
WDW          States-TPPI
SSB                      2
LB        0 Hz
GB        0
```

HSQC-TOCSY spectrum for compound **76**




```
Current Data Parameters
NAME                JZ-N10-43-1
EXPNO                         7
PROCNO                        1

F2 - Acquisition Parameters
Date_             20140714
Time                      3.34
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG      hsqcetgpml
TD                         1024
SOLVENT                   CDCl3
NS                           16
DS                           16
SWH                   4166.667 Hz
FIDRES                4.069010 Hz
AQ                   0.1229300 sec
RG                       189.81
DW                     120.000 usec
DE                        6.50 usec
TE                       300.0 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.47296596 sec
D4                 0.00172414 sec
D9                 0.12000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00003000 sec
L1                           66
ZGOPTNS

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.00 usec
P2                        20.00 usec
P5                        17.34 usec
P6                        26.00 usec
P7                        52.00 usec
P17                     2000.00 usec
P28                        0.10 usec
PLW1                16.00000000 W
PLW10                2.36689997 W
SFO1               400.1313680 MHz

======== CHANNEL f2 ========
CPDPRG2                     garp
NUC2                         13C
P3                        10.00 usec
P4                        20.00 usec
PCPD2                     80.00 usec
PLW2                73.00000000 W
PLW12                1.14059997 W
SFO2               100.6202727 MHz

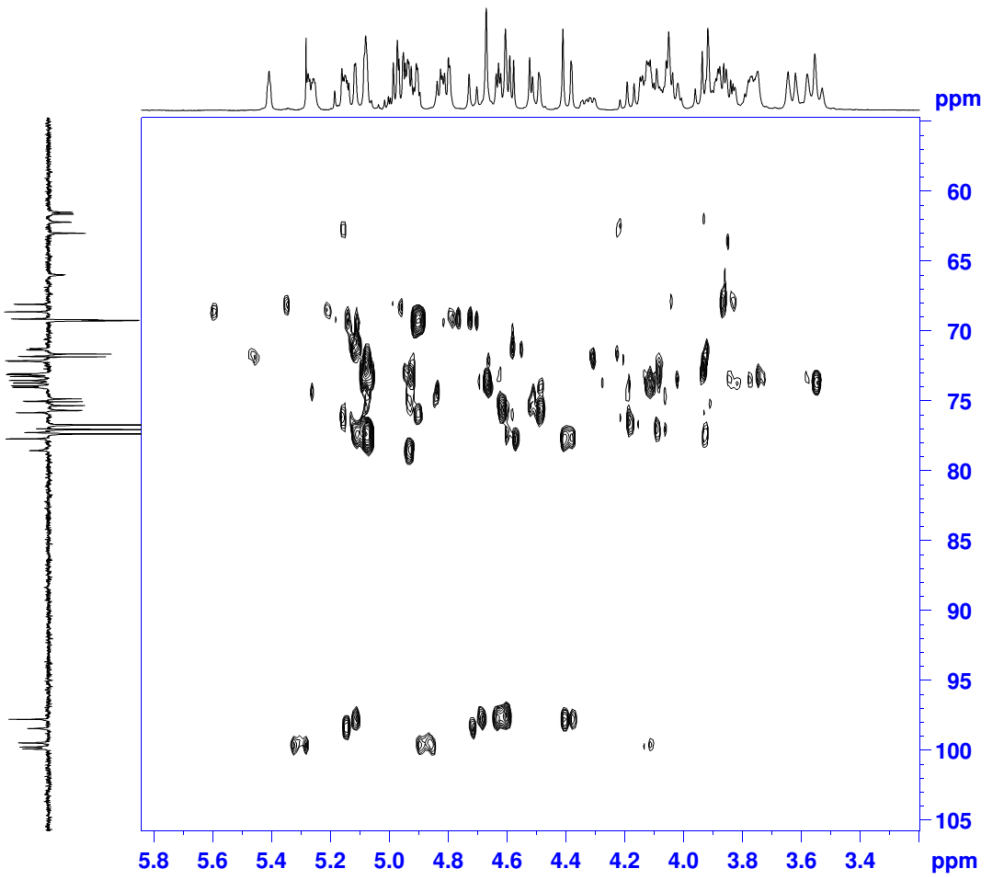
====== GRADIENT CHANNEL =====
GPNAM1              SMSQ10.100
GPNAM2              SMSQ10.100
GPZ1                       80.00 %
GPZ2                       20.10 %
P16                     1000.00 usec

F1 - Acquisition parameters
TD                          256
SFO1                   100.6203 MHz
FIDRES                65.104164 Hz
SW                      165.639 ppm
FnMODE           Echo-Antiecho

F2 - Processing parameters
SI                         1024
SF                 400.1300134 MHz
WDW                        QSINE
SSB                            2
LB              0 Hz
GB              0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2              echo-antiecho
SF                 100.6127591 MHz
WDW                States-TPPI
SSB                            2
LB              0 Hz
GB              0
```

HMBC spectrum for compound **76**




```
Current Data Parameters
NAME                JZ-N10-43-1
EXPNO                         6
PROCNO                        1

F2 - Acquisition Parameters
Date_             20140714
Time                      1.20
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG      hmbcgpndqf
TD                         4096
SOLVENT                   CDCl3
NS                           32
DS                           16
SWH                   4166.667 Hz
FIDRES                1.017253 Hz
AQ                   0.4915700 sec
RG                       189.81
DW                     120.000 usec
DE                        6.50 usec
TE                       300.0 K
CNST13               8.0000000
D0                 0.00000300 sec
D1                 1.39268506 sec
D6                 0.06250000 sec
D16                0.00020000 sec
IN0                0.00002235 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.00 usec
P2                        20.00 usec
PLW1                16.00000000 W
SFO1               400.1313680 MHz

======== CHANNEL f2 ========
NUC2                         13C
P3                        10.00 usec
PLW2                73.00000000 W
SFO2               100.6228138 MHz

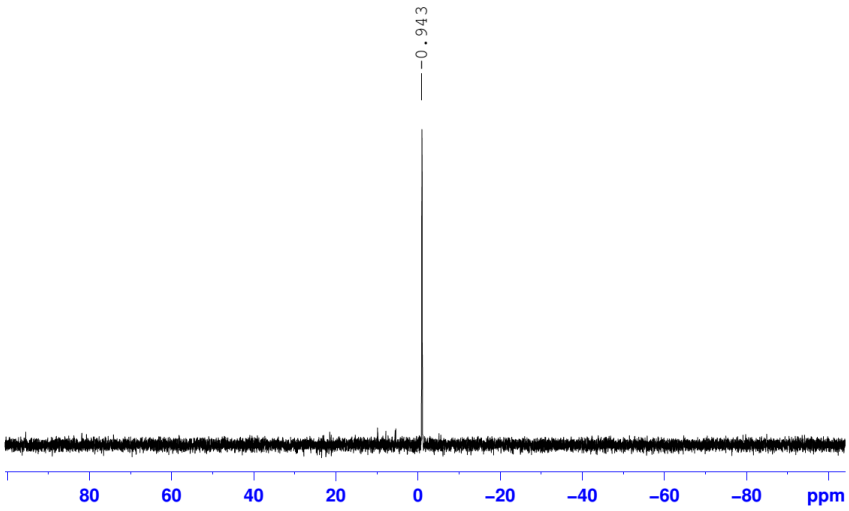
====== GRADIENT CHANNEL =====
GPNAM1              SMSQ10.100
GPNAM2              SMSQ10.100
GPNAM3              SMSQ10.100
GPZ1                       50.00 %
GPZ2                       30.00 %
GPZ3                       40.10 %
P16                     1000.00 usec

F1 - Acquisition parameters
TD                          128
SFO1                   100.6228 MHz
FIDRES               174.592422 Hz
SW                      222.095 ppm
FnMODE                        QF

F2 - Processing parameters
SI                         1024
SF                 400.1300134 MHz
WDW                        SINE
SSB             0
LB              0 Hz
GB              0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2                           QF
SF                 100.6127690 MHz
WDW                      States
SSB             0
LB              0 Hz
GB              0
```

^{31}P NMR spectrum for compound **76**




```
Current Data Parameters
NAME        JZ-N10-43-1
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_           20140713
Time              18.11
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   64
DS                    4
SWH           64102.563 Hz
FIDRES         0.978127 Hz
AQ            0.5112308 sec
RG               189.81
DW                7.800 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                8.00 usec
PLW1        55.00000000 W
SFO1        161.9674942 MHz

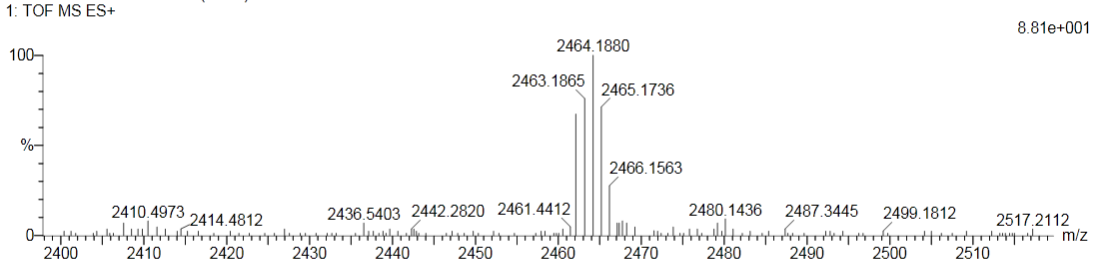
F2 - Processing parameters
SI                32768
SF          161.9755930 MHz
WDW                  EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```

HRESIMS report for compound **76**

Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

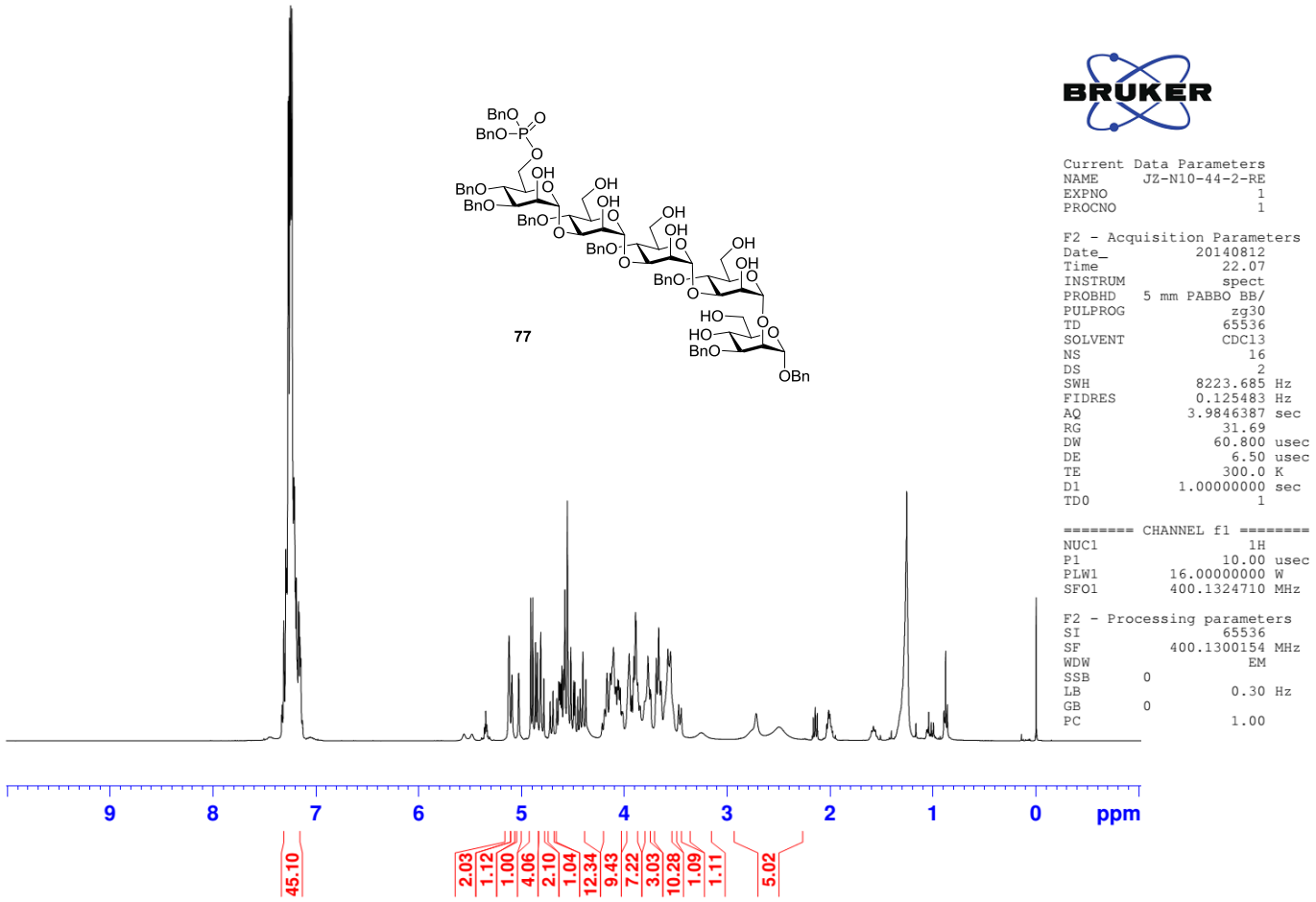
Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 132-132 H: 170-189 O: 35-35 23Na: 0-1 Si: 3-3 P: 1-1

JZ-N10-43-1-20150212 167 (3.269)
1: TOF MS ES+

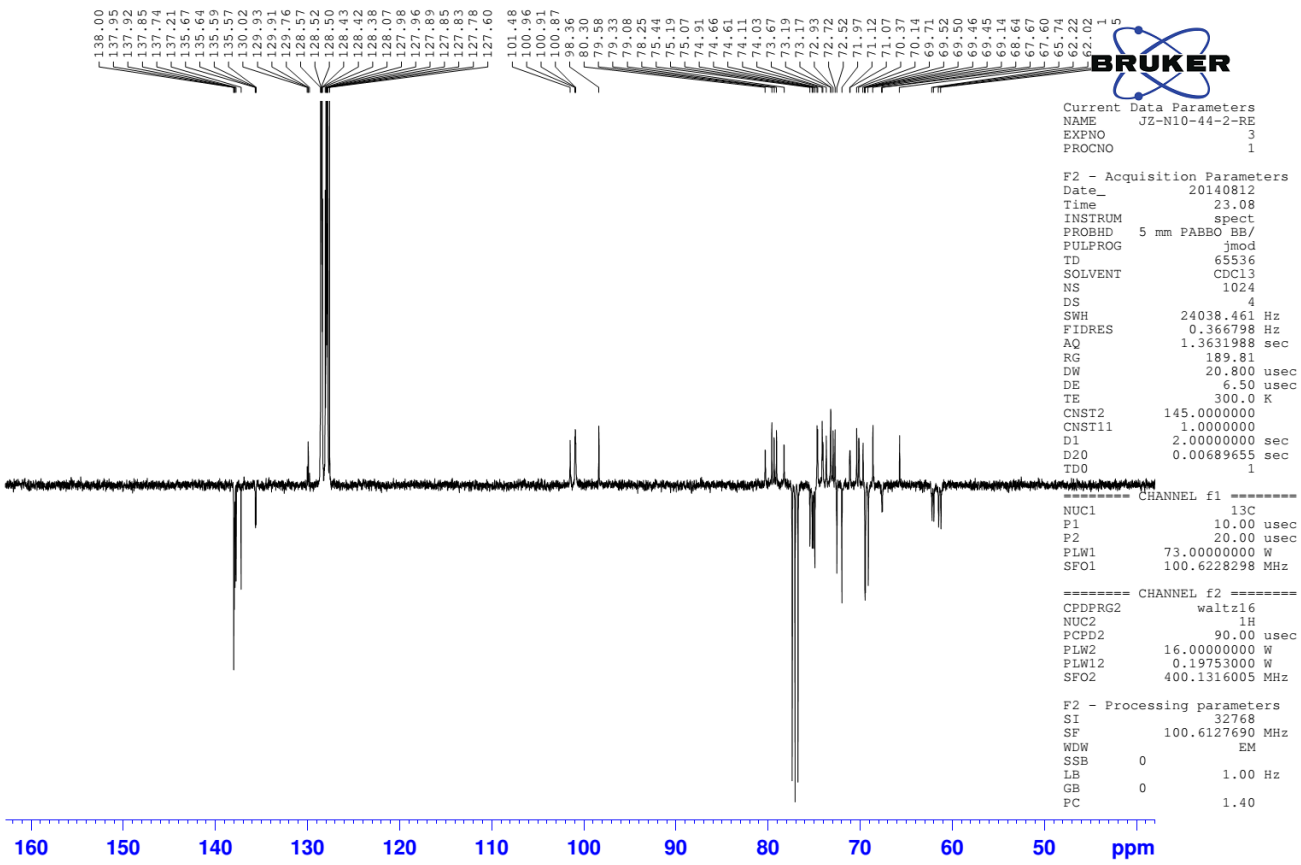


Minimum:				-1.5			
Maximum:		500.0	1000.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
2462.1118	2462.1170	-5.2	-2.1	46.5	16.0	0.0	C132 H179 O35 23Na Si3 P

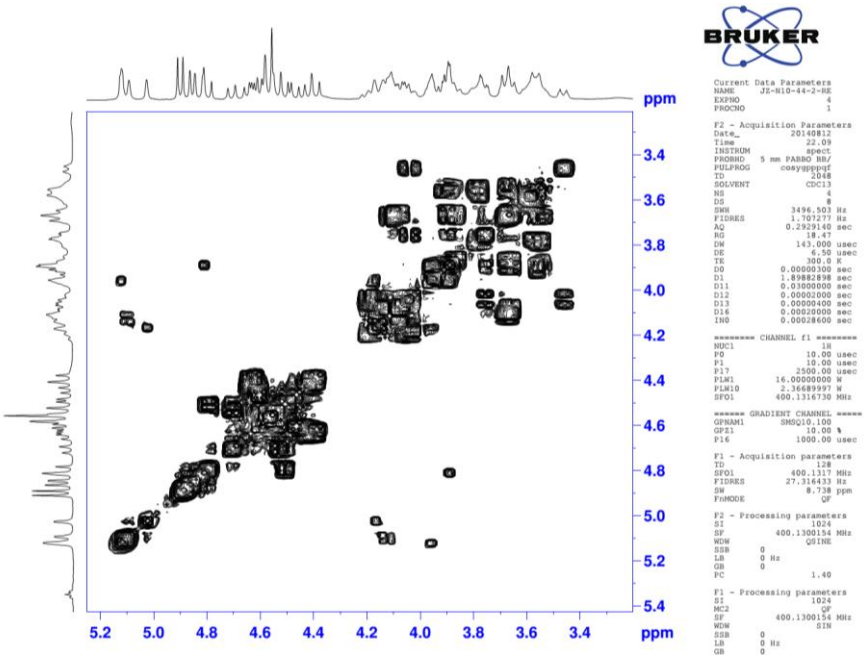
^{1}H NMR spectrum for compound **77**



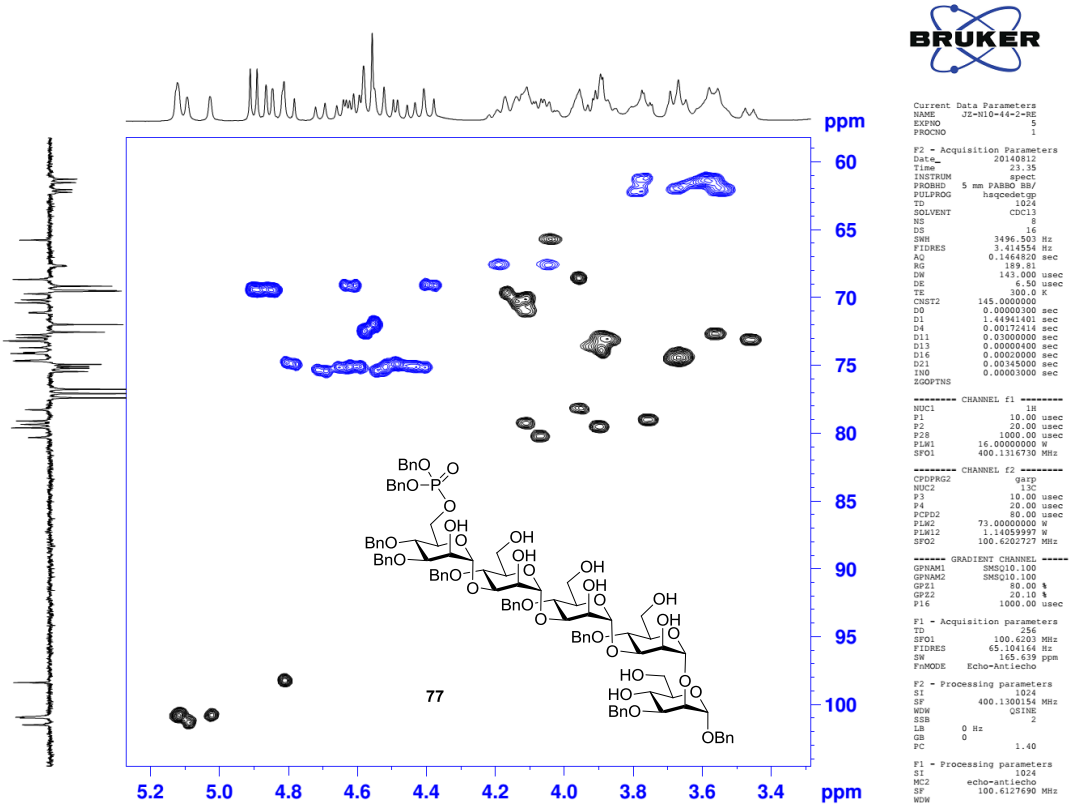
^{13}C-APT NMR spectrum for compound **77**



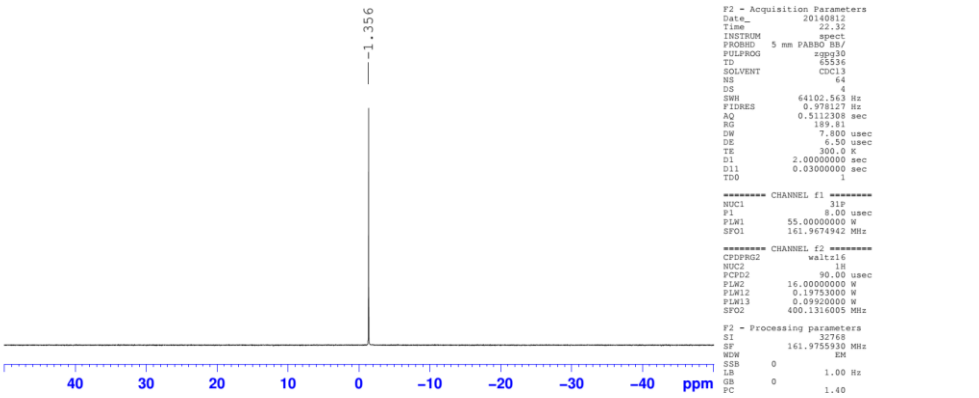
COSY spectrum for compound **77**



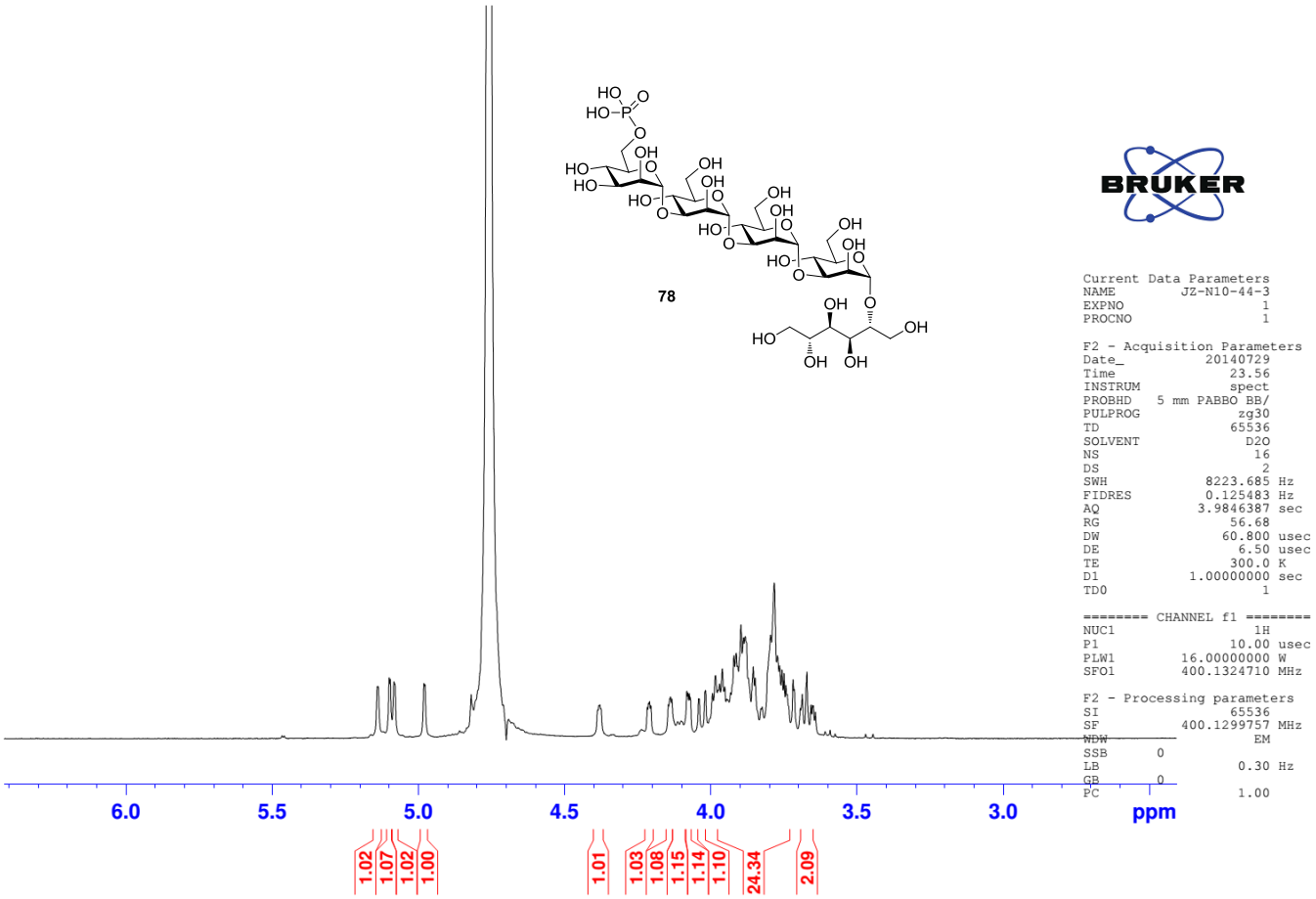
HSQC spectrum for compound **77**



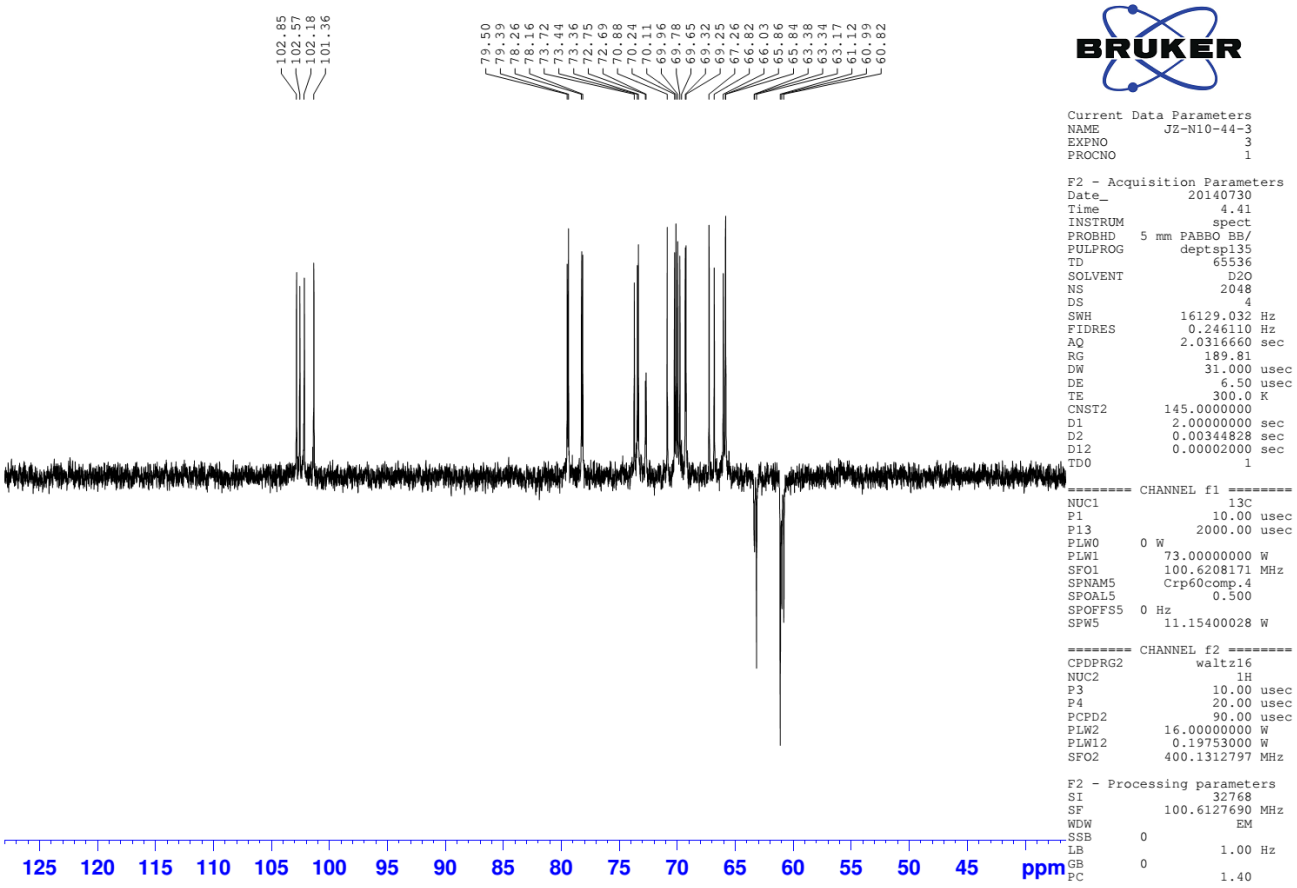
^{31}P NMR spectrum for compound **77**



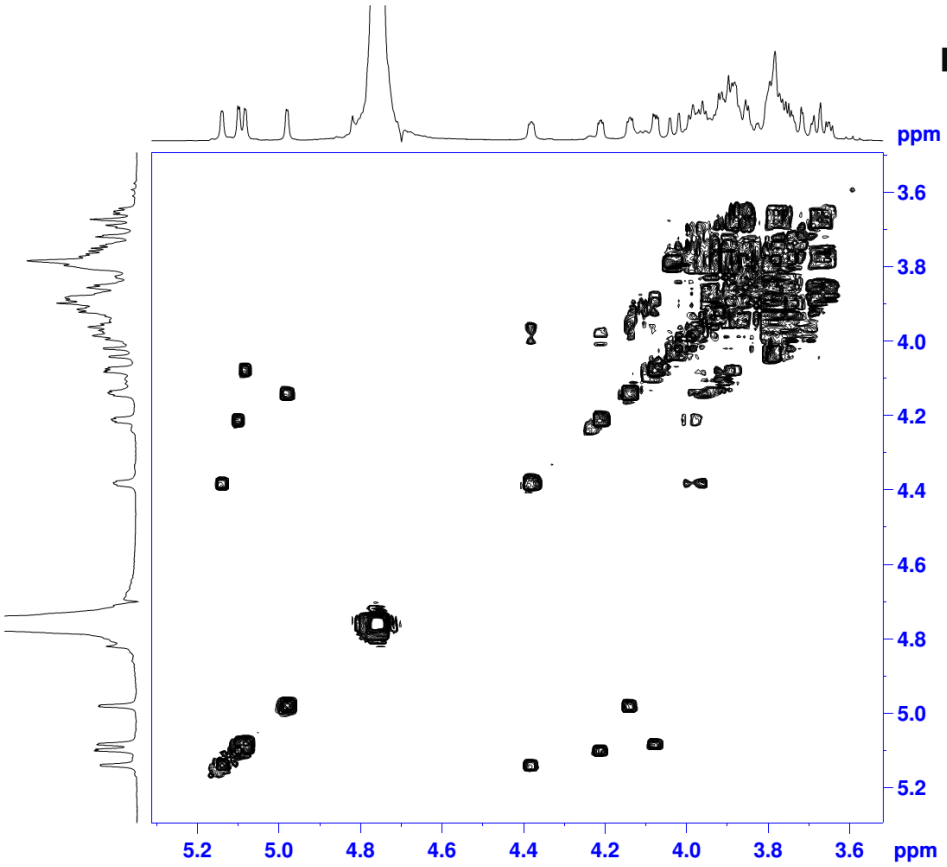
^{1}H NMR spectrum for compound **78**



^{13}C-APT NMR spectrum for compound **78**



COSY spectrum for compound **78**




```
Current Data Parameters
NAME          JZ-N10-44-3
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140730
Time               0.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT             D2O
NS                    4
DS                    8
SWH            2202.643 Hz
FIDRES         1.075509 Hz
AQ           0.4649460 sec
RG               28.13
DW             227.000 usec
DE               6.50 usec
TE              300.0 K
D0          0.00000300 sec
D1          1.72679698 sec
D11         0.03000000 sec
D12         0.00002000 sec
D13         0.00000400 sec
D16         0.00020000 sec
IN0         0.00045400 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                10.00 usec
P1                10.00 usec
P17             2500.00 usec
PLW1        16.00000000 W
PLW10        2.36689997 W
SFO1        400.1319993 MHz

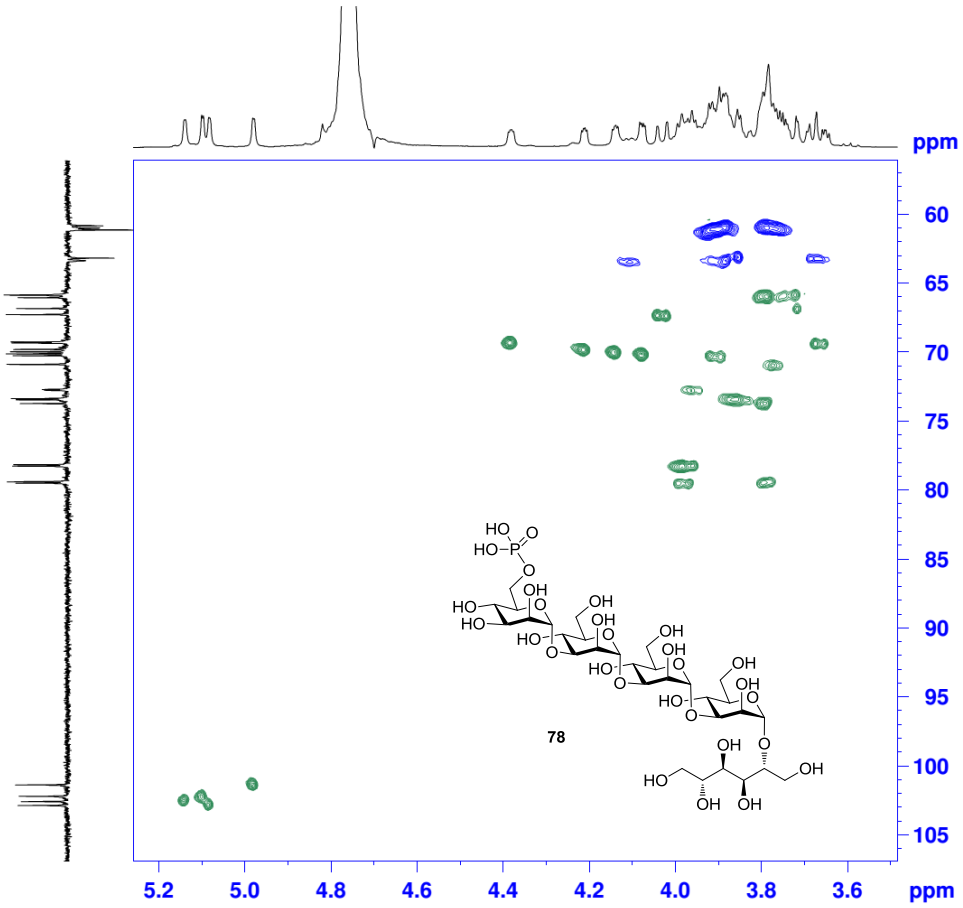
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPZ1               10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1             400.132 MHz
FIDRES        17.208149 Hz
SW                 5.505 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF          400.1299732 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF          400.1299727 MHz
WDW                   SIN
SSB       0
LB        0 Hz
GB        0
```

HSQC spectrum for compound **78**




```
Current Data Parameters
NAME          JZ-N10-44-3
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140730
Time               0.31
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                 1024
SOLVENT             D2O
NS                   16
DS                   16
SWH            2202.643 Hz
FIDRES         2.151019 Hz
AQ           0.2324980 sec
RG               189.81
DW             227.000 usec
DE               6.50 usec
TE              300.0 K
CNST2       145.0000000
D0          0.00000300 sec
D1          1.36339796 sec
D4          0.00172414 sec
D11         0.03000000 sec
D13         0.00000400 sec
D16         0.00020000 sec
D21         0.00345000 sec
IN0         0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P28             1000.00 usec
PLW1        16.00000000 W
SFO1        400.1319993 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2        73.00000000 W
PLW12        1.14059997 W
SFO2        100.6202727 MHz

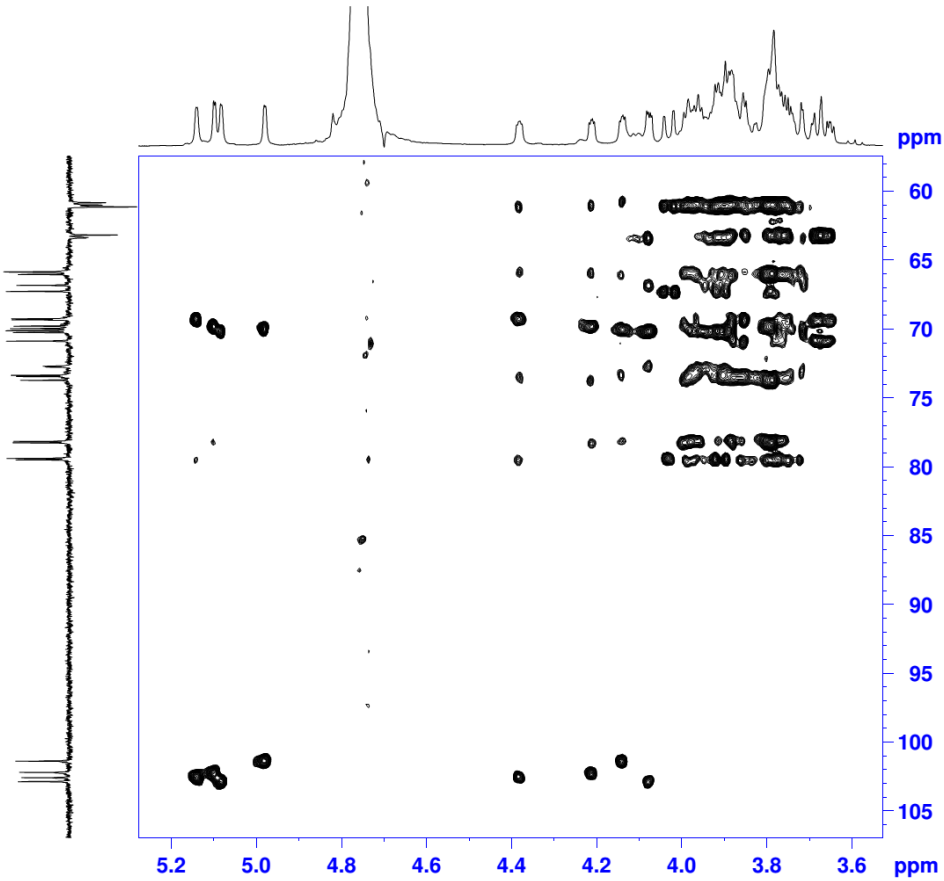
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6203 MHz
FIDRES        65.104164 Hz
SW              165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF          400.1299743 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF           100.6127572 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

HSQC-TOCSY spectrum for compound **78**




```
Current Data Parameters
NAME          JZ-N10-44-3
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140730
Time                4.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpm1
TD                   1024
SOLVENT               D2O
NS                     16
DS                     16
SWH             2202.643 Hz
FIDRES          2.151019 Hz
AQ            0.2324980 sec
RG                 189.81
DW               227.000 usec
DE                  6.50 usec
TE                 300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.36339796 sec
D4            0.00172414 sec
D9            0.12000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00003000 sec
L1                     66
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P5                  17.34 usec
P6                  26.00 usec
P7                  52.00 usec
P17               2500.00 usec
P28               1000.00 usec
PLW1         16.00000000 W
PLW10         2.36689997 W
SFO1         400.1319993 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                   13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

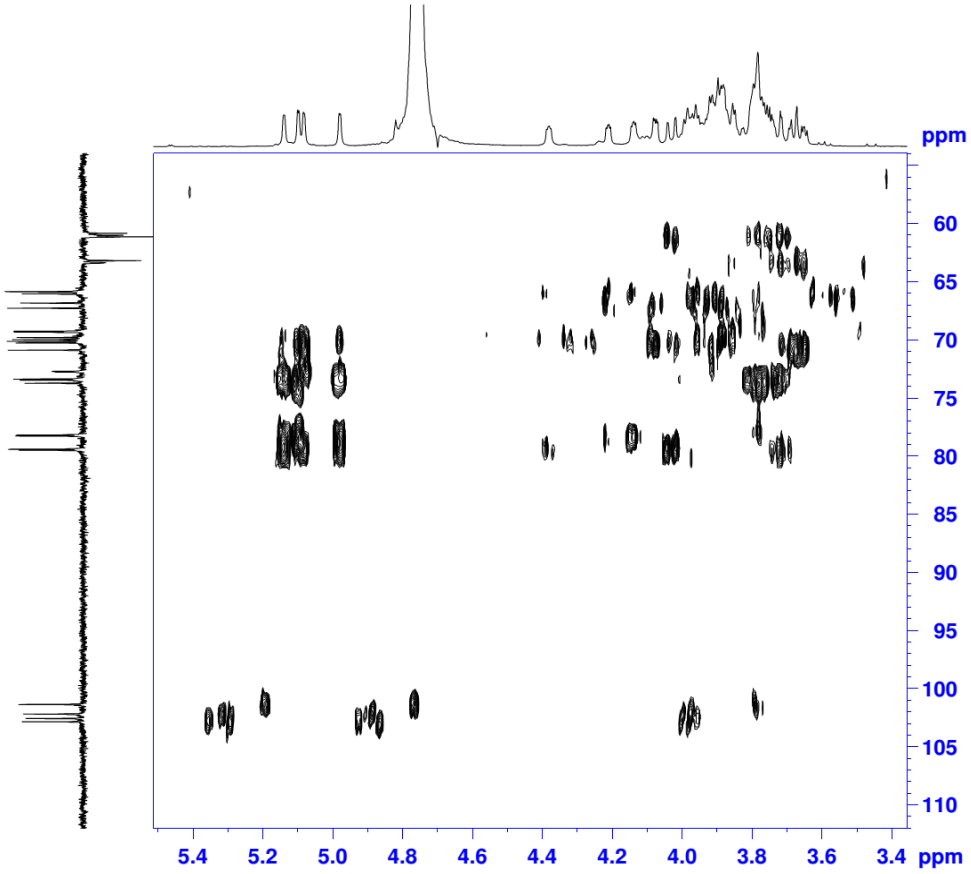
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1         100.6203 MHz
FIDRES        65.104164 Hz
SW              165.639 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF          400.1299765 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF          100.6127622 MHz
WDW         States-TPPI
SSB                     2
LB        0 Hz
GB        0
```

HMBC spectrum for compound **78**




```
Current Data Parameters
NAME          JZ-N10-44-3
EXPNO                   6
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140730
Time                6.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      hmbcgpndqf
TD                   4096
SOLVENT               D2O
NS                     32
DS                     16
SWH             2202.643 Hz
FIDRES          0.537755 Hz
AQ            0.9298420 sec
RG                 189.81
DW               227.000 usec
DE                  6.50 usec
TE                 300.0 K
CNST13         8.000000
D0            0.00000300 sec
D1            0.95441282 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00002235 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
PLW1         16.00000000 W
SFO1         400.1319993 MHz

======== CHANNEL f2 ========
NUC2                   13C
P3                  10.00 usec
PLW2         73.00000000 W
SFO2         100.6228138 MHz

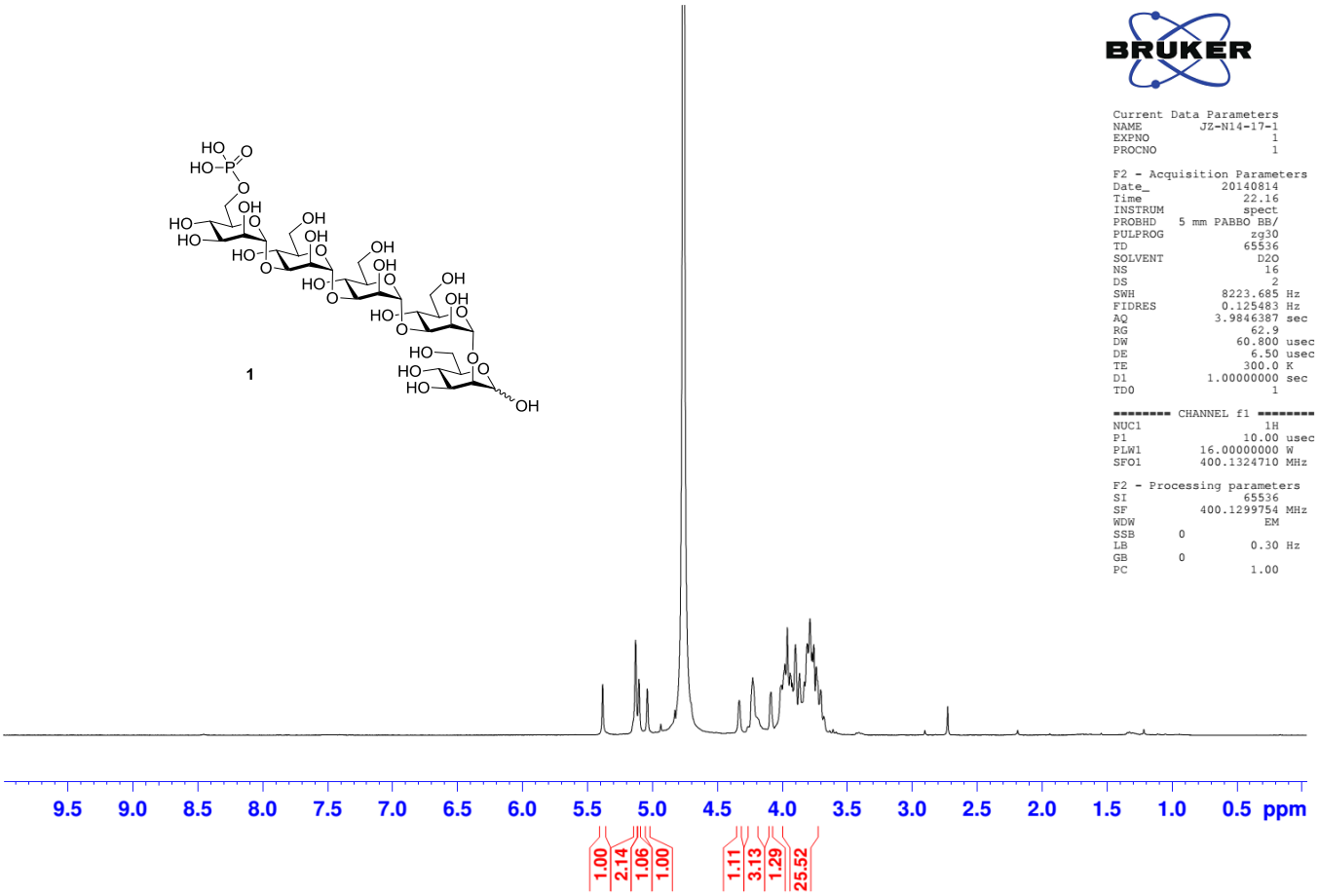
====== GRADIENT CHANNEL =====
GPNAM1       SMSQ10.100
GPNAM2       SMSQ10.100
GPNAM3       SMSQ10.100
GPZ1              50.00 %
GPZ2              30.00 %
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1         100.6228 MHz
FIDRES       174.592422 Hz
SW              222.095 ppm
FnMODE               QF

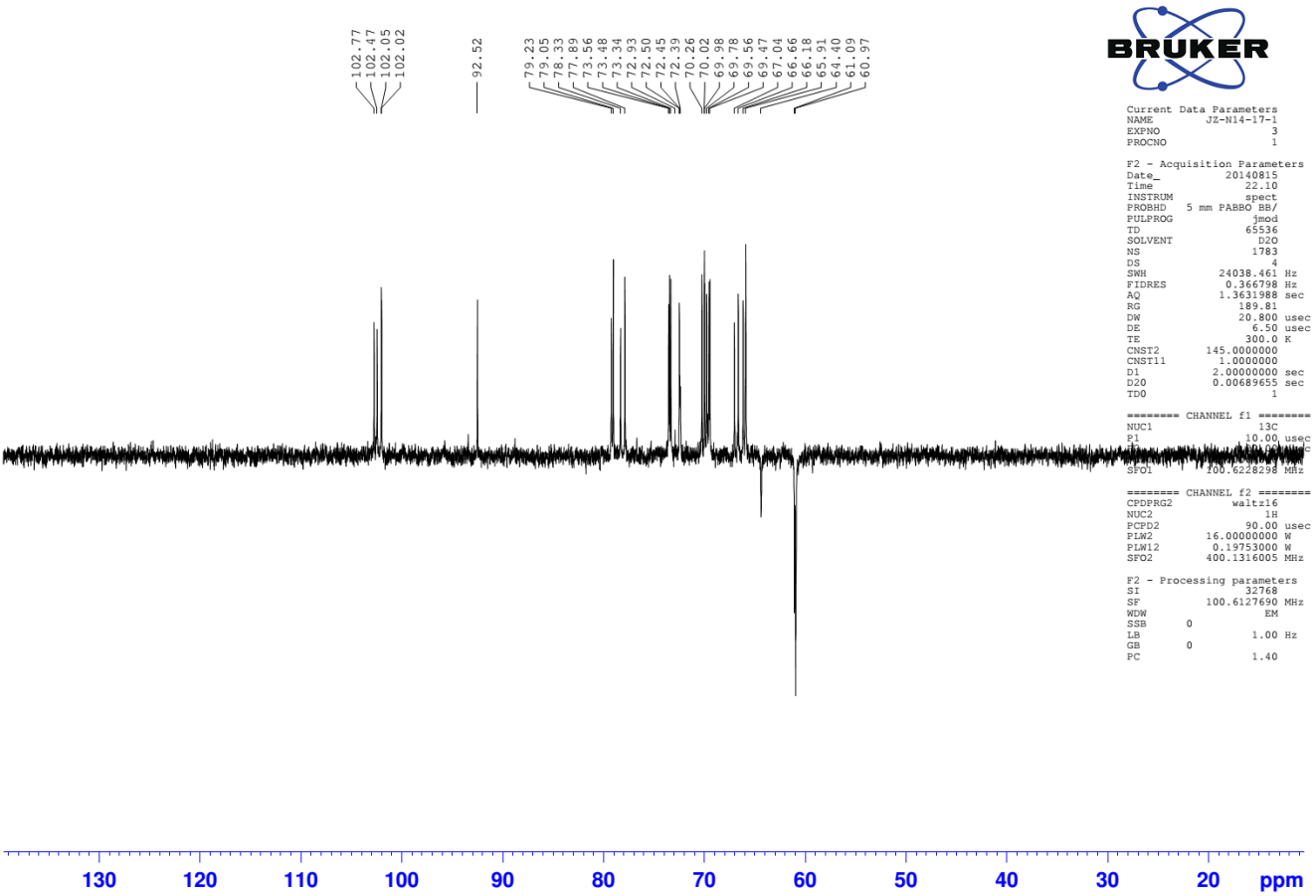
F2 - Processing parameters
SI                   1024
SF          400.1299721 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF          100.6127523 MHz
WDW               States
SSB       0
LB        0 Hz
GB        0
```

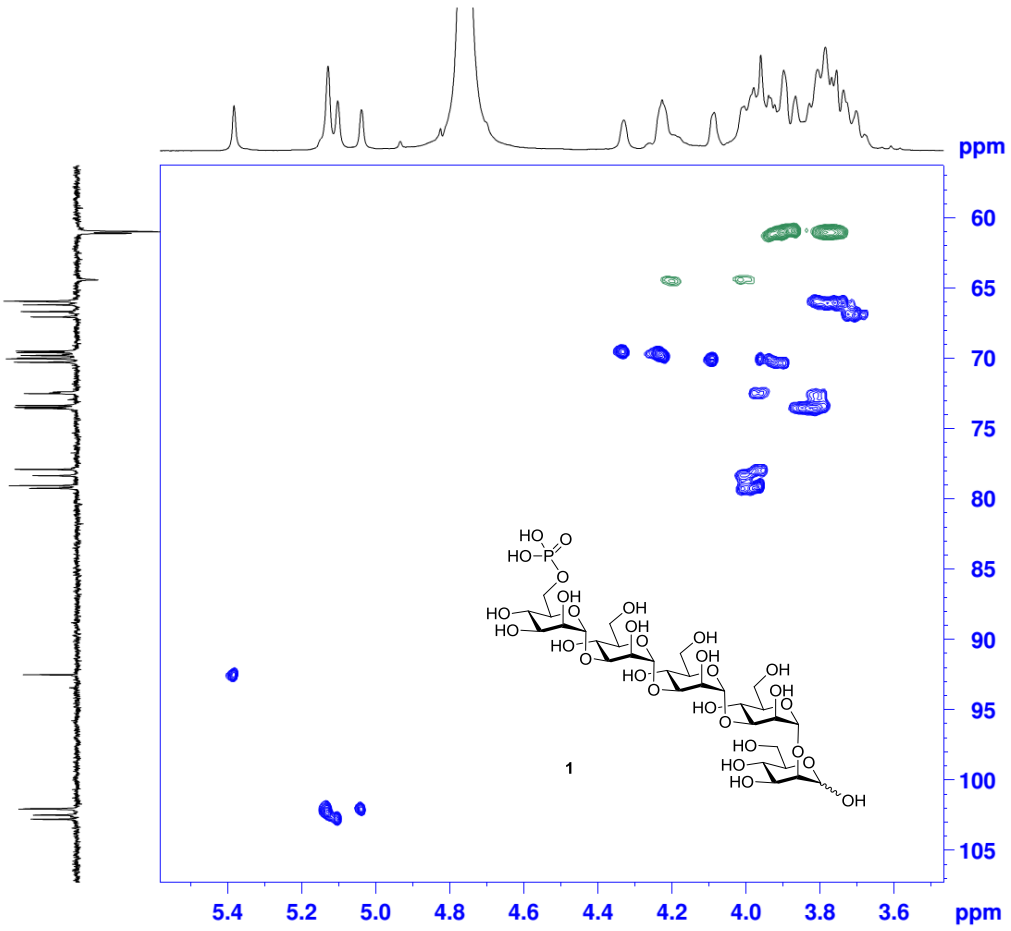
^{1}H NMR spectrum for compound **1**



^{13}C-APT NMR spectrum for compound **1**



HSQC spectrum for compound **1**




```
Current Data Parameters
NAME          JZ-N14-17-1
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140815
Time                23.51
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                   1024
SOLVENT               D2O
NS                     26
DS                     16
SWH             2100.840 Hz
FIDRES          2.051602 Hz
AQ             0.2437620 sec
RG                 189.81
DW                238.000 usec
DE                   6.50 usec
TE                  300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.35213399 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
P2                   20.00 usec
P28                1000.00 usec
PLW1         16.00000000 W
SFO1         400.1320482 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                80.00 usec
PLW2         73.00000000 W
PLW12         1.14059997 W
SFO2         100.6202727 MHz

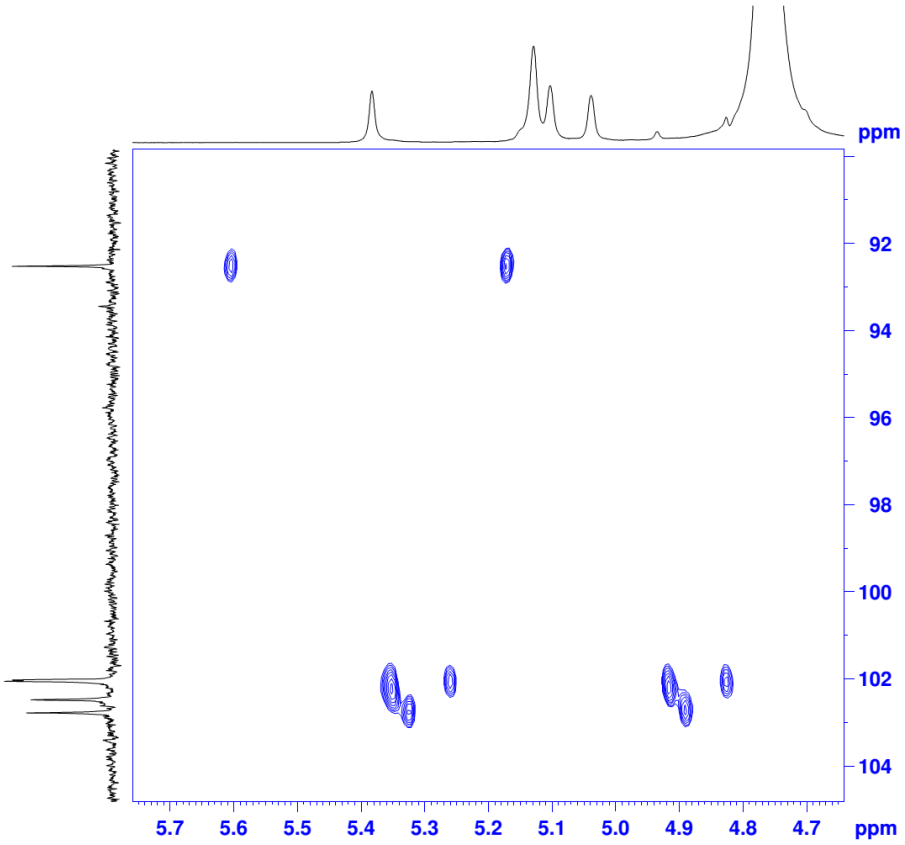
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF            400.1299748 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                     1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF            100.6127586 MHz
WDW           States-TPPI
SSB                       2
LB        0 Hz
GB        0
```

Coupled-HSQC spectrum of compound **1**




```
Current Data Parameters
NAME          JZ-N14-17-1-2
EXPNO                   9
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140816
Time                 2.51
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcedetgp
TD                   1024
SOLVENT               D2O
NS                     16
DS                     16
SWH             2100.840 Hz
FIDRES          2.051602 Hz
AQ             0.2437620 sec
RG                 189.81
DW                238.000 usec
DE                   6.50 usec
TE                  300.0 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.35213399 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D21           0.00345000 sec
IN0           0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
P2                   20.00 usec
P28                1000.00 usec
PLW1         16.00000000 W
SFO1         400.1320482 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                80.00 usec
PLW2         73.00000000 W
PLW12     0 W
SFO2         100.6202727 MHz

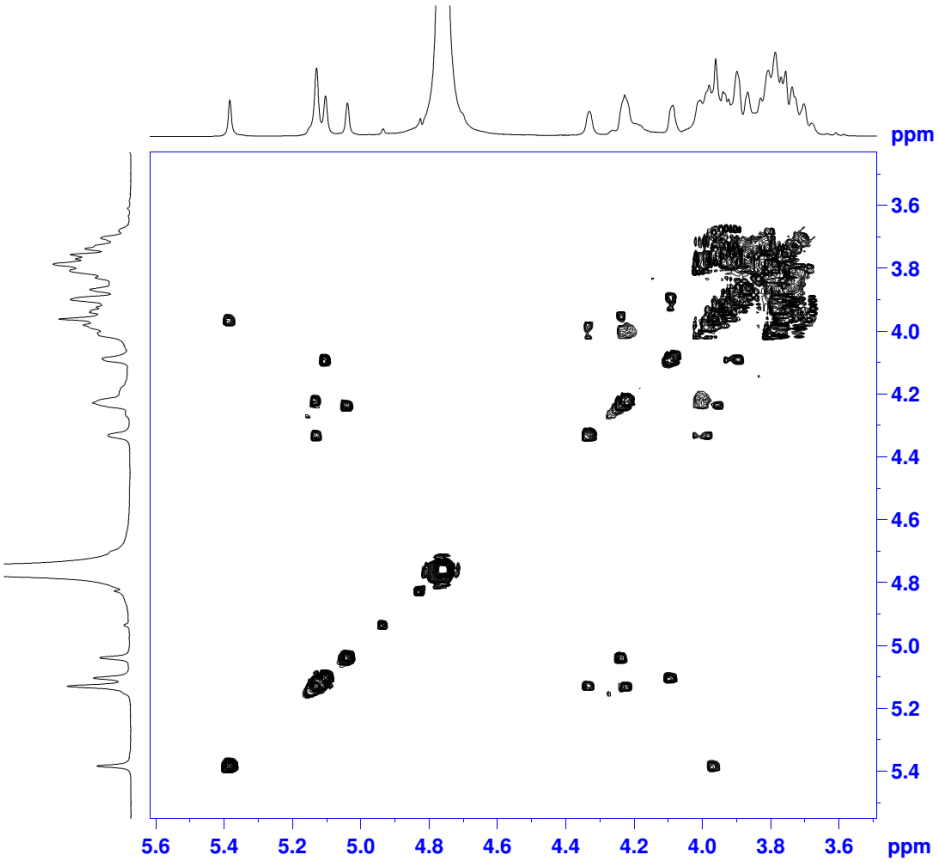
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            100.6203 MHz
FIDRES          65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF            400.1299695 MHz
WDW                   QSINE
SSB                       2
LB        0 Hz
GB        0
PC                     1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF            100.6127581 MHz
WDW
SSB                       2
LB        0 Hz
GB        0
```

COSY spectrum for compound **1**




```
Current Data Parameters
NAME        JZ-N14-17-1-2
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140815
Time               20.31
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT               D2O
NS                      4
DS                      8
SWH             2100.840 Hz
FIDRES          1.025801 Hz
AQ             0.4874740 sec
RG                 26.04
DW                238.000 usec
DE                   6.50 usec
TE                  300.0 K
D0            0.00000300 sec
D1            1.70426905 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00047600 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.00 usec
P1                  10.00 usec
P17                2500.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1         400.1320482 MHz

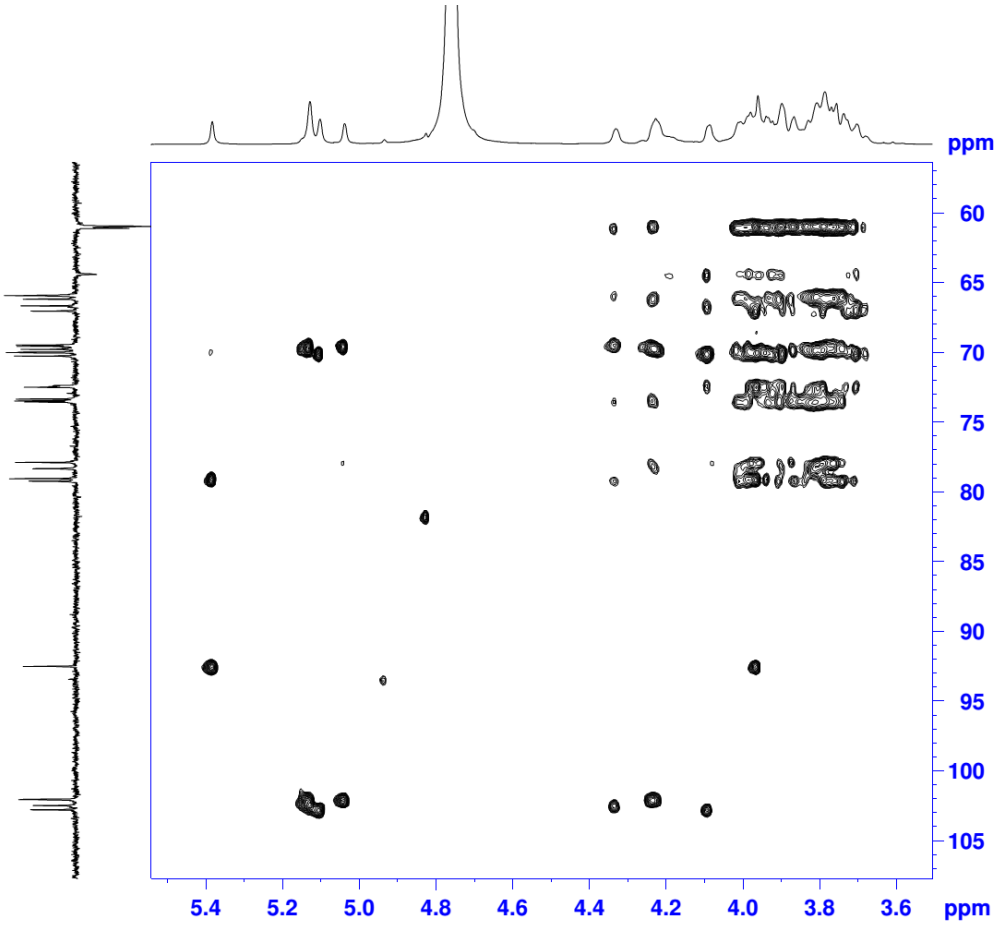
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1              400.132 MHz
FIDRES          16.412815 Hz
SW                 5.250 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF            400.1299722 MHz
WDW                  QSINE
SSB        0
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            400.1299723 MHz
WDW                    SIN
SSB        0
LB         0 Hz
GB         0
```

HSQC-TOCSY spectrum for compound **1**




```
Current Data Parameters
NAME        JZ-N14-17-1-2
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140817
Time                1.48
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG      hsqcetgpml
TD                   1024
SOLVENT               D2O
NS                     30
DS                     16
SWH             2100.840 Hz
FIDRES          2.051602 Hz
AQ             0.2437620 sec
RG                 189.81
DW                238.000 usec
DE                   6.50 usec
TE                  300.0 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.35213399 sec
D4            0.00172414 sec
D9            0.12000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00003000 sec
L1                     66
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P5                  17.34 usec
P6                  26.00 usec
P7                  52.00 usec
P17                2500.00 usec
P28                1000.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
SFO1         400.1320482 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               80.00 usec
PLW2          73.00000000 W
PLW12          1.14059997 W
SFO2         100.6202727 MHz

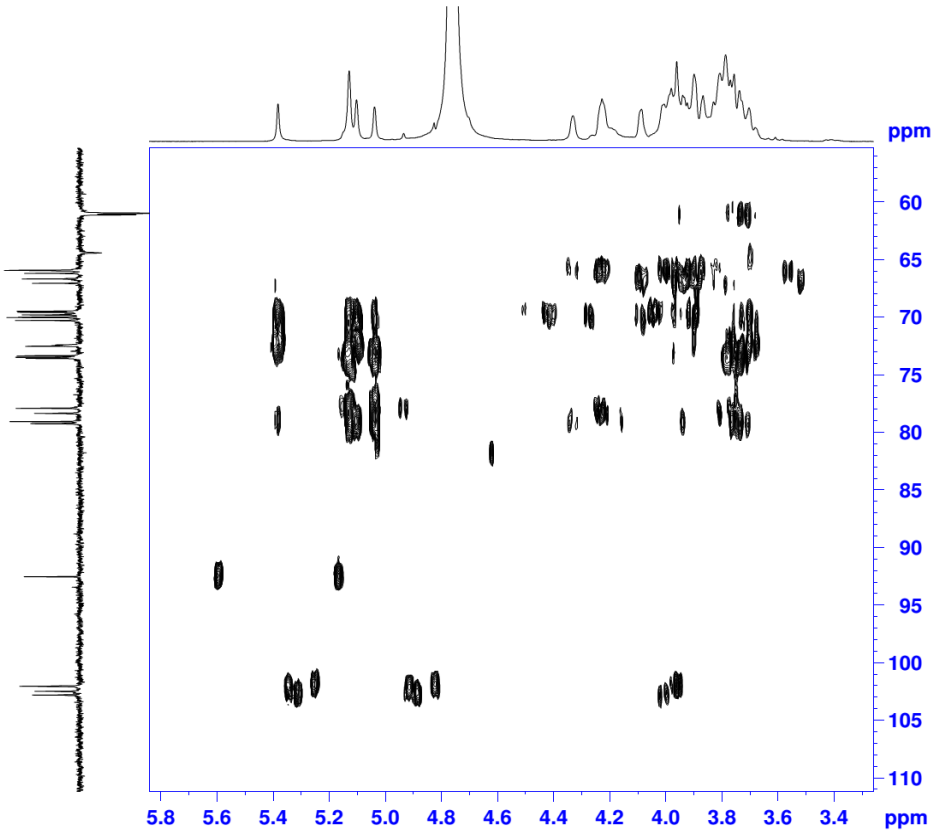
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPNAM2         SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1          100.6203 MHz
FIDRES        65.104164 Hz
SW               165.639 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF            400.1299757 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF            100.6127596 MHz
WDW          States-TPPI
SSB                      2
LB         0 Hz
GB         0
```

HMBC spectrum for compound **1**




```
Current Data Parameters
NAME          JZ-N14-17-1
EXPNO                   6
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140817
Time                 5.32
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       hmbcgpndqf
TD                   4096
SOLVENT               D2O
NS                     58
DS                     16
SWH             2100.840 Hz
FIDRES          0.512900 Hz
AQ              0.9748980 sec
RG                 189.81
DW                 238.000 usec
DE                   6.50 usec
TE                  300.0 K
CNST13          8.0000000
D0             0.00000300 sec
D1             0.90935671 sec
D6             0.06250000 sec
D16            0.00020000 sec
IN0            0.00002235 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
PLW1          16.00000000 W
SFO1         400.1320482 MHz

======== CHANNEL f2 ========
NUC2                  13C
P3                  10.00 usec
PLW2          73.00000000 W
SFO2         100.6228138 MHz

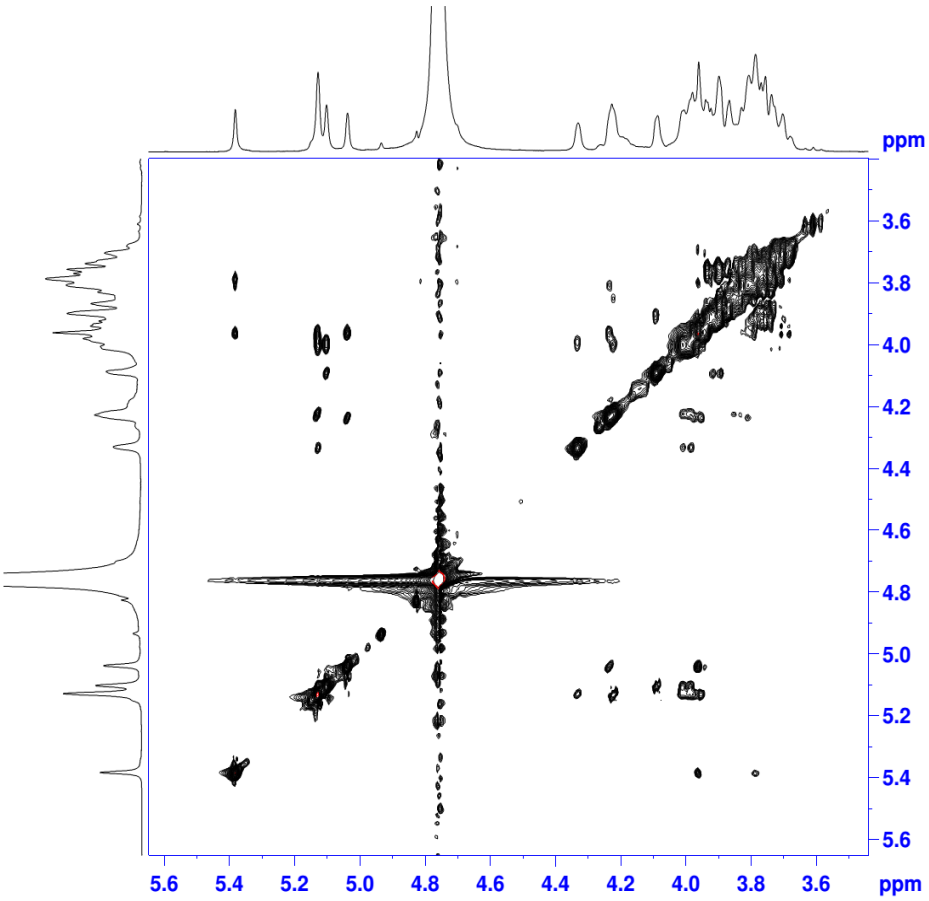
====== GRADIENT CHANNEL =====
GPNAM1        SMSQ10.100
GPNAM2        SMSQ10.100
GPNAM3        SMSQ10.100
GPZ1                50.00 %
GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            100.6228 MHz
FIDRES        178.782639 Hz
SW                222.095 ppm
FnMODE                  QF

F2 - Processing parameters
SI                    1024
SF           400.1299722 MHz
WDW                   SINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF           100.6127690 MHz
WDW                 States
SSB       0
LB        0 Hz
GB        0
```

ROESY spectrum for compound **1**




```
Current Data Parameters
NAME          JZ-N14-17-1
EXPNO                   8
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140816
Time                22.41
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG     roesyphpp.2
TD                   2048
SOLVENT               D2O
NS                     16
DS                     32
SWH             2100.840 Hz
FIDRES          1.025801 Hz
AQ              0.4874740 sec
RG                 22.51
DW                 238.000 usec
DE                   6.50 usec
TE                  300.0 K
D0             0.00022763 sec
D1             1.76325095 sec
D11            0.03000000 sec
D12            0.00002000 sec
IN0            0.00047600 sec
L4                   1587
P15           400000.00 usec

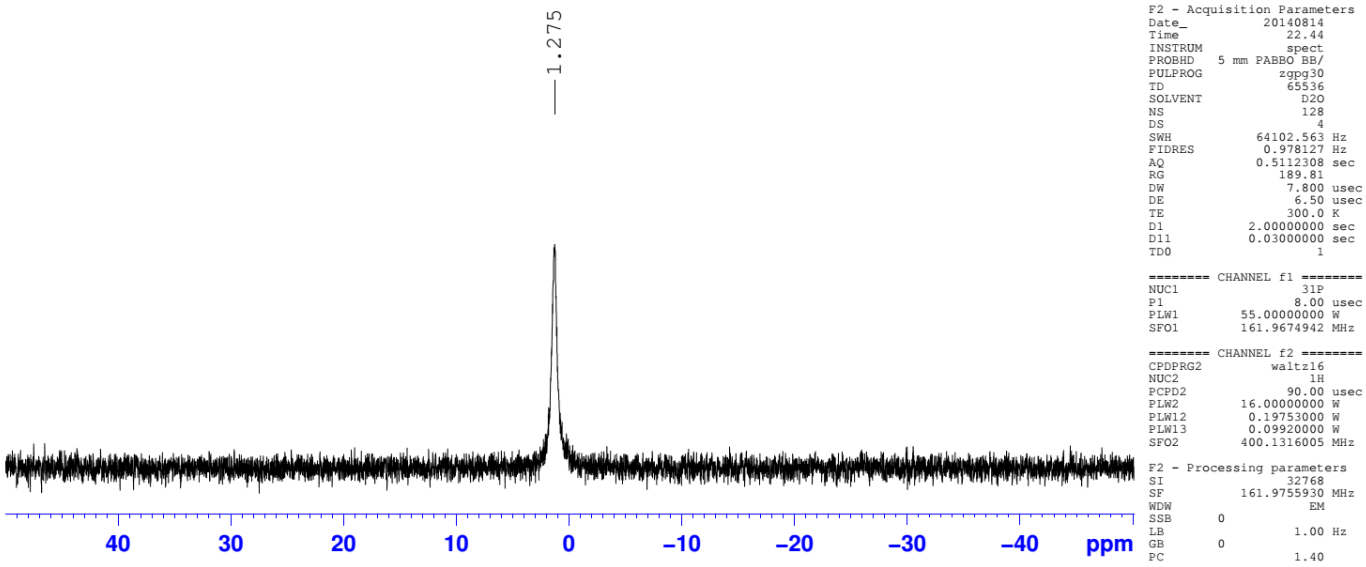
======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
P17               2500.00 usec
P25                126.00 usec
PLW1          16.00000000 W
PLW10          2.36689997 W
PLW27          0.40312001 W
SFO1         400.1320482 MHz

F1 - Acquisition parameters
TD                    256
SFO1            400.132 MHz
FIDRES          8.206408 Hz
SW                 5.250 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                    1024
SF           400.1299759 MHz
WDW                  QSINE
SSB                       2
LB        0 Hz
GB        0
PC                    1.00

F1 - Processing parameters
SI                    1024
MC2          States-TPPI
SF           400.1299750 MHz
WDW
SSB                       2
LB        0 Hz
GB        0
```

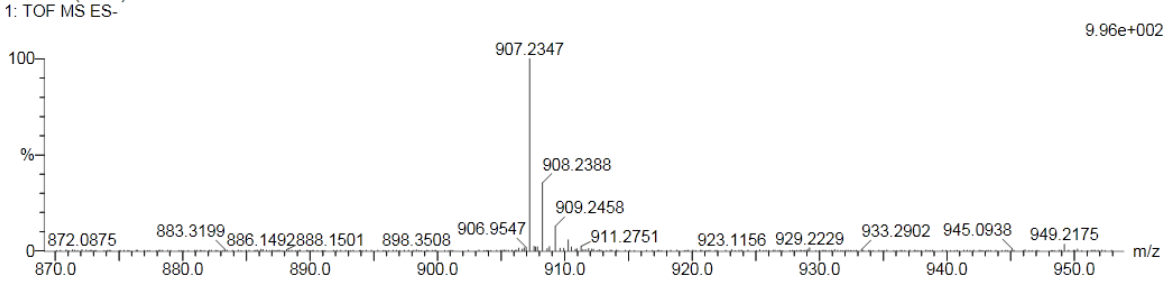
^{31}P NMR spectrum for compound **1**



HRESIMS report for compound **1**

Single Mass Analysis
Tolerance = 1000.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 30-30 H: 52-52 O: 29-29 P: 1-1
TEST1 6 (0.509)
1: TOF MS ES-



Minimum:				-1.5			
Maximum:		1000.0	1000.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
907.2347	907.2332	1.5	1.7	5.5	43.3	0.0	C30 H52 O29 P

2. DFT calculation studies

The structures of plausible intermediates **E, F, C and D** (see Figure S1 for their chemical structures) were used in the computational modeling. The minimum energies of their conformations were determined from fully optimized structures without any conformational restraints. For the calculations, the DFT program package Gaussian 09[1] was employed with 6-31g (d) basis set[2] and the M06 functional.[3] The optimized Gibbs free energy difference between oxacarbenium ions **E** and **F** in vacuum is 13.2 kcal/mol with **F** having the lower energy (Table S1). The iodonium sulfide **D** has the optimized Gibbs free energy of 10.7 lower than **C** in vacuum. A solvation energy is also considered in computational study. The single-point energies for all stationary points have been calculated at M06/lanl2zd[4] level for iodine atom and M06/6-31g (d) level for other atoms with the IEFPCM solvation model[5] and CH_2Cl_2 as the solvent on optimized structures in gas phase. The relative free energy in solvent is calculated in the following way: the solvation free energy is obtained from calculation for each species. The difference in solvation free energy is added to the difference of free energy in gas phase. The relative free energy in solvent is shown in Table 1. The optimized geometries of intermediates **E, F, C** and **D** are also shown below (Figure S2).

Figure S1. Chemical structures of plausible intermediates **C, D, E, F**

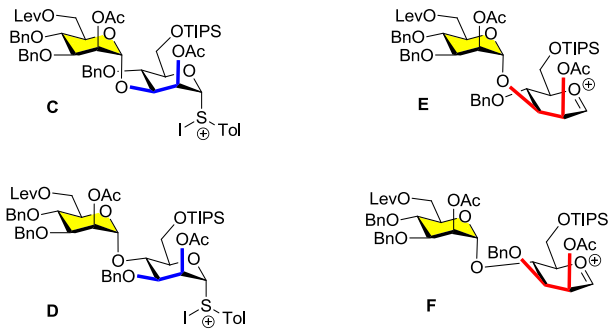
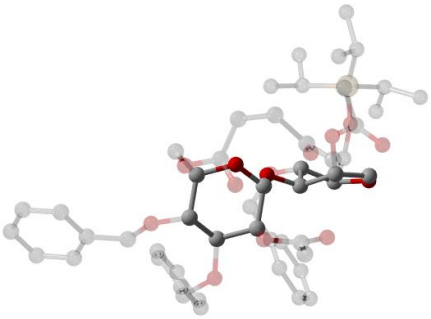
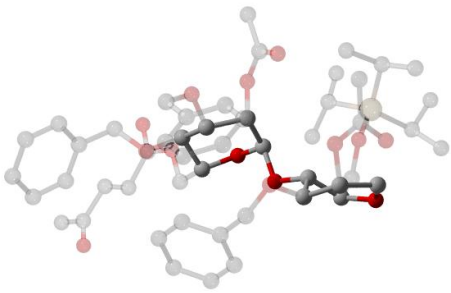


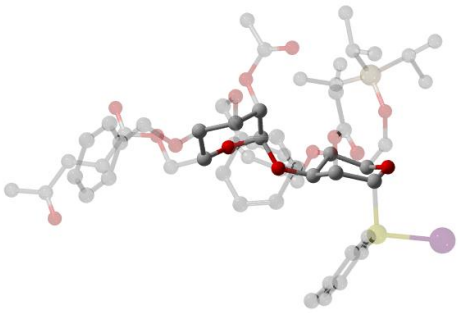
Figure S2. Geometries of of plausible intermediates **C, D, E, F**



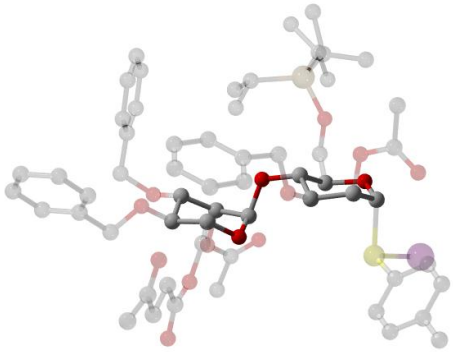
Geometry of oxacarbenium ion E



Geometry of oxacarbenium ion F



Geometry of iodonium sulfide C



Geometry of iodonium sulfide D

Table S1. Energy difference between plausible intermediate analogues

Environment	G(**E**)-G(**F**) (kcal/mol)	G(**C**)-G(**D**) (kcal/mol)
Vacuum	13.2	10.7
CH_2Cl_2	18.6	9.2

Table S2. Tables of atom coordinates for intermediates C, D, E, F

Coordinates for the optimized intermediate C

Elements	X	Y	Z
C	-4.530998	-1.777347	-0.715708
O	-1.698855	1.083152	1.334617
O	-2.068981	3.225213	1.913930
C	-1.754615	2.106520	2.242345
C	-1.382537	1.622634	3.597254
O	-4.419872	-2.091002	0.624167
Si	-4.035056	-3.526272	1.438473
C	-5.698358	-4.299170	1.898240
C	-3.015997	-2.870938	2.889867
C	-3.002626	-4.704953	0.343757
C	-6.572929	-4.402841	0.645442
C	-6.440790	-3.508451	2.974186
C	-2.806901	-3.910752	3.989647
C	-3.539525	-1.560367	3.473973
C	-3.447042	-6.166875	0.443667
C	-1.500491	-4.628854	0.631418
O	-1.744325	-2.130991	-1.241698
C	-0.867745	-3.516419	-2.892819
C	-1.812748	-4.416304	-3.384078
C	-1.480302	-5.754522	-3.563002
C	-0.196533	-6.195913	-3.251028
C	0.750311	-5.301667	-2.758238
C	0.414599	-3.964537	-2.573642
C	-1.258602	-2.106655	-2.583252
H	-4.273535	-2.614214	-1.388931
H	-5.560740	-1.464086	-0.956634
H	-1.564466	2.410580	4.332018
H	-1.942673	0.715237	3.850424
H	-0.321302	1.331562	3.606110
H	-5.504852	-5.315959	2.281499
H	-2.023811	-2.641538	2.455816
H	-3.144519	-4.380193	-0.703495
H	-6.076311	-4.917722	-0.190686
H	-7.506741	-4.944549	0.854051
H	-6.855671	-3.399036	0.293894
H	-5.907232	-3.502000	3.933888

H	-7.439057	-3.933379	3.157337
H	-6.584435	-2.461711	2.665307
H	-2.409881	-4.864219	3.609388
H	-2.100558	-3.534110	4.745352
H	-3.749451	-4.137907	4.510098
H	-3.620720	-0.777934	2.703767
H	-2.856944	-1.210790	4.263546
H	-4.534058	-1.677425	3.927247
H	-4.494152	-6.322249	0.154801
H	-2.828019	-6.799174	-0.210451
H	-3.328975	-6.554969	1.466981
H	-1.105337	-3.605365	0.589187
H	-0.935307	-5.219970	-0.105385
H	-1.268744	-5.039305	1.626336
H	-2.817185	-4.063137	-3.627170
H	-2.218862	-6.453469	-3.951243
H	0.067037	-7.242114	-3.395495
H	1.751689	-5.648581	-2.510166
H	1.142176	-3.262779	-2.159856
H	-0.387520	-1.433889	-2.656559
H	-2.043588	-1.746970	-3.273386
C	-1.831566	1.426208	-0.035036
C	-1.269911	0.270635	-0.864595
C	-2.157356	-0.946017	-0.629947
C	-3.594242	-0.629464	-1.044897
C	-3.323926	1.623119	-0.292632
H	-1.365521	0.570065	-1.928776
H	-1.273363	2.352274	-0.232164
H	-3.651005	-0.403119	-2.126285
H	-3.773813	2.366390	0.374094
H	-2.180689	-1.166279	0.450704
O	-4.090156	0.535526	-0.336631
C	4.032119	-1.111322	-1.299567
O	4.474597	-2.248786	-0.578777
C	5.638418	-2.880814	-0.879956
O	5.919219	-3.882232	-0.276565
C	6.511821	-2.257158	-1.937655
C	7.724123	-3.108616	-2.245938
C	8.619955	-2.476311	-3.287932
C	9.869490	-3.240218	-3.632422
O	8.342397	-1.412639	-3.803221
O	2.206574	0.811075	2.932581
C	2.354937	3.237699	2.516231
C	1.180911	3.837258	2.976060
C	0.656279	4.958047	2.342641
C	1.316287	5.499321	1.242924
C	2.488115	4.912056	0.774890

C	3.002753	3.782534	1.404640
C	2.904586	2.024974	3.216246
O	4.305279	0.835867	0.831975
C	6.511066	1.520943	1.369397
C	6.910143	1.987324	0.114403
C	7.848778	3.005510	0.008407
C	8.399967	3.567842	1.158411
C	8.005452	3.112141	2.410959
C	7.060478	2.094928	2.513875
C	5.502099	0.420358	1.474262
O	1.324131	-1.753819	2.216299
O	-0.247230	-1.397231	3.804386
C	0.661853	-2.056091	3.357694
C	1.183975	-3.331195	3.936985
H	4.829109	-0.362561	-1.411248
H	3.684039	-1.407614	-2.300692
H	5.936801	-2.067542	-2.855326
H	6.834550	-1.257672	-1.603740
H	8.306040	-3.304896	-1.332812
H	7.420265	-4.109277	-2.590086
H	10.532264	-3.289371	-2.757408
H	9.634319	-4.277243	-3.906169
H	10.395972	-2.748782	-4.455246
H	0.693147	3.435810	3.865501
H	-0.259708	5.411566	2.718233
H	0.928037	6.399293	0.764347
H	3.013424	5.341564	-0.077654
H	3.915786	3.311463	1.039136
H	3.974623	1.920927	2.993864
H	2.797762	2.137846	4.302759
H	6.476791	1.545504	-0.784586
H	8.159676	3.358234	-0.973443
H	9.140285	4.361386	1.074361
H	8.431760	3.549284	3.312016
H	6.747976	1.736256	3.495654
H	5.869787	-0.509044	1.000110
H	5.300062	0.178053	2.533205
H	0.788345	-3.468695	4.945792
H	0.860383	-4.168916	3.305459
H	2.278430	-3.338037	3.946797
C	0.653437	-0.984407	0.079311
H	-0.021264	-1.847918	0.053033
O	1.795549	-1.388827	-0.588179
C	0.925212	-0.574892	1.518765
H	0.005141	-0.198238	1.972022
C	3.259685	-0.109573	0.895047
H	3.576886	-1.013865	1.436540

C	2.889816	-0.480360	-0.544261
H	2.623823	0.452154	-1.074899
C	2.027087	0.468970	1.582520
H	1.686656	1.350574	1.005297
O	0.098199	0.131193	-0.623642
S	-3.457671	2.539917	-2.098546
I	-5.872260	3.161605	-2.005202
C	-2.520787	4.015963	-1.944355
C	-1.759076	4.368162	-3.069116
C	-2.494995	4.789762	-0.777433
C	-0.941269	5.482153	-3.002024
H	-1.807147	3.768826	-3.976902
C	-1.665998	5.895821	-0.736599
H	-3.087713	4.527442	0.096000
C	-0.875186	6.257292	-1.837464
H	-0.340401	5.760890	-3.866691
H	-1.629760	6.498813	0.169890
C	0.037337	7.437607	-1.771256
H	1.077136	7.107827	-1.627633
H	0.014404	8.017844	-2.701639
H	-0.216649	8.105601	-0.940779

Coordinates for the optimized intermediate D

ATOM	X	Y	Z
C	2.884105	-2.592163	0.758413
O	2.919906	0.358686	-2.525586
O	4.533605	1.767632	-3.216295
C	3.796287	0.841486	-3.452093
C	3.726320	0.062890	-4.721704
O	2.852773	-3.149994	-0.508386
Si	2.090385	-4.421996	-1.300152
C	0.267382	-4.627024	-0.818555
C	3.073749	-6.010813	-0.965594
C	2.259781	-3.859141	-3.099148
C	-0.658693	-3.574835	-1.428384
C	0.074478	-4.691228	0.697428
C	2.226763	-7.277479	-1.097523
C	3.774906	-5.969511	0.393002
C	1.845683	-4.962030	-4.070983
C	3.671325	-3.357661	-3.396547
O	0.412510	1.182441	-1.357375
C	-1.473956	0.846460	-2.734515
C	-1.750449	2.182290	-3.039025
C	-3.061371	2.613711	-3.202715
C	-4.109401	1.701530	-3.079675
C	-3.843032	0.364498	-2.798112

C	-2.527961	-0.059086	-2.618897
C	-0.059843	0.420226	-2.474845
H	2.080220	-2.939496	1.426482
H	3.842245	-2.813126	1.256757
H	3.988301	0.711932	-5.561266
H	4.463835	-0.748987	-4.677471
H	2.740874	-0.390203	-4.867860
H	-0.021294	-5.608801	-1.238117
H	3.857422	-6.048874	-1.743359
H	1.568038	-3.002634	-3.221831
H	-0.604249	-3.551903	-2.526698
H	-1.708006	-3.771886	-1.156132
H	-0.416807	-2.570257	-1.049753
H	0.749328	-5.406921	1.189787
H	-0.958026	-4.967461	0.955654
H	0.251434	-3.701594	1.140054
H	1.702387	-7.342777	-2.061452
H	2.851241	-8.177839	-1.004853
H	1.465044	-7.335179	-0.305926
H	4.503988	-5.151001	0.451877
H	4.312661	-6.908712	0.588976
H	3.056937	-5.834155	1.217323
H	0.820811	-5.317850	-3.889635
H	1.894531	-4.621070	-5.115577
H	2.515329	-5.831643	-3.987631
H	3.931584	-2.501304	-2.756734
H	3.767758	-3.055873	-4.452057
H	4.426059	-4.139645	-3.222907
H	-0.925289	2.890755	-3.124090
H	-3.287198	3.659050	-3.408229
H	-5.135998	2.047757	-3.201796
H	-4.659995	-0.349666	-2.695406
H	-2.318209	-1.101474	-2.368620
H	-0.024658	-0.659961	-2.266403
H	0.581706	0.614068	-3.348718
C	2.842915	1.087665	-1.303004
C	2.757721	-1.085269	0.628567
C	4.028867	0.618423	-0.465372
H	2.917744	2.161459	-1.519191
H	2.744215	-0.640842	1.639867
H	4.992909	0.792708	-0.957745
O	3.979362	-0.632785	-0.011322
C	-2.405949	2.035452	0.386671
O	-2.750715	2.814858	1.526230
C	-3.488332	3.943974	1.386459
O	-3.649721	4.656593	2.342983
C	-4.090060	4.207238	0.028371

C	-4.818426	5.530595	-0.040088
C	-5.344406	5.825340	-1.426972
C	-6.240841	7.026824	-1.547211
O	-5.061543	5.130658	-2.383875
O	-2.956440	-2.302527	2.825715
C	-4.073152	-3.719714	1.134566
C	-3.527348	-5.002915	1.207969
C	-3.459079	-5.811963	0.078460
C	-3.938014	-5.341364	-1.141957
C	-4.478387	-4.060884	-1.227258
C	-4.542574	-3.252199	-0.095193
C	-4.180571	-2.880121	2.377389
O	-4.095817	-0.208475	1.068647
C	-6.414554	0.248650	0.939321
C	-6.433100	0.648419	-0.399001
C	-7.574461	0.480008	-1.171726
C	-8.718528	-0.083177	-0.609009
C	-8.708895	-0.481234	0.723154
C	-7.558192	-0.322231	1.491650
C	-5.167018	0.428376	1.747522
O	-0.949378	-0.814832	3.836394
O	1.188712	-1.420693	4.207865
C	0.140591	-0.969436	4.614794
C	-0.139491	-0.517987	6.011954
H	-3.267742	1.879200	-0.275294
H	-1.614391	2.537212	-0.187972
H	-3.323237	4.154044	-0.758200
H	-4.786520	3.388930	-0.219380
H	-5.644934	5.568741	0.685070
H	-4.157581	6.357902	0.264373
H	-7.199871	6.821386	-1.051393
H	-5.807083	7.899003	-1.040767
H	-6.427749	7.256893	-2.599754
H	-3.166574	-5.372417	2.169803
H	-3.041565	-6.815455	0.152511
H	-3.897998	-5.976928	-2.025206
H	-4.859331	-3.692043	-2.178900
H	-4.962106	-2.246314	-0.154469
H	-4.951658	-2.111395	2.234853
H	-4.489249	-3.508066	3.223116
H	-5.529541	1.074025	-0.838839
H	-7.574716	0.792271	-2.216043
H	-9.616250	-0.212925	-1.210601
H	-9.598311	-0.925946	1.165910
H	-7.547868	-0.645420	2.533439
H	-4.927764	1.497815	1.888631
H	-5.291290	-0.005241	2.756660

H	0.781378	-0.528510	6.598738
H	-0.580758	0.484652	6.008483
H	-0.874521	-1.189793	6.470916
C	0.009041	-0.372980	1.681039
H	0.903989	-0.100213	2.254937
O	-0.630856	0.832366	1.423707
C	-0.841759	-1.334343	2.510281
H	-0.347554	-2.312665	2.556182
C	-2.848433	-0.097432	1.719151
H	-2.949189	0.418197	2.688319
C	-1.905276	0.684217	0.806401
H	-1.795690	0.115056	-0.131764
C	-2.246290	-1.484118	1.940536
H	-2.145455	-1.968264	0.946104
O	0.355971	-1.080959	0.508593
S	4.112850	1.856107	1.121792
I	6.297735	1.098508	2.050426
C	4.346873	3.453927	0.434105
C	3.599113	4.478660	1.029483
C	5.192799	3.707621	-0.654728
C	3.682102	5.759708	0.506322
H	2.956229	4.267307	1.882612
C	5.257636	4.993004	-1.154749
H	5.783593	2.917770	-1.113888
C	4.509111	6.038015	-0.585720
H	3.098458	6.561357	0.955810
H	5.902562	5.203013	-2.006975
C	4.616190	7.419551	-1.142519
H	3.893510	8.103314	-0.685559
H	5.621143	7.830062	-0.973880
H	4.453144	7.421054	-2.227913
C	1.517124	-0.696081	-0.186020
H	1.544130	-1.331842	-1.083535
C	1.520151	0.767933	-0.617458
H	1.474549	1.399583	0.288800

Coordinates for the optimized intermediate E

ATOM	X	Y	Z
C	3.52055	1.74089	2.19778
O	4.25966	2.65952	1.39902
C	3.65606	3.68615	0.75283
O	4.06058	4.00443	-0.33826
C	2.57704	4.44553	1.48910
C	2.17917	5.67984	0.70105
C	1.58852	5.33523	-0.65130
C	1.87703	6.28860	-1.76776

O	0.89623	4.34288	-0.80445
O	-0.06872	0.38099	0.07778
C	-1.64826	1.53171	-1.39414
C	-2.96478	1.35937	-2.06552
O	-3.65928	0.32366	-2.04280
C	-3.32201	-0.88183	-1.20203
C	-4.64570	-1.24482	-0.56873
O	3.42532	-1.15301	-1.85105
C	3.17920	-3.48420	-1.08104
C	2.48641	-4.28322	-1.99211
C	1.64875	-5.30161	-1.55270
C	1.49442	-5.53187	-0.18856
C	2.17768	-4.73981	0.73078
C	3.01689	-3.72154	0.28744
C	4.08423	-2.39197	-1.57849
O	4.46645	-0.73522	0.94028
C	6.60577	-1.28388	1.81737
C	6.65366	-2.67178	1.67384
C	7.32978	-3.45345	2.60080
C	7.97248	-2.85250	3.68076
C	7.93156	-1.47134	3.83095
C	7.24678	-0.69195	2.90358
C	5.86160	-0.44962	0.82396
O	2.65626	1.51486	-2.03737
O	0.87336	2.13643	-3.26434
C	2.03792	2.28247	-2.95874
C	2.98014	3.29262	-3.51705
O	-1.86241	2.44663	-0.32546
O	-2.05459	4.10480	-1.83584
C	-1.92019	3.77726	-0.68882
C	-1.84114	4.63912	0.52142
O	-5.04662	-0.17779	0.22078
Si	-6.13425	-0.24759	1.52514
C	-7.85659	-0.64165	0.84921
C	-6.06400	1.52477	2.17832
C	-5.54917	-1.60620	2.70524
C	-8.03585	-2.11911	0.49630
C	-8.19344	0.23325	-0.35867
C	-4.66461	2.13966	2.14854
C	-6.68125	1.66199	3.57036
C	-6.52947	-1.83905	3.85793
C	-4.13456	-1.37912	3.23734
O	-1.88391	-1.75716	0.45812
C	-1.10085	-3.17732	-1.39685
C	-2.13448	-4.10849	-1.53147
C	-2.43683	-4.65357	-2.77342
C	-1.70134	-4.27678	-3.89632

C	-0.65752	-3.36668	-3.76885
C	-0.35790	-2.82249	-2.52246
C	-0.81696	-2.56650	-0.05491
H	4.25969	1.17268	2.77221
H	2.85175	2.25346	2.90173
H	1.71496	3.78179	1.62674
H	2.94494	4.71283	2.48969
H	1.41163	6.24662	1.25296
H	3.03199	6.35805	0.57053
H	1.67362	7.32388	-1.46224
H	2.95060	6.23729	-1.99998
H	1.28983	6.03550	-2.65513
H	-0.96615	1.97494	-2.14758
H	-3.39320	2.19722	-2.62624
H	-2.99835	-1.62680	-1.94083
H	-4.47550	-2.17464	0.00241
H	-5.37739	-1.46625	-1.36514
H	2.60995	-4.10093	-3.06136
H	1.10961	-5.91220	-2.27608
H	0.84752	-6.33636	0.15816
H	2.06777	-4.92403	1.79832
H	3.56190	-3.10293	1.00239
H	4.91138	-2.23629	-0.87470
H	4.51555	-2.67406	-2.54640
H	6.15612	-3.14273	0.82422
H	7.36421	-4.53434	2.47826
H	8.50971	-3.46365	4.40347
H	8.43585	-0.99725	4.67093
H	7.21717	0.39278	3.01708
H	6.04233	0.62278	1.00212
H	6.19035	-0.66581	-0.20884
H	2.46210	3.92598	-4.24014
H	3.39227	3.89154	-2.69445
H	3.82641	2.78892	-3.99798
H	-1.81185	5.68763	0.21743
H	-2.71082	4.46299	1.16549
H	-0.94257	4.37725	1.09028
H	-8.56795	-0.39537	1.65855
H	-6.69388	2.10082	1.47688
H	-5.53512	-2.53070	2.09712
H	-7.88135	-2.78534	1.35493
H	-9.04672	-2.31270	0.11005
H	-7.33408	-2.43255	-0.29272
H	-8.11797	1.30670	-0.13990
H	-9.21703	0.04292	-0.71105
H	-7.51778	0.02311	-1.20167
H	-4.22761	2.13072	1.13971

H	-4.69547	3.18342	2.49780
H	-3.96954	1.60234	2.81066
H	-7.68387	1.21635	3.63646
H	-6.77530	2.71909	3.85666
H	-6.05360	1.17921	4.33374
H	-7.55961	-2.01369	3.51774
H	-6.23076	-2.71359	4.45329
H	-6.55291	-0.98034	4.54261
H	-3.38740	-1.28385	2.43611
H	-3.81821	-2.21698	3.87573
H	-4.08367	-0.47226	3.85774
H	-2.70114	-4.40488	-0.64700
H	-3.23959	-5.38237	-2.86824
H	-1.93564	-4.70459	-4.86906
H	-0.06678	-3.08664	-4.63940
H	0.49654	-2.14750	-2.41601
H	-0.70436	-3.34529	0.70830
H	0.11763	-1.98844	-0.07134
C	-2.22341	-0.56259	-0.18349
H	-2.65395	0.08649	0.59716
C	-1.09353	0.20700	-0.85053
H	-0.75021	-0.35779	-1.73950
C	0.99519	1.22341	-0.36049
H	0.58308	2.14783	-0.77701
O	1.71759	1.64054	0.73336
C	1.84797	0.52018	-1.41004
H	1.21801	0.05203	-2.17833
C	3.63292	0.15985	0.23953
H	4.22904	0.92859	-0.27564
C	2.73167	0.81271	1.29502
H	2.27470	0.00909	1.89971
C	2.75189	-0.53138	-0.79280
H	2.10076	-1.25752	-0.26462

Coordinates for the optimized intermediate F

ATOM	X	Y	Z
O	-0.906668	0.047929	1.377197
C	-3.294738	-2.705249	2.001991
C	-4.486094	-1.769158	2.289707
O	-4.233856	-0.56558	2.794822
C	-3.035292	0.191761	2.445103
C	-3.449171	1.52693	1.883234
O	-3.475778	-3.097511	0.607183
O	-5.099078	-1.670976	0.877717
C	-4.45055	-2.43094	0.088454
C	-4.737184	-2.553679	-1.339456

O	-4.012638	1.347715	0.617639
Si	-4.589962	2.626226	-0.343845
C	-5.389577	1.705819	-1.793128
C	-3.107671	3.628896	-0.981201
C	-5.817939	3.647337	0.677009
C	-6.549168	0.809223	-1.361244
C	-4.325026	0.888426	-2.521961
C	-2.210611	4.231734	0.102198
C	-3.554468	4.723603	-1.953977
C	-6.724896	2.79241	1.566722
C	-6.678915	4.544835	-0.216251
O	-0.980689	-2.736708	1.449511
C	1.094069	-2.464693	2.72728
C	0.953096	-1.647383	3.852223
C	1.969212	-0.776547	4.22799
C	3.150536	-0.72579	3.491293
C	3.311752	-1.547379	2.37966
C	2.286432	-2.4092	2.003172
C	-0.004601	-3.38653	2.286325
H	-3.330884	-3.634634	2.577764
H	-5.298448	-2.223092	2.863838
H	-2.506752	0.352816	3.39666
H	-2.542521	2.154628	1.856721
H	-4.15208	1.999733	2.589729
H	-5.653682	-2.019949	-1.599963
H	-3.877977	-2.13895	-1.900216
H	-4.8035	-3.61414	-1.60954
H	-5.784209	2.462649	-2.492066
H	-2.493747	2.905307	-1.549627
H	-5.212652	4.300957	1.331497
H	-7.413655	1.384289	-1.005874
H	-6.901977	0.193534	-2.203873
H	-6.251955	0.133815	-0.54344
H	-3.560447	1.523922	-2.990859
H	-4.760619	0.264415	-3.318636
H	-3.801386	0.209604	-1.828581
H	-1.609442	3.473866	0.623155
H	-1.493895	4.937435	-0.341755
H	-2.784424	4.793871	0.854817
H	-4.241307	4.360534	-2.732118
H	-2.6888	5.1699	-2.462959
H	-4.061216	5.539572	-1.418651
H	-6.177749	2.09424	2.214554
H	-7.344141	3.429019	2.214571
H	-7.414182	2.187134	0.962362
H	-7.310783	3.945567	-0.888603
H	-6.086451	5.223157	-0.842552

H	-7.3548	5.165631	0.388777
H	0.052256	-1.711846	4.465981
H	1.849683	-0.150817	5.11034
H	3.952966	-0.055977	3.796401
H	4.23168	-1.521129	1.797192
H	2.413058	-3.062221	1.13799
H	0.384591	-4.205964	1.667821
H	-0.521131	-3.833411	3.153396
C	-2.127346	-0.605102	1.517681
H	-2.621718	-0.68399	0.535098
C	-1.943933	-1.996531	2.111478
H	-1.711986	-1.885186	3.186468
C	2.602713	2.041065	0.616957
O	2.736369	2.805156	-0.570875
C	3.726218	3.722076	-0.728528
O	3.761091	4.357724	-1.74803
C	4.730442	3.850486	0.385741
C	5.735322	4.952461	0.129202
C	6.820977	4.992958	1.18202
C	7.817275	6.112738	1.058346
O	6.877068	4.165182	2.068229
O	1.046193	-1.723035	-2.186998
C	1.123043	-4.046061	-1.403564
C	-0.26057	-4.211216	-1.479969
C	-0.866292	-5.3046	-0.869246
C	-0.102231	-6.247485	-0.186839
C	1.278939	-6.090303	-0.111497
C	1.88387	-4.991226	-0.712953
C	1.821391	-2.903801	-2.093407
O	3.203258	-0.495576	-0.670611
C	5.376292	-1.020766	-1.415688
C	6.164127	-0.743019	-0.296443
C	7.276131	-1.521837	-0.003503
C	7.615624	-2.587804	-0.833884
C	6.840839	-2.869015	-1.953148
C	5.723932	-2.089061	-2.239356
C	4.152323	-0.203477	-1.68922
O	-0.738322	0.20181	-2.240672
O	-2.140494	-1.455395	-2.868501
C	-1.46055	-0.488565	-3.142578
C	-1.301939	0.094478	-4.505982
H	3.552862	1.568667	0.906639
H	2.254714	2.673819	1.446576
H	4.221287	4.008936	1.347518
H	5.261488	2.894568	0.512354
H	6.200339	4.826	-0.860367
H	5.241988	5.93445	0.070231

H	8.258822	6.134941	0.053362
H	7.318023	7.080619	1.202424
H	8.605325	5.998965	1.807558
H	-0.860549	-3.479476	-2.023475
H	-1.945436	-5.434382	-0.942508
H	-0.580107	-7.108064	0.27834
H	1.885889	-6.82348	0.416545
H	2.966775	-4.864767	-0.653913
H	2.782018	-2.696326	-1.59495
H	2.046849	-3.173026	-3.1357
H	5.899424	0.097801	0.347849
H	7.886248	-1.292224	0.868097
H	8.490041	-3.195195	-0.608287
H	7.106851	-3.697523	-2.60689
H	5.11541	-2.308612	-3.117963
H	4.377676	0.8789	-1.684258
H	3.730394	-0.448323	-2.67878
H	-2.1257	-0.220708	-5.150756
H	-1.231764	1.18584	-4.462182
H	-0.357657	-0.277518	-4.924416
C	-0.719673	0.654557	0.091435
H	-1.616265	1.242481	-0.170688
O	0.316399	1.548261	0.186515
C	-0.513539	-0.422603	-0.974948
H	-1.241383	-1.235109	-0.85413
C	1.932821	0.090728	-0.849906
H	1.906822	0.726957	-1.749384
C	1.600943	0.946557	0.369843
H	1.587566	0.307083	1.270228
C	0.891378	-1.005867	-0.981883
H	0.976611	-1.673868	-0.107879

Table S3. Tables of atom coordinates for intermediates C, D, E, F

Intermediate C

Sum of electronic and zero-point Energies=	-4004.361102
Sum of electronic and thermal Energies=	-4004.285010
Sum of electronic and thermal Enthalpies=	-4004.284065
Sum of electronic and thermal Free Energies=	-4004.476199

Intermediate C-solvent

(Unpolarized solute)-Solvent	(kcal/mol)	=	-38.10
(Polarized solute)-Solvent	(kcal/mol)	=	-43.22
Solute polarization	(kcal/mol)	=	2.80
Total electrostatic	(kcal/mol)	=	-40.42

Cavitation energy	(kcal/mol)	=	109.64
Dispersion energy	(kcal/mol)	=	-56.73
Repulsion energy	(kcal/mol)	=	3.15
Total non electrostatic	(kcal/mol)	=	56.06
DeltaG (solv)	(kcal/mol)	=	15.64

Intermediate D

Sum of electronic and zero-point Energies=	-4004.373956
Sum of electronic and thermal Energies=	-4004.296682
Sum of electronic and thermal Enthalpies=	-4004.295738
Sum of electronic and thermal Free Energies=	-4004.493309

Intermediate D-solvent

(Unpolarized solute)-Solvent	(kcal/mol)	=	-37.20
(Polarized solute)-Solvent	(kcal/mol)	=	-40.66
Solute polarization	(kcal/mol)	=	1.85
Total electrostatic	(kcal/mol)	=	-38.81
Cavitation energy	(kcal/mol)	=	108.38
Dispersion energy	(kcal/mol)	=	-55.59
Repulsion energy	(kcal/mol)	=	3.14
Total non electrostatic	(kcal/mol)	=	55.94
DeltaG (solv)	(kcal/mol)	=	17.13

Intermediate E

Sum of electronic and zero-point Energies=	-3324.295831
Sum of electronic and thermal Energies=	-3324.229577
Sum of electronic and thermal Enthalpies=	-3324.228632
Sum of electronic and thermal Free Energies=	-3324.396442

Intermediate E-solvent

(Unpolarized solute)-Solvent	(kcal/mol)	=	-34.08
(Polarized solute)-Solvent	(kcal/mol)	=	-37.40
Solute polarization	(kcal/mol)	=	1.79
Total electrostatic	(kcal/mol)	=	-35.61
Cavitation energy	(kcal/mol)	=	94.36
Dispersion energy	(kcal/mol)	=	-49.11
Repulsion energy	(kcal/mol)	=	2.48
Total non electrostatic	(kcal/mol)	=	47.73
DeltaG (solv)	(kcal/mol)	=	12.13

Intermediate F

Sum of electronic and zero-point Energies=	-3324.316854
Sum of electronic and thermal Energies=	-3324.251399
Sum of electronic and thermal Enthalpies=	-3324.250454

Sum of electronic and thermal Free Energies=	-3324.417487

Intermediate F-solvent

(Unpolarized solute)-Solvent	(kcal/mol)	=	-38.87
(Polarized solute)-Solvent	(kcal/mol)	=	-43.97
Solute polarization	(kcal/mol)	=	2.79
Total electrostatic	(kcal/mol)	=	-41.19
Cavitation energy	(kcal/mol)	=	93.53
Dispersion energy	(kcal/mol)	=	-48.12
Repulsion energy	(kcal/mol)	=	2.47
Total non electrostatic	(kcal/mol)	=	47.88
DeltaG (solv)	(kcal/mol)	=	6.70

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