Electronic Supplementary Material (ESI) for RSC Advances.
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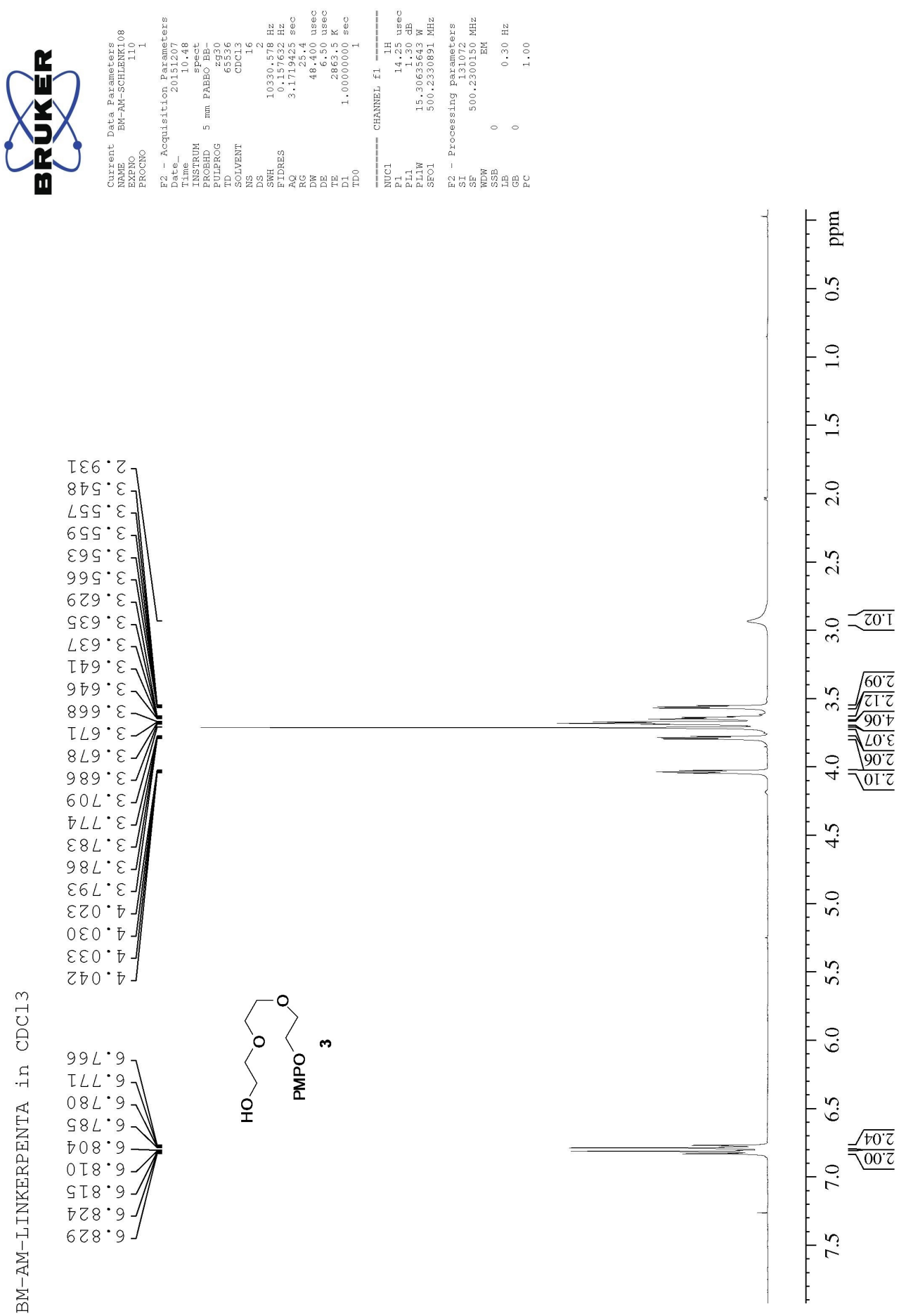
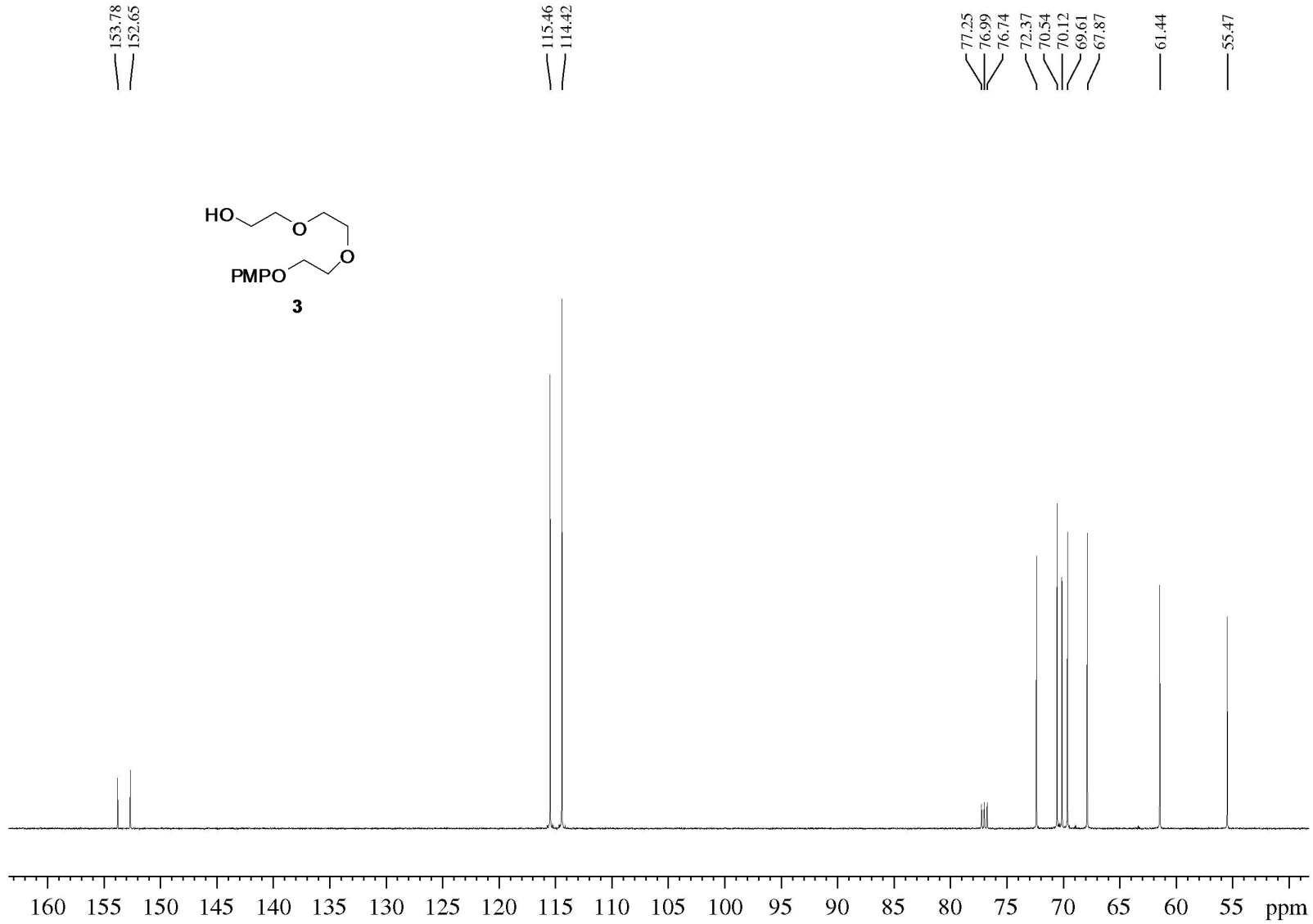
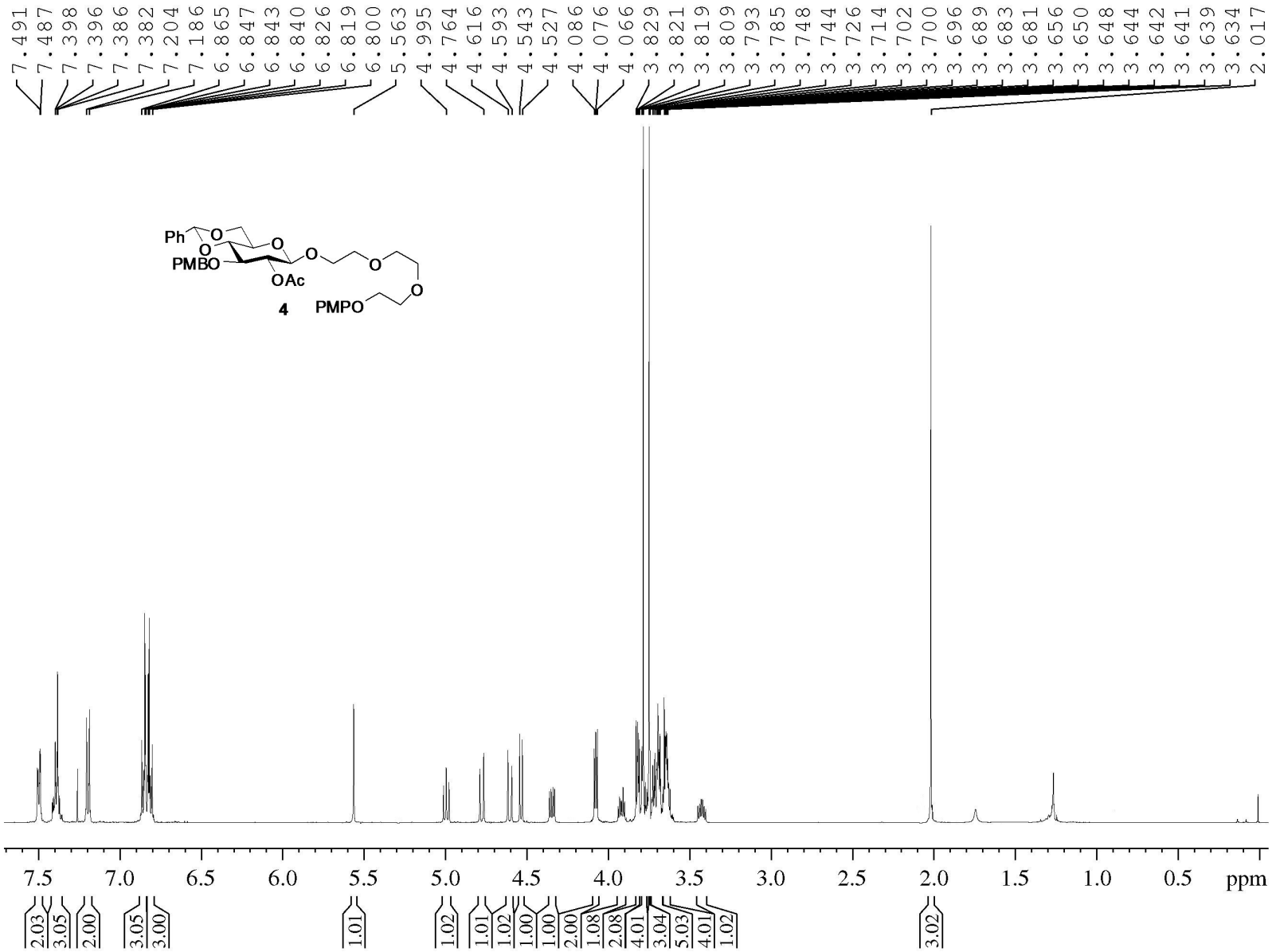


BM-AM-LINKERPENTA in CDCl3




```
Current Data Parameters
NAME      BM-AM-SCHLENK108
EXPNO                  113
PROCNO                   1

F2 - Acquisition Parameters
Date_           20151207
Time              11.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgdc
TD               65536
SOLVENT          CDCl3
NS                 158
DS                   4
SWH          29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG                 203
DW              16.800 usec
DE               6.50 usec
TE             2832.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1               9.50 usec
PL1             -0.50 dB
PL1W       90.18825531 W
SFO1      125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2           80.00 usec
PL2              1.30 dB
PL12            16.00 dB
PL2W       15.30635643 W
PL12W       0.51864696 W
SFO2      500.2320009 MHz

F2 - Processing parameters
SI               32768
SF        125.7829596 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

BM-AM-45PS in CDCl3

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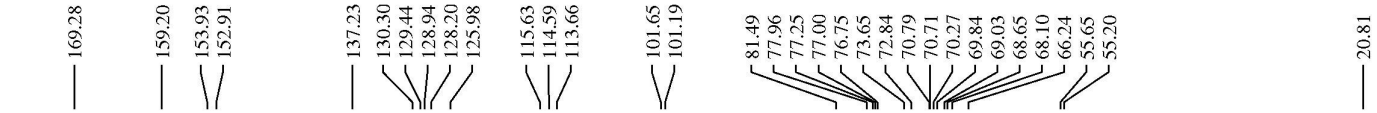
Current Data Parameters
NAME                  BM-AM-45PS
EXPNO                         40
PROCNO                         1

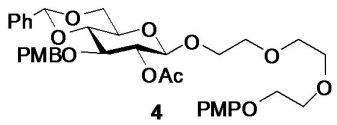
F2 - Acquisition Parameters
Date_                   20150514
Time                       15.07
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             9
DS                             2
SWH                  10330.578 Hz
FIDRES                0.157632 Hz
AQ                    3.1719425 sec
RG                            64
DW                       48.400 usec
DE                        6.50 usec
TE                        1157.6 K
D1                  1.00000000 sec
TD0                            1

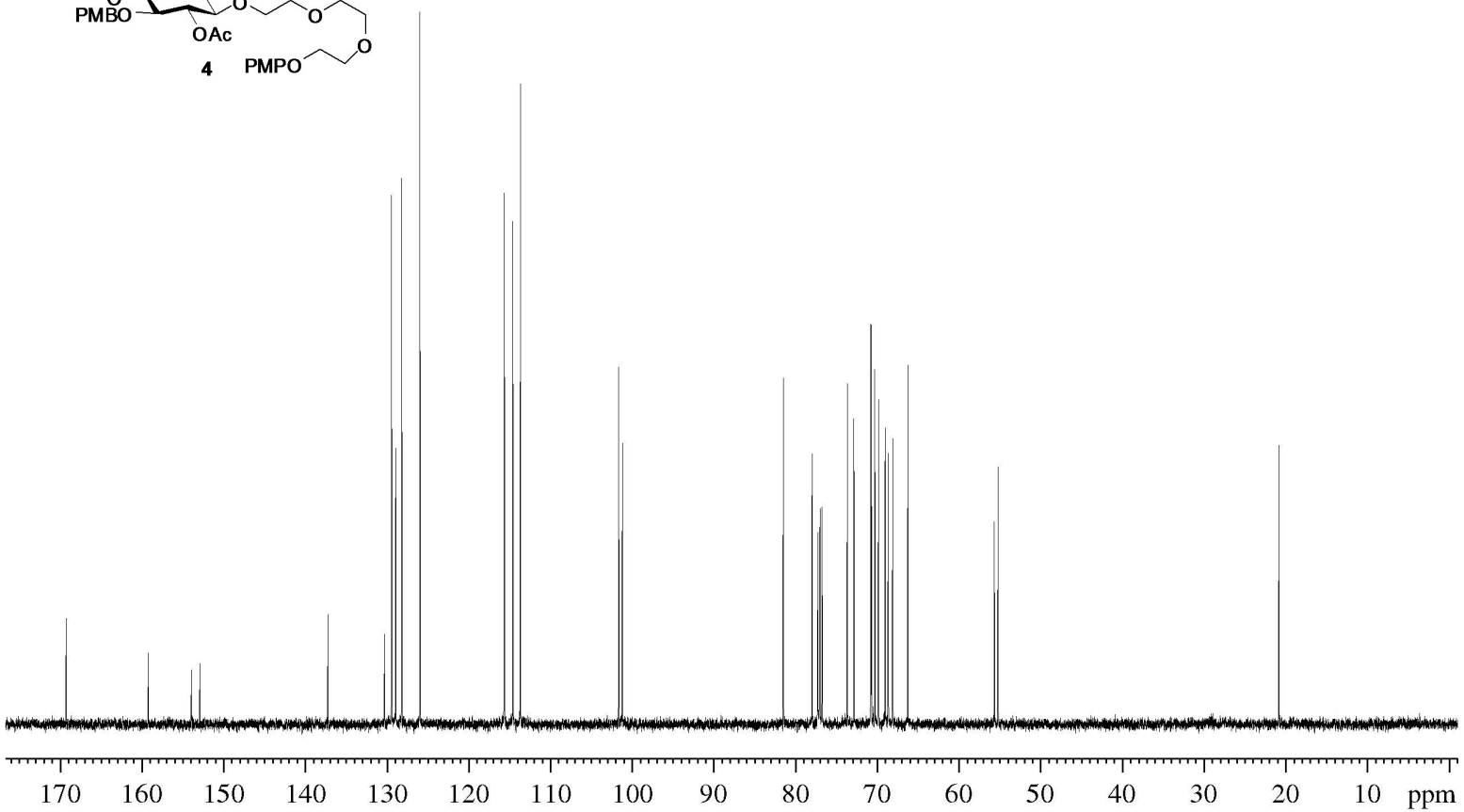
======== CHANNEL f1 ========
NUC1                          1H
P1                       14.25 usec
PL1                       1.30 dB
PL1W                15.30635643 W
SFO1                500.2330891 MHz

F2 - Processing parameters
SI                        131072
SF                  500.2300155 MHz
WDW                           EM
SSB                0
LB                        0.30 Hz
GB                 0
PC                        1.00
```

BM-AM-45PS in CDCl3







Current Data Parameters

NAME	BM-AM-45PS
EXPNO	41
PROCNO	1

F2 - Acquisition Parameters

Date_	20150514
Time	15.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgdc
TD	65536
SOLVENT	CDCl3
NS	130
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010048 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	1156.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
PL1W	90.18825531 W
SFO1	125.7955118 MHz

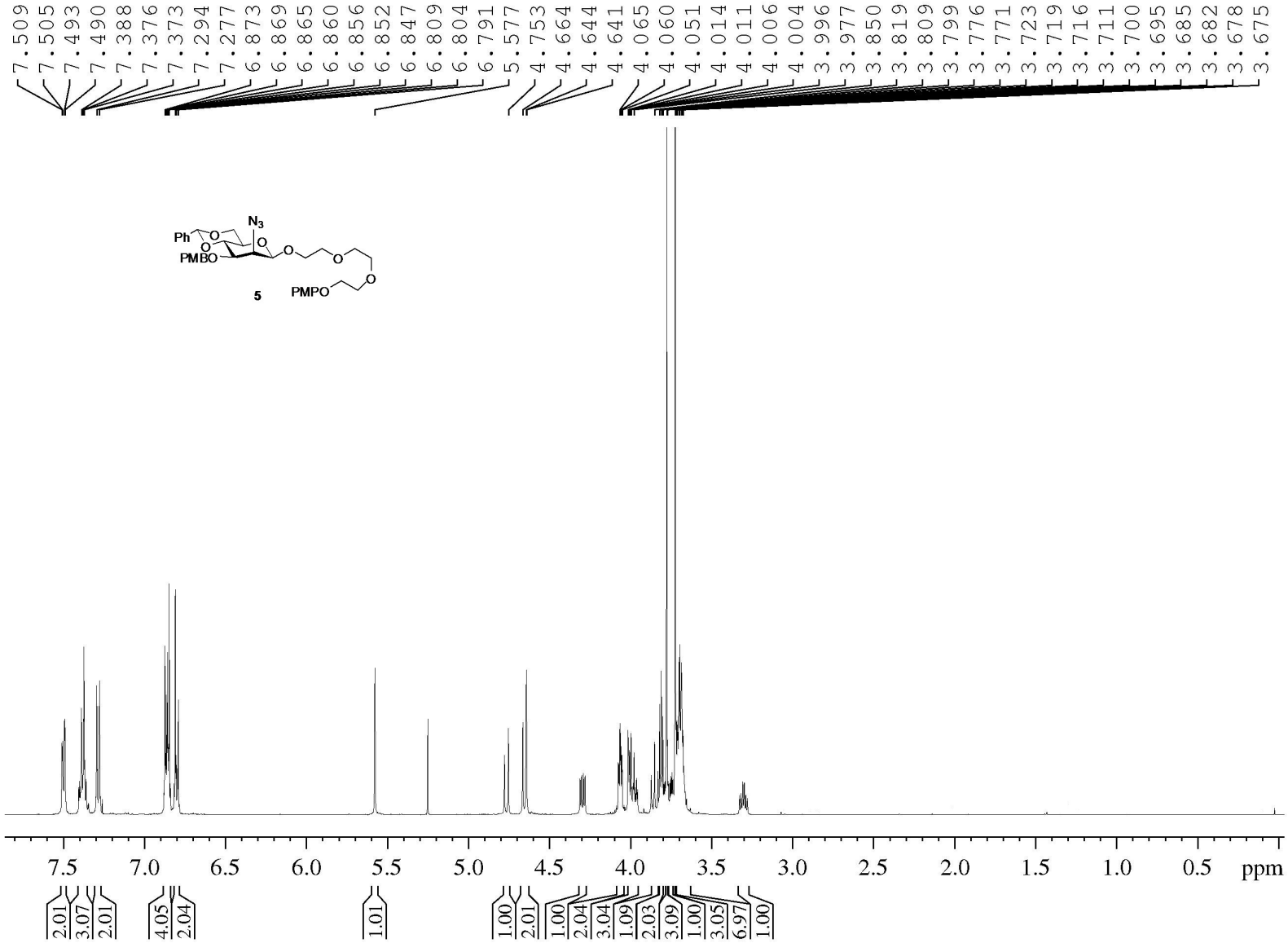
======== CHANNEL f2 ========

CPDPRG[2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.30 dB
PL12	16.00 dB
PL2W	15.30635643 W
PL12W	0.51864696 W
SFO2	500.2320009 MHz

F2 - Processing parameters

SI	32768
SF	125.7829419 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

BM-AM-49PS2 in CDCl3



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Current Data Parameters
NAME          BM-AM-49PS2
EXPNO                 140
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150528
Time               16.24
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719425 sec
RG                 22.6
DW                48.400 usec
DE                 6.50 usec
TE               1232.5 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.25 usec
PL1                1.30 dB
PL1W         15.30635643 W
SFO1         500.2330891 MHz

F2 - Processing parameters
SI                 32768
SF           500.2300150 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```
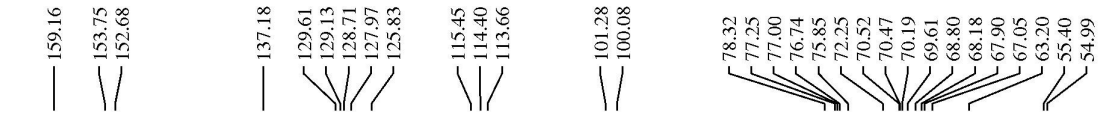
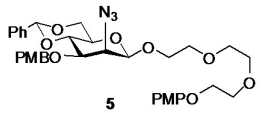

BM-AM-49PS2 in CDCl3





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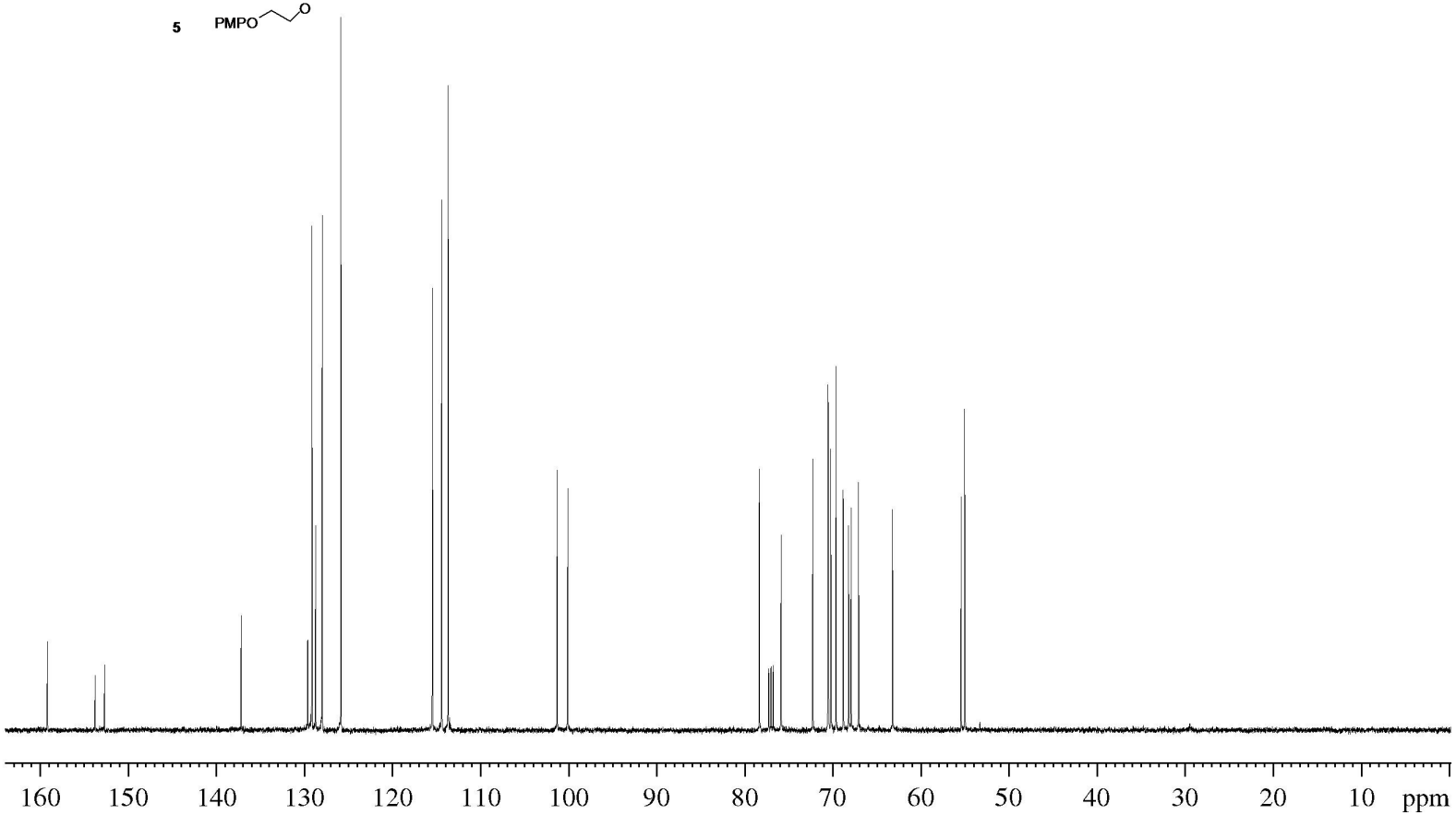
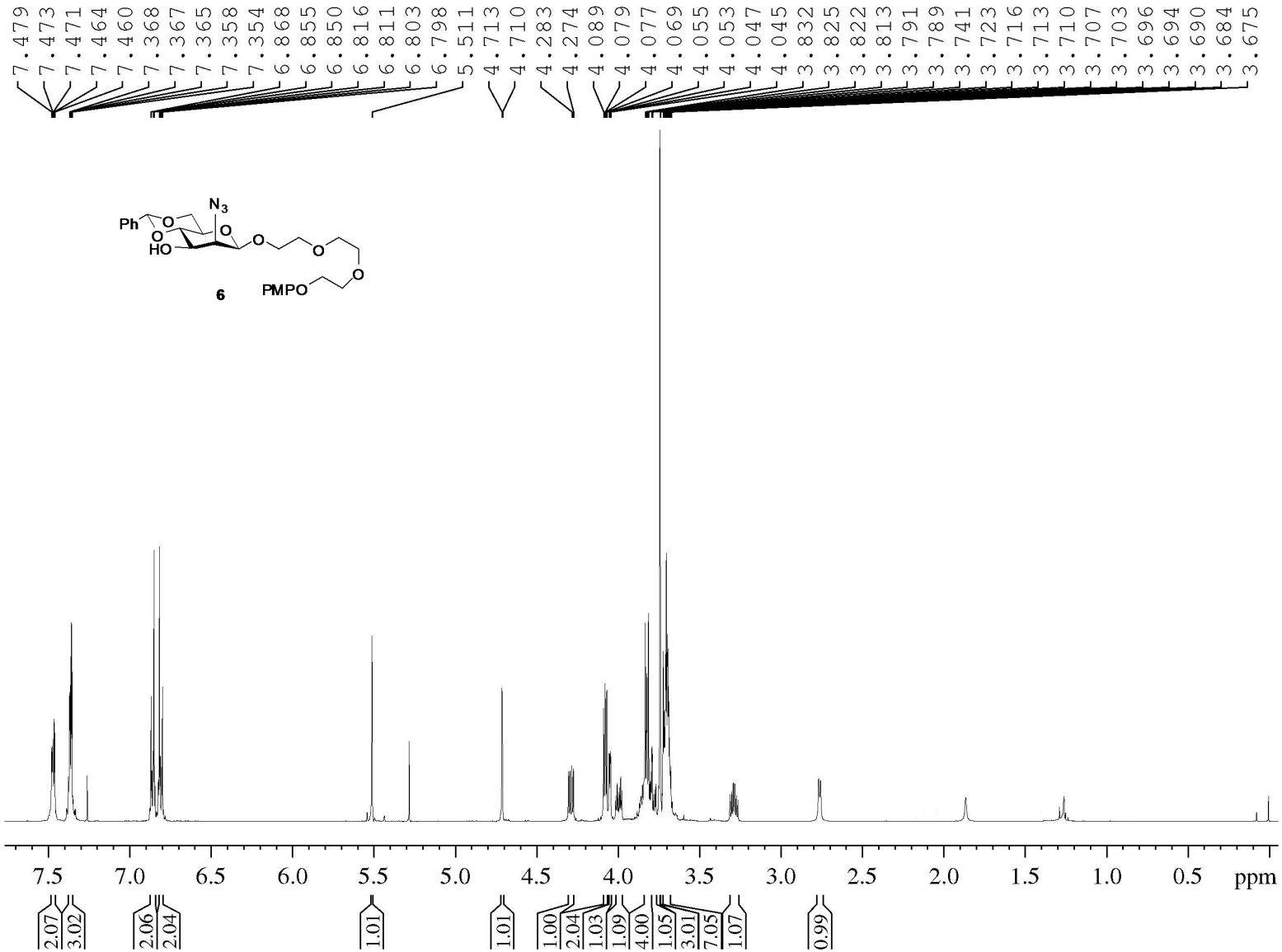
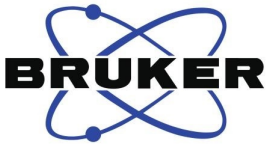



```
Current Data Parameters
NAME          BM-AM-49PS2
EXPNO                 141
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150528
Time               16.27
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zgdc
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  203
DW                16.800 usec
DE                 6.50 usec
TE               1237.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.50 usec
PL1                -0.50 dB
PL1W         90.18825531 W
SFO1         125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 1.30 dB
PL12               16.00 dB
PL2W         15.30635643 W
PL12W         0.51864696 W
SFO2         500.2320009 MHz

F2 - Processing parameters
SI                 32768
SF           125.7829693 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

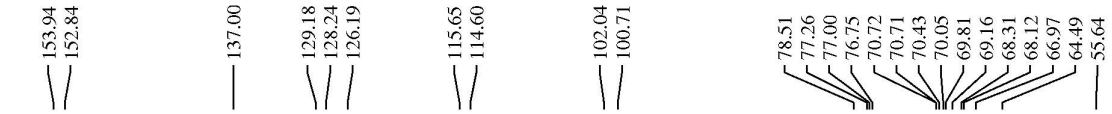
BM-AM-50PS in CDCl3

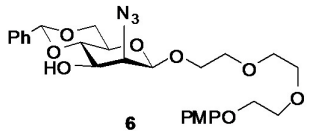





```
Current Data Parameters
NAME                  BM-AM-50PS
EXPNO                        100
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20150529
Time                       15.37
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                   10330.578 Hz
FIDRES                0.157632 Hz
AQ                    3.1719425 sec
RG                         50.8
DW                        48.400 usec
DE                         6.50 usec
TE                        1247.5 K
D1                   1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        14.25 usec
PL1                        1.30 dB
PL1W                15.30635643 W
SFO1                500.2330891 MHz

F2 - Processing parameters
SI                        131072
SF                  500.2300156 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```

BM-AM-50PS in CDCl3





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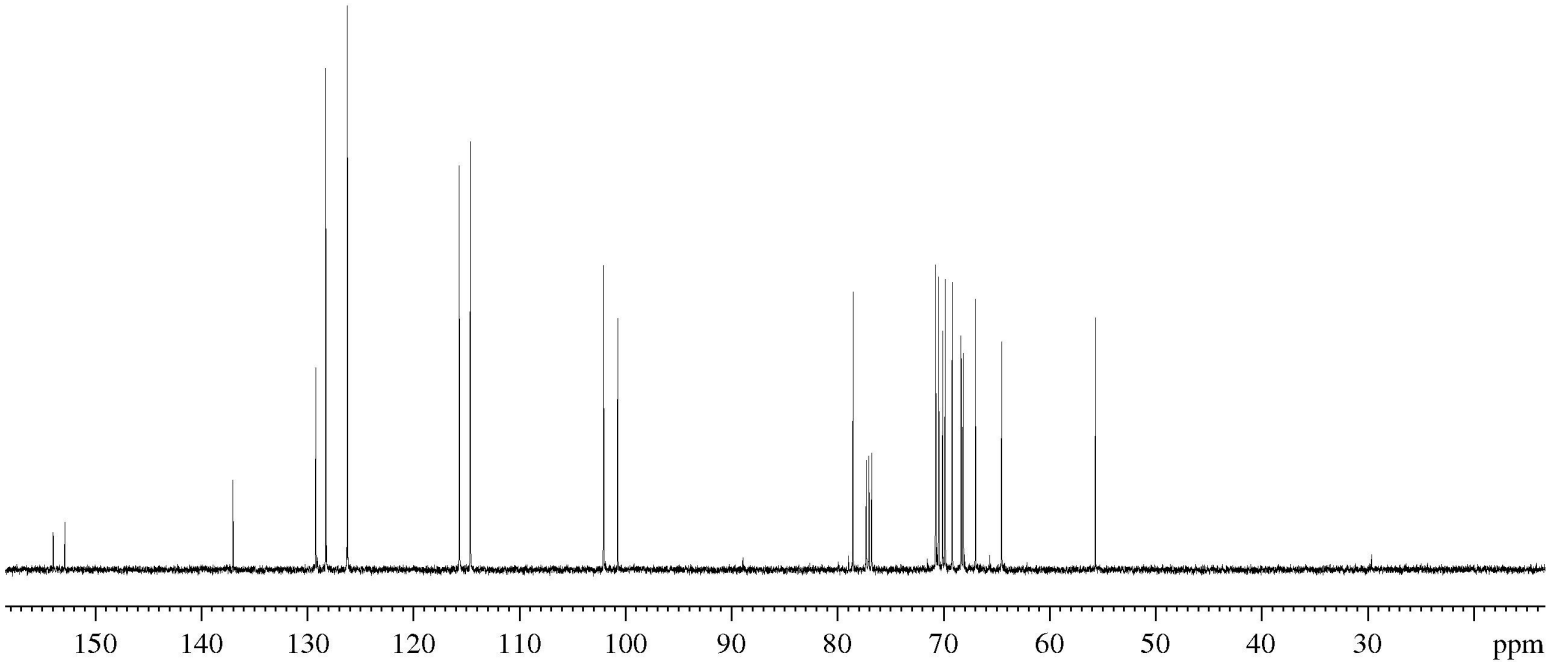
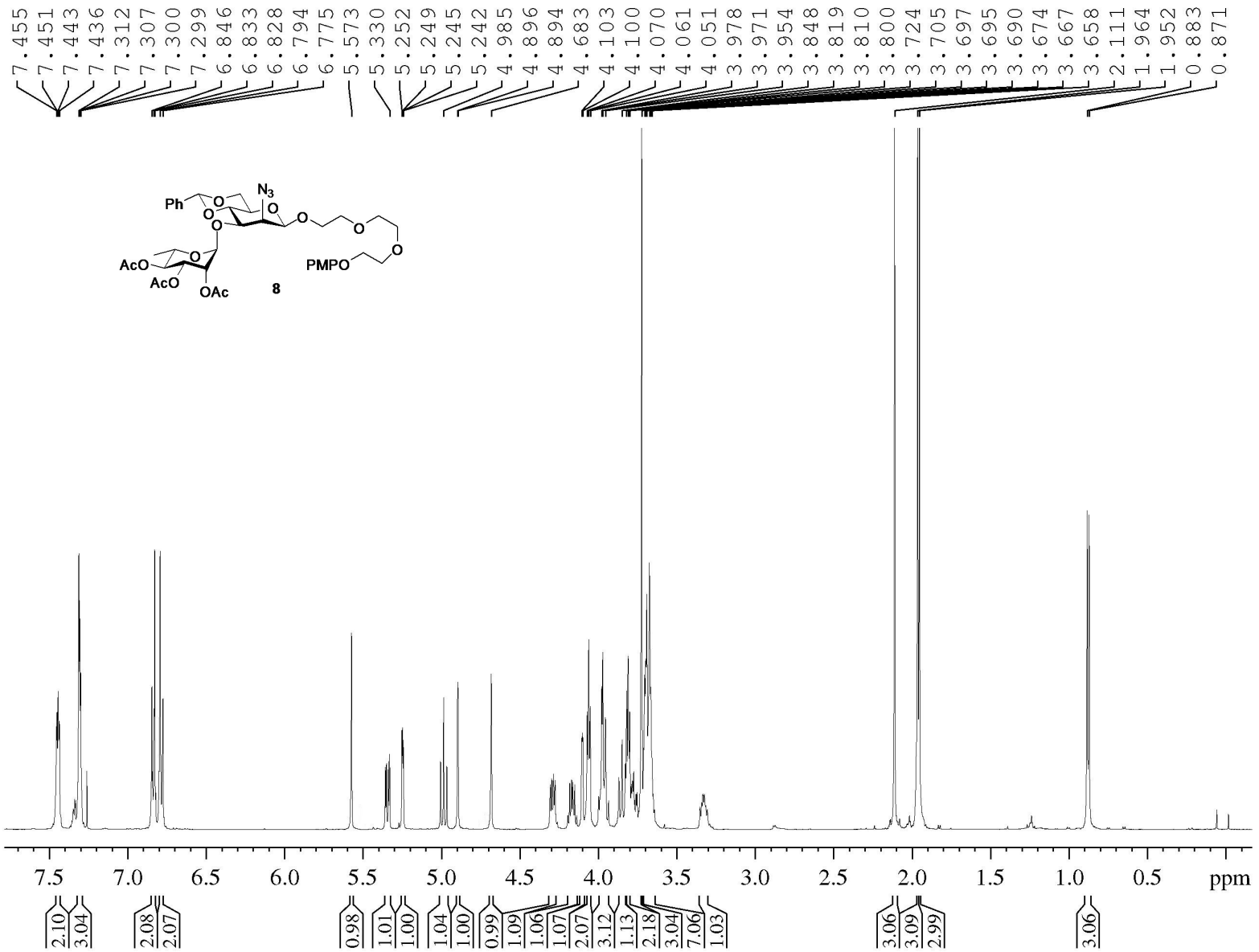
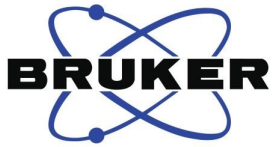



```
Current Data Parameters
NAME                  BM-AM-50PS
EXPNO                        101
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20150529
Time                       15.41
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zgdc
TD                        65536
SOLVENT                   CDCl3
NS                           74
DS                            4
SWH                   29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010048 sec
RG                           203
DW                        16.800 usec
DE                         6.50 usec
TE                       1250.7 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         13C
P1                         9.50 usec
PL1                       -0.50 dB
PL1W                90.18825531 W
SFO1               125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.30 dB
PL12                      16.00 dB
PL2W                15.30635643 W
PL12W                0.51864696 W
SFO2               500.2320009 MHz

F2 - Processing parameters
SI                        32768
SF                 125.7829452 MHz
WDW                          EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```

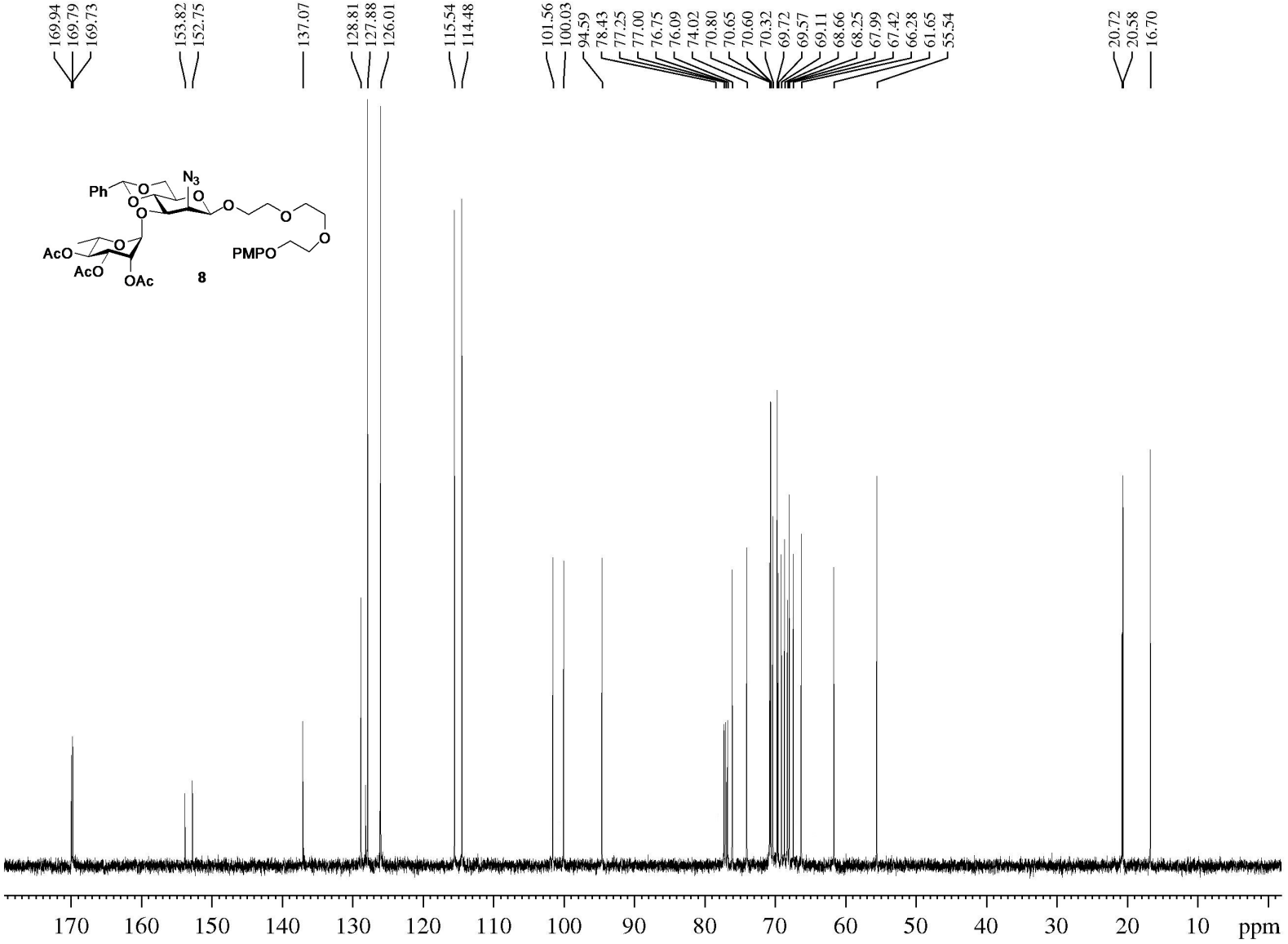
BM-AM-51PS in CDCl3






```
Current Data Parameters
NAME                  BM-AM-51PS
EXPNO                         10
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20150605
Time                       10.02
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            16
DS                             2
SWH                   10330.578 Hz
FIDRES                 0.157632 Hz
AQ                     3.1719425 sec
RG                            36
DW                        48.400 usec
DE                         6.50 usec
TE                        1442.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         14.25 usec
PL1                         1.30 dB
PL1W                15.30635643 W
SFO1                500.2330891 MHz

F2 - Processing parameters
SI                        131072
SF                  500.2330152 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```

BM-AM-51PS in CDCl3



Current Data Parameters
NAME BM-AM-51PS
EXPNO 11
PROCNO 1

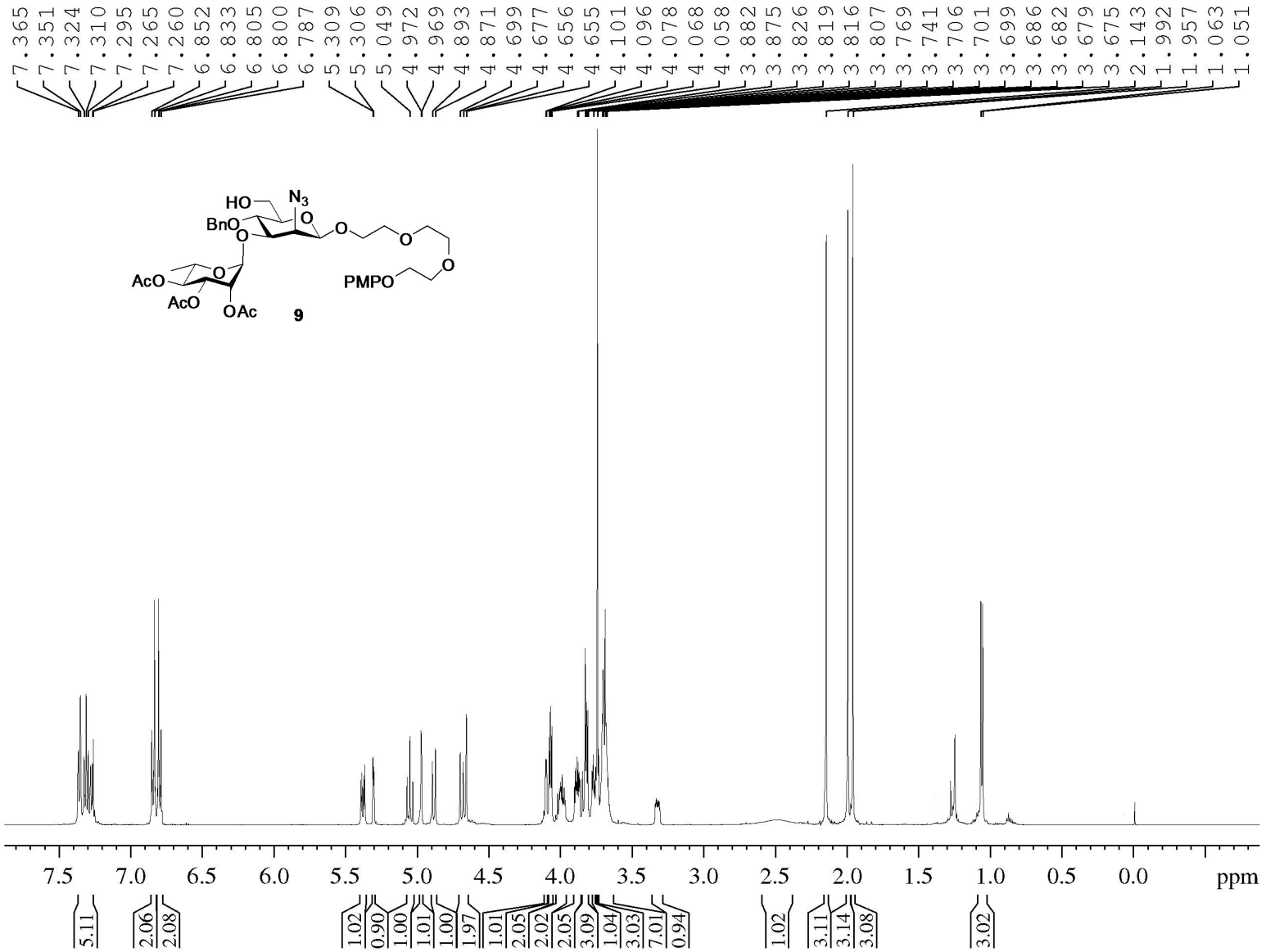
F2 - Acquisition Parameters
Date_ 20150605
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 55
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 1440.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
PL1W 90.18825531 W
SFO1 125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.00 dB
PL2W 15.30635643 W
PL12W 0.51864696 W
SFO2 500.2320009 MHz

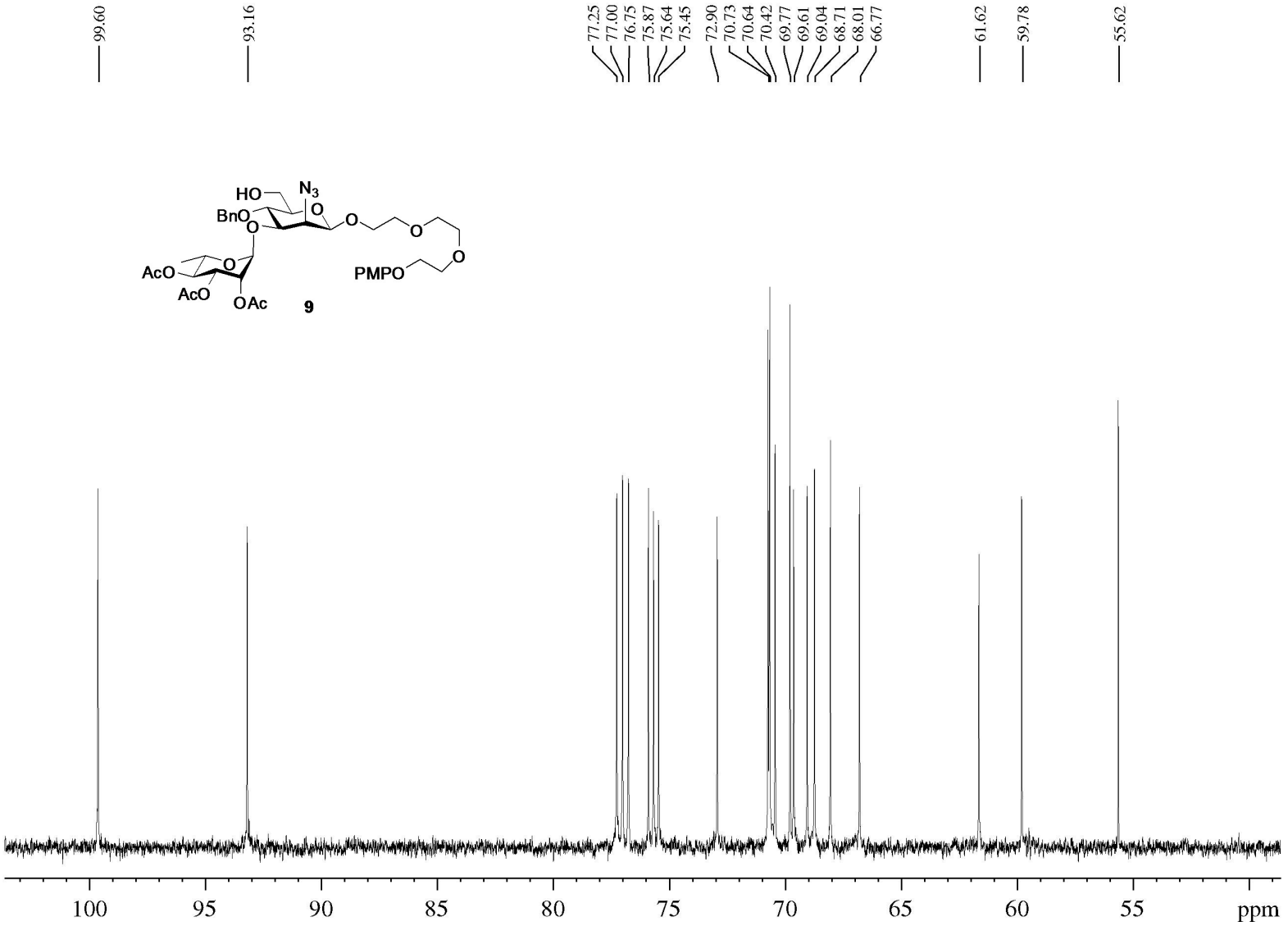
F2 - Processing parameters
SI 32768
SF 125.7829520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

BM-AM-52TCTPS in CDCl3



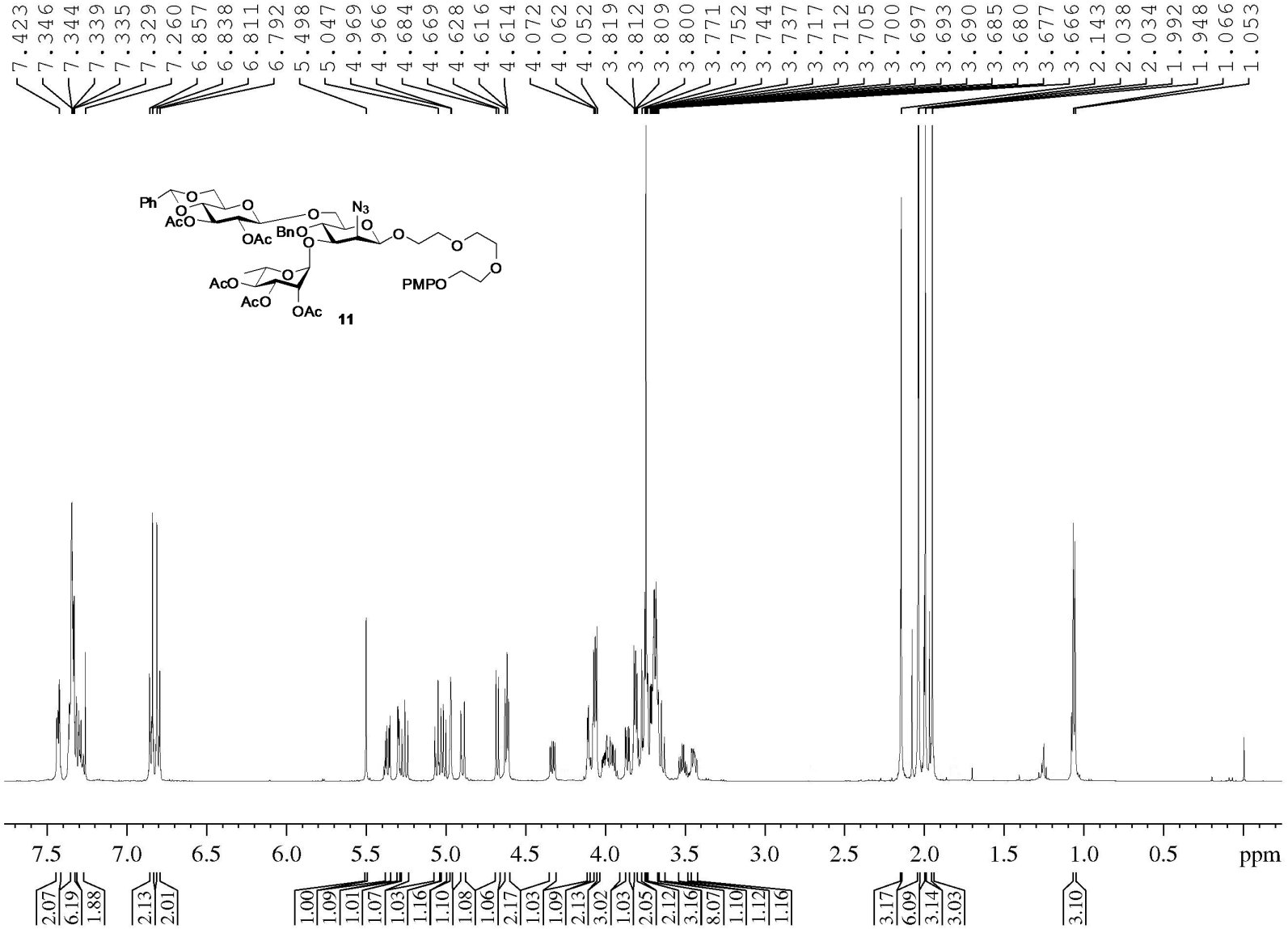

```
Current Data Parameters
NAME       BM-AM-52TCTPS
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150610
Time              10.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719425 sec
RG                 50.8
DW               48.400 usec
DE                6.50 usec
TE               1537.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.25 usec
PL1                1.30 dB
PL1W         15.30635643 W
SFO1         500.2330891 MHz

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

BM-AM-52TCTPS in CDCl3




```
Current Data Parameters
NAME       BM-AM-52TCTPS
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150610
Time               10.31
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                   138
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                1537.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.50 usec
PL1                 -0.50 dB
PL1W         90.18825531 W
SFO1        125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 1.30 dB
PL12               16.00 dB
PL2W         15.30635643 W
PL12W         0.51864696 W
SFO2        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 CDCl3



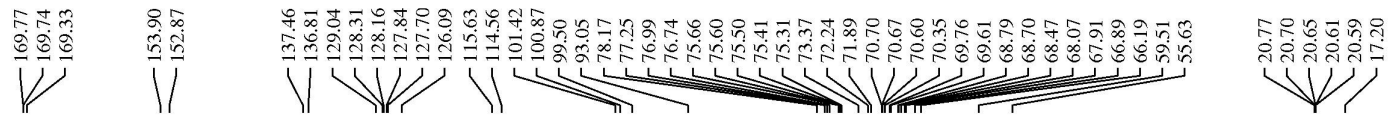
Current Data Parameters
NAME BM-AM-54PS
EXPNO 60
PROCNO 1

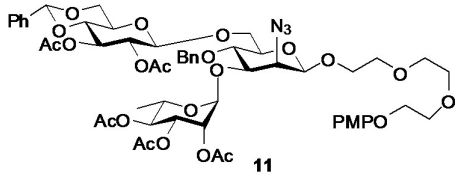
F2 - Acquisition Parameters
Date_ 20150616
Time 11.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 1523.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.25 usec
PL1 1.30 dB
PL1W 15.30635643 W
SFO1 500.2330891 MHz

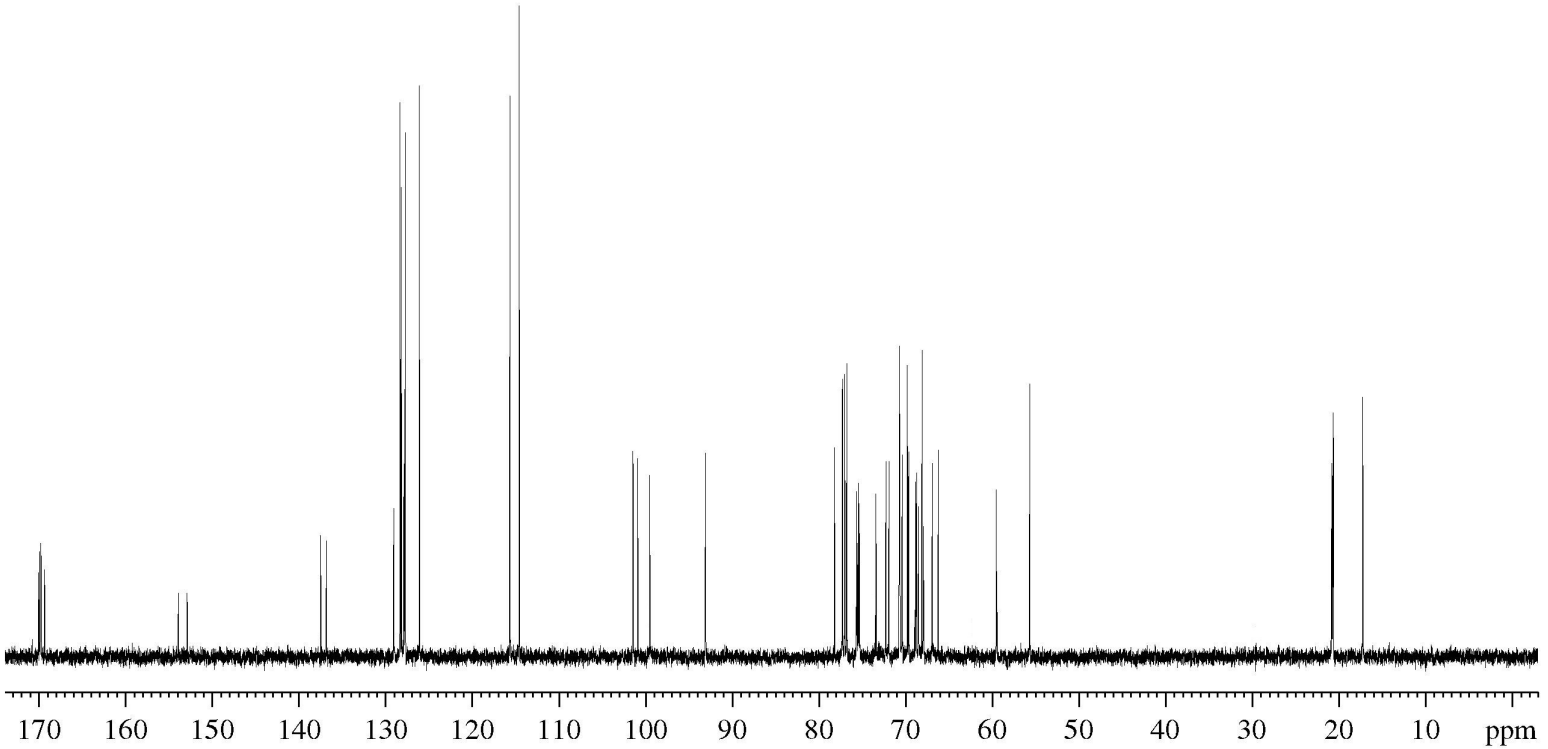
F2 - Processing parameters
SI 131072
SF 500.2300148 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

BM-AM-54PS in CDCl3



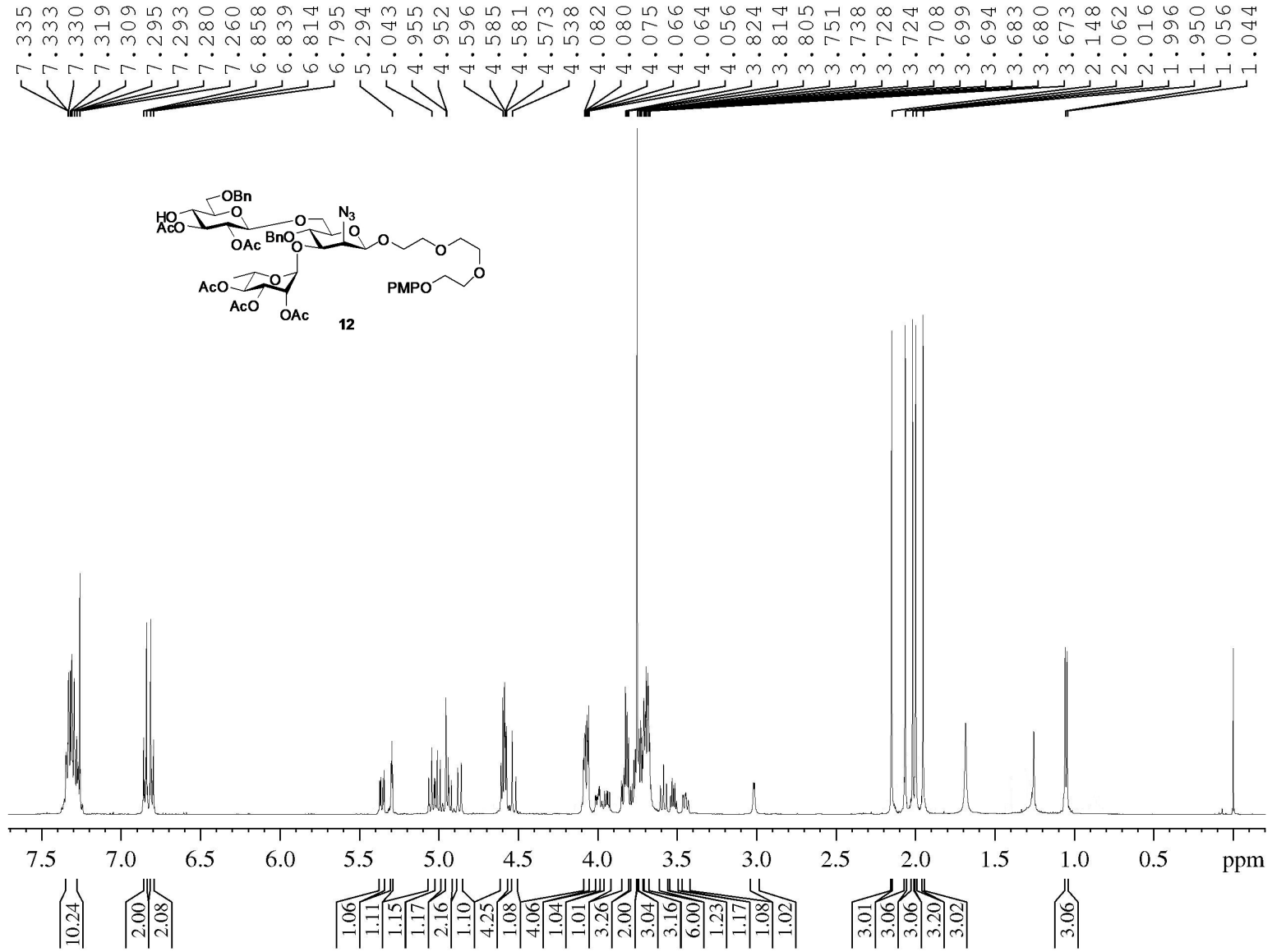


11




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

F2 - Acquisition Parameters
Date_           20150616
Time               11.46
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                   133
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG                   203
DW               16.800 usec
DE                6.50 usec
TE               1523.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.50 usec
PL1                -0.50 dB
PL1W        90.18825531 W
SFO1       125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                1.30 dB
PL12              16.00 dB
PL2W        15.30635643 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
```

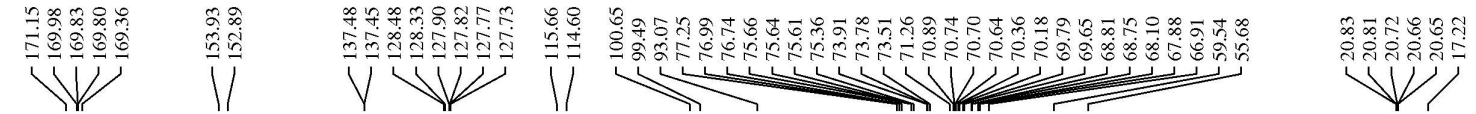
BM-AM-58PS in CDCl3



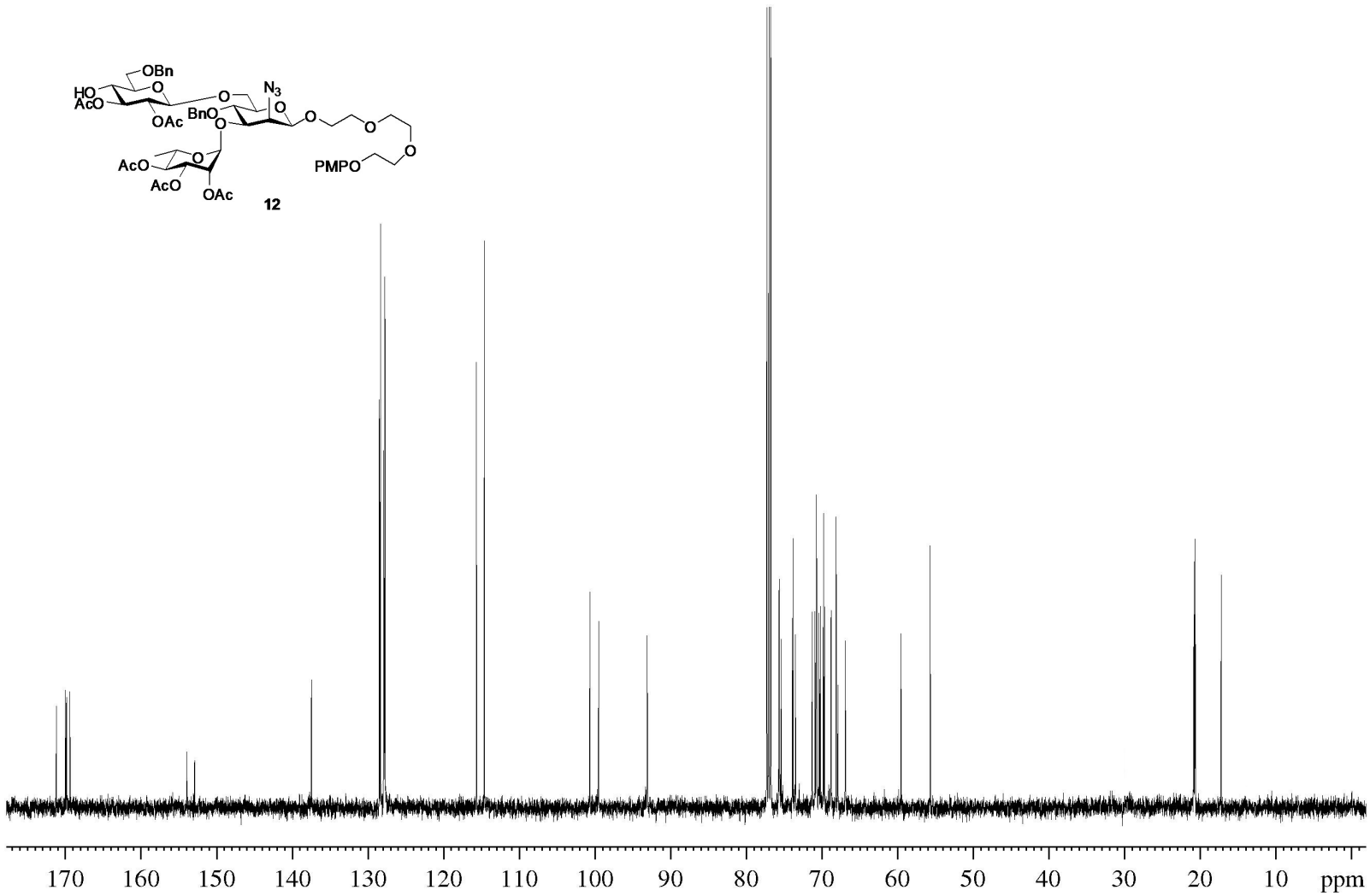
BRUKER

```
Current Data Parameters
NAME                  BM-AM-58PS
EXPNO                         60
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20150728
Time                       12.59
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                 10330.578 Hz
FIDRES                0.157632 Hz
AQ                    3.1719425 sec
RG                          128
DW                       48.400 usec
DE                        6.50 usec
TE                      1493.5 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.25 usec
PL1                       1.30 dB
PL1W              15.30635643 W
SFO1              500.2330891 MHz

F2 - Processing parameters
SI                       131072
SF                500.2300156 MHz
WDW                        EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

BM-AM-58PS in CDCl3

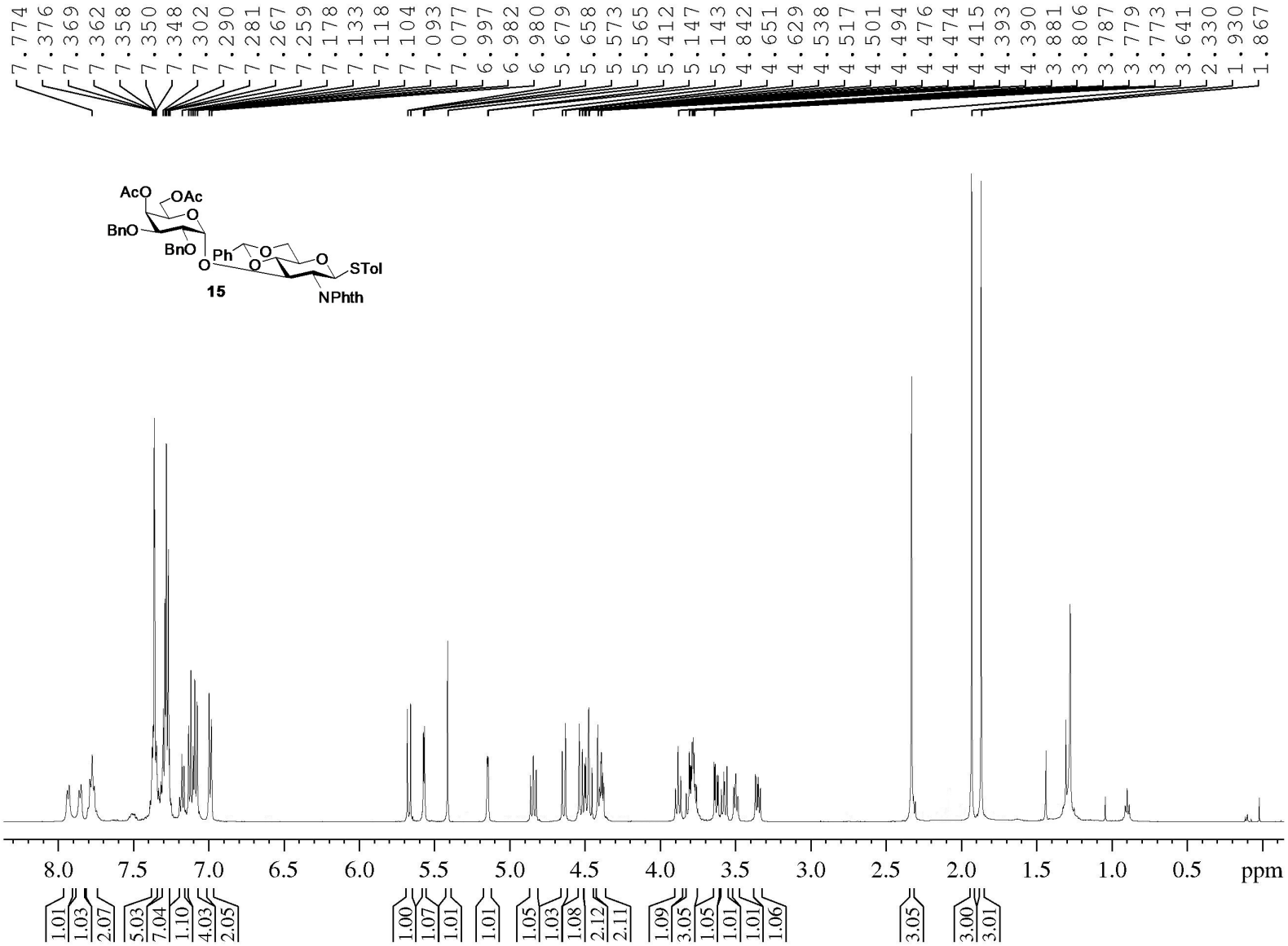


12




```
Current Data Parameters
NAME                  BM-AM-58PS
EXPNO                         63
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20150728
Time                       13.22
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zgdc
TD                        65536
SOLVENT                   CDCl3
NS                          602
DS                            4
SWH                   29761.904 Hz
FIDRES                 0.454131 Hz
AQ                    1.1010048 sec
RG                          203
DW                       16.800 usec
DE                        6.50 usec
TE                       1493.8 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                          9.50 usec
PL1                        -0.50 dB
PL1W                90.18825531 W
SFO1               125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.30 dB
PL12                      16.00 dB
PL2W               15.30635643 W
PL12W               0.51864696 W
SFO2               500.2320009 MHz

F2 - Processing parameters
SI                           32768
SF                 125.7829388 MHz
WDW                             EM
SSB          0
LB                         1.00 Hz
GB           0
PC                         1.40
```

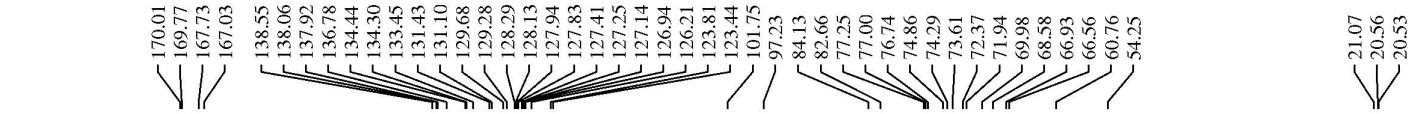
BM-AM-18PENT in CDCl3

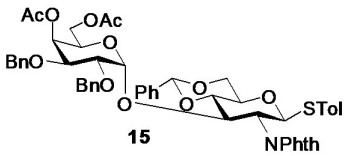


BRUKER

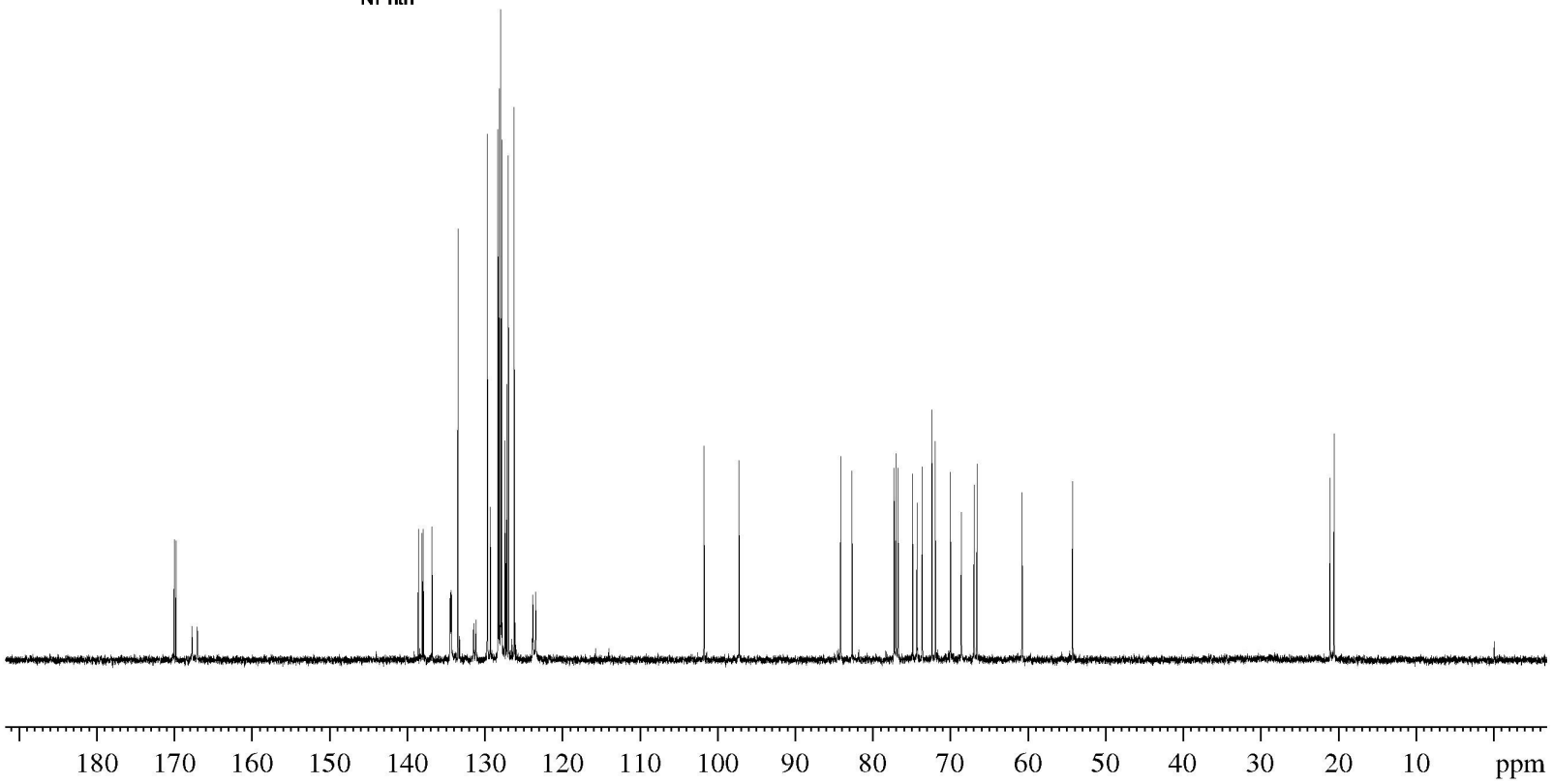
```
Current Data Parameters
NAME        BM-AM-18PENT
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150218
Time               10.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.576 Hz
FIDRES         0.157632 Hz
AQ             3.1719425 sec
RG                    36
DW                48.400 usec
DE                 6.50 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.25 usec
PL1                 1.30 dB
PL1W         15.30635643 W
SFO1         500.2330891 MHz

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

BM-AM-18PENT in CDCl3



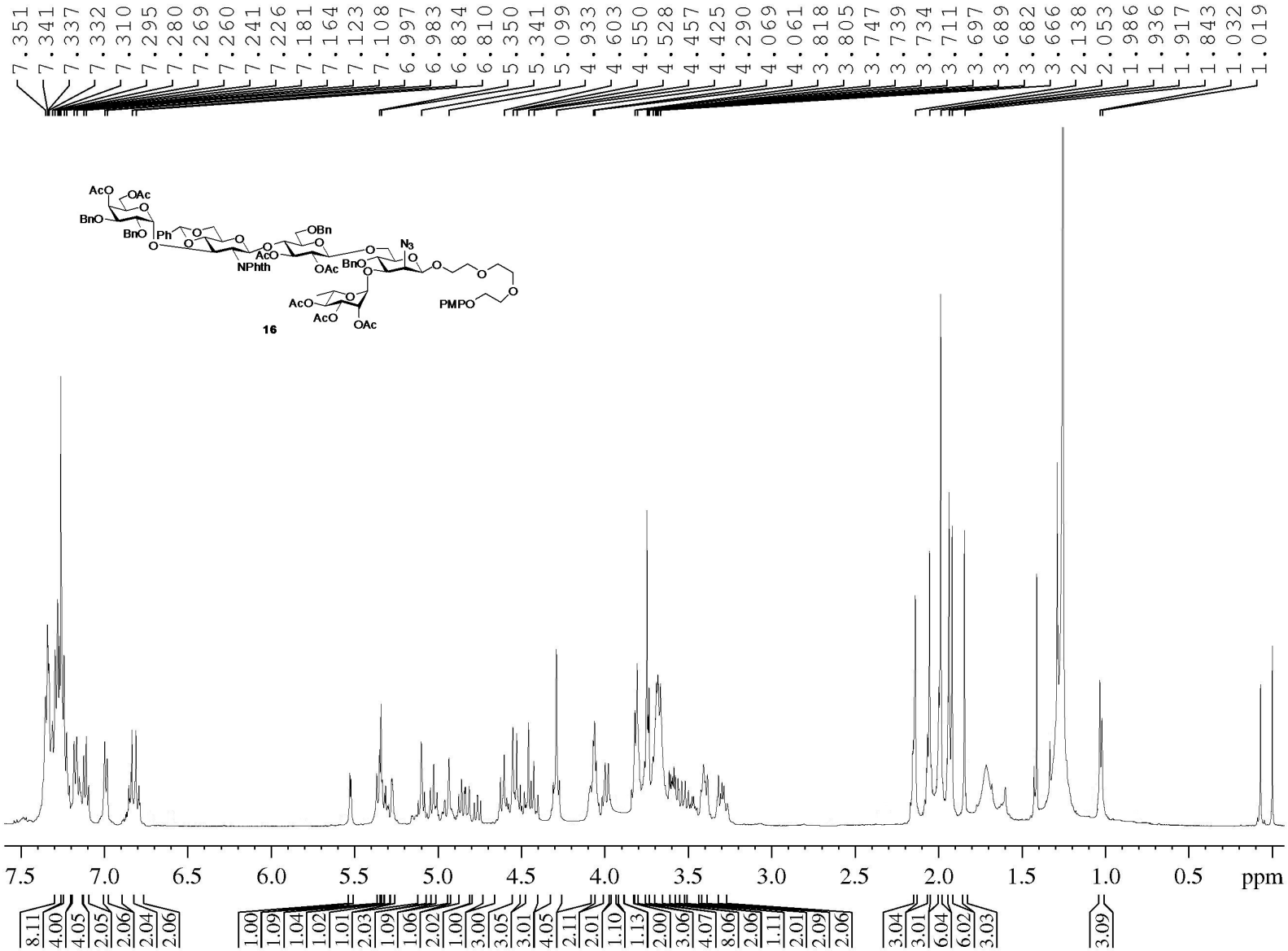


15




```
Current Data Parameters
NAME                  BM-AM-18PENT
EXPNO                           11
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20150218
Time                         10.08
INSTRUM                      spect
PROBHD     5 mm PABBO BB-
PULPROG                      zgdc
TD                          65536
SOLVENT                     CDCl3
NS                            147
DS                              4
SWH                   29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010048 sec
RG                            203
DW                       16.800 usec
DE                        6.50 usec
TE                        300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                          13C
P1                          9.50 usec
PL1                        -0.50 dB
PL1W                90.18825531 W
SFO1                125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2                 waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL2                         1.30 dB
PL12                       16.00 dB
PL2W                15.30635643 W
PL12W                0.51864696 W
SFO2                500.2320009 MHz

F2 - Processing parameters
SI                            32768
SF                  125.7829505 MHz
WDW                              EM
SSB                 0
LB                          1.00 Hz
GB                  0
PC                          1.40
```

BM-AM-60PS4AUG in CDCl3



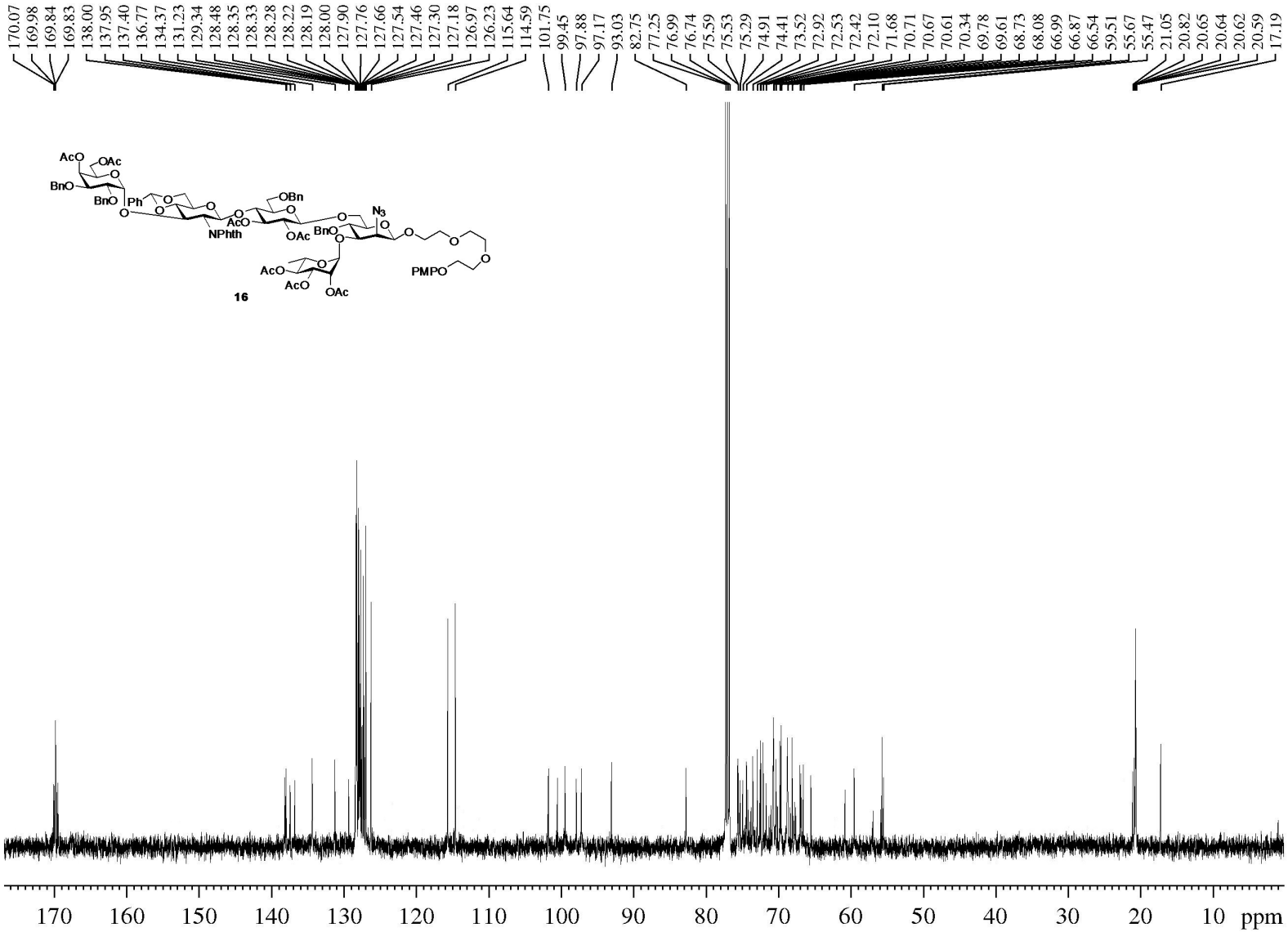
Current Data Parameters
NAME BM-AM-60PS4AUG
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150804
Time 9.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 1613.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.25 usec
PL1 1.30 dB
PL1W 15.30635643 W
SFO1 500.2330891 MHz

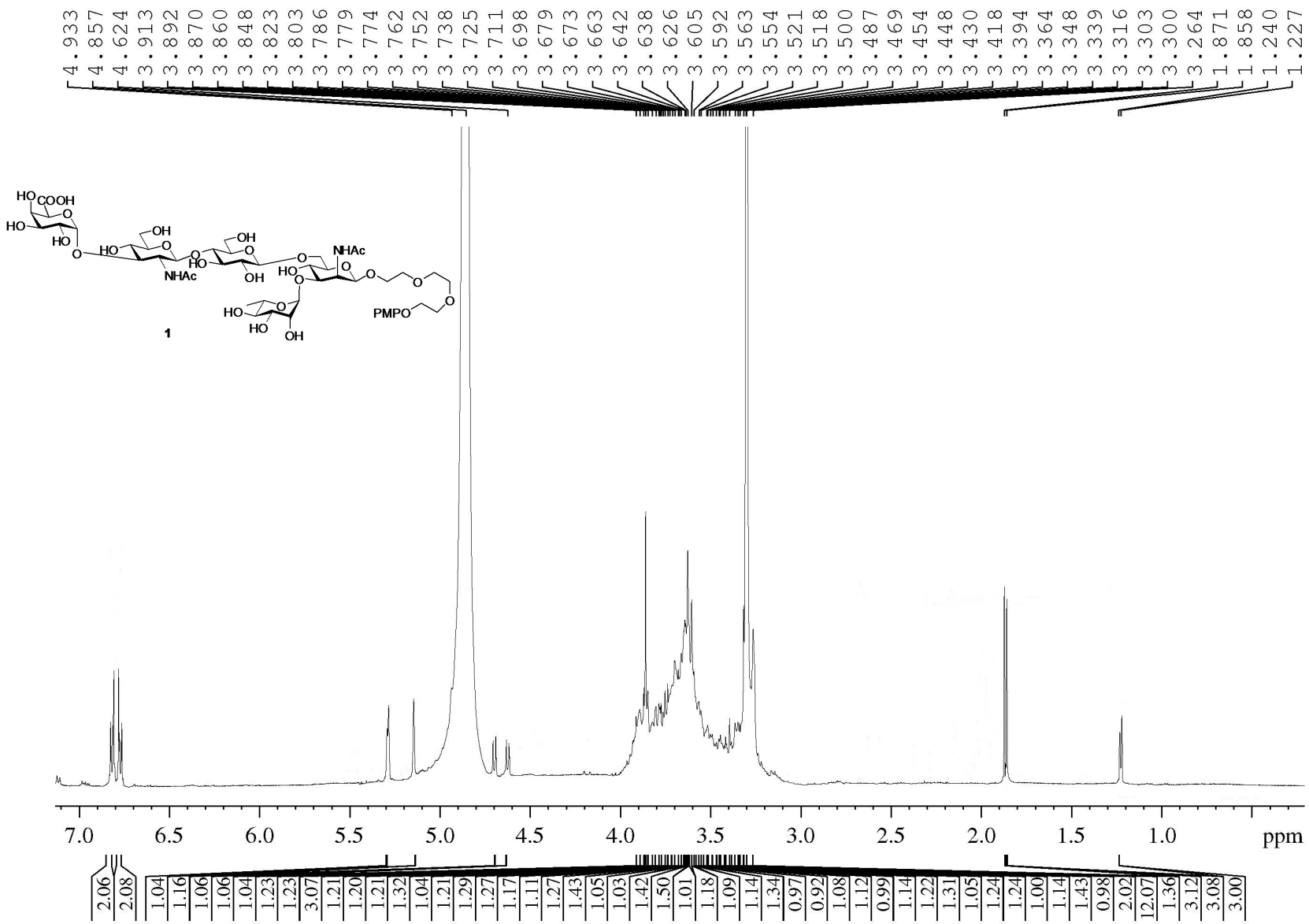
F2 - Processing parameters
SI 131072
SF 500.2300155 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

BM-AM-60PS4AUG in CDCl3



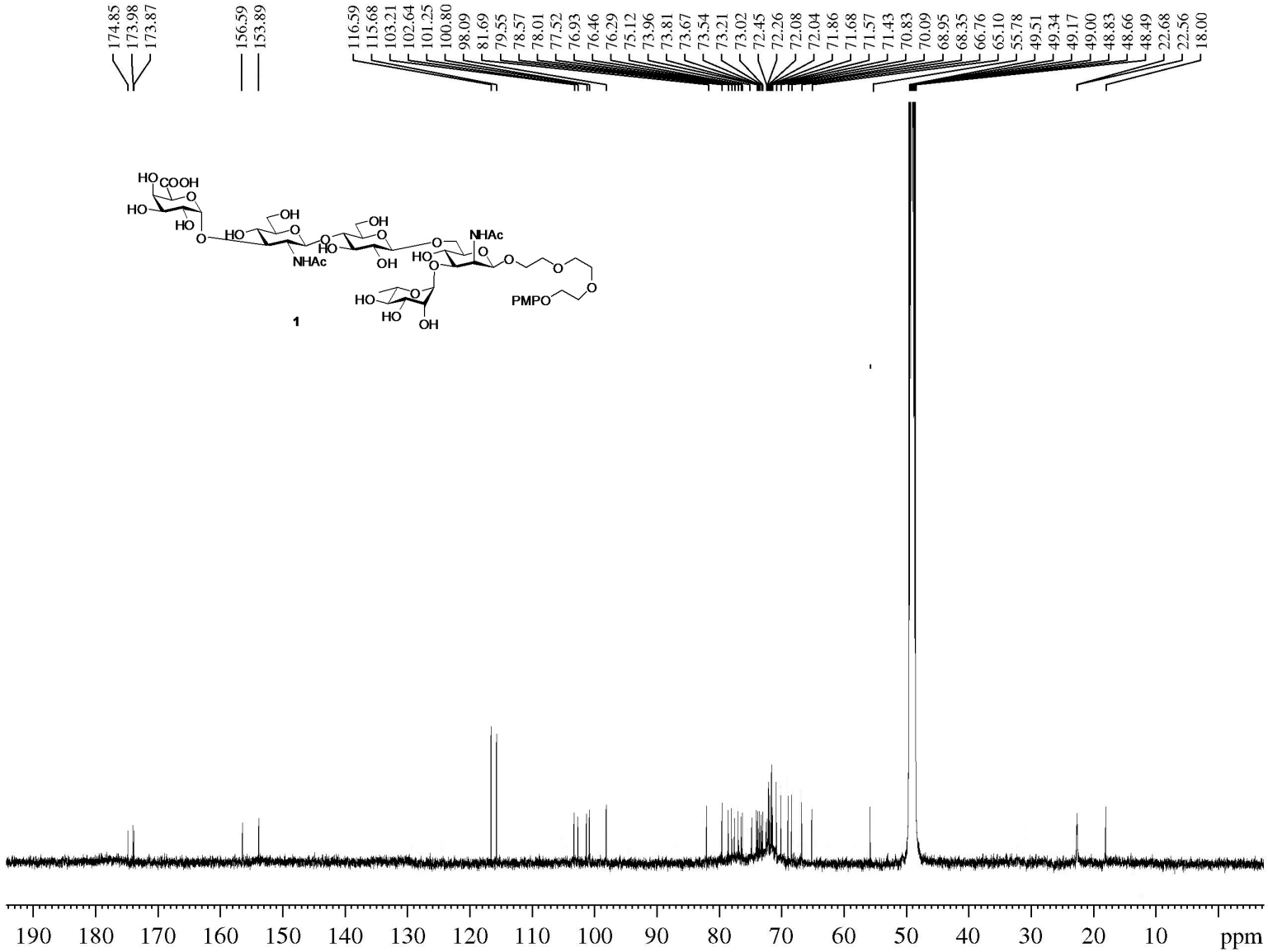

```
Current Data Parameters
NAME      BM-AM-60PS4AUG
EXPNO                 13
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150804
Time              10.23
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zgdc
TD                65536
SOLVENT           CDCl3
NS                  789
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE              1594.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                9.50 usec
PL1              -0.50 dB
PL1W       90.18825531 W
SFO1      125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               1.30 dB
PL12             16.00 dB
PL2W       15.30635643 W
PL12W       0.51864696 W
SFO2      500.2320009 MHz

F2 - Processing parameters
SI                32768
SF          125.7829396 MHz
WDW                 EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

BM-AM-PENTFINAL in MeOD




```
Current Data Parameters
NAME      BM-AM-PENTFINAL
EXPNO                 220
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151105
Time              16.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           MeOD
NS                 128
DS                   2
SWH          10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719425 sec
RG                 128
DW               48.400 usec
DE                6.50 usec
TE              2292.7 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               14.25 usec
PL1               1.30 dB
PL1W        15.30635643 W
SFO1        500.2330891 MHz

F2 - Processing parameters
SI               131072
SF          500.2300178 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

BM-AM-PENTFINAL in MeOD



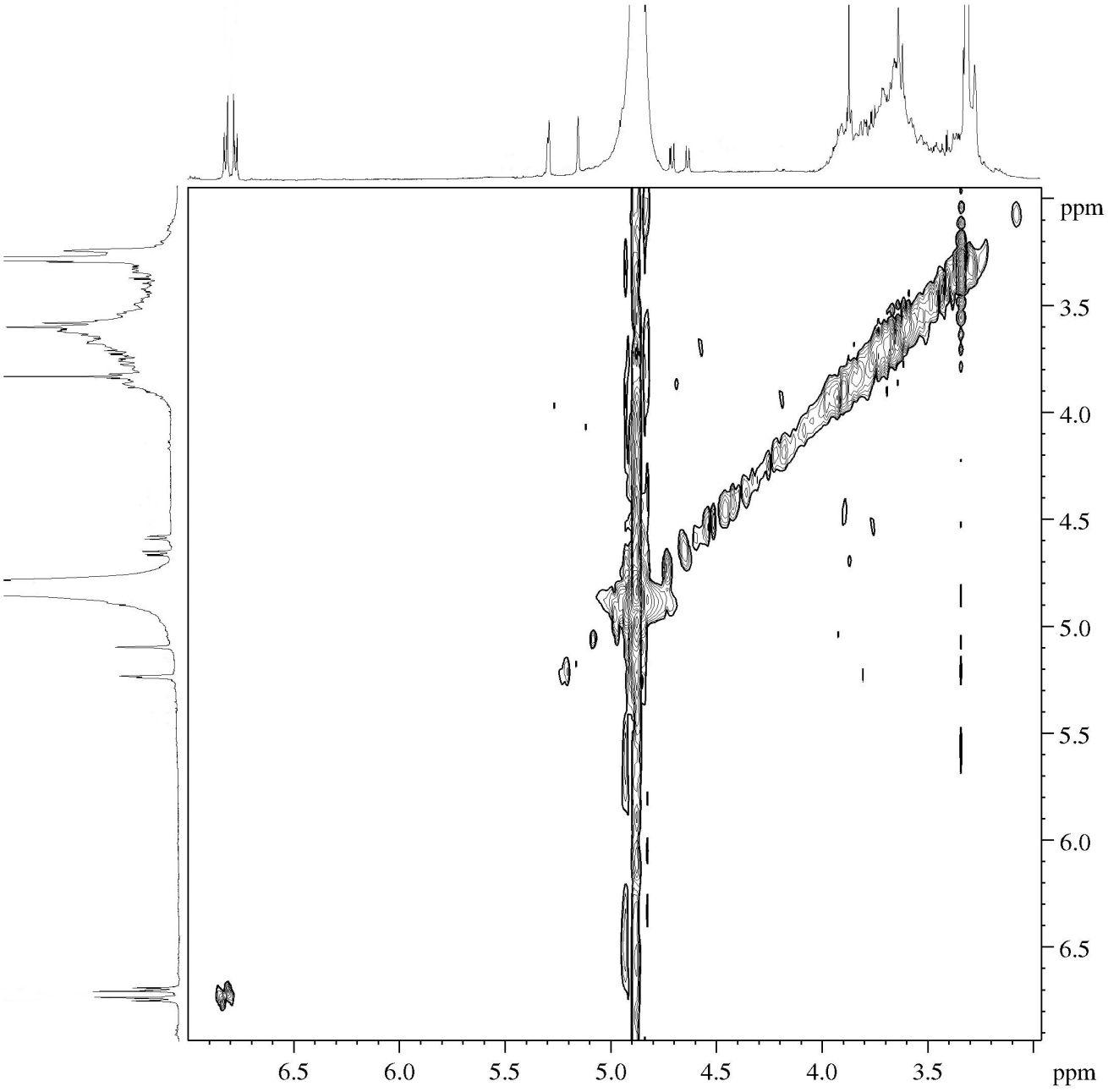
Current Data Parameters
NAME BM-AM-PENTFINAL
EXPNO 221
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151105
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 65536
SOLVENT MeOD
NS 18000
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 2296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
PL1W 90.18825531 W
SFO1 125.7955118 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.00 dB
PL2W 15.30635643 W
PL12W 0.51864696 W
SFO2 500.2320009 MHz

F2 - Processing parameters
SI 32768
SF 125.7827604 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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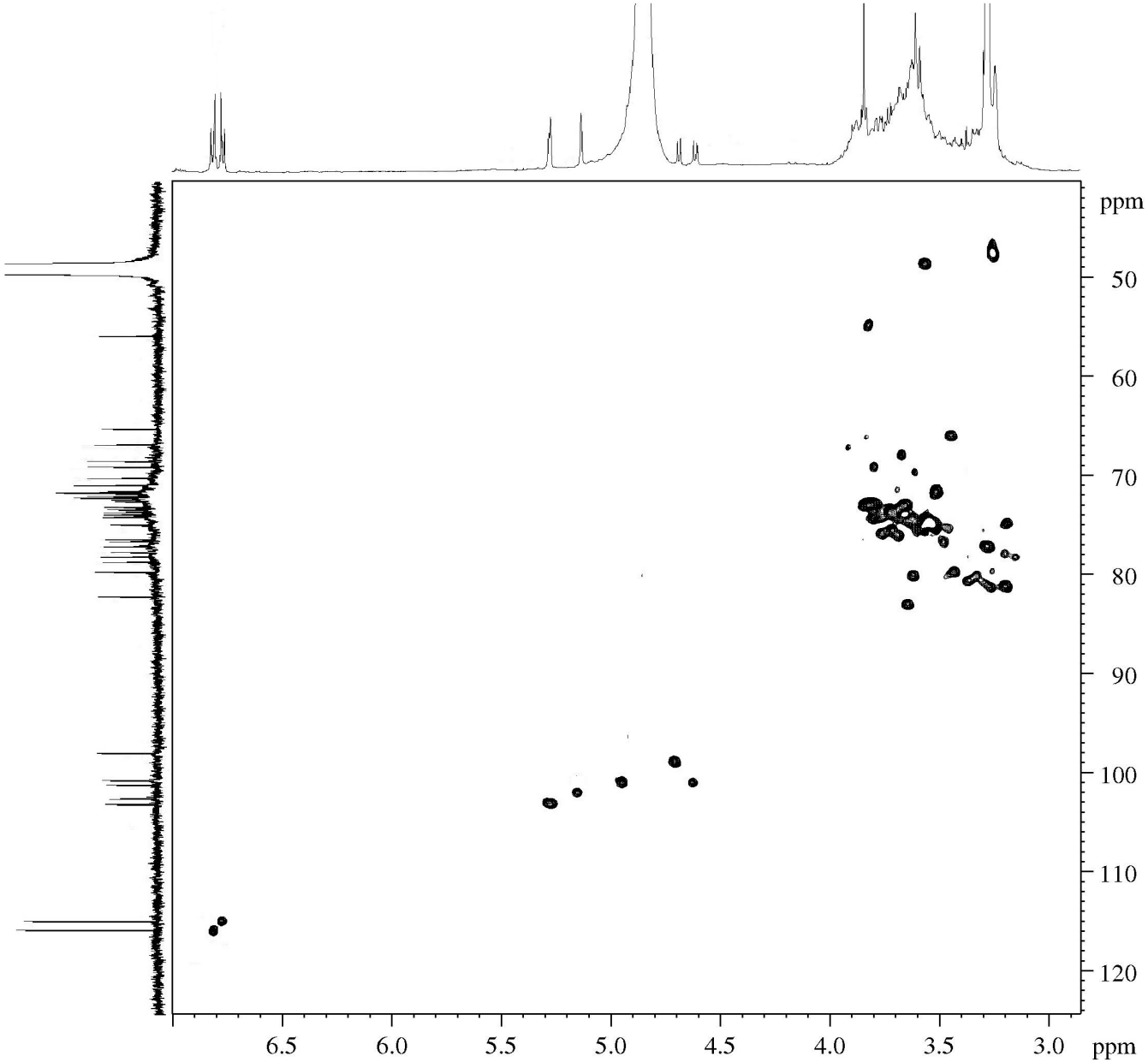
```
Current Data Parameters
NAME      BM-AM-PENTA HSCOSY
EXPNO                  111
PROCNO                   1

F2 - Acquisition Parameters
Date_           20151210
Time               15.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         cosygpqf
TD                 2048
SOLVENT             MeOD
NS                   32
DS                   16
SWH              6684.492 Hz
FIDRES           3.263912 Hz
AQ              0.1531904 sec
RG                   161
DW                74.800 usec
DE                 6.50 usec
TE                2905.1 K
D0             0.00000300 sec
D1             1.48689198 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00014975 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                14.25 usec
P1                14.25 usec
PL1                1.30 dB
PL1W         15.30635643 W
SFO1        500.2330075 MHz

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

F1 - Acquisition parameters
TD                   128
SFO1             500.233 MHz
FIDRES          52.173840 Hz
SW                13.350 ppm
FnMODE                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-AM-PENTA HSCOSY
EXPNO                  112
PROCNO                   1

F2 - Acquisition Parameters
Date_              20151210
Time                  17.40
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG      hsqcetgpsi2
TD                     1024
SOLVENT                MeOD
NS                       96
DS                       16
SWH               6009.615 Hz
FIDRES            5.868765 Hz
AQ               0.0851968 sec
RG                     203
DW                  83.200 usec
DE                    6.50 usec
TE                  3242.5 K
CNST2          145.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D4              0.00172414 sec
D11             0.03000000 sec
D13             0.00000400 sec
D16             0.00020000 sec
D24             0.00086207 sec
IN0             0.00001985 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.25 usec
P2                   28.50 usec
P28                   0.10 usec
PL1                   1.30 dB
PL1W           15.30635643 W
SFO1           500.2330014 MHz

======== CHANNEL f2 ========
CPDPRG[2               garp
NUC2                    13C
P3                    9.50 usec
P4                   19.00 usec
PCPD2                70.00 usec
PL2                  -0.50 dB
PL12                 17.00 dB
PL2W           90.18825531 W
PL12W           1.60379910 W
SFO2           125.7955123 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]          SINE.100
GPNAM[2]          SINE.100
GPNAM[3]          SINE.100
GPNAM[4]          SINE.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              125.7955 MHz
FIDRES           98.277740 Hz
SW                 200.000 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF             500.2300133 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                    1.00

F1 - Processing parameters
SI                    1024
MC2         echo-antiecho
SF             125.7829781 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
```

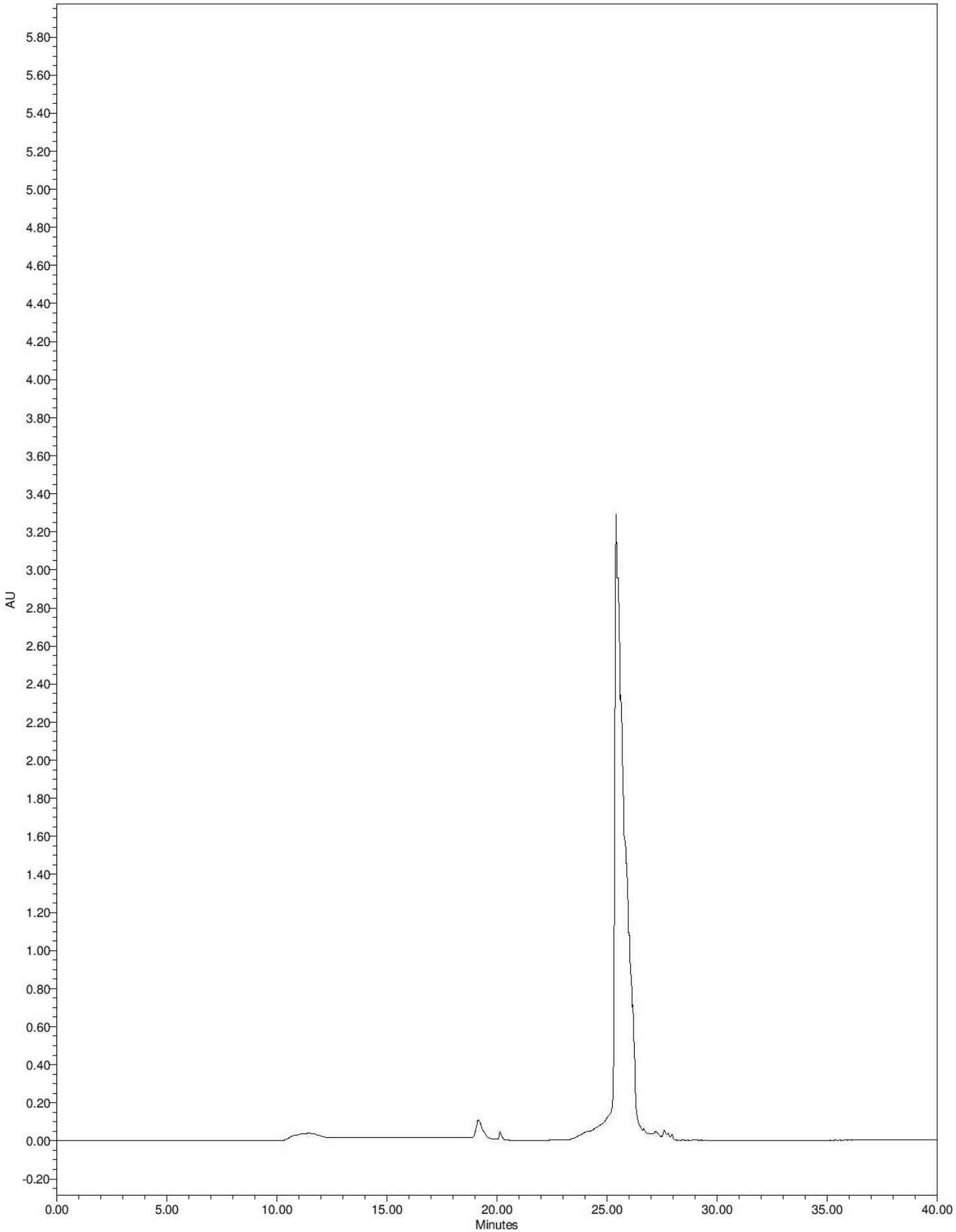


Figure S1: HPLC chromatogram of the target compound 1

Condition: HPLC on a Waters Nova-Pak C18 column (3.9 × 300 mm; 4 µm particle size) with a flow rate of 1mL/min and using a gradient of CH3CN in water (Conditions: 0 to 10% A in B, A = CH3CN, B = water, over 40 min.)

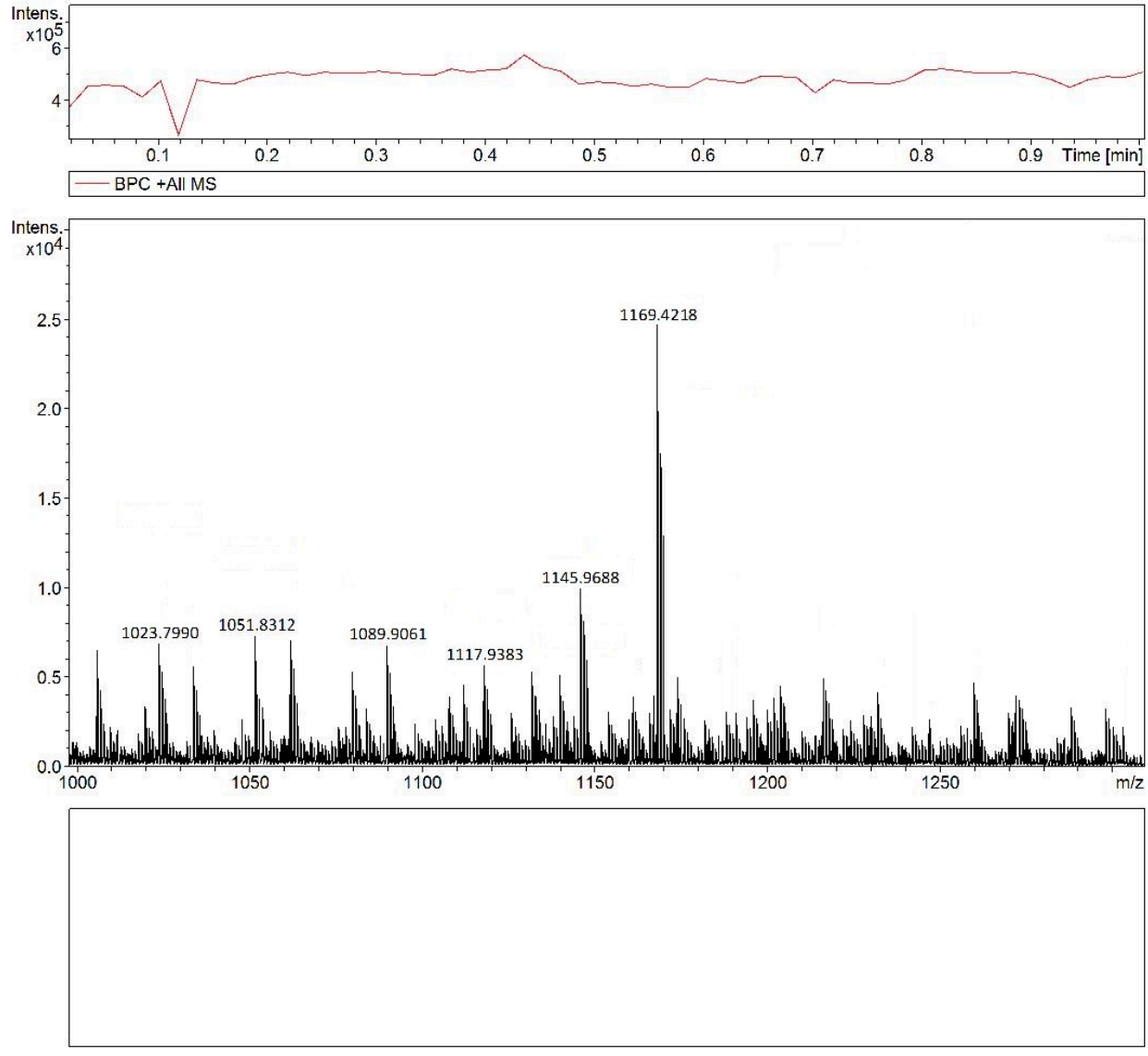
Display Report

Analysis Info

Analysis Name	D:\Data\User data\2016\AUGUST\BM_AM_SAI10.d	Acquisition Date	8/26/2016 4:54:27 PM
Method	Tune_pos_Standard.m	Operator	RAJESH VASHISTH
Sample Name	BM_AM_SAI10	Instrument	maXis impact 8282001.00127
Comment			

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)