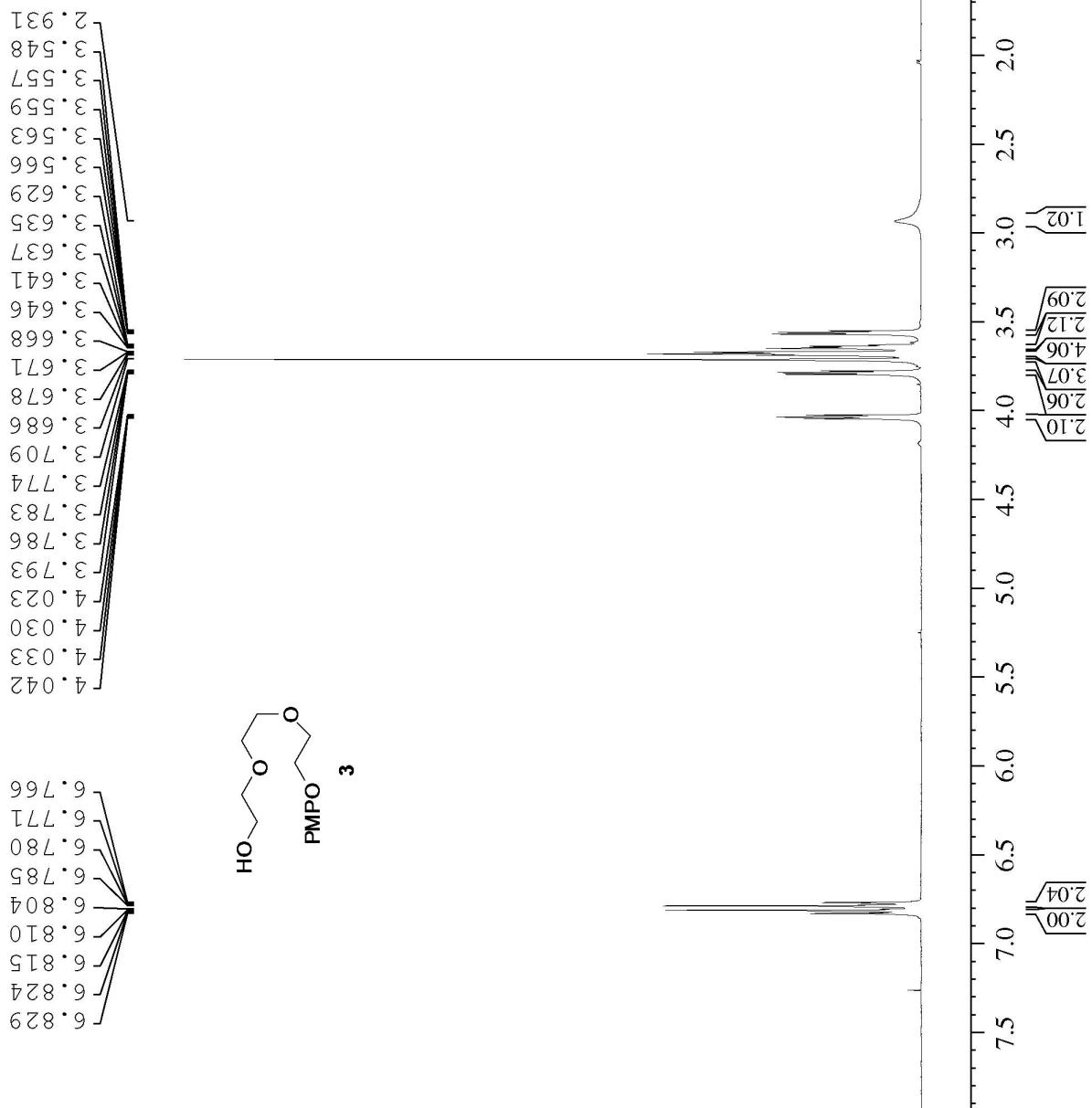
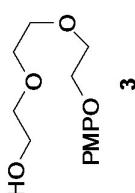
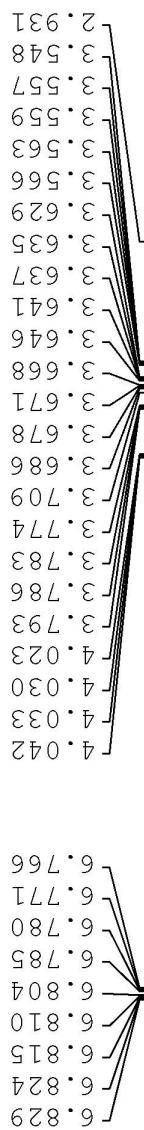




BM-AM-LINKERPENTA in CDCl<sub>3</sub>



Current Data Parameters  
NAME: BM-AM-SCHLENK108  
EPRFC: 110  
PROCBNO: 1  
F2 - Acquisition Parameters  
Date\_20151207  
Time\_10.48  
INSTRUM:spect  
PROBHD: 5 mm PABBO BB-  
PULPROG: zg30  
TD: 65536  
SOLVENT: CDCl<sub>3</sub>  
NS: 16  
DS: 2  
SWH: 10330.518 Hz  
FIDRES: 0.15162 Hz  
AQ: 3.1719423 sec  
RG: 25.4  
DW: 48.400 usec  
DE: 6.50 usec  
TE: 2863.5 K  
D1: 1.0000000 sec  
TD0: 1  
===== CHANNEL f1 =====  
NUC1: 1H  
P1: 14.05 usec  
PL1: 1.30 dB  
P1W: 15.30633643 W  
SFQ1: 500.2330891 kHz  
F2 - Processing Parameters  
SI: 131072  
SF: 500.2300150 MHz  
WDW: EM  
SSB: 0  
LB: 0.30 Hz  
GB: 0  
PC: 1.00

BM-AM-LINKERPENTA in  $\text{CDC}_{13}$

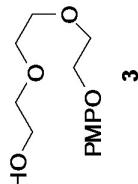


153.78

114.42

77.25  
76.99  
76.74  
72.37  
70.54  
70.12  
69.61  
67.87

55.47



```

Current Data Parameters
NAME      BM-AM-SCHLENN108
EXPTNO    113
PROCNO    1

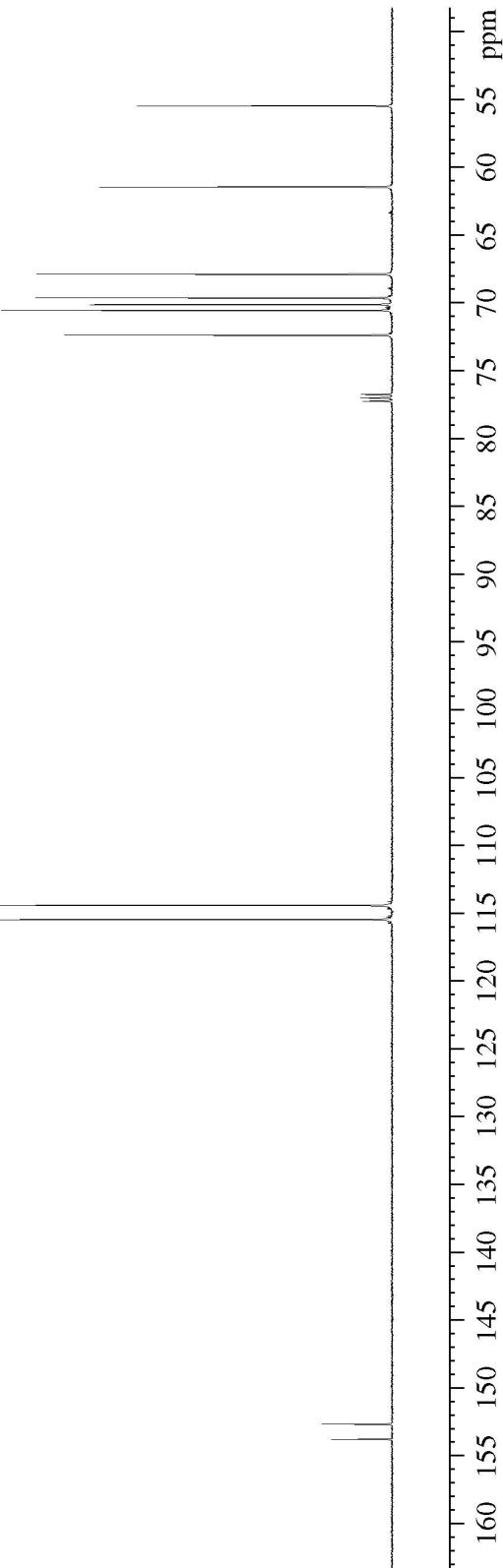
F2 - Acquisition Parameters
Date-    2011207
Time     11:08
INSTRUM  spect
PROBHD  5 mm PABBO BB
PULPROG  zg30
TD      65536
SOLVENT  CDCl3
NS      150
D1      1.4
SWH     29761.904 Hz
ETDRES  0.454111 Hz
AQ      1.1010048 sec
RG      203
FGDLY   16.800 usec
DW      6.50 usec
DE      2832.0 K
T1      2.0000000 sec
D11     0.03000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1      13C
P1       9.50 usec
P1W     -0.50 dB
P1M     90.18835531 W
SP01    125.7955118 MHz

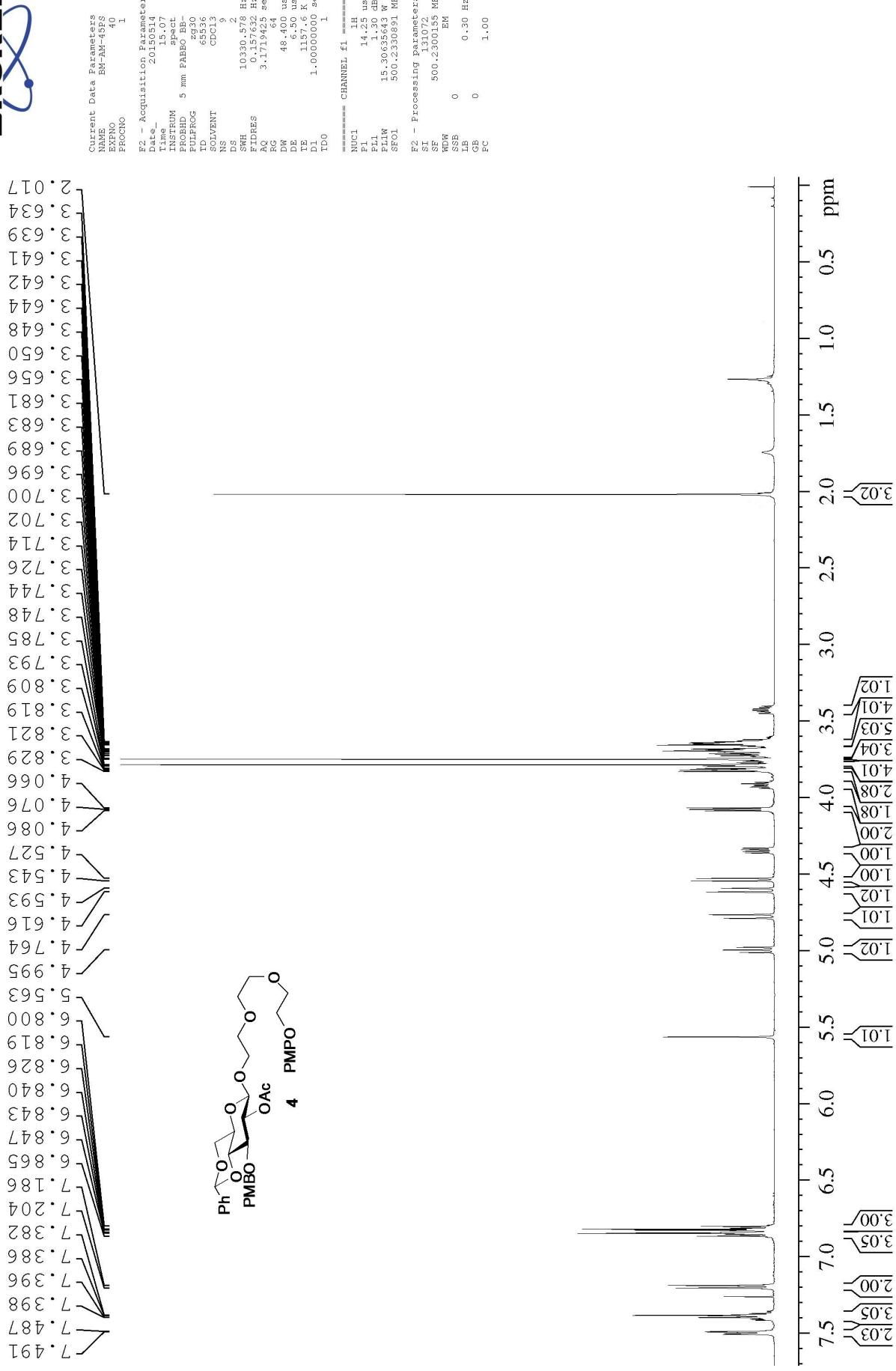
===== CHANNEL f2 =====
NUC2      1H
P0PD2    80.00 usec
P12      1.30 dB
P112    16.00 dB
P12W    15.31665563 W
P112W   0.5184666 W
SP02    500.2320093 MHz

F2 - Processing parameters
SI      32768
SF      125.7823556 MHz
WDW    EM
SSB      0
LB      1.00 Hz
GB      0
PC      1.40

```



BM-AM-45PS in CDCl<sub>3</sub>



BM-AM-45PS in  $\text{CDCl}_3$

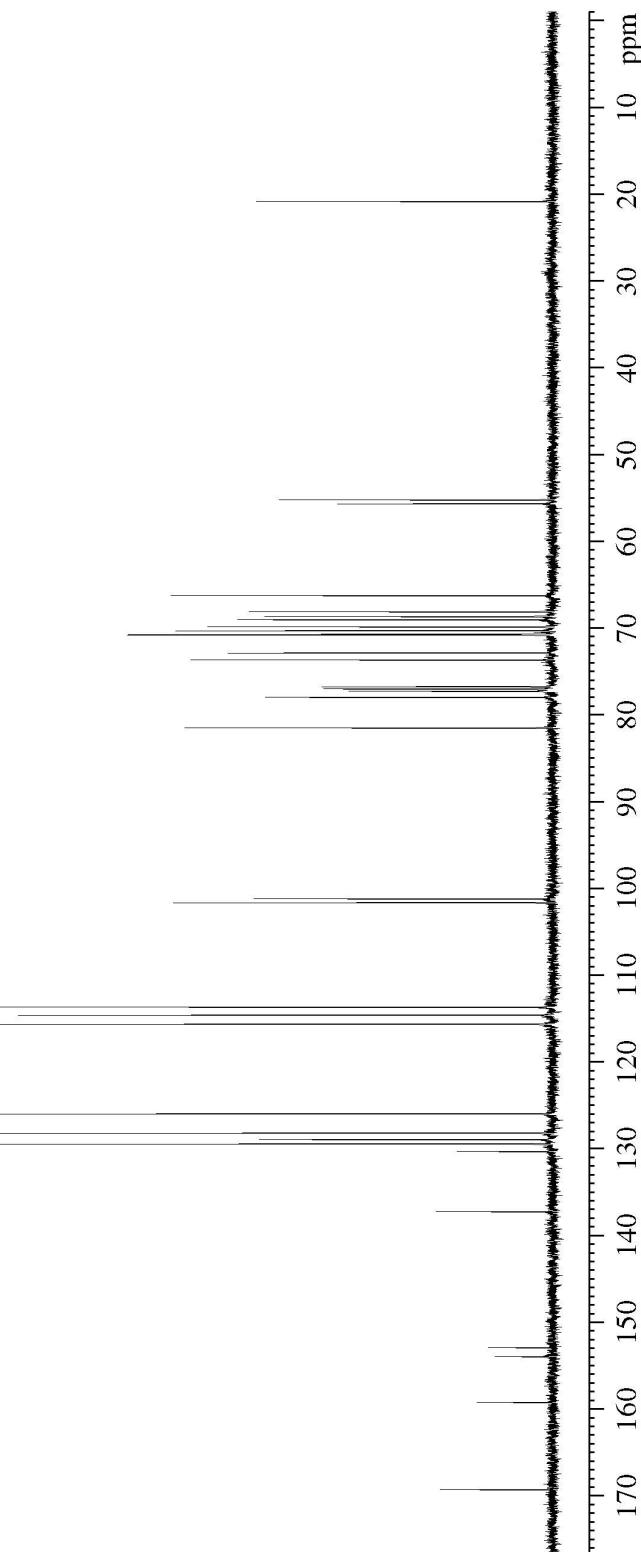
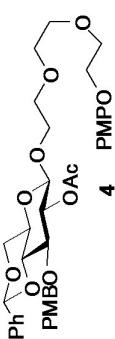


169.28      159.20      153.93      137.23  
130.30      129.44      128.94      128.20  
115.63      114.59      113.66      101.19  
101.15      101.19

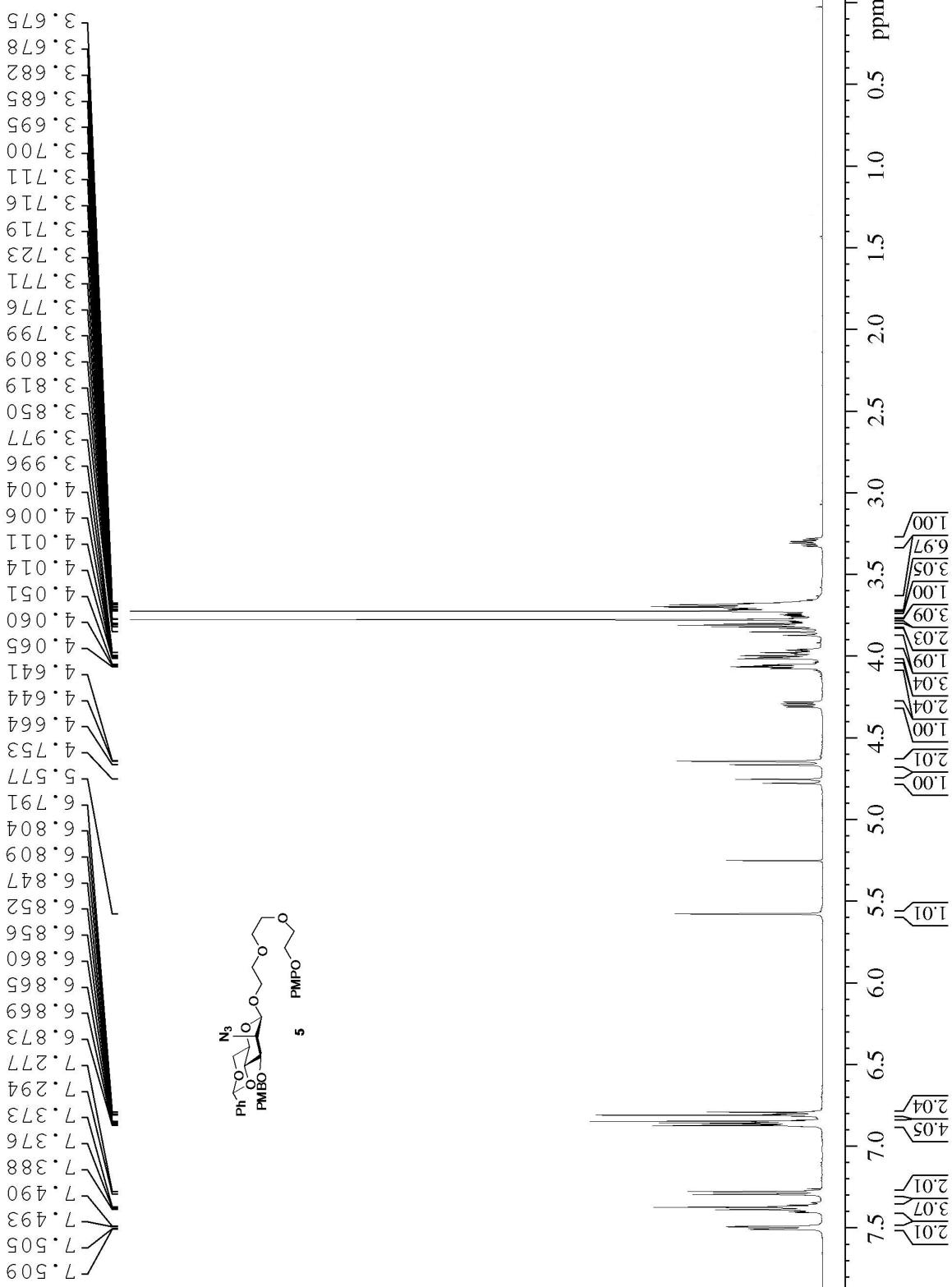
81.49      77.00      77.25      77.96  
76.75      73.65      72.84      70.79  
70.71      70.27      69.84      69.03  
68.65      68.03      68.10      66.24  
65.65      55.65      55.20

Current Data Parameters  
NAME BM-AM-45PS  
EXPNO 41  
PRCNO 1  
  
F2 - Acquisition Parameters  
Date e\_ 20150514  
Time 15.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg3dc  
TD 65536  
SOLVENT CDCl3  
NS 130  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454113 Hz  
AQ 1.1010048 sec  
RG 203  
RGDW 16.800 usec  
DE 6.50 usec  
TE 115.65 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.50 usec  
PL1 90.18825531 W  
PLW1 125.7935118 MHz  
  
===== CHANNEL f2 =====  
CPDPRG12 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 1.30 dB  
PLW2 15.10635643 W  
PL12W 0.51884636 W  
SF01 500.2320009 MHz  
  
F2 - Processing parameters  
ST 32768  
SF 125.7829419 MHz  
WDW 0  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



BM-AM-49PS2 in CDC13

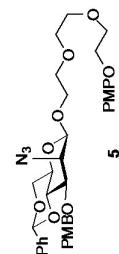


BM-AM-49PS2 in CDC<sub>13</sub>



159.16  
153.68  
137.18  
129.61  
128.71  
127.97  
115.45  
114.40  
113.66  
101.28  
100.08

78.32  
77.25  
77.00  
76.74  
75.85  
72.25  
70.32  
70.47  
70.19  
69.61  
68.80  
68.18  
67.90  
67.05  
63.20  
55.40  
54.99



Current Data Parameters  
NAME BM-AM-49PS2  
EXPNO 141  
PROCNO 1

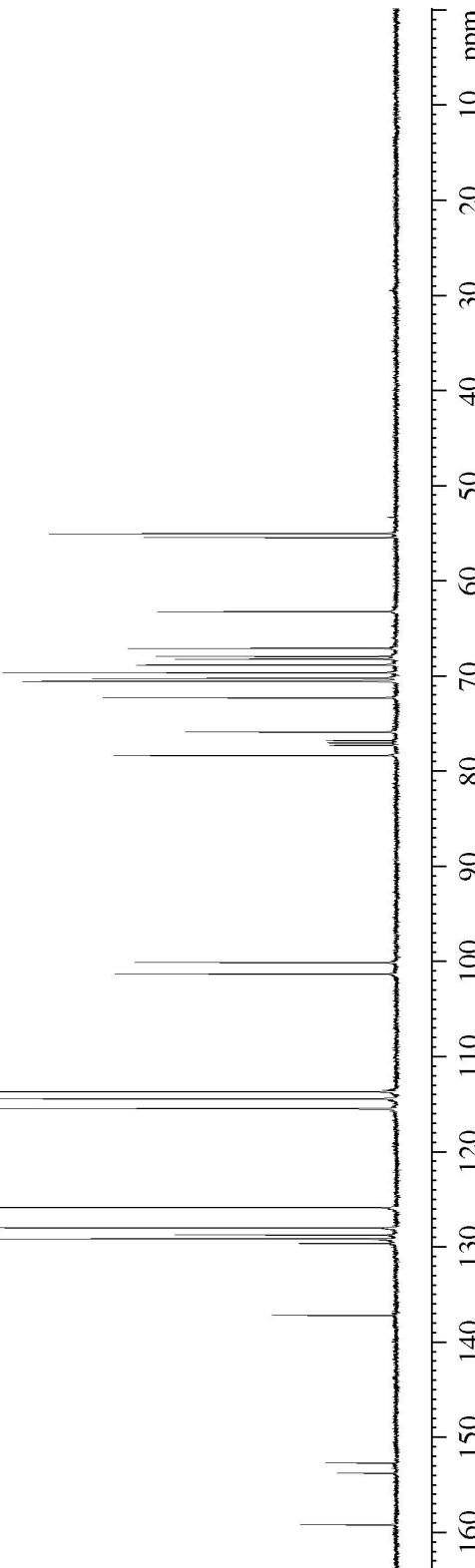
F2 - Acquisition Parameters  
Date\_ 20150528  
Time\_ 16.27

INSTRUM spect  
PROBID 5 mm PABBO BB-  
PULPROG 203  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 40  
DS 29761.904 Hz  
SWH 0.164531 Hz  
AQ 1.101048 sec  
RG 203  
DW 16.800 usec  
DE 6.50 usec  
TE 123.7 K  
D1 2.000000 sec  
D11 0.0300000 sec  
TDO 1

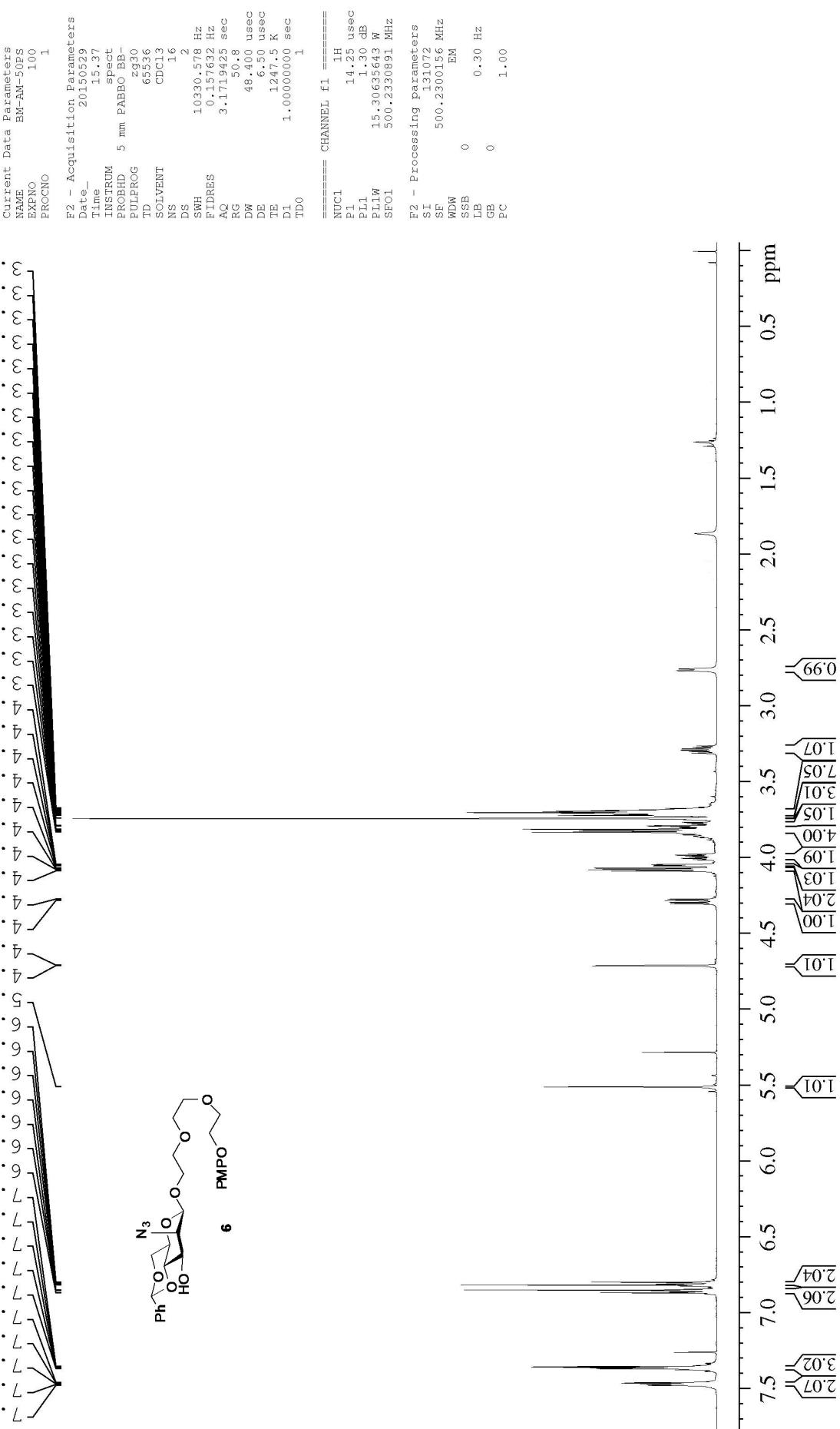
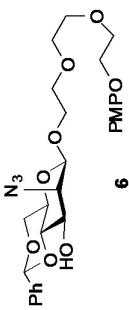
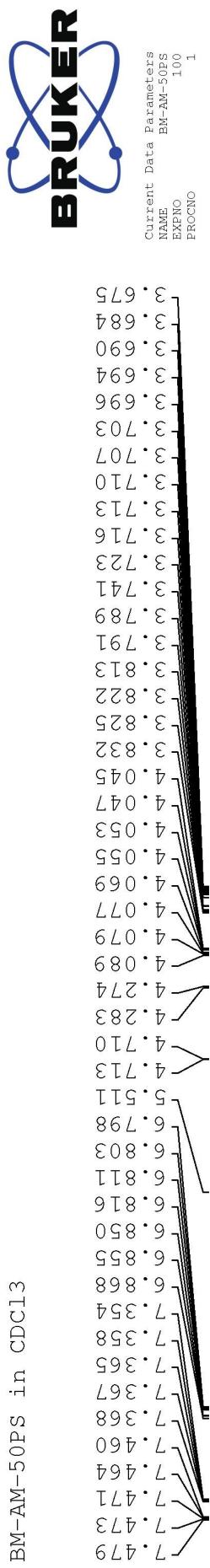
===== CHANNEL f1 =====

NUC1 P1 9.13C usec  
PL1 80.18425531 W  
PL1W SFO1 225.7395116 MHz  
===== CHANNEL f2 =====

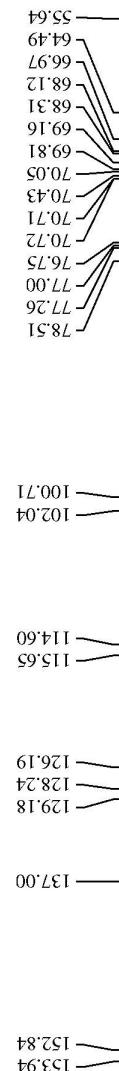
CPDPGRG [2] 1H  
NUC2 PCPD2 80.00 usec  
PL2 PL12 1.30 dB  
PL1W PL12W 15.3093543 W  
PL12W 0.51664596 W  
SF02 500.2320009 MHz  
F2 - Processing Parameters  
SI 32768  
SF 125.7329693 MHz  
WDW 0 EM  
SSB 0 1.00 Hz  
LB 0 1.40



BM-AM-50PS in CDCl<sub>3</sub>



BM-AM-50PS in CDCl<sub>3</sub>



Current Data Parameters  
NAME BM-AM-50PS  
EXPNO 101  
PROCNO 1

F2 - Acquisition Parameters

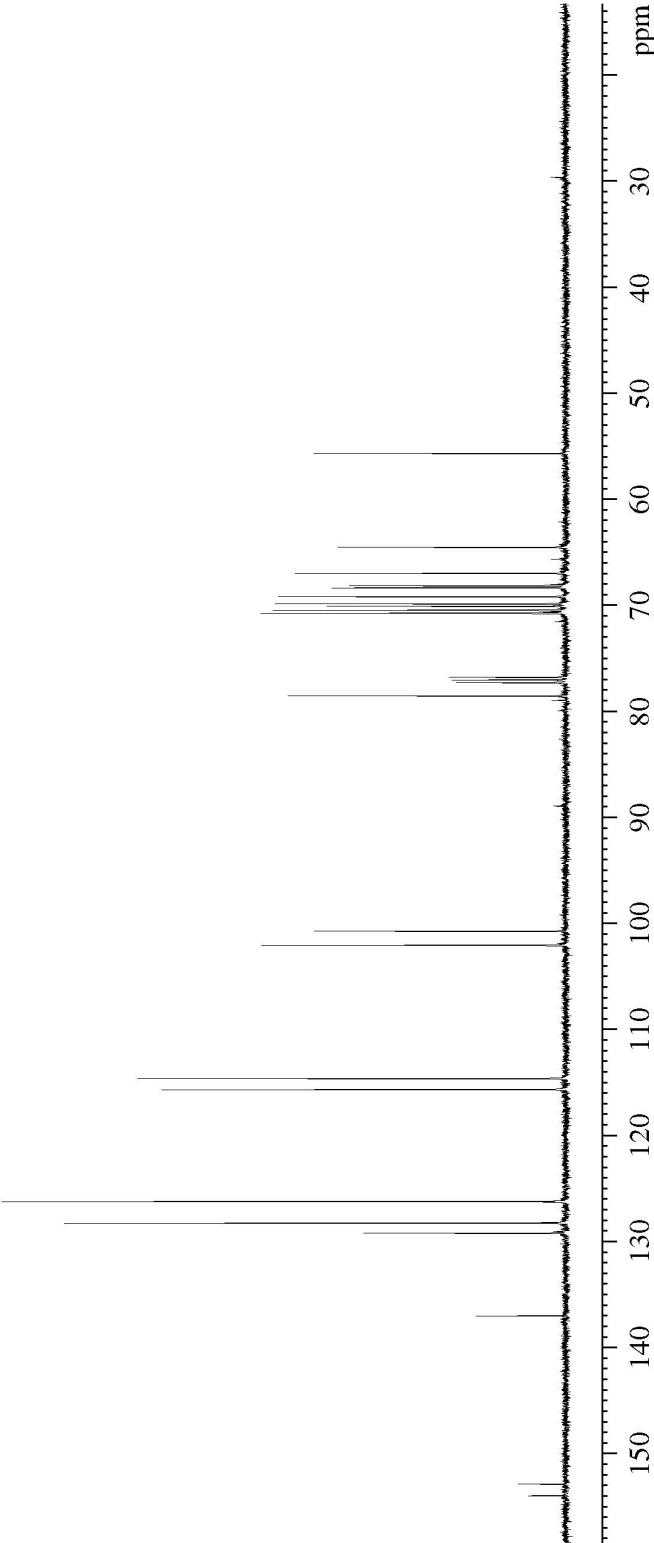
Date\_ 20150529  
Time\_ 15.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 74  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 1.203  
DW 16.800 usec  
DE 6.50 usec  
TE 1250.7 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

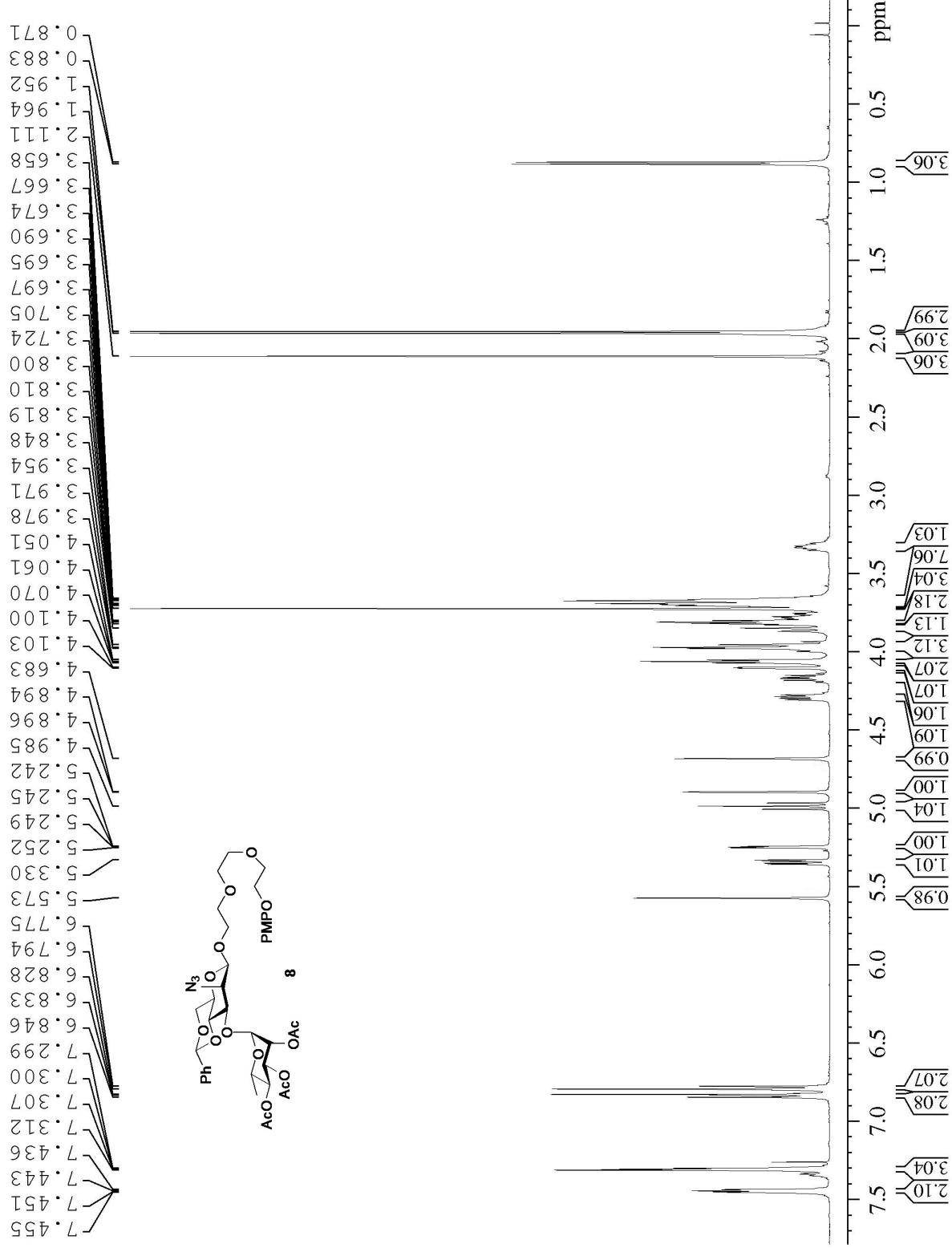
===== CHANNEL f1 =====

NUC1 13C  
P1 9.50 usec  
PL1 -0.50 dB  
PL1W 90.18822531 W  
SF01 125.7795118 MHz

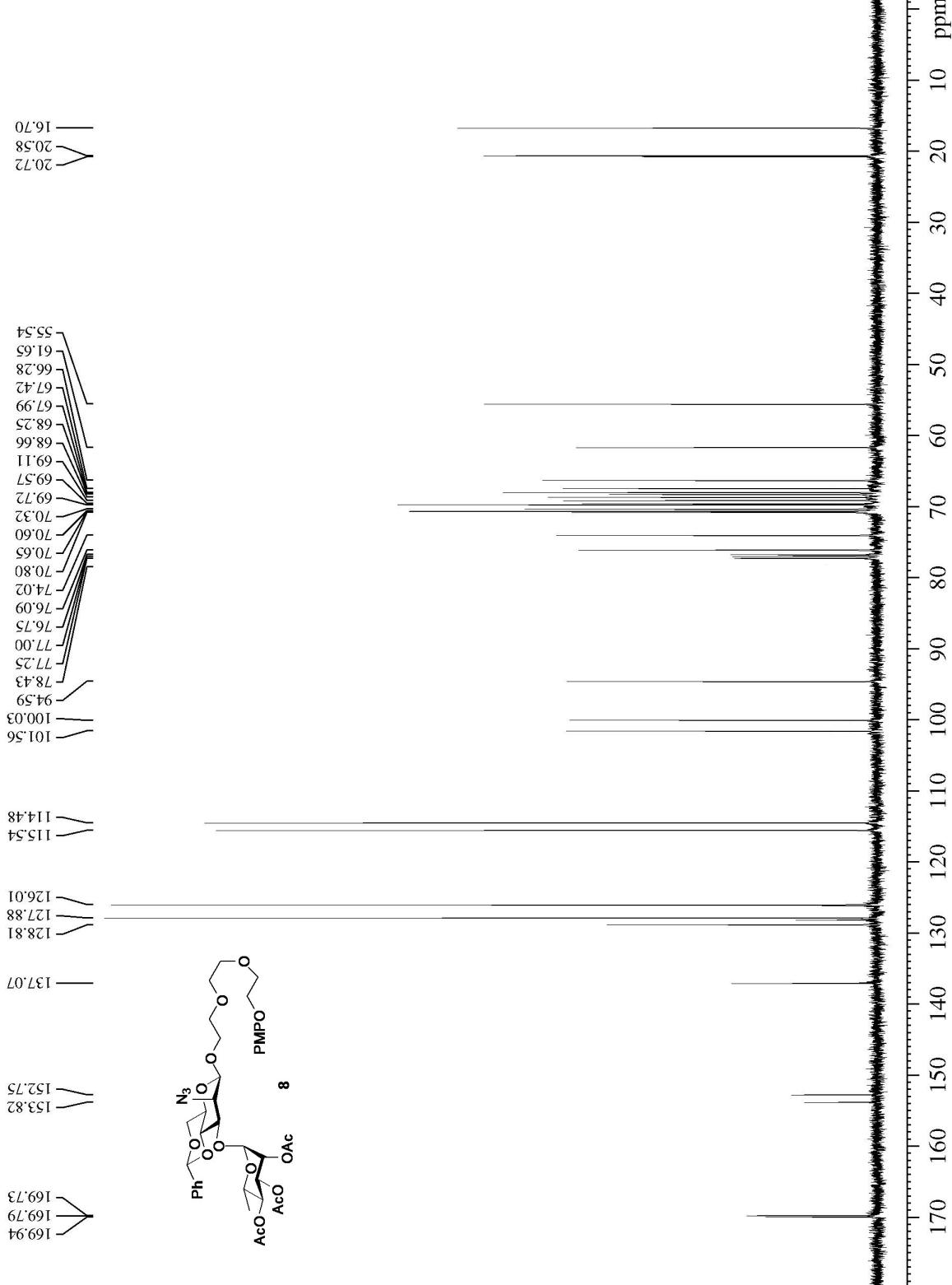
===== CHANNEL f2 =====

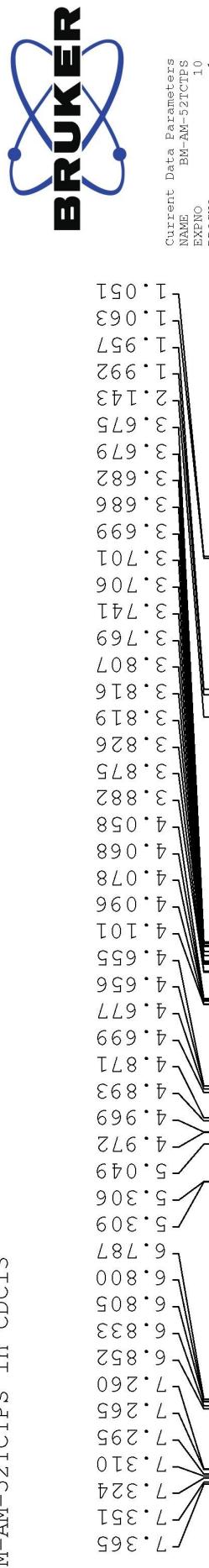
CPDPRG[2  
NUC2 1H  
PCPD2 80.00 usec  
PL2 1.30 dB  
PL12 15.30632643 W  
PL12W 0.51864696 W  
SF02 500.3202009 MHz  
ST 32768  
SF 125.7829452 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





BM-AM-51PS in  $\text{CDCl}_3$





```
Current Data Parameters
NAME BM-AM-52TCTPS
EXPNO 10
PROCNO 1
```

```
F2 - Acquisition Parameters
Date_ 20150610
Time 10:29
INSTRUM spect
PROBID 5 mm PABBO BB-
PULPROG
TD 6536
SOLVENT CD13
SWH 10330.578 Hz
FIDRES 0.157332 Hz
AQ 3.1719425 sec
RG 50.8
DW 48.400 usec
DE 6.50 usec
TE 1537.9 K
D1 1.0000000 sec
TDO 1
```

```
==== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PL1 1.30 dB
PL1W 15.30035643 W
SFO1 500.23300891 MHz
```

```
F2 - Processing Parameters
SI 131072
SF 500.2300154 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 1.00
PC
```

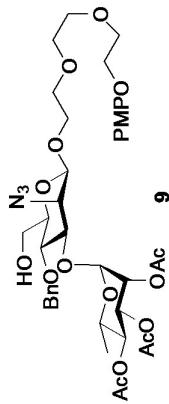


BM-AM-52TCTPS in CDCl<sub>3</sub>

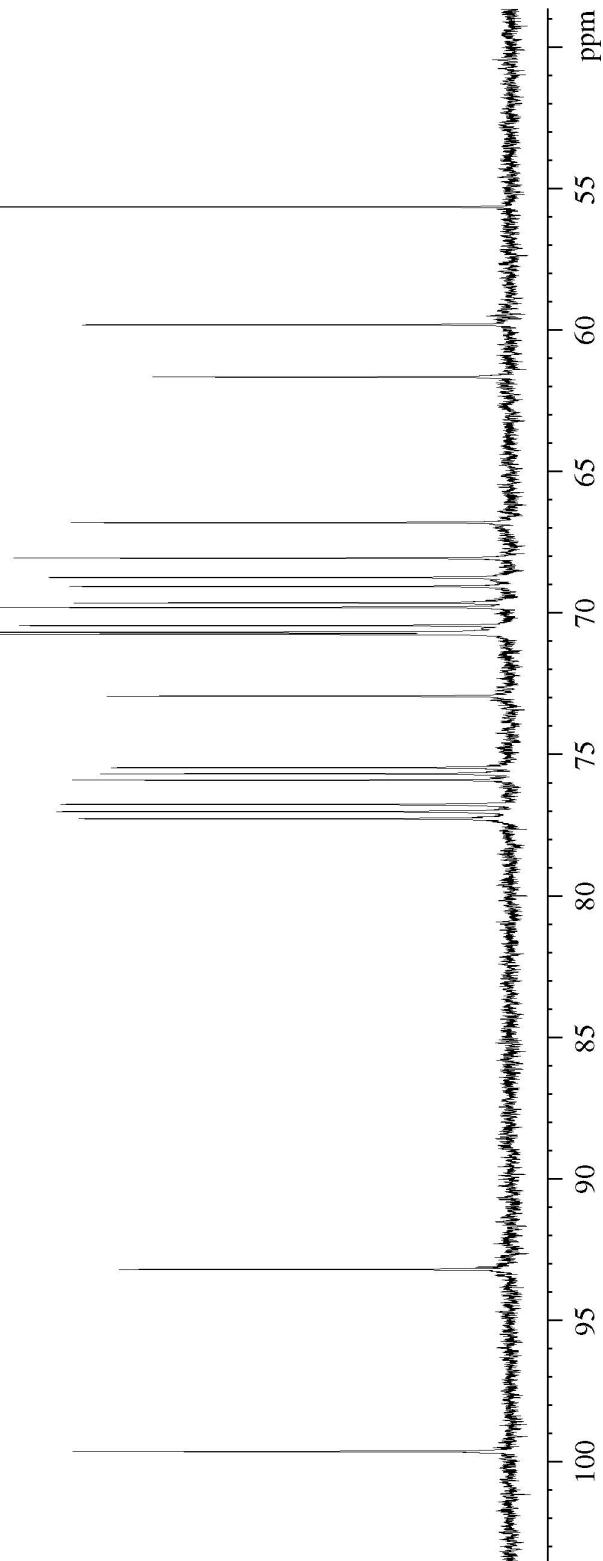


55.62 ——————  
59.78 ——————  
61.62 ——————  
68.01  
68.71  
69.04  
69.16  
69.77  
70.42  
70.64  
70.73  
72.90  
75.45  
75.87  
76.75  
77.00  
77.25  
93.16 ——————  
99.69 ——————

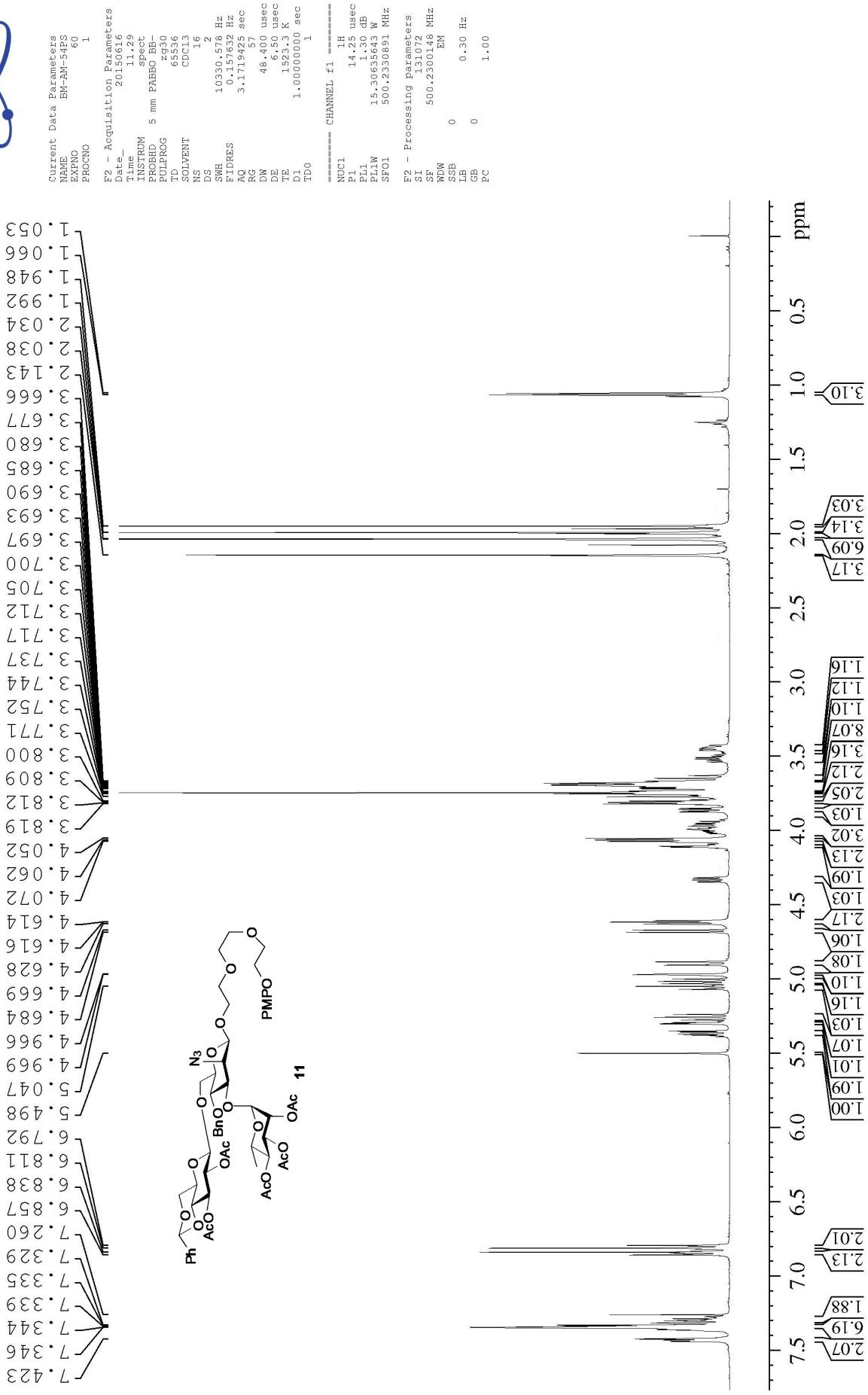
69.77  
68.01  
68.71  
69.04  
69.16  
69.77  
70.42  
70.64  
70.73  
72.90  
75.45  
75.87  
76.75  
77.00  
77.25



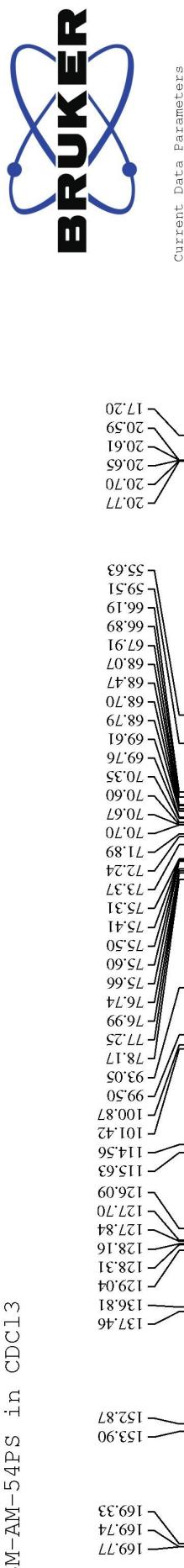
Current Data Parameters  
NAME BM-AM-52TCTPS  
EXPNO 11  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 2015/06/10  
Time 10.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg3dc  
TD 6536  
SOLVENT CDCl<sub>3</sub>  
NS 138  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.101048 sec  
RG 203  
DW 16.800 usec  
DE 6.50 usec  
TE 1537.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
  
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.50 usec  
PL1 -0.50 dB  
PL1W 90.1882/531. W  
SF01 125.1955/118 MHz  
  
===== CHANNEL f2 =====  
CPDRG[2  
NUC2 1H  
FCPD2 80.00 usec  
PL2 1.30 dB  
PL2W 15.3/163.643 W  
PL12W 0.5188/649.6 W  
SF02 500.2320009 MHz  
  
F2 - Processing Parameters  
SI 131072  
SF 125.7829446 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



BM-AM-54PS in CDCl<sub>3</sub>



BM-AM-54PS in CDCl<sub>3</sub>



Current Data Parameters  
NAME BM-AM-54PS  
EXPNO 63  
PROCNO 1

F2 - Acquisition Parameters

Date 2015/06/16  
Time 11.46  
INSTRUM 5 mm PABBO BB-  
PROBHD 2gdc  
PULPROG 65536  
TD 133  
SOLVENT CDCl<sub>3</sub>  
NS 4  
DS 29761,904 Hz  
SWH 0.45/1.131 Hz  
FIDRES 1.1010048 sec  
AQ 203  
RG 16.800 usec  
DE 6.50 usec  
TE 1523.2 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TDO 1

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

NUC1 13C  
P1 9.50 usec  
PL1 -0.50 dB  
PL1W 90.18895531 W  
SF01 125.7955118 MHz  
SFO2 500.2320009 MHz

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

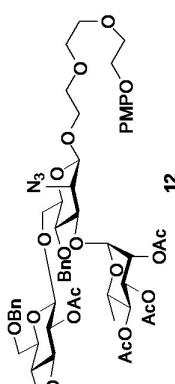
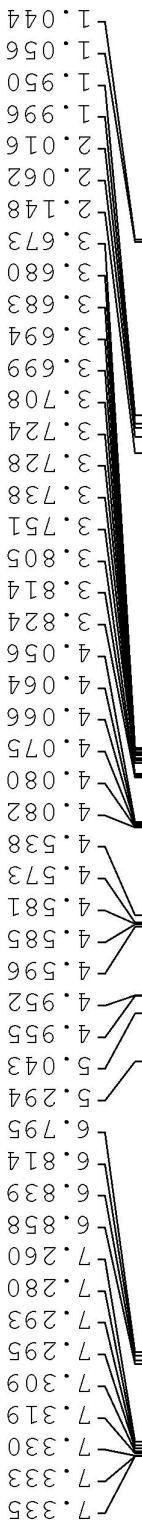
CPDRG [2] waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 1.30 dB  
PL12 16.00 dB  
PL2W 15.30835643 W  
PL12W 0.51864696 W  
SFO2 500.2320009 MHz

F2 - Processing parameters

SI 131072  
SF 125.7829441 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



BM-AM-58PS in CDCl<sub>3</sub>



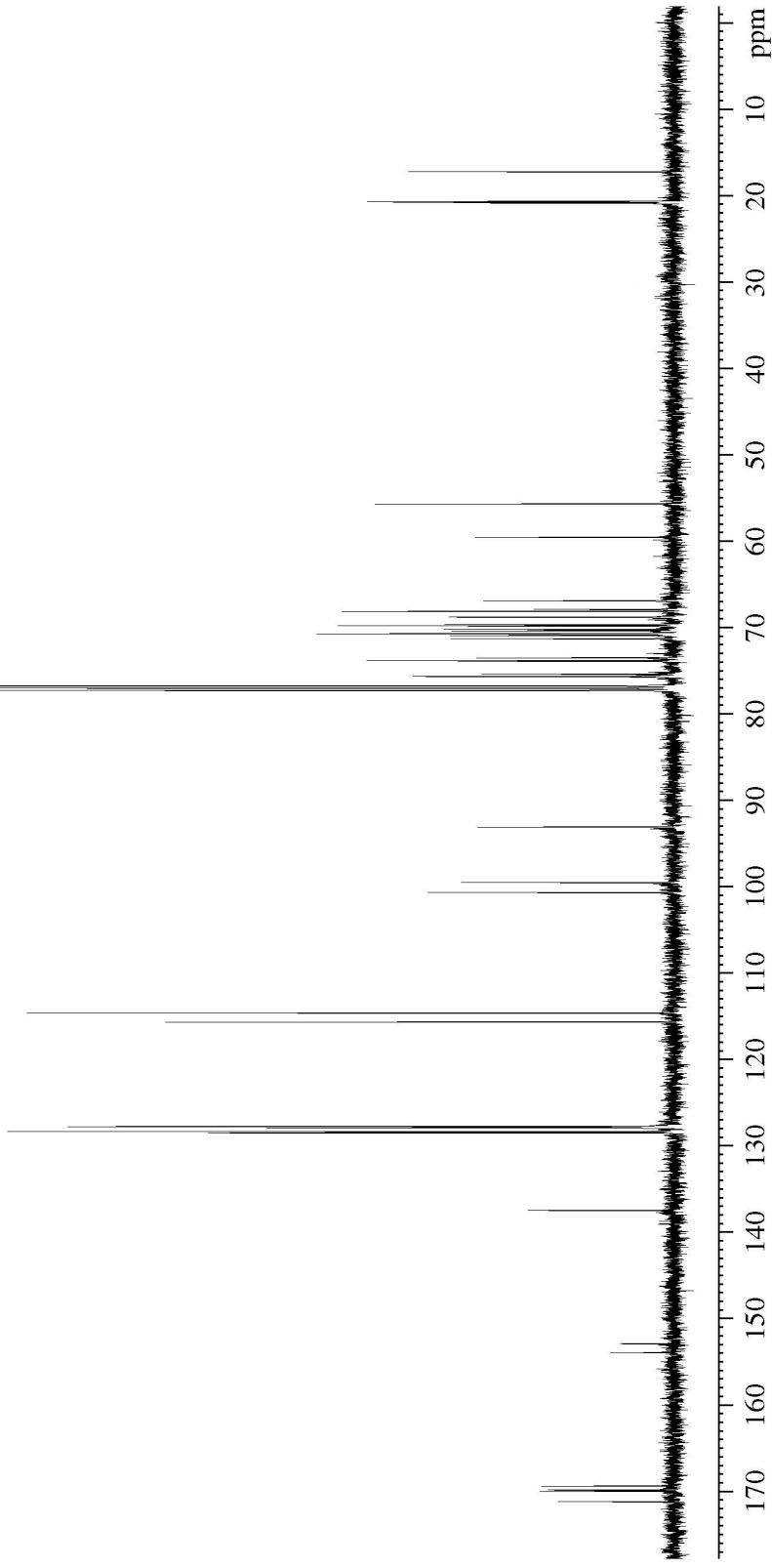
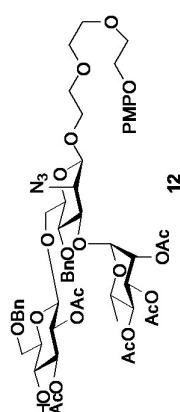
Current Data Parameters  
NAME BM-AM-58PS  
EXNO 60  
PROCNO 1  
F2 - Acquisition Parameters  
Date 20150728  
Time 12:59  
INSTRUM PABBO BB-  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.17632 Hz  
AQ 3.171945 sec  
RG 128  
DW 48.400 usec  
DE 6.50 usec  
TE 1493.5 K  
D1 1.0000000 sec  
TDO 1  
===== CHANNEL f1 ======  
NUC1 1H  
P1 14.25 usec  
PL1 1.130 SB  
PLW 15.30635643 W  
SF01 500.2330831 MHz  
F2 - Processing parameters  
SI 131072  
SF 500.23300156 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

BM-AM-58PS in  $\text{CDCl}_3$



Current Data Parameters  
NAME BM-AM-58PS  
EXPRO 6.3  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 2015/7/28  
Time 13.22  
INSTRUM spect  
PROBID 5 mm PABBO BB-  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 602  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.451131 Hz  
AQ 1.1010048 sec  
RG 203  
DW 16.800 usec  
DE 6.50 usec  
TE 1193.8 K  
D1 2.000000 sec  
D11 0.0300000 sec  
TDO 1  
  
===== CHANNEL f1 =====  
NP01 13C  
P1 9.50 usec  
PL 0.451131 Hz  
SWFO1 90.148825531 W  
SF01 125.7955118 MHz  
  
===== CHANNEL f2 =====  
CPDPFG12  
NPIC2 1H  
PDPD2 30.00 usec  
PR2 1.30 dB  
PT12 15.34635613 W  
PT2W 0.53865656 W  
PT12W 500.2320059 MHz  
SF02 125.7955118 MHz  
  
F2 - Processing parameters  
SI 32768  
SF 125.7955118 MHz  
WDW 0  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

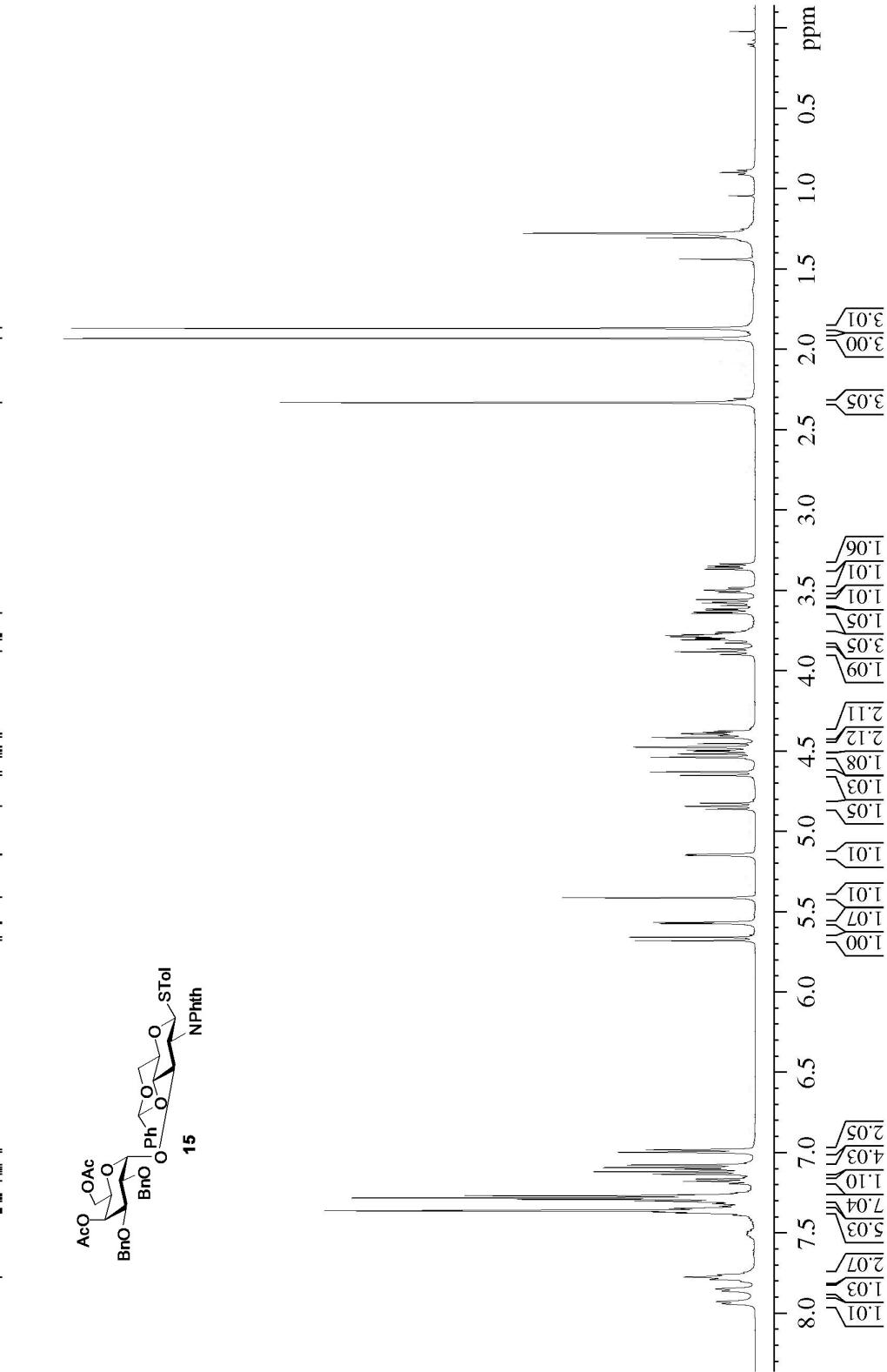
17.22  
20.65  
20.66  
20.72  
20.81  
20.83  
69.72  
69.75  
69.79  
69.81  
69.85  
69.88  
69.91  
69.94  
69.98  
70.10  
70.18  
70.36  
70.64  
70.70  
70.74  
70.89  
71.26  
73.51  
73.78  
73.91  
75.36  
75.61  
75.64  
75.66  
76.74  
76.99  
77.25  
93.07  
99.49  
100.65  
114.60  
115.66  
127.73  
127.77  
127.82  
128.33  
128.48  
137.48  
153.93  
152.89  
169.80  
169.83  
169.85  
171.15



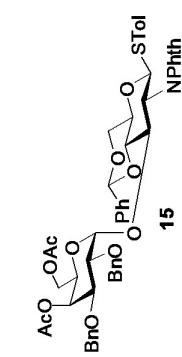
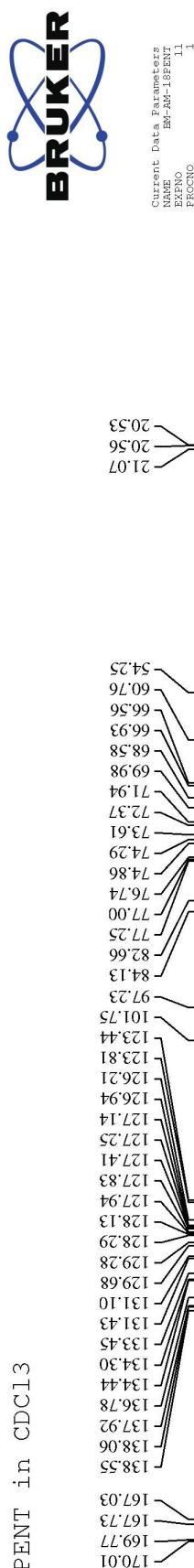
BM-AM-18PENT in CDCl<sub>3</sub>



Current Data Parameters  
NAME BM-AM-18PENT  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20150218  
Time 10:03  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 6536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 10330.576 Hz  
FIDRES 0.157832 Hz  
AQ 3.1719425 sec  
RG 36  
DW 48.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TDO 1  
===== CHANNEL f1 =====



BM-AM-18PENT in CDCl<sub>3</sub>



21.07  
20.56  
20.53



```

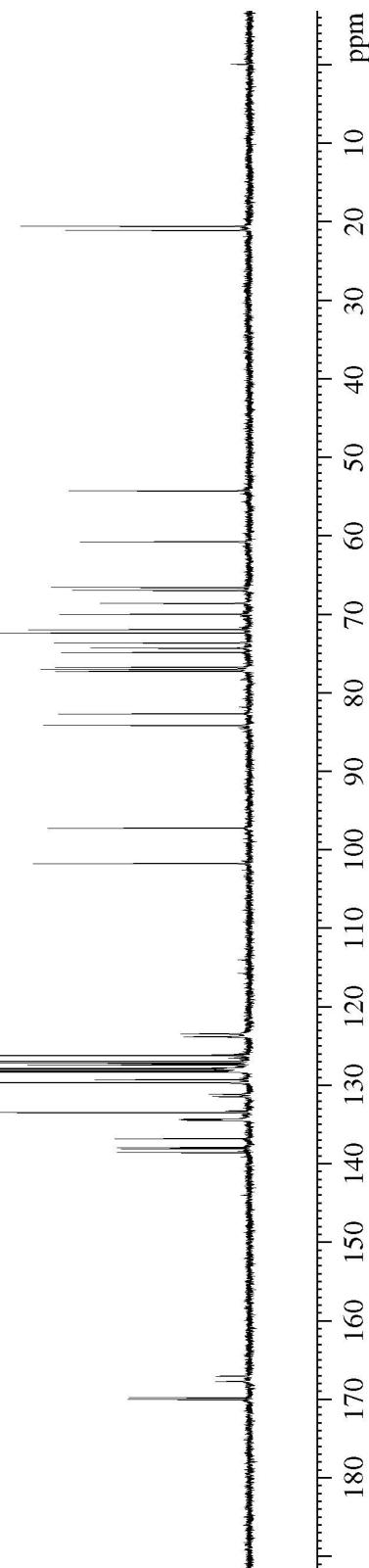
Current Date Parameters
NAME: BM-AM-18PENT
EXNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date: 2015/02/18
Time: 10:08
INSTRUM: spect
PROBOD: 5 mm PARBO BB-
PULPROG: 2edc
TD: 65536
SCV: 147
NS: 1
DS: 1
TE: 2971.61
SWH: 0.454131
RG: 1.1010048
DW: 2.03
DE: 16.000 usec
TE: 6.50
TE: 300.0 K
D1: 2.0000000 sec
D1L: 0.0300000 sec
TDO: 1

===== CHANNEL f1 =====
NO1: 13C
P1: 9.50 usec
PL1: -0.50
PLW: 90.1825531
SPOL: 125.7955118 MHz

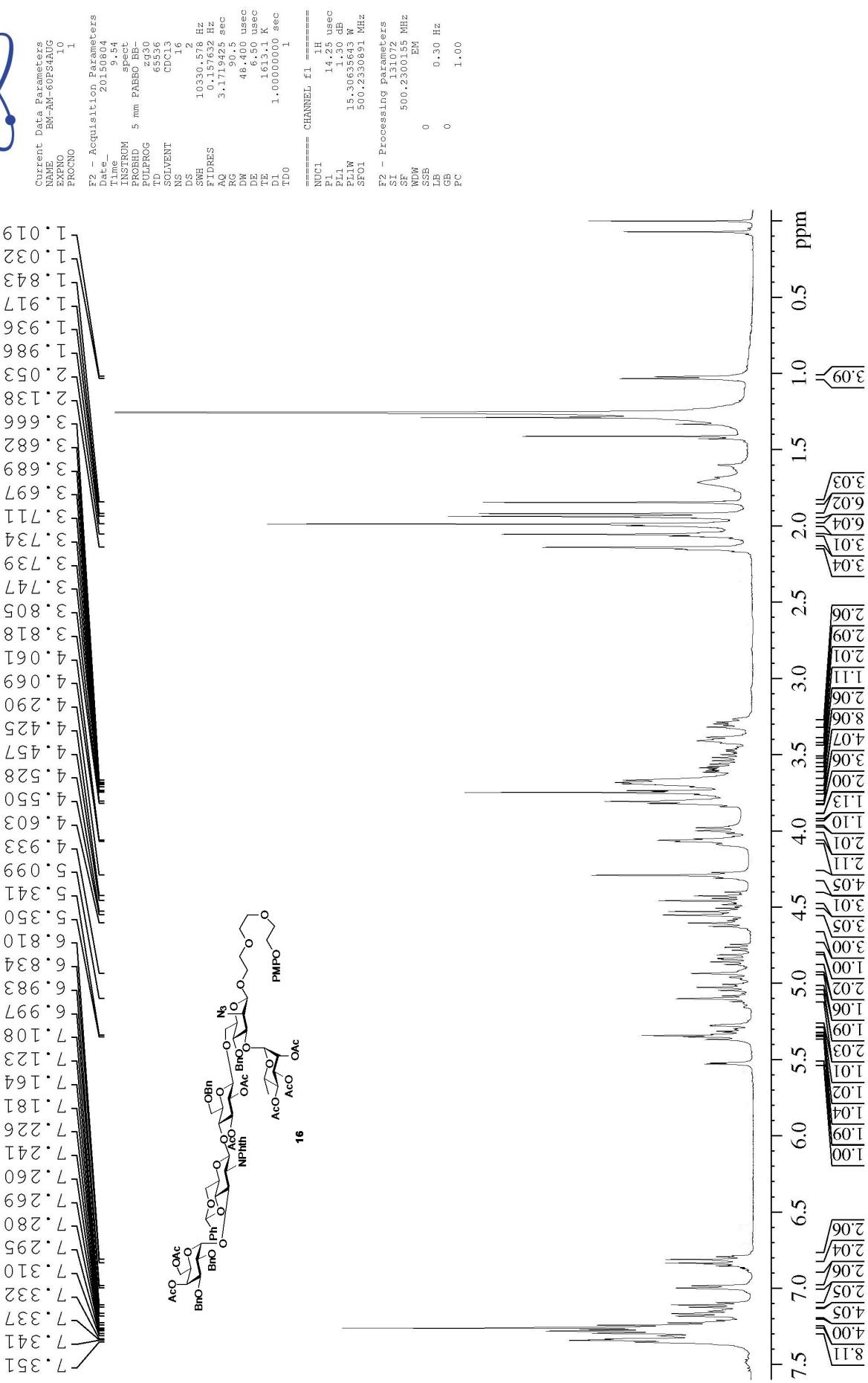
===== CHANNEL f2 =====
CPDPFG12
NO2: 1H
P2: 80.00 usec
PL2: 1.50
PLW: 15.3035643
FW: 0.518645956 Hz
SPOL2: 500.2320009 MHz

F2 - Processing parameters
SI: 32768
SF: 125.782905 kHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

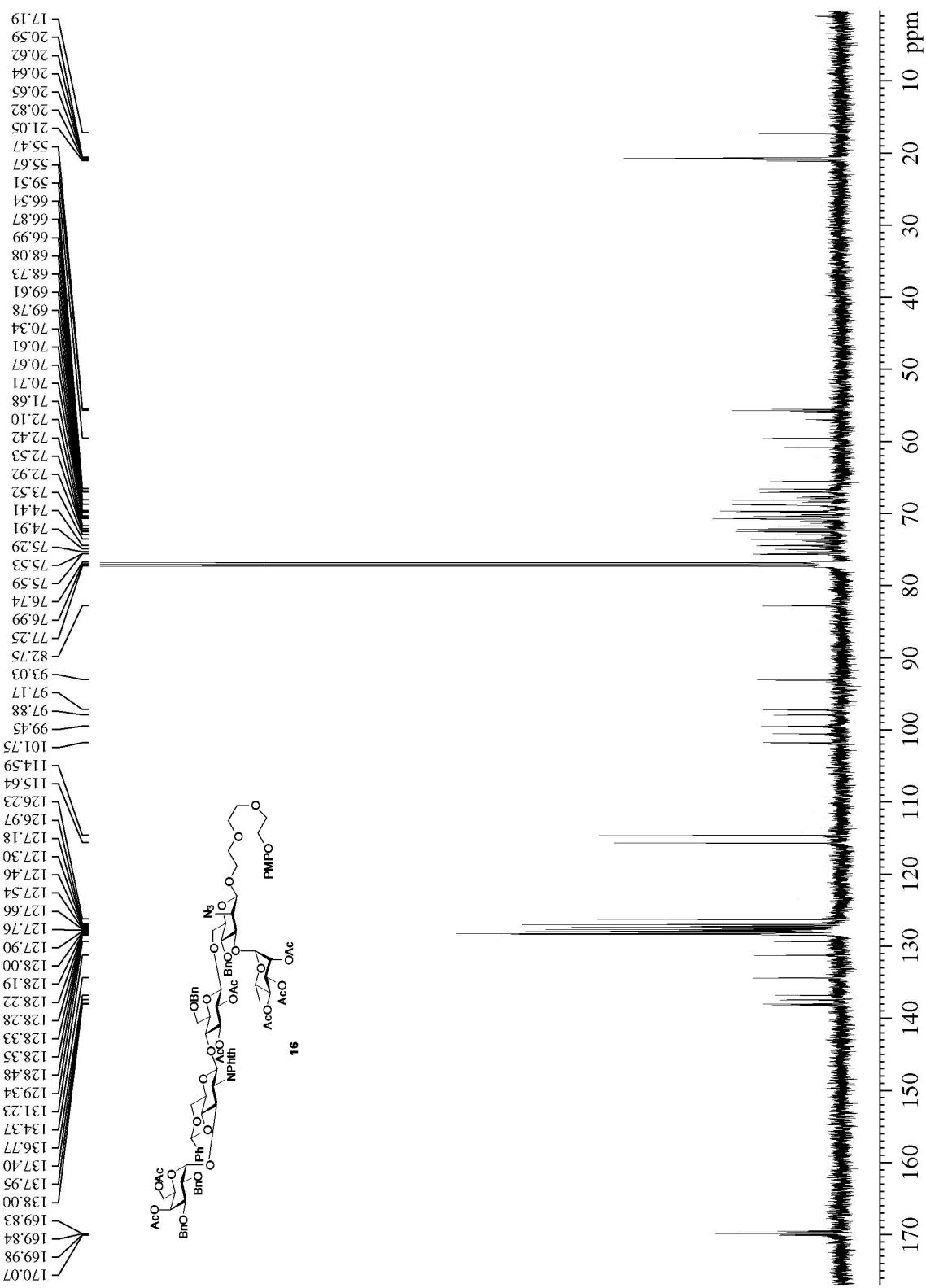
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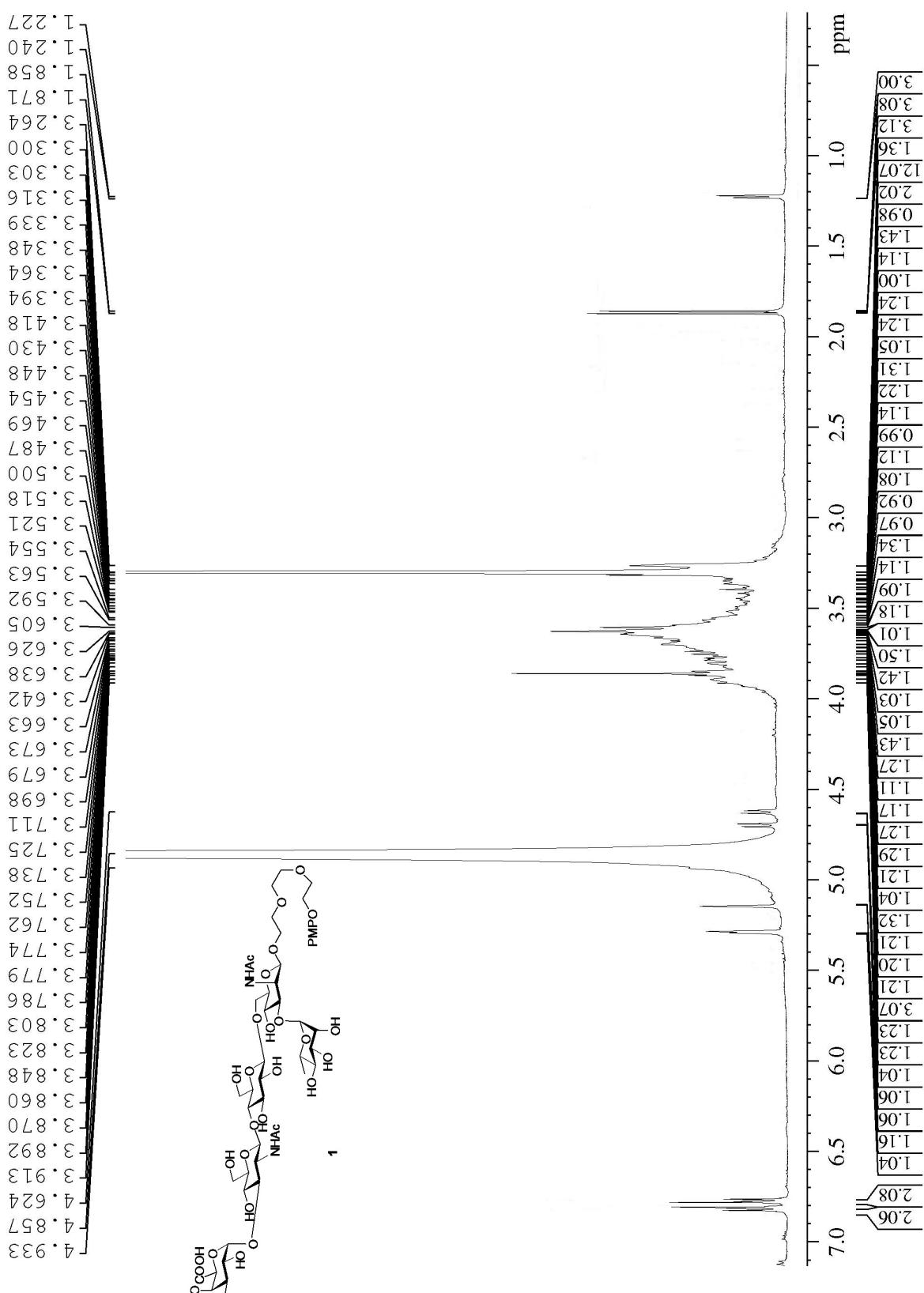
BM-AM-60PS4AUG in CDCl<sub>3</sub>



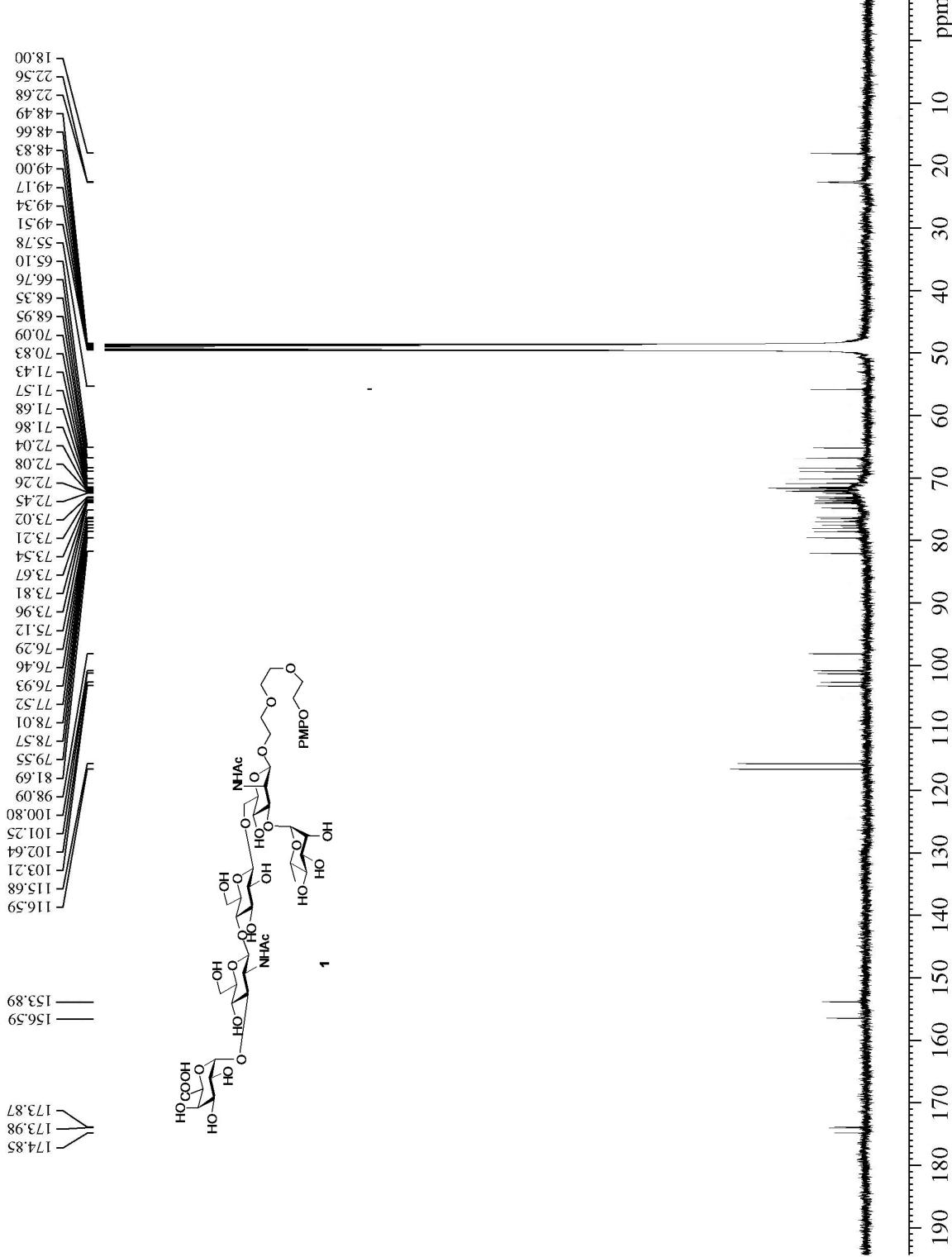
BM-AM-60PS4AUG in CDCl<sub>3</sub>



BM-AM-PENTFINAL in MeOD



BM-AM-PENTFINAL in MeOD





Current Data Parameters  
NAME BM-AM-PINTA\_HSCOSY  
EXPNO 111  
PROCNO 1

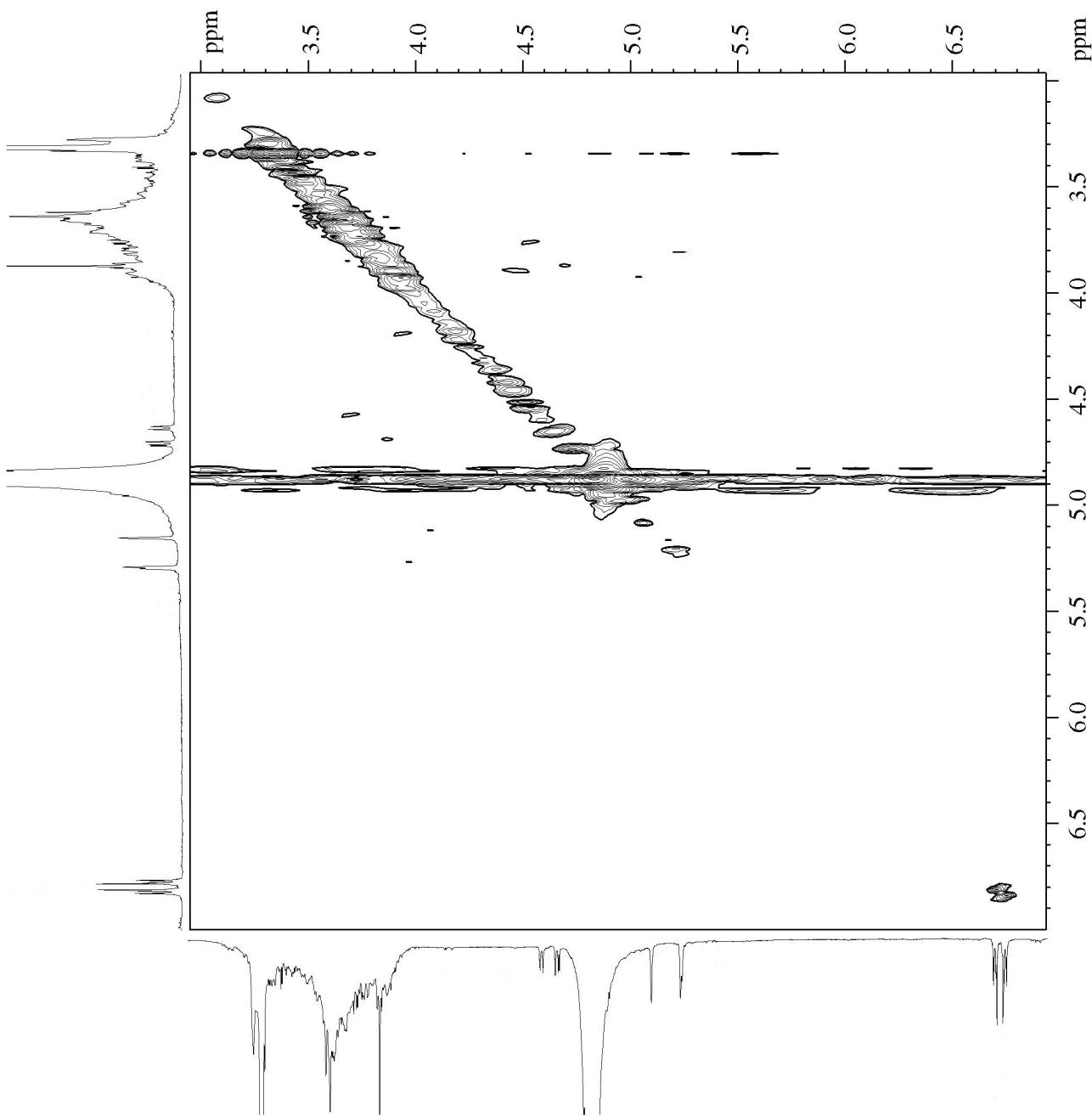
F2 - Acquisition Parameters  
Date\_ 20151210  
Time 15:44  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosyqcf  
TD 2048  
SOLVENT MeOD  
NS 32  
DS 1.6  
SWH 6684.192 Hz  
FIDRES 3.263912 Hz  
AQ 0.1531904 sec  
RG 1.61  
DW 74.800 usec  
DE 6.50 usec  
TE 2905.1 K  
D0 0.0000030 sec  
D1 1.46689198 sec  
D13 0.0000400 sec  
D16 0.0002000 sec  
INO 0.00014975 sec

===== CHANNEL f1 =====  
NUC1 1H  
P0 14.25 usec  
P1 14.25 usec  
PL1 1.30 dB  
PL1W 15.30635643 W  
SF01 500.2330075 MHz  
===== GRADIENT CHANNEL =====  
GPNAME[1] SINE,1.00  
GBZ1 10.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 128  
SF01 500.233 MHz  
FIDRES 52.17340 Hz  
SW 13.350 ppm  
FINMODE QF

F2 - Processing parameters  
SI 1024  
SF 500.2300000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 500.2300000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0





Current Data Parameters

```

NAME      BM-PENTA-BSOFT
EXPROD    1
PROCNO   1

F2 - Acquisition Parameters
Date_     2015/2/10
Time_    17:40
INSTRUM  5 mm PABBO-BB-
PROBID   hqetps-a2
TD       1024
SOLVENT  MeOD
NS      16
DS      600.9, 615. Hz
TE      5,867.65 Hz
PLINES   0, 0.051968 sec
AQ      203
RG      83.200 usec
DW      6.50 usec
DE      32.25 K
CNUST2  145.0000000 sec
DO      0.0000000 sec
D1      1.0000000 sec
D4      0.017414 sec
D11    0.0300000 sec
D13    0.0000400 sec
D16    0.0002000 sec
D24    0.0008267 sec
TIN0   0.00001985 sec
ZGOPTNS

===== CHANNEL f1 =====
NUC1L   1H
P1      14.25 usec
P2      28.50 usec
P28     0.10 usec
PL1    15.3034643 W
SF01   500.233014 MHz

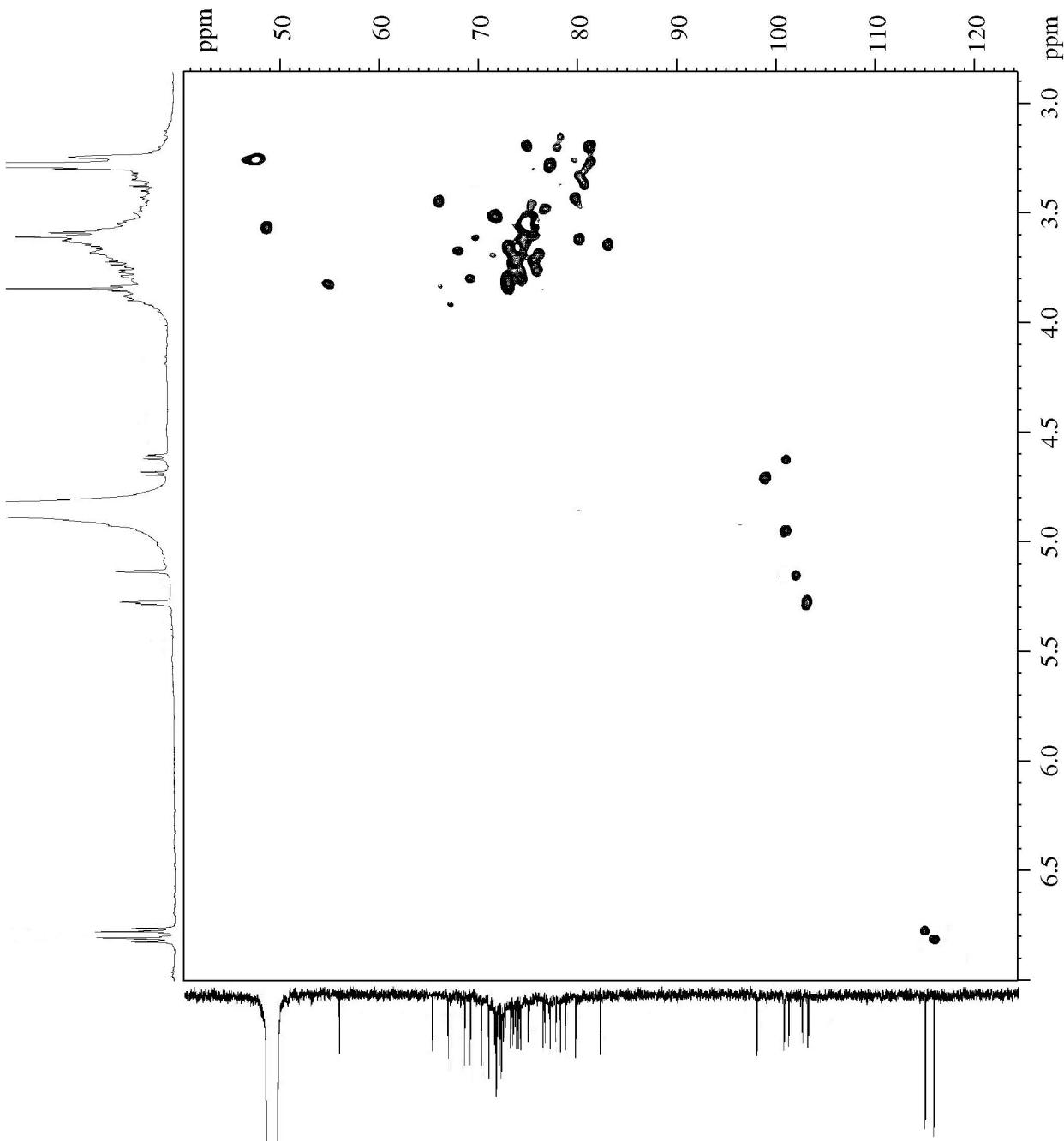
===== CHANNEL f2 =====
OPDPRG [2
NUC2   13C
P1      9.50 usec
P2      13.00 usec
P28     0.10 usec
PL2    17.00 dB
PLW    90.18322511 W
PL2W   1.6073910 W
SF22   125.7351213 MHz

===== GRADIENT CHANNEL =====
GPNAME[1] SINE,100
GPNAME[2] SINE,100
GPNAME[3] SINE,100
GPNAME[4] SINE,100
GP21   80.00 %
GP22   20.10 %
GP23   11.00 %
GP24   -5.00 %
P16    100.00 usec
P19    60.00 usec

F1 - Acquisition Parameters
TD      256
SF01   125.73935 MHz
FIDRES  98.47700 Hz
SW      200.000 Fpm
FIDDEDE Echo-Anticho
F2 - Processing parameters
SI      500.230013 MHz
SF      500.230013 MHz
SSB    0 Hz
LB      0 Hz
PC      1.00

F1 - Processing parameters
SI      1024
SF2   echo-anticho
SF    125.732271 MHz
SSB2  0 Hz
LB2   0 Hz
GB      0

```



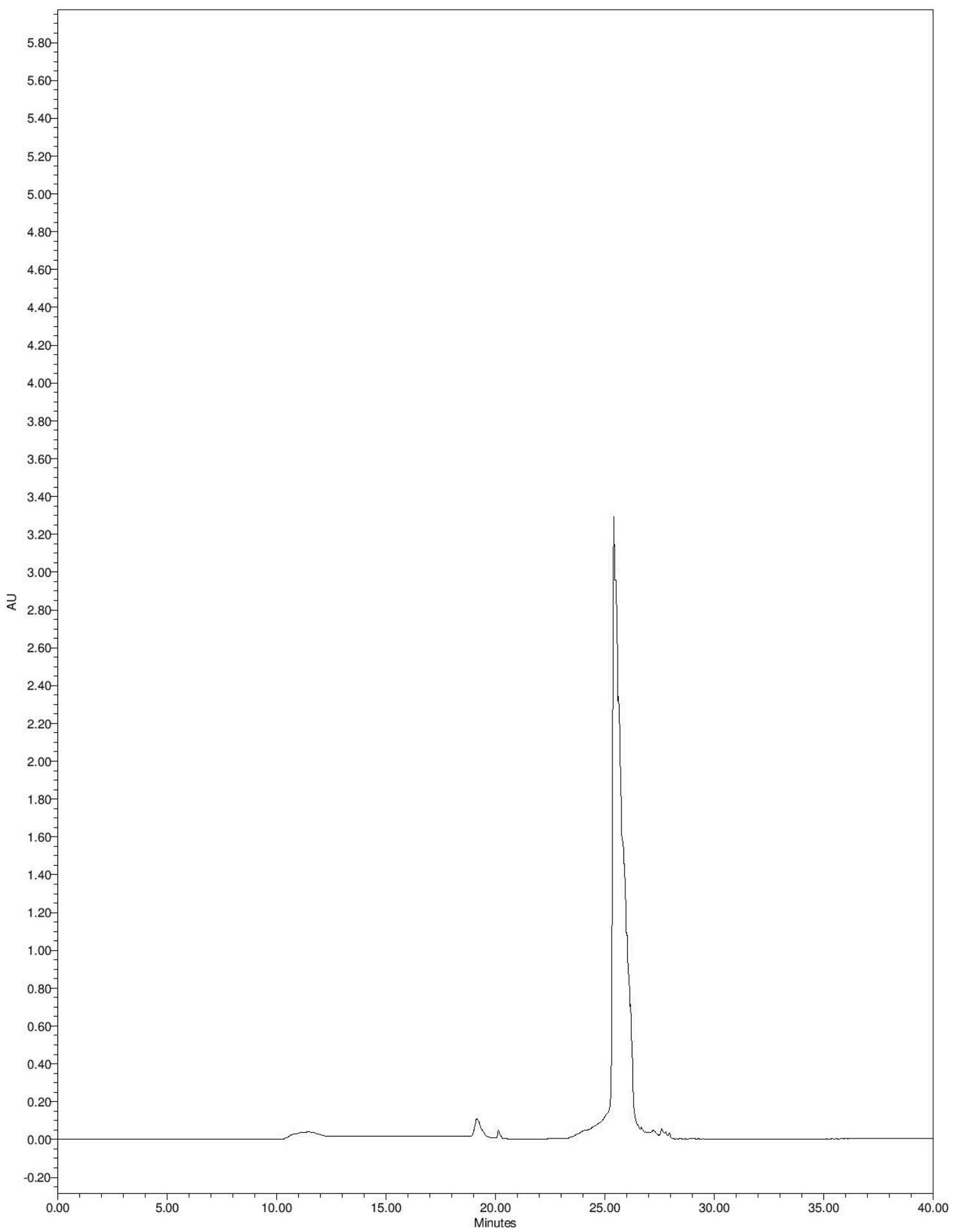


Figure S1: HPLC chromatogram of the target compound 1

Condition: HPLC on a Waters Nova-Pak C18 column (3.9 × 300 mm; 4  $\mu$ m particle size) with a flow rate of 1mL/min and using a gradient of CH<sub>3</sub>CN in water (Conditions: 0 to 10% A in B, A = CH<sub>3</sub>CN, B = water, over 40 min.)

## Display Report

### Analysis Info

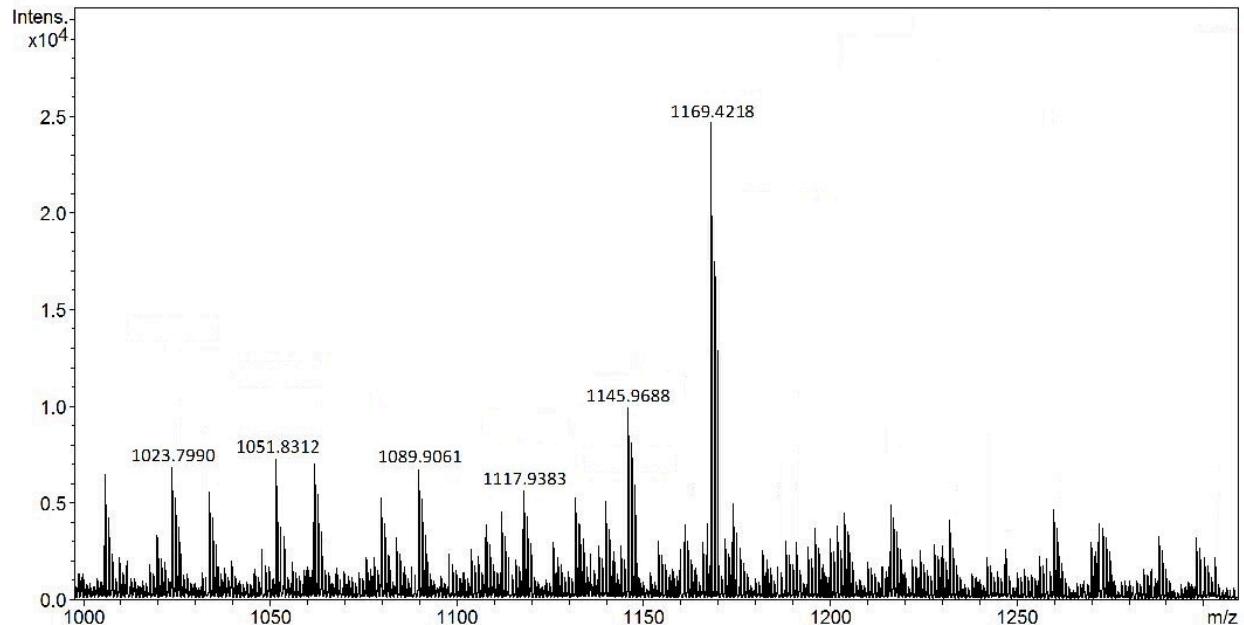
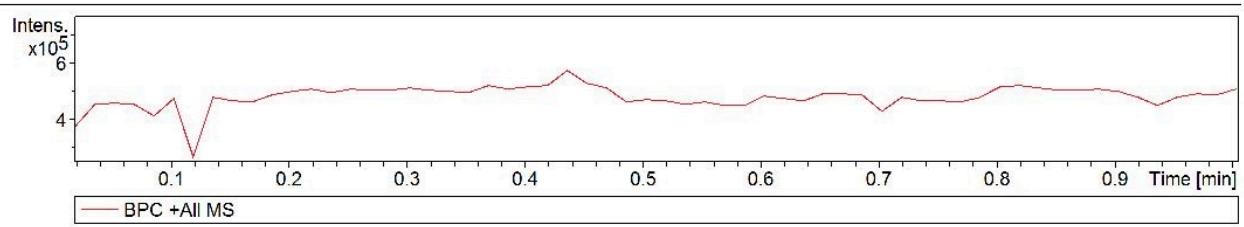
Analysis Name D:\Data\User data\2016\AUGUST\BM\_AM\_SAI10.d  
Method Tune\_pos\_Standard.m  
Sample Name BM\_AM\_SAI10  
Comment

Acquisition Date 8/26/2016 4:54:27 PM

Operator RAJESH VASHISTH  
Instrument maXis impact 8282001.00127

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



BM\_AM\_SAI10.d

RAJESH

Figure S2: ESI-MS of the target compound 1 (data collected on BRUKER Maxis Impact mass spectrometer, ESI (+)ve mode)